Direct numerical simulations of multiphase flow 
with applications to basaltic volcanism and 
planetary evolution

by

Jenny Suckale

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Abstract

Multiphase flows are an essential component of natural systems: They affect the explosivity of volcanic eruptions, shape the landscape of terrestrial planets, and govern subsurface flow in hydrocarbon reservoirs. Advancing our fundamental understanding and predictive capabilities of multiphase flows is a problem of immense importance for both industrial and scientific purposes.

This thesis studies the potential of direct numerical simulations for advancing our fundamental understanding of the multiphase flow dynamics in magmatic flow. It is divided into two parts. The first part investigates gas-fluid coupling during the buoyant ascent of an exsolved gas phase in the conduit of basaltic volcanoes. The second part examines the solidification processes in magma oceans which entail both degassing (gas-fluid coupling) and crystallization (solid-fluid coupling).

For both applications, we find that the fluid dynamics at the length scale of the interfaces has important ramifications for the large-scale behavior of the system. We conclude that direct numerical simulations are an interesting complement to more traditional computational approaches and may provide new insights into the complexity of magmatic systems.

Thesis Supervisor: Linda T. Elkins-Tanton
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1 Introduction

2 Modeling rapidly deforming interfaces in buoyancy-driven flow with large viscosity contrasts

2.1 Introduction.............................................. 43
2.2 Governing equations.................................... 46
2.3 Numerical method........................................ 49
  2.3.1 Ghost-fluid-type fluid solver....................... 49
  2.3.2 Level-set-based Interface solver............... 54
  2.3.3 Coupling of the two solvers...................... 56
2.4 Benchmark problems.................................... 57
  2.4.1 Pressure jump at the interface of a viscous drop ...... 57
  2.4.2 Pressure jump for weak inclusions in pure shear ...... 58
  2.4.3 Rayleigh-Taylor instability........................ 59
  2.4.4 Compositional plume................................ 60
2.5 Results.................................................. 61
  2.5.1 Pressure jump at the interface of a viscous drop ...... 61
  2.5.2 Pressure jump for weak inclusions in pure shear ...... 62
  2.5.3 Rayleigh-Taylor instability........................ 65
  2.5.4 Compositional plume................................ 65
2.6 Discussion.............................................. 66
  2.6.1 Evaluation of the fluid solver..................... 66
  2.6.2 Evaluation of the interface solver.................. 69
5 The possibility of catastrophic magma ocean degassing and implications for the formation of early planetary atmospheres 125

5.1 Introduction 125
5.2 Model 127
  5.2.1 Bubble dynamics at microscopic scales 127
  5.2.2 Degassing at macroscopic scales 134
5.3 Results 136
  5.3.1 Early phase of magma ocean solidification 137
  5.3.2 Late phase of magma ocean solidification 141
5.4 Discussion 144
  5.4.1 Catastrophic degassing of magma oceans 144
  5.4.2 Water hitching its way up to the surface 146
  5.4.3 Extent of early melting might determine the fate of volatiles 147
  5.4.4 Three end-member cases of degassing 148
5.5 Conclusion 151

6 Direct numerical simulations of solid-fluid coupling in crystalline suspensions 153

6.1 Introduction 153
6.2 Governing equations 157
6.3 Numerical method 158
  6.3.1 Mathematical formulation 159
  6.3.2 Navier-Stokes solver 161
  6.3.3 Computation of the linear and angular momenta 162
  6.3.4 Collision forces 163
6.4 Results 165
  6.4.1 Flow over a circular cylinder 167
  6.4.2 Flow over a square cylinder 171
<table>
<thead>
<tr>
<th>Section</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.4.3</td>
</tr>
<tr>
<td>Sedimentation of a single sphere</td>
</tr>
<tr>
<td>6.4.4</td>
</tr>
<tr>
<td>Sedimentation of two interacting spheres</td>
</tr>
<tr>
<td>6.5</td>
</tr>
<tr>
<td>Conclusion</td>
</tr>
<tr>
<td>7</td>
</tr>
<tr>
<td>When crystals collide: Constraints on the fate of terrestrial planets during magma ocean solidification</td>
</tr>
<tr>
<td>7.1</td>
</tr>
<tr>
<td>Introduction</td>
</tr>
<tr>
<td>7.2</td>
</tr>
<tr>
<td>Model</td>
</tr>
<tr>
<td>7.3</td>
</tr>
<tr>
<td>Results</td>
</tr>
<tr>
<td>7.3.1</td>
</tr>
<tr>
<td>Very dilute suspensions</td>
</tr>
<tr>
<td>7.3.2</td>
</tr>
<tr>
<td>Dilute suspensions of equisized crystals</td>
</tr>
<tr>
<td>7.3.3</td>
</tr>
<tr>
<td>Dilute suspensions with heterogeneous crystal-size distributions</td>
</tr>
<tr>
<td>7.4</td>
</tr>
<tr>
<td>Discussion</td>
</tr>
<tr>
<td>7.4.1</td>
</tr>
<tr>
<td>Vesta: Skewed crystal-size distributions may facilitate early crystal settling</td>
</tr>
<tr>
<td>7.4.2</td>
</tr>
<tr>
<td>The Moon: The possibility of crystal settling during the late stages of solidification</td>
</tr>
<tr>
<td>7.4.3</td>
</tr>
<tr>
<td>Conclusions</td>
</tr>
</tbody>
</table>

A Supplement for chapter 2

<table>
<thead>
<tr>
<th>Section</th>
</tr>
</thead>
<tbody>
<tr>
<td>A.1</td>
</tr>
<tr>
<td>Abbreviated derivation of the jump conditions</td>
</tr>
<tr>
<td>A.2</td>
</tr>
<tr>
<td>Pressure jump for weak inclusions at extremely large viscosity contrasts</td>
</tr>
<tr>
<td>A.3</td>
</tr>
<tr>
<td>Convergence tests for benchmark problems 1, 2, and 3</td>
</tr>
<tr>
<td>A.4</td>
</tr>
<tr>
<td>Possible biases related to iterative reinitialization techniques</td>
</tr>
<tr>
<td>A.5</td>
</tr>
<tr>
<td>Subgrid features</td>
</tr>
</tbody>
</table>

B Supplement for chapter 3

<table>
<thead>
<tr>
<th>Section</th>
</tr>
</thead>
<tbody>
<tr>
<td>B.1</td>
</tr>
<tr>
<td>Projection Method</td>
</tr>
<tr>
<td>B.2</td>
</tr>
<tr>
<td>Dependence of breakup time on bubble radii for large bubbles</td>
</tr>
<tr>
<td>B.3</td>
</tr>
<tr>
<td>Resolution restriction for breakup induced by multibubble interactions</td>
</tr>
<tr>
<td>B.4</td>
</tr>
<tr>
<td>Convergence tests</td>
</tr>
</tbody>
</table>
C Supplement for chapter 4 231
    C.1 Bubble and crystal populations in HP magma 231
    C.2 Analytic solution for the stresses in an elliptic plate of moderate thickness with clamped edges 233
    C.3 Numerical approach for plugs with large thicknesses 236
    C.4 Stress concentration at the microscopic scale 236

D Supplement for chapter 5 239
    D.1 Homogeneous nucleation 239

E Supplement for chapter 6 241
    E.1 Adjustment of the collision parameters 241
List of Figures

2-1 Comparison of the standard (top) and ghost fluid (bottom) construction of finite-difference stencils for computing the pressure gradient in the vicinity of the interface. The interface between fluid 1 and 2 is located between grid points \((i, j)\) and \((i + 1, j)\). If the existence of the interface is not taken into account (top), the finite-difference approximation of the derivative \(\partial P/\partial x \approx (p_{i+1,j} - p_{i,j})/\Delta x\) will only be \(O(1)\) accurate. Ghost fluid methods fictitiously extend each fluid into the domain of the other yielding two 'ghost' phases (bottom). After this extension, two values for pressure are associated with grid point \((i + 1, j)\), the physical \(p_{i+1,j}\) and the ghost value \(p_{i+1,j}^+\). The ghost phases fulfill the additional purpose of enforcing the jump conditions at the interface. The jump conditions \([P]_{i,j}\) and \([P]_{i+1,j}\) are computed on both sides of the interface and then interpolated to reflect the subgrid position of the interface. This yields the jump at the interface denoted as \([P]_{i,j}\). The resulting finite-difference stencil \(\partial P/\partial x \approx (p_{i+1,j} - p_{i,j}^- + [P]_{i,j})/\Delta x\) is now order \(O(\Delta x)\) accurate. . . 44
2-2 Illustration of the construction of the asymmetric finite-difference stencil for the second derivative of the velocity field in one dimension. Two neighboring grid cells of size $\Delta x$ are shown. The two fluids are shaded in grey and white, respectively, implying that the interface crosses only the grid cell on the right. The symmetric three-point stencil commonly used to compute the second derivative of the velocity at point $u_{i,j}$ is indicated by crosses. In order to take the subgrid position of the interface explicitly into account, we shift the central point in the symmetric stencil $u_{i,j}$ to coincide with the interface $u_{I,j}$. This leads to an asymmetric stencil indicated by black dots and spanned by the points $u_{i-1,j}$, $u_{I,j}$ and $u_{i+1,j}$.

2-3 Initial and boundary conditions for the Rayleigh-Taylor instability as specified by [296]. The fluids are characterized by different densities $\rho_i$ and viscosities $\mu_i$. The level set function is constructed such that it is negative within the buoyant fluid and positive outside.

2-4 Computation of the pressure jump inside a static drop as a consequence of surface tension (benchmark problem 1). The Bond number (eq. 2.10) is set to $\Pi_3 = 10^{-3}$ to ensure sphericity of the drop. The viscosity contrast is $\Pi_1 = 10^{-6}$. The point-wise visualization of the pressure field illustrates the original resolution of the simulation ($51 \times 51$). The computational domain is a square box of aspect ratio 1.

2-5 Computation of the pressure field associated with a dynamic drop rising under its own buoyancy. The Bond number (eq. 2.10) is set to $\Pi_3 = 10^{-3}$ to ensure sphericity of the drop. The point-wise visualization of the pressure field highlights the original resolution of the simulation ($81 \times 121$). The computational domain is a rectangular box of aspect ratio $2 \times 3$. The pressure field is a combination of the discontinuous jump at the interface and the hydrostatic and dynamic contributions outside.
2-6 The Rayleigh-Taylor instability at \( t = 1500 \) computed by the level set method on a 300\( \times \)330 grid compared to the best results of the four codes compared in [296].

2-7 Comparison of the pressure field obtained numerically (left), computed analytically (middle) and the percentage error of the numerical solution (right) for benchmark problem 2. The average percentage error is \(<1\%\), the maximum is 3.76 \%. For easier comparison with [58], the grid resolution in the computation is set to 280\( \times \)280 and the viscosity contrast between inclusion \( \mu_{\text{in}} \) and surrounding matrix \( \mu_{\text{m}} \) to \( \Pi_1 = \mu_{\text{in}}/\mu_{\text{m}} = 10^{-3} \).

2-8 Detailed comparison of the level set (thin black line) and the marker chain approach (thick grey line) for the isothermal and isoviscous Rayleigh-Taylor instability at nondimensional time \( t = 1500 \). The plotted interfaces represent a zoom onto the instability descending from the top downwards in the middle of the box. The two methods yield an almost identical interface.

2-9 Left: Evolution of the entrainment of the buoyant fluid over time as computed by the five different codes. Right: Evolution of the root mean square velocity of the interface over time as computed by the five different codes. The level set computation was done on a 160 \( \times \) 176 grid.

2-10 Three-dimensional benchmark computation for problem 3, a compositional plume rising from a free-slip surface. The grid resolution is 40 \( \times \) 40 \( \times \) 50. The six snapshots of the dynamic evolution of the plume are shown for non-dimensional times 0, 8.4, 16.8, 25.2, 33.6, and 42. The experimental results by [173] are included as black and white reproduction in the background.
2-11 Setup and results for an example computation highlighting the differences between tracer- and level-set-based approaches for tracking dynamic interfaces. (top) The velocity field is constructed such that the square gradually shrinks onto its center. The sides move inward with velocity 1, the velocity along the main diagonals is set to $\sqrt{2}$, and a cosine taper is used to smooth the transition between these two values. The interface is tracked simultaneously using a level set function, which is illustrated in gray ($\phi < 0$) and white ($\phi > 0$), and 10 000 tracers placed on the initial interface which form a black line in the plot. (bottom) The interface position using (left) a level set function versus (right) tracers. While the level set function correctly outlines a square diminished in size, the tracers have formed spurious tentacles along the edges of the square.

2-12 Zoom onto the isothermal and isoviscous Rayleigh-Taylor instability specified by [296] at time $t = 1500$. In this computation, the interface is tracked simultaneously by a level set function (in grey/white) and by tracers (black line). We only plot the tracers for the lower segment of the interface to highlight the difference between the two interface-representation techniques. In the tracer-based computation, we observe the formation of a thin, elongated peak, reminiscent of the tentacles observed at the edges of the collapsing square in Fig. 2-11.

2-13 Illustration of the mass loss problem associated with interfaces that are entirely below grid resolution. Shown is a single computational cell spanned by the four grid points at the corners. One fluid (shaded in grey) is surrounded by the other fluid (white) such that the interface crosses the cell without interacting with the grid points. Because the level set function is positive at all grid points, the piece of grey fluid will be added to the white phase in the next computational step, leading to mass loss in the grey phase.
3-1 Dependence of the three main non-dimensional domains on bubble radius and magma viscosity. We assume a magma density of $\rho_f = 3500$ kg/m$^3$ and a surface-tension coefficient of $\sigma = 0.3$ N/m. The boundary of regime 1, characterized by spherical bubbles and negligible inertia, is determined only by the size of the bubbles, because $Bo$ does not depend on magma viscosity (see eq. 3.13). Regime 2, in which bubbles become deformable but inertia remains negligible, only exists at sufficiently high viscosity, $\mu \geq 3$ Pa·s.

3-2 Wavelength-dependence of the growth rate $n$ over a wide range of magma viscosities $\mu_f = 1, 10, 100, \text{ and } 1000$ Pa·s. The other parameters used in the computation are $\rho_f = 3500$ kg/m$^3$, $\rho_g = 1.226$ kg/m$^3$, $g = 9.81$ m/s$^2$, and $\sigma = 0.3$ N/m. The vertical grey line delimits the stable size range $a < \lambda_{cr}$. The grey dots indicate the fastest growing wavelength for a specific $\mu_f$ from the approximative expression for $\lambda_{max}$ (eq. 3.19) that is only valid at large viscosities.

3-3 Overview of the non-dimensional regime covered by the 95 simulations (black dots) constraining the stability of isolated gas bubbles at Re > 1 (sec. 3.4.2). The grey shading delimits the domain in which we observe breakup in two dimensions. A comparison with the shape regimes for bubbles during buoyant ascent [95] confirms that we reproduce the expected steady-state shape correctly in our computations. Note that we did not perform simulations for low Bo and high Re, because that case is of little relevance for basaltic magmas.
3-4 Breakup modes of an initially spherical bubble in two dimensions. A: An initially spherical bubble reaches its steady-state shape without breakup ($Re \approx 5$, $Fr \approx 0.4$, $We \approx 90$, and $\Pi_1 = 10^{-6}$). The snapshots shown are at non-dimensional times $t = 0, 1.97, 3.93,$ and $5.90$. B: Gradual breakup during which three small bubbles are torn off each side. The run is characterized by $Re \approx 25$, $Fr \approx 0.3$, $We \approx 800$ and $\Pi_1 = 10^{-6}$. Snapshots are at $t = 0, 1.42, 2.08,$ and $2.48$. C: An extreme example of breakup in the catastrophic regime characterized by $Re \approx 250$, $Fr \approx 0.16$, $We \approx 1350$ and $\Pi_1 = 10^{-6}$. Snapshots are at $t = 0, 0.59, 1.03, 1.58, 1.91, 2.04, 2.26,$ and $2.49$. The grid resolution in all runs is $80 \times 160$.

3-5 Catastrophic breakup of an initially spherical bubble in three dimensions. $Re \approx 16$, $Bo \approx 1150,$ and $\Pi_1 = 10^{-6}$. It is likely that, analogous to Fig. 3-4C, a series of small bubbles is generated during catastrophic breakup in three dimensions, but not resolved due to resolution restrictions. The computation was performed with a grid resolution of $75 \times 75 \times 50$ equidimensional cells. The snapshots shown refer to $t = 0, 1.15, 1.73, 2.88, 3.45,$ and $4.3$.

3-6 Dependence of the breakup time $t_B$ on bubble radius $a$ for gradual breakup. In order to evaluate the dependence of $t_B$, the computation is dimensional with $\rho_f = 3500$ kg/m$^3$, $\rho_g = 1.226$ kg/m$^3$, $g = 9.81$ m/s$^2$, $\sigma = 0.3$ N/m, $\mu_f = 10$ Pa·s, and $\mu_g = 10^{-5}$ Pa·s. The breakup time is expressed in percent of the initial breakup time at $a = 5.4$ cm. The numerical data points are associated with an error bar reflecting the finite time step $\Delta t$ in the computation. The line represents a cubic fit through the data.
Overview of the non-dimensional regime covered by 52 simulations (black dots) investigating the effect of multibubble interactions on breakup at Re > 0 (sec. 3.4.3). The computations have been binned based on their initial conditions, where 1.1 ≤ Π₂ ≤ 2.0, 1.1 ≤ Π₃ ≤ 2.0 and 1.1 ≤ Π₄ ≤ 3.0. The grey shading visualizes our finding that while coalescence and breakup commonly occur in sequence at Re > 0, coalescence dominates at small Re and breakup at large Re.

A three-dimensional computation of two deformable bubbles coming into close contact without coalescing. Non-dimensional numbers are Re ≈ 2, Bo ≈ 166, Π₁ = 10⁻⁶, Π₂ = 1.43, Π₃ = 1.2, and Π₄ = 2.0. Snapshots are at t = 0, 2.04, 3.06, 4.08, 5.10, and 6.12. The resolution is 50 × 50 × 80.

Two breakup sequences as a consequence of differing initial separation distances in the vertical direction Π₄ = 2 (A) and Π₄ = 1.8 (B). Both computations are based on Re ≈ 5, Fr ≈ 0.2, We ≈ 70, Π₁ = 10⁻⁶, Π₂ = 1.43, and Π₃ = 1.16. The snapshots shown for the first computation (top) refer to non-dimensional times t = 0, 1.5, 3.0, 4.5, and 6.0. Those on the bottom to t = 0, 2.32, 3.48, 4.41, and 5.80. C: Multi-bubble interactions for bubbles in the unstable size range (sec. 3.5.1). Non-dimensional numbers are Re ≈ 350, Fr ≈ 0.2, We ≈ 3000, Π₁ = 10⁻⁶, Π₂ = 1.43, Π₃ = 1.16, and Π₄ = 2. Snapshots are at non-dimensional times t = 0, 0.34, 0.51, 0.64, and 0.87. Initially, the deformation of each bubble is reminiscent of the breakup sequence of isolated bubbles (Figure 3-4). The presence of the other bubble only becomes apparent during the late stages of breakup, indicating that unstable bubbles break up more rapidly than they interact. All three computations are based on a grid resolution of 100 × 200.
3-10 Overview of the non-dimensional regime covered by 69 simulations (black dots) to constrain the stability of gas slugs (sec. 3.4.4). For all computations $\Pi_1 = 10^{-6}$ and $\Pi_5 = 0.7$. The grey shading delimits the domain in which we observe breakup in two dimensions.

3-11 A: Gradual breakup analogous to Fig. 3-4B. $Re \approx 10$, $Fr \approx 0.14$, $We \approx 95$, $\Pi_1 = 10^{-6}$, and $\Pi_5 = 0.67$. The snapshots shown are at $t = 0, 0.30, 0.60, 0.90, 1.20$, and 1.47. B: Gradual breakup may occur cyclically. $Re \approx 50$, $Fr \approx 0.16$, $We \approx 100$, $\Pi_1 = 10^{-6}$, and $\Pi_5 = 0.67$. Snapshots are at $t = 0, 0.94, 1.33, 1.56, 1.93$, and 2.20. C: Catastrophic breakup with gradual breakup occurring simultaneously along the walls. $Re \approx 80$, $Fr \approx 0.10$, $We \approx 3000$, $\Pi_1 = 10^{-6}$, and $\Pi_5 = 0.7$. The snapshots shown are at $t = 0, 0.29, 0.59, 0.88, 1.18$, and 1.47. All three computations were performed at grid resolutions of $80 \times 240$.

3-12 Dependence of the steady-state shape of conduit-filling slugs on Re. All computations are based on a spherical initial condition and $\Pi_5 = 0.7$. At finite Re, a dimple forms at the rear of the slug visible on all three interfaces. As Re increases from left to right, the steady-state width of the slug increases and the magmatic films separating interfaces and conduit walls are thinned out. Shear stresses will intensify as the magmatic films thin out and eventually lead to the tearing-off of small droplets similar to gradual breakup of isolated bubbles (Fig. 3-4B).
Comparison of the slug and plug model. A: The slug model assumes that the volcanic conduit is filled with fluid magma (grey) throughout. Each Strombolian eruption is thought to represent the burst of a gas slug of up to 35 m$^3$ [226]. B: Instead of focusing on one vent, the plug model captures the dynamics of the entire crater terrace. It incorporates the dichotomy of Strombolian magma with HP magma residing at shallow and LP magma at large depth. Flow in the LP magma is driven by buoyant ascent of gas bubbles inducing convective flow in the magma. For the first few hundred meters below the free surface, HP magma is crystalline enough to behave as a porous plug at low shear and strain rates.

Illustration of the rheological transitions with increasing crystal fraction. Estimates of melt strength are computed by viscosity $\times$ strain rate. At zero to low crystal fraction, the aggregate is fully liquid (regime A), where the increase in effective viscosity is given by the Einstein-Roscoe relationship. In the transitional regime, B, it is partly liquid and partly solid. The strength of the aggregate increases rapidly through a power-law (Bingham rheology). Beyond a rheologically critical crystal fraction, the aggregate behaves like a solid body (domain C).

Increase in crystallinity with decreasing pressure at 1115°C computed with MELTS based on the bulk composition of Strombolian magma from [80]. The shaded boxes highlight the observed crystallinity of HP magma at Stromboli.

Geometry of the elliptical cylinder representing the plug with semimajor axis $a$, semiminor axis $b$ and thickness $2h$. The coordinate is located at the center of the plate with $z$ corresponding to the vertical direction. The plate is stressed at the lower surface (shaded in grey) by a uniform pressure $p$. 

23
4-5 Overview of the spatial distribution of maximum shear at different depth intervals inside the plug with semimajor axis $a$, semiminor axis $b$ and moderate thickness $h = 70$ m based on the analytical solution for moderately thick plates (Appendix C). The top panel compares the value of maximum shear at the two boundary points furthest from the center, $(a, 0)$ and $(-a, 0)$, the two boundary points closest to the center, $(0, b)$ and $(0, -b)$ and the center throughout the plug. The bottom panels show the spatial distribution of maximum shear at various depths through color shading and five iso-stress contours. All stresses are nondimensionalized by the pressure applied at the lower surface of the plug.

4-6 Comparison of the increase in integrated maximum shear at the edges of the ellipse (in percent with respect to the center of the ellipse) and the vent locations (black dots) from October 1994 to September 2002 as mapped by [104]. The size of the ellipse is adjusted to coincide with the edge of the crater terrace.

4-7 The gas-driven eruption cycle suggested in the plug model. Continuous gas accumulation underneath the plug exerts an increasing pressure onto the overlying material until the critical pressure for failure is reached. Normal eruptions represent ductile failure of the plug during which the gas-rich layer underneath is partially drained. The buoyancy pressure drops, the eruptions ceases and gas accumulation begins again.

5-1 The wetting angle $\theta$ is the angle between the crystal face and the tangent to the bubble surface at the point of contact.

5-2 Relative supersaturations required for heterogeneous nucleation $\Delta P_{het}$ as compared to homogeneous nucleation $\Delta P_{hom}$ for wetting angles from $\theta = 0^\circ$ (no wetting) to $\theta = 180^\circ$ (perfect wetting).
Evolution of the volatile content (top) and saturation pressure (bottom) in a 1000-km-deep magma ocean with the fluid composition derived by [107] and initial volatile content 0.05 % water and 0.01 % carbon dioxide. The solubility behavior is computed based on [205]. The grey domain highlights volatile enrichment levels sufficient for heterogeneous nucleation based on the uncertainty interval given in sec. 5.3.1. The inset in the bottom figure illustrates that the supersaturation pressure corresponds to a depth which increases with increasing volatile enrichment (not plotted to scale).

An example computation of the rate of heterogeneous nucleation \( J \) for variable supersaturations of the melt \( \Delta P \). Nucleation becomes appreciable (i.e. \( J > 1 \text{cm}^{-3}\text{s}^{-1} \)) at \( \Delta P \approx 210 \text{MPa} \). However, in the pressure range \( 210 < \Delta P < 220 \text{MPa} \) the nucleation rate is still too low to trigger a local shift in convective forces and thus little to no degassing is expected. The beginning of catastrophic degassing occurs at \( \Delta P \approx 219 \text{MPa} \). Nucleation may be regarded as instantaneous (i.e. \( J > 10^4 \text{cm}^{-3}\text{s}^{-1} \)) at \( \Delta P > 224 \text{MPa} \).

Comparison of the depth dependence of solubility for water and carbon dioxide based on the solubility model by [205]. The melt composition is assumed to be basaltic (as specified in Table 3, [205]) and \( T = 2000^\circ\text{C} \). In both cases we assume a small amount (0.01 wt %) of the other volatile present in the melt.

Overview of the two phases of magma ocean solidification that are pertinent to catastrophic degassing sequences. Left: Nucleation delayed by insufficient supersaturation and bubble breakup create small bubbles that remain entrained and do not degas. Right: Once bubbles have reached a critical sized required for degassing, compositional convection becomes dominant at shallow depths. Catastrophic degassing may not happen until > 80% solidification for a 1000-km-deep magma ocean as may have existed on terrestrial planets and exoplanets.
Illustration of the three end-member cases of magma ocean degassing. Note that the wiggly arrows in red represent heat flux and not degassing. The first case (A) represents continuous degassing and gradual atmosphere formation. It applies to magma oceans with extremely high initial volatile contents or alternatively, with a content of crystals that are wetted perfectly by at least one of the dissolved volatiles. The second case (B) represents a degassing history characterized by one or several catastrophic degassing events with little or no degassing happening prior or after. Catastrophic degassing leads to the sudden formation of a substantial atmosphere. In the third case (C), the volatile content is never sufficient to trigger degassing and little atmosphere will form during solidification. The initial magma ocean depth is smaller in this case to reflect that this scenario is more likely for shallow magma oceans.

Computational domain for the simplified case of a single sphere sinking in viscous fluid. \( \Omega \) describes the entire computational domain including both solid and fluid phases and \( \partial \Omega \) its boundaries. \( P \) is the portion of the domain occupied by a single or multiple particles and \( \partial P \) is the solid-fluid interface.

Comparison of the wake behind a fixed cylinder at \( \text{Re}_f = 26 \) as observed experimentally (top) by [284] and computed numerically (bottom). The green arrow highlights the position of the second stagnation point in both cases.

Instantaneous out-of-plane vorticity over a fixed cylinder at three different Reynolds numbers showing Von-Kármán-vortex shedding.

Convergence test for the drag on a fixed circular cylinder at \( \text{Re} = 40 \). We investigate the convergence of the viscous \( C_v \) and the pressure contribution \( C_p \) to the drag on the cylinder's surface separately (see eq. 6.28 and [110]). Despite using a second-order fluid solver, the convergence at the fluid-solid interface is only first order.
6-5 Temporal evolution of drag and lift coefficients for flow over a circular cylinder at four different Reynolds numbers. The grid resolution in all four cases is 800 $\times$ 1600. .................................................. 169

6-6 Instantaneous out-of-plane vorticity over a square cylinder at three different rotation angles and $\text{Re} = 410$ showing Von-Kármán-vortex shedding. .... 170

6-7 Temporal evolution of drag and lift coefficients for flow over a square cylinder at $\text{Re} = 500$. Contrary to the case of a circular cylinder, both drag and lift exhibit period doubling as previously observed by [266]. ....... 171

6-8 Solid sphere sinking in viscous fluid at $\text{Re}_p = 90$. The computational domain is $3d \times 3d \times 9d$ and the resolution is $41 \times 41 \times 121$. The local speed of the flow field is represented in colour and the contours of the stream function are shown in white. The colouring of the sphere itself indicates its speed at a given time. .......................................................... 173

6-9 Comparison of the predicted drag coefficient for different Reynolds numbers with the empirical relationship by [50]. .......................... 174

6-10 The four stages of the interaction mode drafting-kissing-tumbling observed for two identical spheres at finite Re. The approximate Re of the computation is 150 based on the maximum settling speed of the spheres. ....... 175

7-1 Convective regimes in a solidifying magma ocean. At the planetary scale flow is driven by thermal convection. Flow is turbulent for most of the depth range of the magma ocean except for a boundary layer at the bottom where flow is rapid but non-turbulent. The conductive boundary layer is not visualized. The degree to which crystals can settle out of suspension in the steady-flow regime at the bottom of the magma oceans depends on the local fluid-dynamical conditions and is therefore dominated by compositional convection at the microscopic scale. .................................. 179
7-2 Body centered cubic (bcc) particle array consisting of spheres with radius \( r \). In this staggered setup, the smallest gap between particles is given by \( g \). The side length of the cell is given by \( a \); a reasonable proxy for a typical separation distance of the crystals.

7-3 Drag coefficient \( C_D \) for a sphere (3D) from \( 1 \leq \text{Re}_p \leq 1000 \) based on the data by Clift et al. (1978). The Stokes drag law, more precisely its Oseen extension [50] is also plotted for comparison purposes.

7-4 Simultaneous settling of 30 identical crystals with \( \text{Re}_p \approx 80 \) in a linear flow field at times 0.6s, 1.05s, 1.65s, 2.25s, 3.9s and 4.5s. The influx speed is set to the equilibrium settling speed of an isolated crystal in stagnant fluid. Since the presence of other crystals increases the drag experienced by each single crystal, the crystals tend to drift backwards over time. The color shading represents the average local flow speed normalized by the influx speed and the white contour lines represent the out-of-plane vorticity. The computations was done at a grid resolution of \( 800 \times 1600 \).

7-5 Temporal evolution of the drag (top) and lift (bottom) force for 30 identical spherical crystals (see Fig. 7-4) normalized by the drag and lift forces in the very dilute limit. The thick red line represents the mean drag and lift at a given time.

7-6 Simultaneous settling of 5 heavy crystals (\( \text{Re}_p \approx 120 \)) amidst 30 light crystals (\( \text{Re}_p \approx 80 \)) in a linear flow field at times 0.38s, 0.9s, 1.5s, 2.25s, 3.75s and 4.5s. The influx speed is set to the equilibrium settling speed of an isolated grey crystal akin to Fig. 7-4. The color shading represents the average local flow speed normalized by the influx speed and the white contour lines represent the out-of-plane vorticity. The computations was done at a grid resolution of \( 800 \times 1600 \).

7-7 Temporal evolution of the drag (top) and lift (bottom) force for the 30 grey crystals (blue and green, respectively) and the 5 black crystals (red) as shown in Fig. 7-6) normalized by the drag and lift force of a single sphere in the very dilute limit.
7-8 Average linear momentum of 5 and 7 heavy spheres ($Re_p \approx 120$) settling amidst 30 and 42 light crystals ($Re_p \approx 80$) at initial separation distances $a = 10r$ and $a = 7.5r$. Spikes in the curve represent rapid changes in momentum due to crystal collisions. Arrows indicate the onset of collisions for either case.

7-9 Two simulations of 30 spheres with equal density but variable size. In both cases, the influx is identical to Figs. 7-4 and 7-6 and the total crystal fraction is identical to Fig. 7-4 to within 0.001%. Contrary to the case of a homogeneous crystal-size distribution, the crystals begin to segregate immediately. Run A (snapshots are taken at times 0.38 (A1), 1.50 (A2), 3.00 (A3), and 4.51 (A4)) is characterized by a smaller deviation in crystal sizes and therefore separation of the crystals is slower than in case B (snapshots are taken at times 0.38 (B1), 1.13 (B2), 3.00 (B3), and 4.13 (B4)). The computations was done at a grid resolution of $800 \times 1600$.

7-10 Illustration of the entrainment of a small dense crystal (black) in the wake of a large and less dense crystal (grey). The settling of the large crystal dominates the local flow field sufficiently to divert the small crystal without colliding with it. The snapshots are details from the computation shown in Fig. 7-11.

7-11 Simultaneous settling of 5 heavy crystals ($Re_p \approx 120$) amidst 30 light crystals with a linear crystal-size distribution in a linear flow field at times 0.38s, 0.90s, 1.50s, 2.25s, 3.00s, and 3.75s. The influx speed is identical to Fig. 7-4 and 7-6. The color shading represents the average local flow speed normalized by the influx speed and the white contour lines represent the out-of-plane vorticity. The computations was done at a grid resolution of $800 \times 1600$.

7-12 Depth dependence of adiabat, liquidus and solidus for Vesta, the Moon and the Earth.
7-13 Relationship of the crystal-size distribution slope to the time variation in nucleation rate [180]. The top row (A) describes a single nucleation event and the middle row (B) a sequence of two nucleation events leading to a kinked crystal-size distribution. The bottom row (C) represents the hypothesized origin of skewed crystal-size distributions in solidifying magma oceans due to numerous nucleation events that are closely spaced in time.

A-1 Numerical (left) and analytical (middle) solution for the pressure field for benchmark problem 2. The viscosity contrast between inclusion and surrounding matrix is 6 (top row) and 10 (bottom row) orders of magnitude. The right panels shows the percentage error for both computations. The grid resolution is $150 \times 150$ in both cases.

A-2 Convergence test for benchmark problem 3. Shown are the numerical solutions for the pressure jump due to surface tension at the interface between a viscous drop and the surrounding fluid at grid resolutions $21 \times 21$ (left), $31 \times 31$ (center), and $41 \times 41$ (right). Each dot represents one grid point. Although the jump as such is resolved sharply without artificial smoothing at all of these resolutions, a minimum of $\approx 15$ grid points in both the x- and y-direction are required inside of the drop to resolve its spherical shape.

A-3 Convergence test for benchmark problem 2. The viscosity contrast is $\Pi_1 = 10^{-3}$ as discussed in the paper, sec. 2.5.2. The shown grid resolutions are $20 \times 20$ (top) and $80 \times 80$ (bottom). In both cases, we contrast numerical (left) and analytical solution (right). The comparison shows that the additional challenge of benchmark problem 2 as compared to benchmark problem 1 lies in fully resolve the magnitude of the pressure jump, for which high resolution is required.
A-4 Left: Convergence test for the isothermal and isoviscous Rayleigh-Taylor instability, benchmark problem 3. A lack of convergence is easiest to identify during the phases of rapid rise of an instability. We illustrate this for the rise of the secondary instability on the right side of the box at time t=1000 and four different grid sizes: 60×66, 80×88, 100×110, and 120×132. We observe convergence for grid sizes above 100×110. Right: Convergence test for the isothermal and isoviscous Rayleigh-Taylor instability, benchmark problem 3. Analogous to Fig. S7, we illustrate this convergence test for the rise of the secondary instability at time t=1000. The four interfaces were computed based on the time steps: $\Delta t = 180\Delta x$, $\Delta t = 90\Delta x$, $\Delta t = 45\Delta x$, and $\Delta t = 25\Delta x$. We observe convergence for time steps $\Delta t \leq 25\Delta x$.

A-5 Illustration of the accumulation of numerical error over time reflected in mass fluctuations. The plot shows the mass of the buoyant phase as a percentage of its initial mass. This plot compares to a similar plot presented by Schmalzl and Lod doch, [2003]. We note that fluctuations < 1% are not unexpected in complex fluid dynamical simulations. Overall, the mass conservation is satisfactory.

A-6 Illustration of the potential bias introduced through an iterative reinitialization procedure. The left figure (A) shows the isothermal and isoviscous Rayleigh-Taylor instability at t=1500 computed with extension velocities. The other two figures (B) and (C) are based on an iterative reinitialization procedure, but different parameters are used in the iteration. For case (B) a single reinitialization iteration is performed at each computational time step $\Delta t$ and $\Delta \tau = 0.9\Delta x$ is used in the numerical solution of equation A.16. For case (C) 20 iterative reinitialization steps were taken at each physical time step $\Delta t$ with $\Delta \tau = 0.9\Delta x/20$. All computations were performed on a 120×132 grid.
The Rayleigh-Taylor instability as computed by the HS-tracer method at time \( t = 1500 \). The equations of motion for this simulation were solved on an \( 81 \times 81 \) grid. The right panel is a zoom onto the peak located left of the descending instability. Each blue dot represents one particle and the grid represents a rough estimate of the scale at which the flow field is approximated correctly.

Dependence of the breakup time \( t_B \) on bubble radius \( a \) for large bubbles. In order to evaluate the dependence of \( t_B \), the computation is dimensional with the same parameters as in Fig. 3-6: \( \rho_f = 3500 \) kg/m\(^3\), \( \rho_g = 1.226 \) kg/m\(^3\), \( g = 9.81 \) m/s\(^2\), \( \sigma = 0.3 \) N/m, \( \mu_f = 10 \) Pa-s, and \( \mu_g = 10^{-5} \) Pa-s. The breakup time is expressed in percent of the initial breakup time at \( a = 5.4 \) cm. The numerical data are no longer compatible with the simple scaling relationship \( t_B \sim a^3 \) (eq. 3.20), which is not unexpected, given the wide fluid dynamical range it spans.

Dependence of multibubble interactions on the initial vertical separation distance. The three simulations show two bubbles passing (top), breaking up (middle), and coalescing (bottom) as a consequence of increasing the non-dimensional vertical distance \( \Pi_3 = 1.16 \) (top), \( \Pi_3 = 1.3 \) (middle), and \( \Pi_3 = 1.4 \) (bottom). The other non-dimensional numbers are identical for the three simulations: \( Re \approx 5 \), \( Fr \approx 0.2 \), \( We \approx 70 \), \( \Pi_1 = 10^{-6} \), \( \Pi_2 = 1.43 \), and \( \Pi_4 = 2 \). Snapshots are taken at non-dimensional times \( t = 0, 1.5, 3.0, 4.5, \) and \( 6.0 \). All three computations were performed with a grid resolution of \( 100 \times 200 \).

Convergence test for the catastrophic breakup of an isolated gas bubble (compares to Fig. 3-4C). Shown are four computations at differing resolutions \( 40 \times 80, 80 \times 160, 160 \times 320, \) and \( 320 \times 640 \).

Convergence test for the catastrophic breakup of a conduit-filling gas slug (compares to Fig. 3-11C). Shown are four computations at differing resolutions \( 40 \times 80, 80 \times 160, 160 \times 320, \) and \( 320 \times 640 \).
B-5 Convergence test for the gradual breakup of an isolated gas bubble (compares to Fig. 3-4B). Shown are four computations at differing resolutions 40×80, 80×160, 160×320, and 320×640. .............................................. 229

B-6 Convergence test for the gradual breakup of a conduit-filling gas slug (compares to Fig. 3-11A). Shown are four computations at differing resolutions 40×80, 80×160, 160×320, and 320×640. .............................................. 230

C-1 Thin-section analysis of Stromboli’s HP magma. .............................................. 232

C-2 Left: Maximum shear stress for a thick elliptical cylinder overlain by the computational grid generated by Distmesh. The stresses are extremely high in the vicinity of the side boundaries. Right: Maximum shear stress for a thick elliptical cylinder with a free-moving side flank. .............................................. 237

C-3 Stress concentration around the bubble interface in a purely extensional stress field. The stress is measured in multiples of the applied stress at the boundary σbc. The black circles surrounding the bubbles correspond to three times the radius of the bubble and denote the range over which the stress concentration due to the presence of the bubble is appreciable (Saint-Venant’s principle). In panel A, the bubbles are spaced closely enough for substantial stress concentration; in panel B, the bubbles are far enough apart to be negligible on the large scale. The purely compressional case is analogous. .............................................. 238

D-1 Illustration of the activation energy for homogeneous nucleation. The blue curve represents the Free Helmholtz energy ΔF_{surf} required for forming a new interface and the red curve the volumetric gain in Free Helmholtz energy ΔF_{vol} from the presence of a bubble. The sum of the two contributions is shown in green. An activation energy of ΔF^* needs to be overcome for spontaneous nucleation to occur. .............................................. 240

E-1 Repulsive force between particles i and j as defined in eq. E.1 [91]. .... 242
List of Tables

2.1 Analytical versus numerical results for the pressure jump due to surface tension at the interface of a static drop. This computation was done dimensionally with $\sigma = 0.0728$ kg/s$^2$ – a representative value for the air/water interface. ................................. 59

2.2 Comparison of the quantitative parameters characterizing the dynamics of the isoviscous Rayleigh-Taylor instability. ......................... 64

3.1 Theoretical prediction of the maximum stable bubble radius $a_{\text{max}}$ in basaltic magma of different viscosities $\mu_f$. Additional parameters used in the computation: $\rho_f = 3500$ kg/m$^3$, $\rho_g = 1.226$ kg/m$^3$, $g = 9.81$ m/s$^2$, surface tension $\sigma = 0.3$ N/m, and viscosity ratio $10^{-6}$. .... 87

5.1 Overview of variables used in the text. ......................... 128

5.2 Supersaturations required for non-zero homogeneous (eq. D.3) and heterogeneous (eq. 5.3) nucleation in a basaltic magma ocean with variable volatile contents. We consider nucleation rates of $J < 1$ cm$^{-3}$ s$^{-1}$ to be negligible. The remaining parameters are $\sigma = 0.3$ N/m, $\rho_m = 3400$ kg/m$^3$, $T = 1100K$, $g = 9.5$ m/s$^2$, $V_{H_2O} \approx 11.5\AA^3$, $V_{CO_2} \approx 4\AA^3$, $D_{H_2O} = 100 \times 10^{-12}$ m$^2$/s [326], and $D_{CO_2} \approx 13 \times 10^{-12}$ m$^2$/s [315, 326, 313]. In order to take both water and carbon dioxide into account for the computation of the forefactor $J_0$, we take the weighted mean of the parameters characterizing water and carbon dioxide, respectively. ................................. 137
5.3 Overview of expected bubble sizes in a magma ocean including their
dynamical behavior. .................................................. 141

6.1 Mean drag coefficient $C_D$ for flow over a circular cylinder at different
Reynolds numbers based on the simulations in Fig. 6-5. .......... 167

6.2 Strouhal numbers for flow over a fixed cylinder at different Reynolds
numbers based on the simulations in Fig. 6-3. ................. 167

6.3 Mean drag coefficient $C_D$ for flow over a square cylinder. ....... 172

7.1 Order-of-magnitude estimates for the key non-dimensional parameters
characterizing flow in magma oceans. ............................... 178

7.2 Approximate physical parameters for a theoretical magma ocean. .. 178

7.3 Overview of different types of suspensions grouped according to the
crystal fraction and the corresponding non-dimensional gap between
crystals as defined in Fig. 7-2. ................................. 183
Chapter 1

Introduction

This dissertation consists of six self-contained studies linked together through their focus on multiphase flow problems and their computational methodology. Broadly speaking, all fluid systems in which different liquid, gaseous or solid phases are simultaneously present may be considered multiphase. Without further specification, however, nearly all of fluid dynamics would fall under this generic label. In the sense in which the term multiphase flow is commonly used, it denotes a more specific class of problems typically tied together by the context in which they arise rather than by an abstract similarity in their properties. This thesis is no exception: The commonality of the multiphase systems investigated here is their relevance for magmatic flow.

A large number of problems in Earth science are related to the solidification processes in molten rocks. Examples range from the propagation velocity of hazardous lava flows to the differentiation of cooling magma oceans and the disputed origin of layering in igneous intrusions. We are well equipped to model the two end-member cases of the solidification process, i.e. the early stages in which the aggregate is largely molten and the final stages in which it is mostly solid. The greatest challenge is posed by the intermediary stages in which crystallized minerals, exsolved gas bubbles and highly viscous magma may all contribute significantly to the dynamics of the aggregate. The goal of this thesis is to extend the reach of our numerical models a little further into this complex regime of solid-fluid-gas interactions.
Much of the complexity of modeling multiphase flow stems from the dynamic interaction of the various fluid and solid phases that are simultaneously moving through the system. This complexity limits the usefulness of purely analytical approaches. Laboratory experiments provide a compelling alternative, but may not always offer the necessary degree of control over the length scales and the physical parameters characterizing the flow. Numerical simulations are thus an essential complement to experiments and, for certain problem, they may be the only available tool for investigating multiphase dynamics.

Computational methods for multiphase flows are as varied as the problems for which they are intended. Here we consider a class of approaches that are commonly referred to as direct numerical simulations. These types of methods are direct in the sense that they fully resolve the physics of the problem from first principles instead of relying on effective constitutive laws, approximate settling speeds, or similar simplifying assumptions. Direct numerical simulations are thus particularly advantageous for complex flow problems for which it is typically not possible to specify effective ensemble properties a priori.

The added sophistication of fully resolving the fluid dynamic interaction of all suspended phases limits the reach of direct numerical simulations to length scales commensurate to the length scales of the interfaces in the flow. Particularly in the Earth sciences, where the relevant flow systems may span whole planets, this limitation highlights that direct numerical simulations are a complement to more traditional approaches such as large-scale convection simulations rather than an alternative. They offer the possibility to gain more detailed insights into the complex fluid-dynamical interactions at small scales and can thus inform the inputs required for large-scale computations such as rheology, effective viscosity or settling velocities of suspended particles.

Another role that direct numerical simulations may play in Earth science is to help forge a closer connection between petrological observations and numerical models. Integrating data on the bubble content, the types of mineral phases or the crystal size distribution characterizing a given flow system into geodynamical models has proven
challenging, because the physical ramifications of these observations are often not
obvious. Direct numerical simulations may shed some light on these complex con-
nections and thereby contribute to creating a tighter link between field observations,
experiments and modeling.

This thesis studies the potential of direct numerical simulations for advancing our
fundamental understanding and predictive capabilities of the multiphase dynamics
of cooling magmatic flow. This task implies both a methodological and an applied
focus. The usefulness of direct numerical simulations is inevitably tied to the insights
that these computations can reliably provide for complex three dimensional systems.
The choice of numerical scheme has a profound influence on the tractability, accuracy,
robustness, and efficiency of the simulation. Even a state-of-the-art numerical model,
however, is useless if it does not make a significant contribution to our understanding
of some of the important open questions in Earth science.

Here we discuss two specific examples in which the results from direct numer-
ical simulations provide a new perspective. The first example is the dynamics of
an exsolved gas phase ascending in basaltic lava, which is critical for understanding
the mechanism of explosive eruptions in basaltic volcanoes. The key methodologi-
ical challenge in this suite of computations is the accurate treatment of the rapidly
deforming interface between two fluids, gas and magma, with drastically different
viscosity. The second example is crystal settling in cooling magma oceans, which
is essential for constraining the later evolution of the planet including the onset of
convective overturn and early volcanism. The key methodological challenge for this
series of simulations is the full dynamic coupling of solid and fluid phases for various
densities, shapes and crystal size distributions. The thesis is broadly divided into two
parts by the discussion of basaltic volcanism (chapters 2–4) and planetary evolution
(chapters 5–7).

In chapter 2 we develop and benchmark the computational methodology for fully
resolving the interface dynamics of buoyancy-driven flow in the presence of large
viscosity contrasts. Our implementation relies on the combination of three numerical
methods, an extended ghost fluid type discretization which we extend to the Stokes
regime, the level set method, and the extension velocity technique, to tackle the three main challenges in these types of computations, i.e. the accurate solution of the equations of motion in the presence of large viscosity contrasts, the representation of strongly deforming interfaces between different fluids, and the accurate coupling of fluid and interface solver.

Chapter 3 applies this numerical approach to investigate the bubble dynamics in basaltic volcanoes in general and Stromboli volcano in particular. The main finding is that conduit-filling gas pockets, also referred to as slugs, are prone to dynamic instabilities that lead to their rapid breakup during ascent. This insight sheds some doubts on the current paradigm positing that normal Strombolian eruptions are caused by the burst of large gas slugs.

In chapter 4 we study the slug model for normal Strombolian activity in more detail. We conclude that an analysis of the petrological data for Stromboli substantiates doubts about one of the key assumptions behind the slug model, namely that the magma in the upper conduit is a Newtonian fluid. We draft an alternative framework, the plug model, which is compatible both with the petrological data and with the fluid dynamical constraints on conduit dynamics discussed in chapter 3.

The insight that the vigor of the flow field has important ramifications for the stability of entrained gas bubbles is relevant not only for degassing in basaltic volcanoes but also for the degassing processes in solidifying magma oceans. Chapter 5 explores these ramifications. By blending fluid dynamical arguments with a simplified model of nucleation and bubble growth, we identify the possibility that magma oceans may degas catastrophically and build their primordial atmosphere very rapidly. We also analyze which physical and chemical parameters determine the degassing history of magma oceans and conclude that a wide range of degassing histories ranging from continuous to catastrophic and negligible degassing are possible.

Chapter 6 develops and benchmarks a computational methodology for direct numerical simulations of solid-fluid coupling in crystalline suspensions. We rely on distributed Lagrange multipliers to enforce rigid body motion in the solid phase, which adds minimal computational overhead as compared to a pure fluid solver. The key
novelty of our implementation is an analytical treatment of the integration necessary
to compute the hydrodynamic forces on the solid interfaces. This innovation boosts
the accuracy and efficiency of the computation.

In chapter 7 we study the fluid dynamics of crystal settling in a solidifying magma
ocean using the computational approach discussed in chapter 6. The main finding
is that crystal collisions play a crucial role for settling or flotation, because they
transfer kinetic energy from fast to slow moving crystals and to the fluid itself. This
mechanism is particularly consequential for suspensions consisting of approximately
equal shares of buoyant and heavy crystals with similar sizes. The importance of
crystal collisions has important ramification for magma oceans on the Moon and on
Vesta. While our simulations point to very efficient crystal settling during the early
phase of solidification, at least on Vesta and the Moon, we suggest that significant
re-melting of the magma ocean must occur to delay the otherwise inevitable cessation
of crystal settling towards the late stages. For the Moon, we hypothesize that the
heat provided by impactors and tidal forces may suffice to lower the crystal fraction in
suspension and allow for plagioclase flotation during the late stages of magma ocean
solidification.
Chapter 2

Modeling rapidly deforming interfaces in buoyancy-driven flow with large viscosity contrasts

2.1 Introduction

Numerical modeling is an indispensable tool for understanding geophysical processes and an important complement to analytical models, which are inevitably simplified versions of the original problem. Although numerical models often approximate the original problem directly, each specific method comes with its own limitations and advantages. Thus, numerical benchmark studies are an important tool to evaluate and compare the performance of various approaches. The goal of this chapter is to develop and test a numerical tool that correctly captures the complex flow dynamics of systems with large viscosity contrasts and strongly deforming interfaces. The emphasis of this study is on buoyancy-driven flow. This exclusive focus on buoyancy is justified by the fact that it is a common element in numerous geodynamical processes including

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Figure 2-1: Comparison of the standard (top) and ghost fluid (bottom) construction of finite-difference stencils for computing the pressure gradient in the vicinity of the interface. The interface between fluid 1 and 2 is located between grid points \((i, j)\) and \((i + 1, j)\). If the existence of the interface is not taken into account (top), the finite-difference approximation of the derivative \(\partial P/\partial x \approx (p_{i+1,j} - p_{i,j})/\Delta x\) will only be \(O(1)\) accurate. Ghost fluid methods fictitiously extend each fluid into the domain of the other yielding two 'ghost' phases (bottom). After this extension, two values for pressure are associated with grid point \((i + 1, j)\), the physical \(p_{i+1,j}\) and the ghost value \(p_{i+1,j}^-\). The ghost phases fulfill the additional purpose of enforcing the jump conditions at the interface. The jump conditions \([P]_{i,j}\) and \([P]_{i+1,j}\) are computed on both sides of the interface and then interpolated to reflect the subgrid position of the interface. This yields the jump at the interface denoted as \([P]_{i,j}\). The resulting finite-difference stencil \(\partial P/\partial x \approx (p_{i+1,j} - p_{i,j}^- + [P]_{i,j})/\Delta x\) is now order \(O(\Delta x)\) accurate.

salt diapirs (e.g. \([323, 248, 228, 124]\)), lithospheric instabilities (e.g. \([119, 76, 52, 251, 117, 64]\)), interactions between compositional plumes (e.g. \([244]\)), trench motion in the context of self-consistent subduction models (e.g. \([235, 249]\)), magma mixing (e.g. \([179, 21]\)), lava dome growth (e.g. \([28, 102, 101]\)), and bubble dynamics in magmatic flow (e.g. \([172]\)). Although temperature plays an important role in many of these processes, isothermal models are valuable as long as the time scale of thermal interaction is large compared to the time scale of buoyant ascent.
From a numerical perspective, simulations of buoyancy-driven flow pose three main challenges: (1) The computation of the flow field is complicated by the jump conditions at the interface. The material parameters (i.e., viscosity and density) jump discontinuously across the interface. These discontinuities in the coefficients of the equations of motion are paralleled by jumps in their solution (i.e., pressure and stresses). Since all of these jumps occur directly at the interface, numerical errors associated with the jump computation will translate quickly into less accurate interface dynamics. (2) The time-evolution of the interface needs to be tracked without restricting the deformability of the interface in the flow field and without violating mass conservation in either of the two fluids or affecting the discontinuous jumps in fluid properties across the interface. (3) The two solvers, fluid and interface solver, need to be fully and accurately coupled. We stress that this requirement is of special significance for buoyancy-driven flow in which motion is driven actively by the interface as compared to, for example, passive advection of an interface in a thermally-driven convection cell.

Here, we combine three tools, a ghost fluid type approach [72, 133, 157], the level set method [201], and the extension velocity technique [168, 5] to tackle each of the above three challenges. We deal with the first challenge, the incorporation of the jump conditions in a sharp manner, by developing an extended discretization scheme for the multi-phase Stokes equation based on a ghost fluid type approach. Our implementation was inspired by [133] and [157]. To our knowledge, it provides the first application of ghost fluids to the Stokes equation. We address the second challenge by representing the interface through a level set function. We address the second challenge by representing the interface through a level set function. The third challenge, the accurate coupling of flow and interface solver, is tackled through the velocity-extension procedure pioneered by [168] and later improved upon by [5] and [42, 43]. As discussed in detail elsewhere [281, 5, 43, 134] the construction of extension velocities ensures that our method is not prone to problems such as mass loss and spurious interface repositioning, which commonly plague codes relying on iterative re-initialization [282, 281, 280].

Together, these three tools equip us with an accurate method of simulating buoyancy-
driven flow in the presence of large viscosity contrasts. We have selected four benchmark problems to validate its different aspects and to compare its performance to other approaches: (1) The pressure jump due to surface tension at the interface of a spherical drop, (2) the jump in pressure and normal stresses at the interface of a circular inclusion which is several orders of magnitude less viscous than the surrounding rock matrix [250, 58], (3) the isothermal Rayleigh-Taylor instability as specified by [296], and (4) a compositional plume rising from a free-slip surface as investigated by [173]. The first two benchmark problems serve as a verification for the accuracy of our multi-phase Stokes solver and its ability to resolve the various types of jump conditions that might arise in complex flow fields. The third benchmark problem, the isothermal Rayleigh-Taylor instability specified by [296], allows us to study the relative advantages and disadvantages of our interface tracking technique in comparison to four other approaches for representing interfaces. Finally, we choose a compositional plume as our fourth and only three-dimensional benchmark problem in order to validate our computations with respect to experimental [173] and numerical data [173, 247].

2.2 Governing equations

The dynamics of buoyancy-driven flow involving two incompressible fluids with zero chemical diffusivity and negligible inertia are described by the Stokes equation

$$-\nabla p + \nabla \cdot (\mu(\Gamma)(\nabla \mathbf{v} + (\nabla \mathbf{v})^T)) + g\rho(\Gamma) = 0,$$

(2.1)

with the incompressibility constraint,

$$\nabla \cdot \mathbf{v} = 0,$$

(2.2)

and the advection equation for composition

$$\frac{\partial \Gamma}{\partial t} + (\mathbf{v} \cdot \nabla)\Gamma = 0.$$

(2.3)
Figure 2-2: Illustration of the construction of the asymmetric finite-difference stencil for the second derivative of the velocity field in one dimension. Two neighboring grid cells of size $\Delta x$ are shown. The two fluids are shaded in grey and white, respectively, implying that the interface crosses only the grid cell on the right. The symmetric three-point stencil commonly used to compute the second derivative of the velocity at point $u_{i,j}$ is indicated by crosses. In order to take the subgrid position of the interface explicitly into account, we shift the central point in the symmetric stencil $u_{i,j}$ to coincide with the interface $u_{I,j}$. This leads to an asymmetric stencil indicated by black dots and spanned by the points $u_{i-1,j}$, $u_{I,j}$ and $u_{i+1,j}$.

In these equations $p$ denotes the pressure, $\mu$ the viscosity, $\rho$ the density, $\mathbf{v}$ the velocity field, $\mathbf{g}$ the gravitational acceleration and $\Gamma$ the composition, which captures the spatial dependence of $\rho$ and $\mu$ in the presence of multiple fluid phases.

Additionally, the jump conditions at the interface due to the combined effect of surface tension and stresses need to be fulfilled:

$$
\begin{bmatrix}
\mathbf{n} \\
\mathbf{t}_1 \\
\mathbf{t}_2
\end{bmatrix} (pI - \tau) \mathbf{n}^T =
\begin{bmatrix}
\sigma \kappa \\
0 \\
0
\end{bmatrix},
$$

where $I$ is the identity matrix, $\sigma$ the surface tension coefficient, $\tau$ the stress tensor, $\kappa$ the curvature of the interface, and $\mathbf{n}, \mathbf{t}_1, \mathbf{t}_2$ the normal and two tangential vectors to the interface. Note that we use square brackets to denote a jump in a given quantity throughout.

Instead of tracking the discontinuous composition function $\Gamma$, we introduce an
auxiliary function called the level set function \( \phi \). The level set function \( \phi \) will be properly defined in section 2.3.2. At this point, we simply note that the spatial variation of material parameters can be written in the form \( \rho(\Gamma) = \rho(\phi) \) and \( \mu(\Gamma) = \mu(\phi) \).

In the absence of surface tension, the dynamics of the system are fully described by two non-dimensional numbers,

\[
\Pi_1 = \frac{\mu_2}{\mu_1} \quad \text{and} \quad (2.5)
\]

\[
\Pi_2 = \frac{gd^3 \Delta \rho^2}{\mu_{ref}^2} \quad (2.6)
\]

where \( \Delta \rho \) represents the density difference between the two fluid phases and either of the two viscosities can be chosen for \( \mu_{ref} \). \( \Pi_2 \) represents the ratio of buoyancy forces to viscous drag. Introducing the characteristic length \( d \), we substitute the following characteristic quantities \( x = dx' \), \( v = \Delta \rho gd^2/\mu_{ref} v' \), \( \mu = \mu_{ref} \mu' \), \( \rho = \Delta \rho \rho' \), and \( p = \mu_{ref}^2/(\Delta \rho d^2) p' \) into eq. 2.1, drop the primes, and obtain the non-dimensional Stokes equation

\[
-\nabla p + \Pi_2 \nabla \cdot (\rho(\phi)(\nabla v + (\nabla v)^T)) + \Pi_2 \rho(\phi) \hat{z} = 0, \quad (2.7)
\]

where \( \hat{z} \) is the unit vector in vertical direction and

\[
\rho(\phi) = \begin{cases} 
\rho_1/\Delta \rho & \text{for } \phi < 0 \\
\rho_2/\Delta \rho & \text{for } \phi \geq 0,
\end{cases} \quad (2.8)
\]

and

\[
\mu(\phi) = \begin{cases} 
\Pi_1 & \text{for } \phi < 0 \\
1 & \text{for } \phi \geq 0.
\end{cases} \quad (2.9)
\]

In the presence of surface tension, we additionally introduce the Bond number,

\[
\Pi_3 = \frac{\Delta \rho gd^2}{\sigma} \quad (2.10)
\]
which represents the ratio of buoyancy to surface tension forces.

2.3 Numerical method

2.3.1 Ghost-fluid-type fluid solver

Ghost fluid methods

Considering only finite-difference approaches on structured grids, the different numerical strategies that exist for capturing the jump conditions at dynamic interfaces can be grouped into three categories [38]: regularization (i.e., discontinuities in the coefficients and in singular sources are smeared out over one or more grid points), dimension-un-splitting (i.e., discontinuities are represented in a sharp manner based on a local Taylor-series expansion in multiple dimensions), and dimension-splitting techniques (i.e., discontinuities are represented in a sharp manner based on multiple local Taylor-series in one dimension thus representing the original problem as a combination of one-dimensional problems).

The disadvantages of regularization approaches include artificial smearing of the jump conditions, formation of spurious oscillations for large jump magnitudes, and their limitation to first order accuracy in two or higher dimensions [293]. Discretizations based on dimension un-splitting, on the other hand, typically match the jump conditions to second order at the interface (e.g. the immersed-interface method [153]). We note that an adaptation of the immersed-interface method to Stokes flow exists [154]. One drawback of dimension-un-splitting is that the construction of the finite-difference stencils is not a trivial undertaking, particularly in three dimensions. Ghost-fluid methods are part of the third category, dimension-splitting techniques. Since they rely on a combination of local Taylor-series expansions in one dimension, stencils typically consist of only three points in each dimension (e.g. [133, 157]) instead of $3^d$ grid points in $d$ dimensions as required for dimension-un-splitting. The main drawback is that the splitting of dimensions requires projecting the jump conditions in the derivatives onto the direction normal to the interface. As a consequence,
the jumps in the normal derivative are captured correctly and in a sharp manner, but those in the tangential derivative are still smeared out (e.g. [157, 38]).

The key idea behind ghost-fluid techniques – and the origin of their name – is the fictitious extension of the physical domain of each fluid into the physical domain of the other fluid (e.g. [89, 183, 184, 72, 133, 157]). We build the ghost phases through linear extrapolation of the physical phase [133, 157]. They fulfill two purposes (see Figure 2-1): (1) They are used to construct more accurate stencils in the vicinity of the interface, which consist of a mixture of ghost and physical points. The gain in accuracy is related to the fact that the interface was essentially removed from the stencil by constructing the linear extension of the fluid. (2) They are used to enforce the jump conditions at the interface, which are determined by harmonic interpolation taking the subgrid location of the interface into account. Thus, ghost-fluid methods locally decouple a single two-phase flow problem into two single-phase flow problems that are then merged back together based on the jump conditions at the interface.

Figure 2-1 illustrates the construction of finite-difference stencils for the pressure gradient (eq. 2.7). Although the strategy for building the stencils for the viscous term in equation 2.7 is similar in essence, we use asymmetric stencils for additional accuracy around the interface [133, 157]. Figure 2-2 explains the construction of the asymmetric three-point stencils approximating the second derivative of the velocity. The central point $u_{i,j}$ of the standard symmetric stencil is shifted to coincide exactly with the interface $u_{I,j}$. The viscosity of the 'asymmetric' stencil point $u_{I,j}$ is computed through harmonic interpolation [133, 157]

$$\mu = \frac{\mu_1 \mu_2}{\mu_2 \theta + \mu_1 (1 - \theta)},$$

where $\theta$ denotes the subgrid position of the interface.

**Jump conditions**

Evidently, the accuracy of ghost-fluid methods hinges critically on the accuracy with which the jump conditions are computed. Three types of jump conditions need to be
considered (eq. 2.4): (1) the jump in pressure due to surface tension, (2) the jump in pressure due to viscous stresses, and (3) the jump in stresses. As noted by [133], the pressure jump in equation 2.4 can be rephrased more simply as

\[ p = \sigma \kappa + 2\mu (\nabla u \cdot \mathbf{n}, \nabla v \cdot \mathbf{n}, \nabla w \cdot \mathbf{n}) \cdot \mathbf{n}. \]  

(2.12)

The first term in equation 2.12 is the surface-tension-related contribution to the pressure jump and the second term represents the viscous contribution. In addition to the pressure, stresses may also be discontinuous across the interface, implying that jump conditions need to be considered when approximating the second derivative of the velocity field. The computation of the stress jumps is based on the insight that the discontinuity of normal stresses can be avoided through a coordinate transform [153]. Hence, we compute the stress jump in the coordinate system spanned by the normal and the two tangential vectors at each point of the interface, yielding a matrix of jump conditions that is then rotated back into the computational domain. This strategy leads to the following expression [133]

\[
\begin{pmatrix}
\mu u_x & \mu u_y & \mu u_z \\
\mu v_x & \mu v_y & \mu v_z \\
\mu w_x & \mu w_y & \mu w_z \\
\end{pmatrix}
\begin{pmatrix}
\nabla u \\
\nabla v \\
\nabla w \\
\end{pmatrix}
= \mu
\begin{pmatrix}
0 \\
t_1 \\
t_2 \\
\end{pmatrix}^T,
\begin{pmatrix}
0 \\
t_1 \\
t_2 \\
\end{pmatrix}
\begin{pmatrix}
\nabla u \\
\nabla v \\
\nabla w \\
\end{pmatrix}^T
\]

(2.13)

We note that contrary to the discontinuous derivatives on the left, the derivatives on the right hand side of equation 2.13 are spatially continuous and thus amenable to a finite-difference approximation [133]. For a detailed derivation of equations 2.12 and 2.13, please refer to Appendix A.

As is evident from equations 2.12 and 2.13, the jump conditions themselves depend on the velocity field. Therefore, it is not obvious how to compute the jump conditions without knowing the solution to the equations of motion beforehand. In their ghost-
fluid method for solving the multi-phase Navier-Stokes equation, [133] suggest using the numerical estimate of the velocity field from the previous time step to compute the jump conditions at the current time step. This strategy is not an option for the Stokes equation, because it conflicts with the assumption of quasi-stationarity inherent to Stokes flow. Instead, we solve for the jump conditions at each time step as explained next.

Discretization of the multi-phase Stokes equation in a ghost framework

We use finite differences on a staggered grid in Cartesian coordinates to approximate the non-dimensionalized multi-phase Stokes equation (eq. 2.7). The coefficients of the Stokes equation (i.e., density and viscosity) are assigned at each time step based on the new position of the interface, which yields a sharp representation of the discontinuity in material properties without introducing artificial smearing (eqs. 2.8 and 2.9).

As discussed in section 2.3.1, the basic idea of ghost-fluid methods is to locally decouple a single multi-phase flow computation into multiple single-phase computations. One key advantage of this strategy is that the incompressibility constraint (eq. 2.2) can be used to simplify the viscous term

\[ \nabla \cdot (\mu(\phi)(\nabla \mathbf{v} + (\nabla \mathbf{v})^T)) = \mu(\phi)\nabla^2 \mathbf{v} \]  

which leads to a standard saddle-point problem

\[ \begin{pmatrix} -\mu(\phi)\nabla^2 & \text{grad} \\ -\text{div} & 0 \end{pmatrix} \begin{pmatrix} \mathbf{v} \\ p \end{pmatrix} = \begin{pmatrix} g\rho(\phi) \\ 0 \end{pmatrix} \]  

when ignoring the jump conditions. The three jump conditions, the pressure jump due to surface tension \([p]_{st}\), the viscous contribution to the pressure jump \([p]_v\), and
the jump in the stresses $[\nabla v]$, scale differently (see eqs. 2.12 and 2.13)

$$[p]_{st} \sim \kappa,$$
$$[p]_v \sim \nabla v, \text{ and}$$
$$[\nabla v] \sim \nabla v,$$

where $\kappa$ is the curvature of the interface. Since $[p]_{st}$ does not depend on the velocity field, it can be incorporated into the linear system 2.15 as a source term on the right hand side [133, 157]. The other two jumps, $[p]_v$ and $[\nabla v]$, however, need to be solved for at each time step (sec. 2.3.1) yielding the linear system

$$
\begin{pmatrix}
-\mu(\phi)\nabla^2 \text{grad} & [\nabla v] & [p]_v

-\text{div} & 0 & 0
\end{pmatrix}
\begin{pmatrix}
\nabla v \\
0 \\
0
\end{pmatrix} =
\begin{pmatrix}
\nabla v \\
0
\end{pmatrix}
- \begin{pmatrix}
[p]_{st}
\end{pmatrix}.
$$

It is worth mentioning that the three jump conditions are not equally challenging to resolve numerically. The easiest jump to compute is $[p]_{st} = \sigma \kappa$ because it does not depend on the velocity field and because the accurate computation of the curvature $\kappa$ is ensured by representing the interface through a level set function (sec. 2.3.2). The viscous contribution to the pressure jump

$$[p]_v = 2[\mu](\nabla u \cdot n, \nabla v \cdot n, \nabla w \cdot n) \cdot n,$$

and the stress jumps $[\nabla v]$ (eq. 2.13) are more challenging.

We note that in the presence of viscosity contrasts of several orders of magnitudes and/or jump conditions of several orders of magnitude, the condition number of the extended Stokes matrix in the linear system (eq. 2.19) can become a concern. Most computations in this chapter are based either on backslash or the direct solver PARDISO [245, 246]. In terms of iterative solvers, GMRES or stabilized BICG in combination with an incomplete-LU preconditioner seem to be reliable alternatives.
2.3.2 Level-set-based Interface solver

Interface-tracking methods can be divided into two classes, explicit and implicit. Before delving into the details, we attempt to offer an intuitive motivation for these two types of approaches following [254]: Suppose our task were to track the coastline of a lake that experiences strong variations with water level. One possibility would be to monitor the driftwood along the lake shore. However, if water-level variations were large and rapid and the lake-bed topography was rough, the driftwood would partly wash ashore and a large amount of driftwood would be necessary to obtain an accurate estimate of the coastline. The level set method takes a different approach. Instead of tracking the shore of the lake directly, we draw a topographic map of the lake bed. We adjust the datum of this map such that the coastline always corresponds exactly to the zero-elevation contour.

This example illustrates that instead of finding an explicit representation of the interface (i.e., placing markers along it), the level set method takes an implicit approach and embeds the interface into a higher-dimensional function (i.e., the topographic map) such that it corresponds to the zero-contour of that function. The main advantage of this implicit formulation is that geometric complexities of highly convoluted interfaces or topological changes resulting from merging or ripping of interfaces can be captured easily. Also, the approach generalizes in a straightforward manner to higher dimensions, contrary to some explicit front representations (e.g. marker chains) for which three dimensions represent a substantial challenge.

In a static problem, the only property required for the auxiliary higher-dimensional function is that its zero-contour must correspond to the real interface. In a seminal paper, [201] developed a framework for adding dynamics to implicit surfaces. Dynamics pose new constraints on the auxiliary higher-dimensional function. In particular, it turns out to be advantageous if the level set function is constructed as a signed distance function. This entails that it is negative in one fluid, positive in the other, and zero exactly at the interface. Furthermore, its absolute value at any point corresponds to the minimum distance of that point to the interface. Functions that fulfill
these properties will be referred to as level set functions denoted by $\phi$. From this definition it follows that a level set function $\phi$ is normalized

$$|\nabla \phi| = 1. \quad (2.21)$$

Given a velocity field $v$, the propagation of the level set function $\phi$ is described by the advection equation:

$$\frac{\partial \phi}{\partial t} + v \cdot \nabla \phi = 0, \quad (2.22)$$

also referred to as the level set equation [201]. Equation 2.22 shows that the level set method turns a Lagrangian front propagation problem into an Eulerian initial value partial differential equation. At this point we have intentionally not specified the nature of the velocity field $v$ in equation 2.22. One of our goals will be to construct an appropriate velocity field that maintains the signed distance property (eq. 2.21) as the level set function moves (sec. 2.3.3), while continuing to link the zero level set to the proper interface motion.

The numerical solution of equation 2.22 requires high-order schemes. For the spatial discretization we implement the 5th-order-accurate WENO scheme [158, 129, 128] and for the temporal discretization the 3rd-order-accurate, Total-Variation-Diminishing (TVD) Runge-Kutta scheme [260].

The time step used in the computation is restricted through the Courant-Friedrichs-Lewy (CFL) criterion associated with equation 2.22

$$\Delta t < \frac{\Delta x}{|v|_{\text{max}}}, \quad (2.23)$$

where $\Delta t$ and $\Delta x$ are the temporal and spatial grid spacing and $|v|_{\text{max}}$ is the maximum velocity. In the computations we typically use $\Delta t = 0.5 \, \Delta x/|v|_{\text{max}}$ unless convergence requires higher temporal resolution.
Figure 2-3: Initial and boundary conditions for the Rayleigh-Taylor instability as specified by [296]. The fluids are characterized by different densities $\rho_i$ and viscosities $\mu_i$. The level set function is constructed such that it is negative within the buoyant fluid and positive outside.

2.3.3 Coupling of the two solvers

Both the fluid (sec. 2.3.1) and the interface (sec. 2.3.2) solver are Eulerian and each is based on a Cartesian grid with the same grid resolution $\Delta x$. Thus, one might expect that the coupling of the two solvers should be straight-forward, which is only partially true. While the forward coupling of the new interface position into the fluid solver works in the obvious way (i.e. by updating eqs. 2.8 and 2.9), the coupling of the flow field back to the interface solver requires more subtlety in the context of level set methods.

Let us return to the question of which velocity field $\mathbf{v}$ to use in equation 2.22. Intuitively, the most obvious choice might be the physical velocity field resulting from the solution of the Stokes equation. However, as pointed out by [256], using the fluid velocity itself to update the level set function is often a poor choice, since it necessarily creates shearing and distortion of the level set function unless the strain tensor of the flow field vanishes. While possible, continuous restoration of the level set function through an iterative re-initialization procedure such as described by [282]...
leads to several numerical problems such as spurious mass loss and artificial front repositioning [5, 256, 43, 134]. A more detailed study of the potential bias introduced through iterative re-initialization is available in Appendix A.

The need to re-initialize the level set function is a consequence of choosing the physical velocity field for solving the level set equation 2.22, but this is certainly not the only valid choice. In fact, the velocity field used to advect the level set function need be that given by the physics of the problem only for the zero contour – not for any other contour. Thus, analogous to the procedure of embedding the interface into the higher-dimensional level set function, we are free to embed the velocity of the interface into a higher-dimensional velocity function, called the extension velocity field. It is constructed based on two criteria [5]: (1) The extension velocity at the zero contour has to be identical to the physical velocity, and (2) the extension velocity for all other points is chosen such that it ensures maintenance of the normalization criterion (eq. 2.21). It is straight-forward to show (e.g. [256]) that the normalization condition will be maintained if

\[ \nabla \phi \cdot \nabla v_{\text{ext}} = 0. \tag{2.24} \]

Numerically, we compute the extension velocity function as recommended by [5] through the fast-marching method [253, 255].

2.4 Benchmark problems

2.4.1 Pressure jump at the interface of a viscous drop

Surface tension causes pressure to jump at the interface of a spherical drop as can be derived either from thermodynamic free energy considerations or from the Young-Laplace equation. For a static drop of radius \( a \) and surface tension \( \sigma \) the pressure jump is given by

\[ [p]_{st} = \frac{2\sigma}{a}. \tag{2.25} \]
Figure 2-4: Computation of the pressure jump inside a static drop as a consequence of surface tension (benchmark problem 1). The Bond number (eq. 2.10) is set to $\Pi_3 = 10^{-3}$ to ensure sphericity of the drop. The viscosity contrast is $\Pi_1 = 10^{-6}$. The point-wise visualization of the pressure field illustrates the original resolution of the simulation ($51 \times 51$). The computational domain is a square box of aspect ratio 1.

This expression highlights that the effect of surface tension is small for medium-sized drops, but may become substantial as the drop radius decreases.

We investigate the pressure jump (eq. 2.25) both for the case of a static drop and that of a dynamic drop rising under its own buoyancy in a hydrostatic ambient pressure field. In the first case, the pressure jump should be given by a discontinuous step function; in the second case, there will be an additional contribution from the ambient pressure field. We use 'periodic' boundary conditions on the sides of the computational domain and 'no slip' on the top and bottom walls. The viscosity contrast is set to $\Pi_1 = 10^{-6}$ and the Bond number to $\Pi_3 = 10^{-3}$ to ensure sphericity.

2.4.2 Pressure jump for weak inclusions in pure shear

[250] derived analytical solutions for the pressure and velocity fields of elliptical inclusions that are subject to shearing. A viscosity contrast of several orders of magnitude
Table 2.1: Analytical versus numerical results for the pressure jump due to surface tension at the interface of a static drop. This computation was done dimensionally with $\sigma = 0.0728 \text{ kg/s}^2$ – a representative value for the air/water interface.

<table>
<thead>
<tr>
<th>$r$</th>
<th>$p_{st}$ in Pa (analyt.)</th>
<th>$p_{st}$ in Pa (numer.)</th>
<th>Deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 dm</td>
<td>1.456</td>
<td>1.458</td>
<td>&lt; 1%</td>
</tr>
<tr>
<td>1 cm</td>
<td>14.56</td>
<td>14.59</td>
<td>&lt; 1%</td>
</tr>
<tr>
<td>1 mm</td>
<td>145.6</td>
<td>146.0</td>
<td>&lt; 1%</td>
</tr>
<tr>
<td>0.1 mm</td>
<td>1456</td>
<td>1462</td>
<td>&lt; 1%</td>
</tr>
</tbody>
</table>

is assumed between the inclusion and the surrounding rock matrix. The shear boundary condition in combination with the viscosity contrast creates a discontinuous jump in stresses $\left[ \nabla \mathbf{u} \right]$ and pressure $\left[ p \right]$, as derived in eqs. 2.13 and 2.20.

We compute the pressure and velocity field around a circular inclusion of non-dimensional radius $r = 0.1$ inside a $1 \times 1$ computational domain. The boundary conditions in the far-field are set to pure shear with a strain rate of $\dot{\varepsilon} = 1$. The velocity at the four edges of the computational domain is computed analytically based on equations 23-26 in [250]. We investigate viscosity contrasts of $\Pi_1 = 10^{-3} - 10^{-6}$, where the inclusions is assumed to have the lower viscosity. The density is constant in both domains. We compare our computations both to the analytical solution and to the numerical results by [58].

### 2.4.3 Rayleigh-Taylor instability

[296] performed a careful benchmark study of the Rayleigh-Taylor instability. The dynamics are specified through the two non-dimensional numbers $\Pi_1$ and $\Pi_2$ derived in section 2.2. Here, we focus on the isoviscous case ($\Pi_1 = 1$). The dimensions of the computational domain are $[0, \lambda] \times [0, 1]$ where $\lambda = 0.9142$ is chosen such that a harmonic perturbation with wavelength $2\lambda$ yields the largest growth rate. The thickness of the buoyant layer is $d = 0.2$ and the initial deflection of the interface between the two layers is $w = 0.02 \cos(\pi x / \lambda)$. The boundary conditions of the box are assumed to be 'no slip' on the top and bottom of the box and 'reflective' on the side walls. These initial and boundary conditions for the Rayleigh-Taylor instability
are illustrated in Figure 2-3.

[296] defined four quantitative parameters characterizing the dynamics of the Rayleigh-Taylor instability: (1) the initial growth rate $\gamma$, which is computed based on the growth of the amplitude $h$ of the interface

$$h(t) = h(0)e^{\gamma t}, \quad (2.26)$$
evaluated at $t \simeq 0$, (2) the maximum of the root-mean-square velocity

$$v_{\text{rms}} = \sqrt{\frac{1}{V} \int_V \|v\|^2}, \quad (2.27)$$

where $V$ is the area of the computational domain, (3) the time $t(V_{\text{max}})$ at which the maximum root-mean-square velocity $v_{\text{rms}}$ is achieved, and (4) the relative entrainment $e$ of the source layer above a specified height $d = 0.2$

$$e = \frac{1}{\lambda d} \int_d^1 \Gamma \, dV. \quad (2.28)$$

2.4.4 Compositional plume

[173] studied the rise of a compositional plume from a free-slip surface both experimentally and through two-dimensional boundary-element simulations. The experiments were performed with colored corn syrup in colorless glycerine and are reported in terms of non-dimensional times [173]. The initial condition is a semi-spherical blob resting on the free-slip surface. In addition to the experimental and numerical data by [173], [247] presented a numerical solution to this problem in three dimensions.

The computational domain in our simulation is a rectangular box of non-dimensional size $4 \times 4 \times 5$. The initial condition is a semi-spherical blob of radius 1 placed in the center of the box. The density and viscosity contrasts between the two fluids are set to 0.15 and 1, respectively. The boundary conditions are 'periodic' on all four sides of the box and 'free slip' on the top and bottom wall. The 'free-slip' condition is implemented as $v \cdot n = 0$ and $\nabla v \cdot t_1 = \nabla v \cdot t_2 = 0$. 

60
2.5 Results

2.5.1 Pressure jump at the interface of a viscous drop

The linear dependence of the pressure jump \([p]_{st}\) on drop radius (eq. 2.25) is straightforward to reproduce numerically. Table 2.1 details a dimensional comparison of the analytical pressure jump based on equation 2.25 and our numerical results. An example computation of a static drop with Bond number \(\Pi_3 = 10^{-3}\) and viscosity ratio \(\Pi_1 = 10^{-6}\) in a constant ambient pressure field is shown in Figure 2-4. Despite the relatively low resolution of the computation \((51 \times 51)\), the pressure jump is resolved as a sharp discontinuity without artificial smearing or spurious oscillations. A more detailed convergence test for this case is included in Appendix A.

Figure 2-5 shows the equivalent computation for a dynamic drop rising under its own buoyancy. The Bond number (eq. 2.10) is set to \(\Pi_3 = 10^{-3}\) to ensure sphericity of the drop. The point-wise visualization of the pressure field highlights the original resolution of the simulation \((81 \times 121)\). The computational domain is a rectangular box of aspect ratio \(2 \times 3\). The pressure field is a combination of the discontinuous jump at the interface and the hydrostatic and dynamic contributions outside.
own buoyancy. The pressure field reflects the hydrostatic and dynamic contributions to pressure as well as the effect of surface tension. Contrary to Figure 2-4, we now not only observe a jump in pressure itself, but also a jump in the first derivative of pressure. We note that the dynamic case is more challenging than the static case, because it requires both approximating the static pressure jump correctly and maintaining it as a sharp discontinuity over time.

2.5.2 Pressure jump for weak inclusions in pure shear

Figure 2-7 shows the pressure field for a circular inclusion with a viscosity contrast of $\Pi_1 = 10^{-3}$ compared to the surrounding rock matrix. The left panel represents the numerical solution and the middle panel the analytical solution by [250]. Visually, there is no discernable difference between the numerical and the analytical solution. The right panel in Figure 2-7 shows the percentage error of the numerical with respect to the analytical solution. Not surprisingly, the highest error occurs at the interface, more specifically at finite inclinations with respect to the axes $x = 0$ and $y = 0$. This error is not unexpected given that the tangential component of the stress jump is not captured in a sharp manner, but instead smeared over the length of a grid cell (see section 2.6.1). At the given grid resolution of $280 \times 280$, the percentage error drops to below 1% in locations where only the normal component contributes to the stress jump as compared to a maximum percentage error of 3.7% where the tangential component contributes significantly. The average percentage error in the computational domain is $< 1\%$.

In comparison to a previous study of the inclusion problem [58], three aspects of our numerical solution merit attention: (1) Contrary to [58], there are no spurious pressure oscillations at the interface of the inclusion, not even at minimal resolution (Appendix A). This aspect is of greatest importance for dynamic problems as spurious oscillations tend to build up over time. (2) We are able to reproduce a sharp transition from a highly variable pressure field in the matrix to a constant pressure field inside the inclusion. We do not observe any artificial distortions to the constant pressure field inside the inclusion as is the case in [58]. (3) The overall error is lower in
Figure 2-6: The Rayleigh-Taylor instability at $t = 1500$ computed by the level set method on a $300 \times 330$ grid compared to the best results of the four codes compared in [296].
Our computation implying that less resolution is required to accurately resolve the pressure field. In fact, a grid resolution of $80 \times 80$ is sufficient to achieve a lower overall L2-error than the best performing method by [58] at a grid resolution of $280 \times 280$.

In comparison to benchmark problem 1 (sec. 2.5.1), our simulations confirm that the jump conditions $[p]_e$ and $[\nabla v]$ are more challenging to resolve than $[p]_{st}$ (sec. 2.3.1). As detailed in Appendix A, the additional challenge lies in computing the local magnitude of the jump along the interface correctly.

Table 2.2: Comparison of the quantitative parameters characterizing the dynamics of the isoviscous Rayleigh-Taylor instability.

<table>
<thead>
<tr>
<th>Code</th>
<th>Grid</th>
<th>Growth Rate</th>
<th>$t(\text{max } v)$</th>
<th>max $v$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Level sets</td>
<td>120x132</td>
<td>0.01252</td>
<td>211.2</td>
<td>0.00301</td>
</tr>
<tr>
<td>Marker chains</td>
<td>80x80</td>
<td>0.01225</td>
<td>207.05</td>
<td>0.00309</td>
</tr>
<tr>
<td>Marker chains</td>
<td>80x80</td>
<td>0.01207</td>
<td>210.75</td>
<td>0.00305</td>
</tr>
<tr>
<td>Tracers HS</td>
<td>81x81</td>
<td>0.01118</td>
<td>208.99</td>
<td>0.00309</td>
</tr>
<tr>
<td>Tracers CND</td>
<td>48x48</td>
<td>0.01106</td>
<td>208.5</td>
<td>0.00309</td>
</tr>
<tr>
<td>Field SK</td>
<td>160x160</td>
<td>0.01179</td>
<td>207.84</td>
<td>0.00289</td>
</tr>
</tbody>
</table>
2.5.3 Rayleigh-Taylor instability

We were able to reproduce the evolution of the Rayleigh-Taylor instability as specified by [296] to high precision. Figure 2-6 shows a comparison of the isoviscous Rayleigh-Taylor instability computed by five different codes. The top plot is our level-set-based code at a grid resolution of 300×330. A detailed convergence study is available in Appendix A. The other four plots are reconstructed based on the work published in [296]. The authors kindly made the data available online.

We observe the closest agreement of our results with those computed by the marker-chain method. A detailed comparison of the two interfaces is given in Figure 2-8. The temporal evolution of the root-mean-velocity $v_{\text{rms}}$ and the entrainment $e$ (Fig. 2-9) confirms the visual impression that the two methods match well. Table 2.2 provides an overview of the quantitative parameters characterizing the evolution of the instability, i.e. initial growth rate $\gamma$, maximum root-mean-square velocity, and the time $t(v_{\text{max}})$ at which it is achieved. The cited values are from Table 1 in [296]. The long-term evolution of the isothermal Rayleigh-Taylor instability in the non-isoviscous case is more challenging to resolve, not so much because of the viscosity contrast itself, but rather because of the fact that the interface thins out rapidly. Simulations of buoyancy-driven flow require a full two-way coupling of fluid and interface solver, implying that the minimal resolution required is determined by the thickness of the fluid film. Thus, the computational expense scales inversely with the minimal thickness of the fluid film. For additional details, please refer to Appendix A.

2.5.4 Compositional plume

Figure 2-10 gives snapshots of our three-dimensional simulation of an initially semi-spherical compositional plume rising from a free-slip surface. The computation was performed on a $40 \times 40 \times 50$ grid. The experimental results by [173] are included for comparison purposes in the background. Qualitatively, experimental and numerical results match well, with the possible exception of the initial condition. This slight deviation resulting from non-zero surface tension in the experiment has little conse-
Figure 2-8: Detailed comparison of the level set (thin black line) and the marker chain approach (thick grey line) for the isothermal and isoviscous Rayleigh-Taylor instability at nondimensional time $t = 1500$. The plotted interfaces represent a zoom onto the instability descending from the top downwards in the middle of the box. The two methods yield an almost identical interface.

sequence for the long-term evolution of the instability [173]. Our computations also agree well with prior numerical results by [173] and [247].

2.6 Discussion

2.6.1 Evaluation of the fluid solver

To our knowledge, the extended ghost-fluid-type discretization of the multi-phase Stokes equation presented in this study provides the first adaptation of a ghost-fluid-type scheme to the multi-phase Stokes equation. Benchmark problem 1 (sec. 2.4.1 and 2.5.1) demonstrates that our method is able to resolve the pressure jump resulting from surface tension acting at the interface of a spherical drop in both a static (Fig. 2-4) and a dynamic (Fig. 2-5) setting even at low grid resolutions (see Appendix A).

Benchmark problem 2 (sec. 2.4.2 and 2.5.2) establishes the ability of our ghost-fluid-type fluid solver to resolve a pressure jump of multiple orders of magnitude at the
Figure 2.9: Left: Evolution of the entrainment of the buoyant fluid over time as computed by the five different codes. Right: Evolution of the root mean square velocity of the interface over time as computed by the five different codes. The level set computation was done on a $160 \times 176$ grid.

interface of a circular inclusion. Contrary to previous methods [58], our numerical solution does not suffer from spurious pressure oscillations and introduces neither smearing in the pressure jump nor erroneous deviations from the constant pressure field inside the inclusion. In addition, the overall numerical error is lower implying that less resolution is required to obtain a satisfactory level of accuracy.

Another important difference between the regularization-type methods discussed by [58] and the ghost-fluid-type method developed in this study is how error scales with increasing viscosity contrast. While the accuracy of regularization methods typically decreases with increasing viscosity contrast, ghost fluid methods can handle viscosity contrasts of numerous orders of magnitude. The reason for this favourable scaling lies in the discretization of the jump conditions (eqs. 2.13 and 2.12): In both of these equations, the viscosity jump $[\mu]$ is separated out from the velocity-dependent contribution to the jump. Since the velocity-dependent contribution is not discontinuous at the interface, it can be approximated through finite differences and a larger viscosity contrast will not affect the accuracy with which this term is resolved. Consequently, the maximum percentage error of the computed pressure field is largely independent of the viscosity contrast so long as the condition number of the associ-
Figure 2-10: Three-dimensional benchmark computation for problem 3, a compositional plume rising from a free-slip surface. The grid resolution is $40 \times 40 \times 50$. The six snapshots of the dynamic evolution of the plume are shown for non-dimensional times 0, 8.4, 16.8, 25.2, 33.6, and 42. The experimental results by [173] are included as black and white reproduction in the background.

...ted linear system (eq. 2.19) does not render it un-solvable (please refer to Appendix A for more details). The absence of any signs of numerical diffusion and/or spurious oscillations is notable in Figure 2-5, Figure 2-7 and also in benchmark problems 3 and 4. The absence of numerical diffusion is largely related to the level set representation of the interface and will be discussed in that context (sec. 2.6.2). The formation and possible build-up of spurious oscillations as a consequence of dispersive errors is avoided through a combination of three tools: (1) the construction of more accurate, ghost-fluid-based stencils in the immediate vicinity of the interface (sec. 2.3.1), which reduce dispersive error and implicitly enforce the jump conditions in the flow field,
(2) the level set representation of the interface in combination with the extension-velocity-based advection of the level set function (sec. 2.6.2 for more details) and (3) the usage of Total-Variations-Diminishing (TVD) discretization schemes for the level set advection (eq. 2.22).

Overall, we conclude that our extended ghost-fluid-type method is a useful new tool for geodynamics, specifically for problems involving large viscosity contrasts and interfaces at which pressure and stresses may jump discontinuously. We note that the tangential component in the stress jump is not resolved equally well as the normal component, but the error introduced by that inaccuracy is typically small to negligible, particularly in the context of buoyancy-driven flow.

2.6.2 Evaluation of the interface solver

The appeal of benchmark problem 3, the isothermal Rayleigh-Taylor instability by [296] (sec. 2.4.3 and 2.5.3), is that it allows for a direct comparison of the various strategies for representing interfaces (sec. 2.3.2). Out of the four other approaches, we find the poorest agreement with the results obtained by the field approach (Fig. 2-6). The field method works by tracking a characteristic function $F$, usually referred to as the composition function, which is zero on one side of the interface and one on the other. The advective-transport equation is solved for the time evolution of this composition function. This is a straightforward method, in part because it is naturally adaptive – the front is defined on the same Eulerian mesh used in the computation – and also because it easily extends to three dimensions. However, the advective update of a discontinuous function can be problematic since considerable artificial smoothing can occur due to numerical diffusion in the composition function update (e.g. the supposedly sharp interface has spread out into a fictitiously continuous transition between the two fluid phases in Fig. 2-6). Furthermore, the advection of a discontinuous function is prone to dispersive errors, which result in spurious oscillations. Consequently, most implementations smear out the interface over several grid cells, thereby compromising the accuracy with which the fluid dynamics in the vicinity of the interface are resolved. Thus, one is often led to a higher grid resolution than desired in
Figure 2-11: Setup and results for an example computation highlighting the differences between tracer- and level-set-based approaches for tracking dynamic interfaces. (top) The velocity field is constructed such that the square gradually shrinks onto its center. The sides move inward with velocity 1, the velocity along the main diagonals is set to $\sqrt{2}$, and a cosine taper is used to smooth the transition between these two values. The interface is tracked simultaneously using a level set function, which is illustrated in gray ($\phi < 0$) and white ($\phi > 0$), and 10 000 tracers placed on the initial interface which form a black line in the plot. (bottom) The interface position using (left) a level set function versus (right) tracers. While the level set function correctly outlines a square diminished in size, the tracers have formed spurious tentacles along the edges of the square.
Figure 2-12: Zoom onto the isothermal and isoviscous Rayleigh-Taylor instability specified by [296] at time $t = 1500$. In this computation, the interface is tracked simultaneously by a level set function (in grey/white) and by tracers (black line). We only plot the tracers for the lower segment of the interface to highlight the difference between the two interface-representation techniques. In the tracer-based computation, we observe the formation of a thin, elongated peak, reminiscent of the tentacles observed at the edges of the collapsing square in Fig. 2-11.

order to ameliorate the smoothing. Nonetheless, dispersive errors commonly prevail even for smeared interfaces (e.g. [48], [295]). While remedies correcting the consequences of numerical diffusion (e.g. [8]) and dispersion exist (e.g. [152]), we choose to focus on and construct numerical approaches which keep the interface sharp, thus avoiding both the smearing and artificial attempts to 're-sharpen' it. The level set method (sec. 2.3.2) avoids numerical diffusion of discontinuities, because it supersedes the advection of a discontinuous function. Instead, the advection equation (eq. 2.22) is solved for the higher-dimensional level set function, which will not result in numerical diffusion because the level set function has slope one by construction (eq. 2.21).

The evaluation of the differences between the interface as computed through level sets and that obtained from the two particle or tracer methods (see Fig. 2-6) is subtle. Tracer approaches differentiate between two fluids by placing a large number of
Lagrangian particles in one or both of the phases (e.g. [191, 86, 87]). While this Lagrangian representation of compositional differences is attractive for its avoidance of the numerical-diffusion problems of field approaches and its maintenance of mass conservation, the tracer method is prone to 'sampling errors': Although the fluid velocity is typically computed on an underlying mesh, evolving marker particles can create unreal and non-physical subgrid results, far below the actual accuracy of the computation, and these can create misleading and non-existent fingering, as well as thin, sub-cell structures. These structures result from the use of interpolation functions to move the sub-grid markers. An additional difficulty is that there is no natural adaptivity to this approach. Particles must be added and subtracted as the interface stretches, shrinks, and contorts. Finally, three-dimensional implementations become computationally very expensive, because a large number of particles is required to obtain sufficient accuracy. For example, [247] estimated that an increase of tracer particles on the order of $10^3$ is necessary when adding another dimension to a previously two-dimensional problem. As a remedy to this problem, [283] suggested using a so-called 'tracer ratio' method, but computational efficiency remains a concern even then [156].

It is often regarded as one of the advantages of particle approaches that they can provide sub-grid resolution. After all, both implementations of the particle method presented in [296] find an elongated fine-scale structure accompanying the instability sinking in the center of the computational domain. However, there is also ample fine-scale structure that differs for the two approaches (see Fig. 2-6). An example illustrating how tracer-based interface tracking can lead to the formation of spurious fine-scale structures at the interface is shown in Figure 2-11. A collapsing square is tracked simultaneously through a level set function (displayed in grey/white) and 10 000 tracers located on the initial interface (Fig. 2-11, top). While the level set function yields a correct approximate solution, the tracers have formed long tentacles at the edges of the square (Fig. 2-11, bottom). This well-known behavior of tracer approaches is related to the fact that tracers move with the local velocity while imbedded surfaces (e.g. fluid interfaces) move with the local fluid velocity in the
normal direction. Despite the tracer method's appeal to indicate possible fine-scale structures, subgrid resolution comes at the risk of not being able to distinguish a geophysical structure from a numerical artifact. Figure 2-12 highlights the challenges associated with tracking deforming interfaces accurately. It shows a computation in which we track the evolution of the isoviscous Rayleigh-Taylor instability [296] simultaneously via level sets and tracers. In order to highlight the part of the interface where the two solutions differ, we only plot the tracers on the lower segment of the interface. Although the underlying resolution at which the equations of motion are solved is identical by construction, the tracer-based interface shows a thin tentacle, while the same structure on the level-set-based interface remains much less elongated. For a more detailed discussion of subgrid structures, please refer to Appendix A.

Finally, marker-chain approaches track the interface by linking together a chain of particles. Contrary to the tracer method, these particles are only placed directly on the interface. This reduces computational cost, while keeping the advantage of
the tracer method, namely its relative non-diffusivity. We note that the marker-chain solution to benchmark problem 3 is almost identical to our level-set-based results (Figs. 2-6 and 2-8) and that the thin tentacle accompanying the center instability is smaller than for both tracer approaches. The main challenges of the marker-chain method are the geometric intricacies related to its three-dimensional implementation, in which one is required to track an evolving two-dimensional mesh of linked fluid particles. While possible, adaptive algorithms for grid refinement and simplifications are required [247]. Overall, we conclude that the three main advantages of an interface solver based on the level set method are that: (1) It is naturally adaptive and able to handle strongly deforming interfaces and topological changes in the interface (i.e. rupturing or merging) without compromising accuracy or increasing computational cost. (2) It is computationally efficient and maintains this efficiency even for very complex interfaces and in three dimensions (Fig. 2-10). In the computations for benchmark problems 3 and 4, only about 5% of the computational time at each time step is spent on advecting the interface. Since less computational effort is required for the interface solver, more resources are available for the more accurate solution of the equations of motion. (3) Level sets propagate like surfaces with the local fluid velocity normal to the interface and avoid many problems commonly encountered in explicit approaches as illustrated in Figure 2-11.

2.6.3 Coupling of the solvers

The level set method avoids many problems commonly associated with tracking dynamic interfaces (sec. 2.6.2) as long as the normalization of the level set function (eq. 2.21) is maintained throughout the computation. In our implementation, the coupling between fluid and interface solver is facilitated by the fact that both solvers are based on the same grid. As a consequence, we will not resolve any subgrid features in our computations. In fact, if one of the fluids is thinned out to below grid resolution, mass loss will occur. This is illustrated in Figure 2-13. It shows a single computational cell spanned by four grid points located in the corners. In this constellation the level set function is positive $\phi > 0$ at all grid points. Thus, the piece
of grey fluid shown will be added to the white fluid in the next computational step, resulting in mass loss in the grey phase. We stress that this mass loss is an indication of insufficient resolution in the computation. In fact, mass loss is closely related to the accumulation of numerical error and can thus be used to evaluate numerical error over the course of the simulation. We monitor mass balance throughout our computations. For an example of the evolution of the mass balance over time, please refer to Appendix A. We note that the level set method has been extended for problems in which the passive tracking of subgrid features might be desirable \cite{70, 71}, but since these are not relevant for buoyancy-driven problems, we will not discuss them further.

2.7 Conclusion

The combination of three complementary methods, the ghost-fluid, level set, and extension velocity methods yields a versatile and accurate method for simulating buoyancy-driven flow in the presence of large viscosity contrasts. Each of the three components targets one of the main challenges associated with the numerical description of complex flows, namely (1) the solution of the multi-phase Stokes equation in the presence of discontinuities in the coefficients, solution, and source terms, (2) the accurate advection of a dynamically deforming interface such that no restrictions on interface geometry are imposed, and (3) the full and accurate coupling of fluid and interface solver while ensuring that discontinuities remain sharp over time and that mass is conserved in both phases. We validate our approach through four carefully selected benchmark problems in both two and three dimensions. We find excellent agreement in all four cases. Deviations from results obtained with different interface-representation techniques, as for the isothermal Rayleigh-Taylor instability by \cite{296}, are not unexpected and explained by methodological differences.

Based on its methodology and performance for the selected benchmarks, we argue that our method is particularly interesting for the following types of geodynamical problems: (1) Problems that are characterized by sharp discontinuities in material parameters, pressure, stresses, or a source term. An example could be compositional
plumes impinging on the lithosphere or a compositional discontinuity in the Earth's mantle. (2) Flow for which surface tension needs to be taken into account, such as magma bubbles (e.g. [170, 171]). (3) Problems with strongly and/or rapidly deforming interfaces such as multiple plume overturn in the Earth's mantle or lava-dome formation [28].
Chapter 3

Bubble dynamics in basaltic volcanoes and ramifications for modeling normal Strombolian activity

3.1 Introduction

Many basaltic volcanoes erupt substantial amounts of gas while expelling comparatively little degassed magma. This observation suggests that gas segregation must have occurred prior to eruption and warrants attributing the existence of explosive basaltic volcanism to the presence of exsolved volatiles. Since the exsolution of gas is largely suppressed in the case of sufficiently deep sea-floor volcanism, explosive basaltic activity should be very rare at mid-ocean ridges [108] and expected to occur primarily at subaerial volcanoes, in agreement with observations.

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Substantial progress has been made in understanding the early stages of eruptions in basaltic volcanoes, i.e., bubble nucleation and growth (e.g. [274, 176, 123, 292, 85, 192, 219]), and its late stages, i.e., fragmentation (e.g. [275, 175, 204, 327, 277, 196]). However, the complex fluid dynamical interactions that may arise between these two stages still pose many open questions [94].

This study complements prior work [170, 172, 171] by not only examining two-phase flow in the Stokes, but also in the Navier-Stokes regime at low to moderate Reynolds number (Re). Analyzing flow behavior at finite Re is of interest for Strombolian-type eruptions because inertia is not generally negligible. Inertial effects become important because of (1) the low viscosity of basaltic magma as compared to more silicic counterparts and (2) the high rise speed of gas pockets in the meter range, which are thought to cause normal Strombolian activity [25, 300, 301, 302, 104].

Refining our understanding of bubble dynamics in basaltic flow is important to (1) inform the interpretation of vesicle morphology and bubble size distributions observed in thin sections and the conclusions drawn for the flow conditions at quenching, (2) identify meaningful assumptions about interface dynamics used in two-phase-flow models, which refrain from resolving the gas-magma interface directly, and (3) verify how the gas dynamics observed in laboratory experiments change at scales representative of volcanic systems. We devote special attention to identifying the ramifications of our results for the two commonly used models of explosive basaltic volcanism, the Rise-Speed-Dependent (RSD) model pioneered by [321] and the Collapsing-Foam (CF) model [303, 125, 126].

Both models agree in relating normal Strombolian style eruptions to the presence of a segregated gas phase. More precisely, both models assume that normal Strombolian activity is caused by the bursting of large gas slugs at the free surface, an idea pioneered by [25] and refined in a large number of subsequent studies. They differ, however, in the presumed location where this gas slug is thought to form. The CF model assumes that gas accumulation occurs in the magma chamber or, more generally, under a large roof area in the conduit, implying that the gas slug originates at moderate to great depth and ascends stably through the volcanic conduit.
Figure 3-1: Dependence of the three main non-dimensional domains on bubble radius and magma viscosity. We assume a magma density of $\rho_f = 3500 \text{ kg/m}^3$ and a surface-tension coefficient of $\sigma = 0.3 \text{ N/m}$. The boundary of regime 1, characterized by spherical bubbles and negligible inertia, is determined only by the size of the bubbles, because Bo does not depend on magma viscosity (see eq. 3.13). Regime 2, in which bubbles become deformable but inertia remains negligible, only exists at sufficiently high viscosity, $\mu \geq 3 \text{ Pa-s}$.

In contrast, the RSD model asserts that the gas slug forms gradually during ascent through a cascade of coalescence, implying that slug formation occurs at comparatively shallow depth. To compare these contrasting views and to verify the regimes for which they are applicable, we investigate the following two questions numerically: (1) How likely is a coalescence cascade, as suggested by the RSD model, and under which conditions could interactions between multiple bubbles lead to coalescence and formation of a single large gas slug? (2) How likely is it that large pockets of gas can ascend stably over long distances, as suggested by the CF model, and under which circumstances is that to be expected?
3.2 Governing equations and scaling analysis

The flow in each domain (i.e. gas and magma) satisfies the Navier-Stokes equation

\[
\rho \left( \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{v} \right) = -\nabla p + \nabla \cdot [\mu (\nabla \mathbf{v} + (\nabla \mathbf{v})^T)] + \rho \mathbf{g} .
\]  

(3.1)

and the incompressibility constraint

\[
\nabla \cdot \mathbf{v} = 0.
\]  

(3.2)

Throughout the chapter we denote the velocity field by \( \mathbf{v} = (u, v, w)^T \), the pressure by \( p \), the density by \( \rho \), the dynamic viscosity by \( \mu \), and the gravitational acceleration by \( \mathbf{g} \). The boundary conditions at the gas-magma interface are a discontinuous step in both density

\[
\rho(\phi) = \begin{cases} 
\rho_g & \text{for } \phi < 0 \\
\rho_f & \text{for } \phi \geq 0 ,
\end{cases}
\]  

(3.3)

and viscosity

\[
\mu(\phi) = \begin{cases} 
\mu_g & \text{for } \phi < 0 \\
\mu_f & \text{for } \phi \geq 0 ,
\end{cases}
\]  

(3.4)

where the subscripts refer to either 'gas' or 'fluid' and \( \phi \) is the level set function used to represent the interface (see chapter 2).

Additionally, the jump condition at the interface needs to be fulfilled:

\[
\begin{bmatrix}
\mathbf{n} \\
\mathbf{t}_1 \\
\mathbf{t}_2
\end{bmatrix}
\left( \rho I - \tau \right) \mathbf{n}^T = 
\begin{bmatrix}
\sigma \kappa \\
0 \\
0
\end{bmatrix} ,
\]  

(3.5)

where \( I \) is the unit matrix, \( \sigma \) the surface tension, \( \tau \) the stress tensor, \( \kappa \) the curvature of the interface, and \( \mathbf{n}, \mathbf{t}_1, \mathbf{t}_2 \) the normal vector and the two tangential vectors to the interface moving with the local fluid velocity.

Using the sign of the level set function \( \phi \) as an indicator for the two different phases in the manner defined above (eqs. 3.3 and 3.4), we combine the governing
equations for the two phases into one

\[ \rho(\phi) \left( \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} \right) = -\nabla p + \nabla \cdot \left[ \mu(\phi) \left( \nabla \mathbf{v} + (\nabla \mathbf{v})^T \right) \right] \]

\[ + g \rho(\phi) - \sigma \kappa(\phi) \delta(\phi) \mathbf{n} \]  

(3.6)

where the delta function \( \delta(\phi) \) implies that surface tension only acts at the interface.

The two-phase flow systems investigated here span a wide range of fluid dynamical regimes. In order to non-dimensionalize the governing equation (eq. 3.6), we define the following set of characteristic scales

\[ x = a x', \quad v = v_0 v', \quad t = a t', \quad p = v_0^2 p', \quad \rho = \rho \rho', \]

\[ \mu = \mu_f \mu'. \]  

(3.7)

where \( v_0 \) denotes the rise speed of the bubble or gas pocket, \( a \) the radius of the bubble, and \( \mu_f \) the viscosity of the magma. Substituting these characteristic quantities into equation 3.6, rearranging, and dropping the primes yields the non-dimensional multiphase Navier-Stokes equation

\[ \rho(\phi) \left( \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} \right) = -\nabla p + \frac{1}{\text{Re}} \nabla \cdot \left[ \mu(\phi) \left( \nabla \mathbf{v} + (\nabla \mathbf{v})^T \right) \right] \]

\[ + \frac{\rho(\phi)}{\text{Fr}} \hat{z} - \frac{1}{\text{We}} \kappa(\phi) \delta(\phi) \mathbf{n}, \]  

(3.8)

where \( \hat{z} \) denotes the unit vector in vertical direction. The boundary and jump conditions are non-dimensionalized accordingly.

Equation 3.8 highlights that the relevant non-dimensional numbers are

\[ \text{Re} = \frac{\rho_f v_0 a}{\mu_f} \quad \text{(Reynolds number)} \]  

(3.9)

\[ \text{Fr} = \frac{v_0^2}{g a} \quad \text{(Froude number)} \]  

(3.10)

\[ \text{We} = \frac{\rho_f a v_0^2}{\sigma} \quad \text{(Weber number)} \]  

(3.11)

\[ \Pi_1 = \frac{\mu_f}{\mu_g} \quad \text{(viscosity ratio)} \]  

(3.12)
In the special case where \( \text{Re} = 0 \), the non-dimensional groups determining the dynamics of the system reduce to the Bond or Eötvös number

\[
\text{Bo} = \frac{\Delta \rho g a^2}{\sigma}
\]  

(3.13)

and \( \Pi_1 \) as defined previously. We use the variable \( \Pi \) to denote non-dimensional numbers, which do not bear specific names. In section 3.4, we introduce additional non-dimensional ratios to characterize the initial condition, the relative position, and the size ratio of two bubbles.

The non-dimensional numbers (eqs. 3.9, 3.10, 3.11, and 3.13) have intuitive physical interpretations: \( \text{Re} \) is a measure of the relative importance of inertia to viscous forces. \( \text{Fr} \) is the ratio of inertia to buoyancy forces and \( \text{We} \) the ratio of inertia to surface tension. \( \text{Bo} \) is used to quantify the degree to which bubbles are able to deform in the Stokes regime. It corresponds to the ratio of viscous to surface tension forces, such that \( \text{Bo} \gg 1 \) describes the case in which surface tension becomes largely negligible, resulting in extreme bubble deformability. In the special case of buoyancy-driven flow, the Capillary number \( \text{Ca} \) is identical to \( \text{Bo} \), which can be seen when substituting the Stokes rise speed into the expression for \( \text{Ca} \), yielding \( \text{Ca} = \frac{\mu v}{\sigma} = \frac{\Delta \rho g a^2}{\sigma} = \text{Bo} \).

A wide range of flow regimes may arise in basaltic volcanism, because both the bubble radius and the viscosity of basaltic magma may vary by several orders of magnitude. The three main non-dimensional regimes are illustrated in Figure 3-1. They are characterized by gas bubbles that are (1) spherical with negligible inertia (\( \text{Bo} < 1 \) and \( \text{Re} < 1 \)), (2) deformable with negligible inertia (\( \text{Bo} > 1 \) and \( \text{Re} < 1 \)), and (3) deformable with non-negligible inertia (\( \text{Bo} > 1 \) and \( \text{Re} > 1 \)). In the interest of completeness, we note that a non-dimensional regime defined by (\( \text{Bo} > 1 \) and \( \text{Re} < 1 \)) is conceivable theoretically, but of little relevance in a geophysical context, because it would imply an unrealistically low magma viscosity. All simulations presented in this chapter were computed on a Cartesian grid using finite differences. The grid resolution of the computations is included in the respective figure captions and corresponds to the number of grid cells in the \( x \)-, \( y \)-, and \( z \)-direction, if applicable. Detailed
Figure 3-2: Wavelength-dependence of the growth rate $n$ over a wide range of magma viscosities $\mu_f = 1$, 10, 100, and 1000 Pa·s. The other parameters used in the computation are $\rho_f = 3500$ kg/m$^3$, $\rho_g = 1.226$ kg/m$^3$, $g = 9.81$ m/s$^2$, and $\sigma = 0.3$ N/m. The vertical grey line delimits the stable size range $a < \lambda_{cr}$. The grey dots indicate the fastest growing wavelength for a specific $\mu_f$ from the approximative expression for $\lambda_{max}$ (eq. 3.19) that is only valid at large viscosities.

convergence tests are included in Appendix B. In the Stokes regime, we employ our recently developed method for resolving buoyancy-driven interface dynamics in the presence of large viscosity contrasts described in chapter 2. Our Navier-Stokes solver is based on the projection method pioneered by [44], combined with a ghost-fluid-based representation of the material discontinuities and jump conditions [133, 157]. An abbreviated description of the discretization scheme can be found in Appendix B.

### 3.3 Theoretical estimates of bubble breakup

Theoretically, one would expect that the stable size of gas bubbles in stagnant fluids should be limited, because the stabilizing effect of surface tension on the bubble surface decreases rapidly with increasing bubble radius and because the large density
contrast between gas and magma will cause perturbations to grow by a Rayleigh-Taylor instability. The latter tendency is counteracted by viscous forces slowing the rate of growth of unstable interfacial waves (e.g. [20, 96]).

A disturbance of wavelength \( \lambda \) on the bubble surface will be suppressed by surface tension if \( \lambda \) is smaller than the critical value

\[
\lambda_{cr} = 2\pi \sqrt{\frac{\sigma}{g \Delta \rho}}.
\]  

(3.14)

Thus, \( \lambda_{cr} \) provides a lower bound for identifying potentially unstable wavelengths. A reasonable upper bound is half the circumference of the fluid particle

\[
\lambda_{up} = \pi a,
\]  

(3.15)

because a surface perturbation cannot exceed the bubble itself in size [96]. Together, \( \lambda_{cr} \) and \( \lambda_{up} \) yield an estimate of the maximum stable bubble radius

\[
a_{cr} = 2 \sqrt{\frac{\sigma}{g \Delta \rho}},
\]  

(3.16)

implying that gas bubbles with radii in the mm-range or larger (\( a > a_{cr} \)) would be prone to breakup in basaltic liquid if the effect of viscosity was neglected.

For small accelerations, Rayleigh-Taylor instabilities form only when a more dense fluid overlies a lighter one. Hence, it is the leading surface of the bubble where the first indentation of wavelength \( \lambda > \lambda_{cr} \) forms. Splitting of the bubble, however, requires that this indentation grows fast enough to reach the trailing surface of the bubble before it is swept around to the equator of the bubble and stops growing through a Rayleigh-Taylor instability [49, 96]. Growth of a disturbance occurs in several stages. During the early phase, while the amplitude of a disturbance is small with respect to its wavelength \( \lambda \), growth is exponential and characterized by growth rate \( n \). We assume that breakup only occurs if the instability reaches the base of the bubble during its exponential growth period. It follows that the maximum stable bubble size can be estimated by requiring that the time available for growth, \( t_a \), exceeds that
required for growth, \( t_g \) [96].

The time available for growth, \( t_a \), depends on how fast a Rayleigh-Taylor instability in the center of the leading bubble surface is swept outwards by viscous forces. The tangential velocity of the perturbation is determined by the terminal velocity of the bubble [96] yielding the approximate expression

\[
t_a \approx \frac{a}{v_0} \ln \left( \cot \left( \frac{\lambda}{8a} \right) \right)
\]  

(3.17)

in the limit of \( \mu_f \gg \mu_g \) and for \( \lambda_{cr} < \lambda < \lambda_{up} \). We estimate the terminal velocity in eq. 3.17 based on the empirical correlations summarized in [96].

The time required for growth, \( t_g = 1/n \), depends on viscous damping of the interfacial waves and may be estimated, to a first approximation, from linearized stability theory (e.g. [20]). For magmatic systems where \( \mu_f \gg \mu_g \), we can use the simplified expression [215]

\[
n^2 + 2 \frac{\mu_f}{\rho_f} k^2 n - \frac{\Delta \rho}{\rho_f + \rho_g} g k + \frac{\sigma k^3}{\rho_f + \rho_g} = 0, 
\]  

(3.18)

where \( k = 2\pi/\lambda \) is the wavenumber. Figure 3-2 summarizes the numerical solutions of equation 3.18 over several orders of magnitude in \( \mu_f \). The dashed vertical line delimits the stable size regime where \( a < \lambda_{cr} \). The grey dots indicate the surface wavelength which is expected to grow fastest for a given magma viscosity based on the approximative approach by [215]

\[
\lambda_{max} = 4\pi \left( \frac{\mu_f^2}{\rho_f^2} \frac{\rho_f + \rho_g}{g \rho_f - \rho_g} \right)^{1/3}. 
\]  

(3.19)

[96] compared experimentally observed and theoretically predicted breakup times and concluded that gas bubbles rising through stagnant fluid break up if \( t_a > 3.8t_g \). Although their analysis was performed at much lower viscosities, we adopt this empirical criterion to estimate the maximum stable bubble radius for a wider range of magma viscosities (see Table 3.1). Given the semi-empirical nature of the model and the
simplifications it is based on [16], the values in Table 3.1 should be treated with some caution. For a detailed comparison of theoretical and computed bubble sizes see sec. 3.5.

3.4 Simulations

3.4.1 Modeling approach

The main objective of our study is to analyze bubble dynamics in basaltic conduits in which flow is driven primarily by gas. Since bubble ascent is only dynamically important if the bubble rise speed is large relative to the characteristic flow speed in the surrounding fluid, we only consider stagnant fluids in our computations. Our numerical model is set up as follows. First, we do not consider bubble nucleation or diffusive growth of the gas bubbles. This simplification is motivated by the fact that fluid dynamical interactions between bubbles become most relevant once the bubbles have reached sufficiently large radii to deform (Bo > 1) (see also [170, 171]). At this stage, diffusive bubble growth (limited by the initial volatile content and the bubble number density) is thought to have slowed substantially and starts to come to a halt: For an initial water content of 0.5 wt.%, [274] estimated a maximum bubble radius of ~5 mm. Similarly, [220] obtained a maximum size of 6-8 mm for bubbles originating from magma with 1.52 - 3.03 wt.% water. Decompression growth is incorporated in our model (see eq. 3.8). Second, all of our simulations are isothermal, because our computational domain is only several bubble radii in size. On such small spatial scales, temperature is typically not expected to vary dramatically. In addition, we note that (1) [274] demonstrated that the expansion of gas bubbles by decompression can be approximated as an isothermal process due to a balance of cooling resulting from work done in expanding and conductive heat transfer and (2) that a vertical temperature gradient is unlikely to have an important effect on bubble stability [232].

Third, we assume flow to be incompressible in both the liquid magma and the gas. Although gas compressibility plays a significant role for the dynamics on the
Table 3.1: Theoretical prediction of the maximum stable bubble radius $a_{\text{max}}$ in basaltic magma of different viscosities $\mu_f$. Additional parameters used in the computation: $\rho_f = 3500 \text{ kg/m}^3$, $\rho_g = 1.226 \text{ kg/m}^3$, $g = 9.81 \text{ m/s}^2$, surface tension $\sigma = 0.3 \text{ N/m}$, and viscosity ratio $10^{-6}$.

<table>
<thead>
<tr>
<th>Magma viscosity $\mu_f$ [Pa·s]</th>
<th>Maximum bubble radius $a_{\text{max}}$ [m]</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>0.06</td>
</tr>
<tr>
<td>25</td>
<td>0.12</td>
</tr>
<tr>
<td>50</td>
<td>0.18</td>
</tr>
<tr>
<td>75</td>
<td>0.24</td>
</tr>
<tr>
<td>100</td>
<td>0.29</td>
</tr>
<tr>
<td>250</td>
<td>0.53</td>
</tr>
<tr>
<td>500</td>
<td>0.84</td>
</tr>
<tr>
<td>750</td>
<td>1.10</td>
</tr>
<tr>
<td>1000</td>
<td>1.33</td>
</tr>
</tbody>
</table>

length scale of the entire conduit, its effect at the scale of the bubble radius is small. Very large gas pockets are possible exceptions and our simulations might underestimate their expansion. While further study is needed to anticipate the dynamic consequences in detail, two recent numerical studies [53, 217] indicate that taking the gas compressibility into account will tend to destabilize gas bubbles. Thus, our estimates of maximum bubble size and breakup time are likely upper-bound estimates.

Fourth, we assume that both the volatile phase and the surrounding basaltic magma have Newtonian rheology (sec. 3.2). For the gas phase, this assumption is straightforward. The Newtonian behavior of basaltic melts has been well-established from experiments (e.g. [258, 241]). Rheological complexities arising from the presence of gas bubbles in the melt are fully resolved in our simulations. The effect of crystals, however, is only included by defining an effective viscosity, which implies that the crystals are assumed to be small compared to the bubbles.

Finally, by basing our simulations on the Navier-Stokes equation, we model both phases as continua. Molecular interactions such as the effect of surfactants (i.e. 'surface active agents') are not resolved. Although they may play an important role just prior to coalescence or breakup, their properties are essentially unknown for gas bub-
Figure 3-3: Overview of the non-dimensional regime covered by the 95 simulations (black dots) constraining the stability of isolated gas bubbles at Re \(> 1\) (sec. 3.4.2). The grey shading delimits the domain in which we observe breakup in two dimensions. A comparison with the shape regimes for bubbles during buoyant ascent [95] confirms that we reproduce the expected steady-state shape correctly in our computations. Note that we did not perform simulations for low Bo and high Re, because that case is of little relevance for basaltic magmas.

In the absence of resolving the details of the molecular interactions upon microscopic approach of two interfaces, we 'define' coalescence to occur in our simulations once the distance between two interfaces has decreased to below grid resolution \(\Delta x\). This coalescence condition is corroborated by field studies that have shown that thin magmatic films become unstable in the \(\mu m\) range [136].

Before proceeding to the specific setup of our simulations, a few comments on comparing simulations with different dimensions might be in order. We argue that there is a merit in performing both two- and three-dimensional computations. While simulations in three dimensions are appealing for being a more realistic representation of the physical problem at hand, two-dimensional simulations offer the possibility of resolving the dynamics with greater accuracy because they can be performed at higher numerical resolution. However, caution is advised in comparing interface dynamics in two and three dimensions, not only because of differences in the flow field (the direct
three-dimensional analogue of a two-dimensional bubble is a cylinder of infinite extent, not a sphere), but also because surface energy scales as $\sim ML/T^2$ in two dimensions and as $\sim ML^2/T^2$ in three dimensions. Kinetic energy on the other hand, scales as $\sim ML^2/T^2$ in both cases. Thus, the scaling of a fluid dynamical system might differ notably between two and three dimensions.

### 3.4.2 Stability analysis of isolated gas bubbles

We investigate the shape and stability of an isolated gas bubble rising in basaltic magma over the three non-dimensional regimes identified in Figure 3-1. The boundary conditions are 'no-slip' on top and bottom and 'periodic' on the sides, implying that an infinite number of bubbles are juxtaposed in the conduit. The viscosity ratio is set to $\Pi_1 = 10^{-6}$ in all simulations.

The setup of the computation implicitly assumes that the gas flux in the conduit is low enough for isolated gas bubbles to exist in the flow. The maximum gas flux to which this scenario applies is approximately given by the gas flux in the modeled computational domain. Out of the three types of simulations considered in this study, the case of isolated gas bubbles implies the lowest overall gas flux.

### 3.4.3 Impact of multibubble interactions on stability and interface dynamics

The second sequence of simulations aims at constraining the role of the dynamic interaction between multiple bubbles on coalescence, breakup, and deformation over the three non-dimensional regimes in Figure 3-1. In addition to the non-dimensional numbers derived in sec. 3.2, we use the bubble size ratio $\Pi_2 = a_1/a_2$ and the non-dimensional separation distances in vertical and horizontal direction, $\Pi_3 = d_z/a_1$ and $\Pi_4 = d_x/a_1$, to characterize the different initial conditions. We focus on interactions between bubbles that are comparable in size, i.e. $\Pi_2 = O(1)$. If the radius of one of the bubbles is significantly larger than the other, the large difference in rise speed will limit the time scale of interaction. Similarly, we consider sufficiently small separation
distances, i.e. $\Pi_3 = O(1)$ and $\Pi_4 = O(1)$. Analogous to the case of an isolated bubble, we use 'periodic' boundary conditions on both sides and 'no-slip' on top and bottom. Due to the presence of multiple bubbles in the computational domain, the gas flux in the model system is several times higher than that assumed in the previous case (sec. 3.4.2).

### 3.4.4 Stability analysis of conduit-filling gas pockets

If the gas flux in the magmatic system is increased further as compared to the low (section 3.4.2) and moderate (section 3.4.3) gas fluxes considered so far, bubbly flow will transform into slug flow (e.g. [195, 164]). In the slug regime, flow is no longer dominated by bubbles, but instead by conduit-filling pockets of gas. For clarification purposes, we note that in the engineering literature these conduit-filling pockets of gas are referred to as 'Taylor bubbles' while 'slug' denotes the bubbly mixture in between. In contrast, it is common in the geophysical literature to use 'slug' to refer to the conduit-filling gas pocket itself. We abide by the convention of the geophysical literature.

The third group of simulations is targeted at investigating the stability and dynamic behavior of slugs. A key difference of this case compared to the computations outlined in sections 3.4.2 and 3.4.3 is that while the first two sequences of simulations are independent of the conduit geometry, we now have to assume an explicit conduit geometry: We model the conduit as being vertical with rectangular 'no-slip' walls.

In order to track the behavior of the gas slug over a longer segment of the conduit, we define more elongated computational domains. The non-dimensional number $\Pi_5 = \frac{ds}{w} = O(1)$ captures the relative size of the initial diameter of the gas pocket, $ds$, to the conduit width, $w$. We continue to use a spherical initial condition because it is the most stable.
3.5 Results

3.5.1 Dynamic instability of isolated gas bubbles during ascent

A spherical drop is an exact steady solution to the Stokes equation [17]. [138] was the first to investigate the stability of this solution experimentally and demonstrated that small disturbances to the spherical shape of a dynamical drop can lead to highly distorted shapes, even in the Stokes regime. These findings were confirmed soon afterwards through numerical studies [137, 216]. In agreement with these investigations, we observe that gas bubbles stabilize to a spherical shape in the first regime (Bo < 1 and Re < 1) independent of the initial perturbations to the interface. In the second regime (Bo > 1 and Re < 1), however, a wide range of distorted interfaces can develop, depending on the initial condition of the bubble. In the extreme case, the bubble can break up if either the initial distortions of the interface are sufficiently large or if surface tension is negligible. These findings are in agreement with prior studies [216]. Under flow conditions representative of the third regime (Bo > 1 and Re > 1), the breakup of an isolated bubble occurs even in the absence of any distortions of the initial interface position. We performed a total of 95 simulations in this regime (Fig. 3-3). We observe two breakup mechanisms of an initially spherical bubble during buoyancy-driven ascent: (1) gradual breakup in which small droplets are torn off the rear of the bubble (Fig. 3-4B) and (2) catastrophic breakup in which the bubble collapses rapidly into a large number of bubbles with intermediate to small sizes (Fig. 3-4C).

Fig. 3-4A shows a bubble reaching its steady-state shape, a dimpled ellipsoidal cap (e.g. [50]), without breaking up. Fig. 3-4B illustrates a gradual-breakup sequence. As the bubble deforms into steady state, the interface thins out predominantly at the periphery of its trailing surface. A thin layer of gas develops which eventually becomes unstable and is torn up into several small droplets. The sizes and number of these satellite drops increase with Re. Both the formation of a thin sheet of
Figure 3-4: Breakup modes of an initially spherical bubble in two dimensions. A: An initially spherical bubble reaches its steady-state shape without breakup (Re ≈ 5, Fr ≈ 0.4, We ≈ 90, and Π₁ = 10⁻⁶). The snapshots shown are at non-dimensional times t = 0, 1.97, 3.93, and 5.90. B: Gradual breakup during which three small bubbles are torn off each side. The run is characterized by Re ≈ 25, Fr ≈ 0.3, We ≈ 800 and Π₁ = 10⁻⁶. Snapshots are at t = 0, 1.42, 2.08, and 2.48. C: An extreme example of breakup in the catastrophic regime characterized by Re ≈ 250, Fr ≈ 0.16, We ≈ 1350 and Π₁ = 10⁻⁶. Snapshots are at t = 0, 0.59, 1.03, 1.58, 1.91, 2.04, 2.26, and 2.49. The grid resolution in all runs is 80 × 160.
gas trailing the bubble (referred to as 'skirt') and the breaking-off of small satellite
drops are commonly observed in experiments (e.g. [316] and references therein). An
extreme example of catastrophic breakup in two dimensions is illustrated in Fig. 3-
4C. This mechanism initially resembles the gradual variant: A small dimple forms
at the rear of the bubble and grows rapidly in magnitude over time. Contrary to
the case of gradual breakup, however, the leading surface of the bubble also begins
to deform soon after the onset of motion and small-wavelength perturbations $\lambda \ll a$
are apparent well before breakup (Fig. 3-4C, panel 3). Eventually, the gas bubble
breaks up, first along the perturbations on the leading surface (Fig. 3-4C, panel 4)
and subsequently along the sides (Fig. 3-4C, panel 5-8).

In three dimensions, we observe the same sequence of breakup regimes from grad-
dual to catastrophic. In the case of gradual breakup, a ring of smaller droplets is torn
off the rear of the original bubble as it deforms into its steady-state shape. Dur-
ing catastrophic breakup, the rapid growth of the dimple in the rear of the bubble
first leads to the formation of a torus, which then breaks apart azimuthally into sev-
eral bubbles (Fig. 3-5). This type of breakup (i.e. torus formation and subsequent
azimuthal breakup) has been observed both numerically and experimentally for sed-
imenting drops at low to intermediate Re (e.g. [167]). Interestingly, we find that
for a given Bo, the onset of catastrophic breakup occurs at much lower Re in three
compared to two dimensions.

An analysis of our simulations indicates that bubble breakup in basaltic systems
is controlled primarily by Re. The other non-dimensional numbers play a minor role,
although they may delay or enhance breakup slightly. The onset of gradual breakup
occurs approximately at $Re > 5$. With increasing Re ($Re \sim O(10)$), the location of
initial breakup shifts from the sides of the bubble surface more and more upwards
and the sizes and number of broken-off bubbles increase. Thus, breakup becomes
increasingly 'efficient' at intermediate Re, by which we mean that the radius of the
largest bubble after breakup is significantly smaller than the original bubble radius.
If Re exceeds the onset of breakup ($Re \approx 5$) by more than an order of magnitude, the
mode of breakup changes to catastrophic. During a catastrophic breakup sequence,
Figure 3-5: Catastrophic breakup of an initially spherical bubble in three dimensions. \( \text{Re} \approx 16, \text{Bo} \approx 1150, \text{and } \Pi_1 = 10^{-6} \). It is likely that, analogous to Fig. 3-4C, a series of small bubbles is generated during catastrophic breakup in three dimensions, but not resolved due to resolution restrictions. The computation was performed with a grid resolution of \( 75 \times 75 \times 50 \) equidimensional cells. The snapshots shown refer to \( t = 0, 1.15, 1.73, 2.88, 3.45, \) and 4.3.
the original radius of the bubble is reduced dramatically. For example, the area of the largest bubble after breakup in Figure 3-4C is only \( \approx 33 \% \) of the initial bubble area.

In both two and three dimensions, we find that for a given set of material parameters of magma and gas, the tendency for a bubble to break up depends sensitively on its size. This strong size-dependence of the breakup time can be understood through the following simple scaling argument. The relevant physical parameters for breakup are: bubble radius \( a \sim L \), surface tension \( \sigma \sim M/T^2 \), density difference \( \Delta \rho \sim M/L^3 \), dynamic viscosity \( \mu \sim M/LT \) and gravitational acceleration \( g \sim L/T^2 \) (where \( M \) stands for mass, \( L \) for length, and \( T \) for time) yielding

\[
t_B \sim \frac{\sigma a^3 \Delta \rho^2}{\mu^3},
\]

when requiring that \( t_B \sim T \). We are able to confirm the hypothesized dependence of breakup time on bubble radius \( t_B \sim a^3 \) only for gradual breakup and only during its initial stages (\( Re \ll O(100) \), see Fig. 3-6). At larger \( Re \), we observe a more complex correlation between breakup time and bubble radius (Appendix B). Independent of the exact scaling of \( t_B \) with \( a \), however, breakup occurs very rapidly, typically before the bubble has travelled a distance comparable to its own diameter.

### 3.5.2 Effect of multibubble interactions on breakup

At higher gas fluxes than those considered in the preceding section, the interaction between bubbles plays an increasingly important role. This is particularly true when bubbles are deformable, i.e., in regimes two (\( Bo > 1 \) and \( Re < 1 \)) and three (\( Bo > 1 \) and \( Re > 1 \)). One well-known consequence of bubble deformability is enhanced coalescence in the Stokes regime [170, 171]. In this section we demonstrate that coalescence is only one aspect of multibubble interactions, because deformability enhances not only coalescence but also breakup. Since multibubble interactions play a marginal role for interface dynamics in the first regime (\( Bo < 1 \) and \( Re < 1 \)), we will not discuss this regime further. The second regime (\( Bo > 1 \) and \( Re < 1 \)) is more interesting,
Figure 3-6: Dependence of the breakup time $t_B$ on bubble radius $a$ for gradual breakup. In order to evaluate the dependence of $t_B$, the computation is dimensional with $\rho_f = 3500 \, \text{kg/m}^3$, $\rho_g = 1.226 \, \text{kg/m}^3$, $g = 9.81 \, \text{m/s}^2$, $\sigma = 0.3 \, \text{N/m}$, $\mu_f = 10 \, \text{Pa-s}$, and $\mu_g = 10^{-5} \, \text{Pa-s}$. The breakup time is expressed in percent of the initial breakup time at $a = 5.4 \, \text{cm}$. The numerical data points are associated with an error bar reflecting the finite time step $\Delta t$ in the computation. The line represents a cubic fit through the data.

Figure 3-7: Overview of the non-dimensional regime covered by 52 simulations (black dots) investigating the effect of multibubble interactions on breakup at $\text{Re} > 0$ (sec. 3.4.3). The computations have been binned based on their initial conditions, where $1.1 \leq \Pi_2 \leq 2.0$, $1.1 \leq \Pi_3 \leq 2.0$ and $1.1 \leq \Pi_4 \leq 3.0$. The grey shading visualizes our finding that while coalescence and breakup commonly occur in sequence at $\text{Re} > 0$, coalescence dominates at small Re and breakup at large Re.
because, while small deformations impede coalescence [233, 231], large deformations enhance coalescence [170, 171]. For easily deformable bubbles (Bo > 50) of comparable size (Π2 = O(1)), multibubble interactions can manifest themselves in three ways in the Stokes regime, depending on Bo and the non-dimensional separation distance Π4 as analyzed in detail by [330]: (1) At large horizontal distances Π4, the two bubbles will pass each other without topological change of the interface. (2) In a certain range of horizontal distances Π4, the interaction of the bubbles will lead to breakup of either one or both bubbles. Typically, breakup proceeds by a small drop being torn off an ascending bubble because of the presence of a trailing drop [329, 330, 55, 145]. (3) At even smaller distances Π4, the two bubbles coalesce with each other [170, 171]. In our investigation of multibubble interactions at finite Re, we focus on bubbles in the stable regime (Re < O(10)). The reason is that bubbles in the unstable size range will be rare in a typical flow field, because of their rapid breakup (sec. 3.5.1). Figure 3-7 gives an overview of the non-dimensional range covered by our simulations. Qualitatively, we observe a similar range of dynamic interactions at low Re as compared to Re = 0 [330]. Quantitatively, however, we find that the range of non-dimensional separation distances over which coalescence occurs decreases with increasing Re. For example, at intermediate (Re ~ O(10)), two bubbles coalesce only if they lie approximately within the line of ascent of each other (i.e. Π4 < 1.2). At low Re (Re ~ O(1)), coalescence is observed over a much wider range of initial separation distances. Figure 3-8 shows an example of a three-dimensional computation of two deformable bubbles passing each other despite their small initial separation. It should be noted at this point that three-dimensional computation of bubble interactions are challenging because of the high resolution required to accurately resolve the fluid dynamics in the thin magmatic film separating the two bubbles. Therefore, we primarily focus on two dimensions in this section. Please refer to Appendix B for a more detailed discussion or resolution restrictions.

On the basis of our simulations, we identify two other important characteristics of multibubble interactions at finite Re: (1) We are no longer able to identify a 'typical' breakup sequence as for the case of an isolated bubble (sec. 3.5.1) or in the
Figure 3-8: A three-dimensional computation of two deformable bubbles coming into close contact without coalescing. Non-dimensional numbers are $\text{Re} \approx 2$, $\text{Bo} \approx 166$, $\Pi_1 = 10^{-6}$, $\Pi_2 = 1.43$, $\Pi_3 = 1.2$, and $\Pi_4 = 2.0$. Snapshots are at $t = 0$, 2.04, 3.06, 4.08, 5.10, and 6.12. The resolution is $50 \times 50 \times 80$.

Figure 3-9 shows two examples of breakup at $\text{Re} > 0$ for slightly different horizontal separation distances ($\Pi_4 = 2$ (A) and $\Pi_4 = 1.8$ (B)), highlighting that the exact breakup process is very sensitive to initial conditions. (2) Coalescence and breakup are clearly not mutually exclusive. In fact, we find that breakup and coalescence occur in sequence in the majority of simulations, sometimes repeatedly (see Fig. 3-9B). The balance between coalescence and breakup depends primarily on $\text{Re}$ (as long as $\text{Bo} \sim O(100)$ or larger) with coalescence more commonly observed at small $\text{Re}$ and breakup more commonly observed at large $\text{Re}$ (see Fig. 3-7).

One important ramification of the observed balance between coalescence and breakup is that multibubble interactions can destabilize bubbles that would not have broken up when isolated, even in the Stokes regime as long as $\text{Bo}$ is sufficiently high.
(Bo > 10). A comparison of the time scale of breakup induced by multibubble interactions to that of breakup for isolated bubbles indicates that unstable bubbles break up more rapidly than they interact (see Fig. 3-9).

### 3.5.3 Dynamic instability of slugs

As mentioned previously (sec 3.4.4) slugs scale differently than isolated bubbles, implying that the three scaling regimes illustrated in Fig. 3-1 are no longer necessarily meaningful. Most importantly, the limiting case of high surface tension forces (Fig. 3-1, regime 1) does not apply, because slugs only move if they are sufficiently deformable, namely if

\[
\frac{\rho_f g a^2}{\sigma} \approx \text{Bo} > 0.842
\]  

as has been determined experimentally [30]. Thus, a diameter of several mm is typically required for slugs in basaltic magma to ascend under their own buoyancy.

Since our main goal is to investigate the stability of conduit-filling slugs, we focus on Re > 1 (Fig. 3-10). Analogous to the case of isolated gas bubbles (sec. 3.5.1), we observe two regimes of breakup, gradual and catastrophic (Fig. 3-11). Gradual breakup results in small droplets being torn off the gas pocket in the vicinity of the walls. Contrary to the case of isolated gas bubbles, where multiple droplets are commonly torn off the original bubble simultaneously (sec. 3.5.1), gradual breakup of slugs tends to occur repeatedly. Figure 3-11A shows an example of a single sequence of gradual breakup and Figure 3-11B a double sequence of gradual breakup. We observe repeated breakup for most slugs in the unstable regime. The number of breakup cycles and the size of torn-off bubbles increase with Re.

An extreme case of catastrophic breakup is illustrated in Figure 3-11C. Initially, it proceeds similarly to the case of an isolated bubble: A dimple forms in the rear of the slug and grows over time. However, the dimple does not reach the upper surface of the slug, because of the large volume of gas confined in a narrow conduit. Instead, rupture akin to gradual breakup occurs along the sides. Simultaneously, a Rayleigh-Taylor instability forms on the upper surface, propagates through the gas volume, and
A. Sequence of breakup

B. Sequence of coalescence and breakup

C. Sequence of breakup for unstable bubbles

Figure 3-9: A and B: Two breakup sequences as a consequence of differing initial separation distances in the vertical direction $\Pi_4 = 2$ (A) and $\Pi_4 = 1.8$ (B). Both computations are based on Re $\approx$ 5, Fr $\approx$ 0.2, We $\approx$ 70, $\Pi_1 = 10^{-6}$, $\Pi_2 = 1.43$, and $\Pi_3 = 1.16$. The snapshots shown for the first computation (top) refer to non-dimensional times $t = 0, 1.5, 3.0, 4.5, \text{ and } 6.0$. Those on the bottom to $t = 0, 2.32, 3.48, 4.41, \text{ and } 5.80$. C: Multi-bubble interactions for bubbles in the unstable size range (sec. 3.5.1). Non-dimensional numbers are Re $\approx$ 350, Fr $\approx$ 0.2, We $\approx$ 3000, $\Pi_1 = 10^{-6}$, $\Pi_2 = 1.43$, $\Pi_3 = 1.16$, and $\Pi_4 = 2$. Snapshots are at non-dimensional times $t = 0, 0.34, 0.51, 0.64, \text{ and } 0.87$. Initially, the deformation of each bubble is reminiscent of the breakup sequence of isolated bubbles (Figure 3-4). The presence of the other bubble only becomes apparent during the late stages of breakup, indicating that unstable bubbles break up more rapidly than they interact. All three computations are based on a grid resolution of $100 \times 200$. 

100
leads to breakup of the remaining gas slug into two equally sized segments. Similar to the isolated case, the onset of catastrophic breakup is not discontinuous. Small-wavelength perturbations are apparent on the leading surface of the slug well before the regime of catastrophic breakup is reached. Therefore, cyclical breakup may be interpreted as a more moderate variant of catastrophic breakup.

A special consideration when investigating slug breakup is the vicinity of the solid wall and the role it plays for breakup. Not surprisingly, we find that at $\Pi_5 > 0.8$ breakup is observed at all Re and clearly results from the close proximity of the initial interface to the boundary. However, lowering the fill factor to $\Pi_5 \leq 0.7$ eliminates this bias. Figure 3-12 demonstrates that the breakup behavior described in this section is not a boundary artifact. It shows the steady-state shapes of three gas slugs of equal volume and initial shape at varying Re. As expected, the steady-state width of the slug increases with increasing Re, which leads to an increase in shear stresses in the magmatic film separating the slug from the conduit walls and facilitates dynamic instabilities. To further clarify the role of the proximity of the conduit walls for breakup, we compare the onset of breakup for a gas slug to an isolated gas bubble of identical size. We find that conduit walls have a slightly stabilizing effect, which seems to be primarily the consequence of the lower rise speed of the slug (and potentially also of the different steady-state shape of the slug, see Fig. 3-12). Therefore, although we observe slug breakup at approximately the same Re as bubble breakup, this Re is representative of a slightly larger volume of gas in the case of a slug.

3.6 Discussion

3.6.1 Comparison of theoretical and numerical constraints on bubble breakup

Despite the seemingly obvious differences between gradual and catastrophic (Fig. 3-4) breakup, we argue that they are both manifestations of the breakup mechanism outlined in section 3.3. In the case of catastrophic breakup, the connection to the
Figure 3-10: Overview of the non-dimensional regime covered by 69 simulations (black dots) to constrain the stability of gas slugs (sec. 3.4.4). For all computations $\Pi_1 = 10^{-6}$ and $\Pi_5 = 0.7$. The grey shading delimits the domain in which we observe breakup in two dimensions.

Theoretical breakup model is evident: Small-wavelength perturbations are apparent on the leading surface of the bubble (Fig. 3-4C, panel 2) and growth of these Rayleigh-Taylor instabilities eventually leads to breakup of the bubble surface (Fig. 3-4C, panel 3). For breakup sequences at intermediate Re, surface perturbations can still be distinguished visually, although they no longer grow fast enough to cause breakup along the leading surface. The slower growth can be explained by dispersive viscous damping. As plotted in Figure 3-2, barely unstable wavelength grow very slowly at high viscosities ($\mu \geq 100 \text{Pa·s}$).

The conclusion that both gradual and catastrophic breakup fit well into the theoretical framework (sec. 3.3) warrants a brief comparison of predicted (Table 3.1) to computed maximum stable bubble sizes. We perform this comparison only in two dimensions, because the semi-empirical model itself relies on a linearized stability analysis in two dimensions [96, 215]. In our computations, we use the same physical parameters as in Table 3.1 with $\mu_f = 10 \text{ Pa·s}$. We find good agreement between predicted and numerical results. The bubble size, $a_{\text{grad}}$, that marks the onset of the
regime of gradual breakup is smaller than the predicted maximum bubble size by approximately $a_{\text{grad}} \approx 0.85 a_{\text{max}}$. Clearly, the critical radius for the onset of gradual breakup is not a very good proxy for the maximum stable bubble size, because the size of the bubble changes only marginally during this moderate variant of breakup. The extreme form of catastrophic breakup is observed for bubble radii of $a_{\text{cat}} \approx 2.2 a_{\text{max}}$. During these more violent breakup sequences, the initial bubble size is typically reduced by at least 50%, leaving a bubble of approximately the size predicted in Table 3.1.

A noteworthy deviation of our simulations from the breakup model (sec. 3.4.1) is that instabilities do not necessarily disappear once they have reached the periphery of the bubble surface, as would be expected for a Rayleigh-Taylor instability. The cyclical breakup of gas slugs in Fig. 3-11B is an example. We hypothesize that breakup in this case might be the result of the combined effect of a Rayleigh-Taylor and a Kelvin-Helmholtz instability. As the initial Rayleigh-Taylor instability is advected along the leading surface of the slug, it approaches the conduit walls, and shearing intensifies. The surface perturbation may then grow through a Kelvin-Helmholtz instability and eventually trigger breakup along the sides of the slug. The onset of a Kelvin-Helmholtz instability is determined by the Richardson number, $R_i = Fr^{-1}$. Although $R_i$ for bubbles and slugs in basaltic systems is typically too high to expect the spontaneous formation of a Kelvin-Helmholtz instability, a pre-existing perturbation could still grow through this mechanism.

### 3.6.2 Non-dimensional conditions for a coalescence cascade

The RSD model assumes that the gas slugs representative of normal Strombolian activity form through progressive coalescence of gas bubbles. It relies on two main assumptions about the fluid dynamical interactions between magmatic and gaseous phase: (1) It assumes that a large bubble coalesces with all smaller bubbles lying within the vertical line of ascent of the large bubble [322, 206] and (2) it proposes that coalescences can lead to a run-away situation resulting in the formation of a single large bubble. On the basis of our numerical experiments, we conclude that the
Figure 3-11: A: Gradual breakup analogous to Fig. 3-4B. Re $\approx 10$, Fr $\approx 0.14$, We $\approx 95$, $\Pi_1 = 10^{-6}$, and $\Pi_5 = 0.67$. The snapshots shown are at $t = 0, 0.30, 0.60, 0.90, 1.20$, and $1.47$. B: Gradual breakup may occur cyclically. Re $\approx 50$, Fr $\approx 0.16$, We $\approx 100$, $\Pi_1 = 10^{-6}$, and $\Pi_5 = 0.67$. Snapshots are at $t = 0, 0.94, 1.33, 1.56, 1.93$, and $2.20$. C: Catastrophic breakup with gradual breakup occurring simultaneously along the walls. Re $\approx 80$, Fr $\approx 0.10$, We $\approx 3000$, $\Pi_1 = 10^{-6}$, and $\Pi_5 = 0.7$. The snapshots shown are at $t = 0, 0.29, 0.59, 0.88, 1.18$, and $1.47$. All three computations were performed at grid resolutions of $80 \times 240$. 

104
first assumption is justified for deformable bubbles of comparable size ($\Pi_2 \sim O(1)$).
In fact, the assumption is rather conservative because the range of initial separation
 distances in the horizontal direction which result in bubble coalescence is $\Pi_4 > 1$ at
$Re < O(10)$ (sec. 3.5.2). Judging from our simulations, the second assumption is
less straight-forward, because both coalescence and breakup are commonly observed
in free flow at finite $Re$ (provided that $Bo \gg 1$). As discussed in section 3.5.2,
the balance of coalescence and breakup depends primarily on $Re$. Once bubbles
grow sufficiently such that $Re > O(10)$, breakup dominates, gradually reducing the
average bubble size. In that case, continued breakup and coalescence of bubbles
would yield a bubble population with a maximum bubble radius comparable to the
critical radius for gradual breakup of isolated bubbles (sec. 3.5.1). Evidently, this
rationale only applies to free flow, where the average bubble radius $a \ll d$, with $d$
representing the half width of the conduit. We conclude that it is possible for gas
slugs to form through a coalescence cascade only if the viscosity is sufficiently high
and/or the conduit sufficiently narrow such that bubbles are characterized by $Bo > 1$
and $Re < O(1)$ throughout the evolution of the cascade.

For Stromboli, the volume of the slug is thought to be on the order of $V \approx
20 - 35 \text{ m}^3$ [226]. Since the characteristic radius in our computations is based on
the spherical initial condition, a Strombolian slug would thus be represented by an
effective radius of several meters ($r \approx 1.7 - 2 \text{ m}$). Given the large size of the slug, we
estimate that a minimal magma viscosity on the order of $\mu_f \approx 5 \times 10^4 \text{ Pa-s}$ would be
required for a coalescence cascade in the upper conduit. Estimates for the viscosity
of Strombolian lava vary from $50 - 500 \text{ Pa-s}$ [302] for the samples acquired by [31]
and [79] to $10^{1.5} - 10^4 \text{ Pa-s}$ in a more recent study evaluating viscosity at Stromboli
as a function of temperature and water content [189]. Most commonly, values in the
range of $O(100) \text{ Pa-s}$ are used (e.g. [25, 301, 302]). Nonetheless, it might not be
unrealistic to expect that the effective viscosity in the upper conduit is significantly
elevated ($\mu_f \sim O(10^4) \text{ Pa-s or larger}$) because of its high phenocryst content (e.g.
[22, 81, 230]). An important caveat is that our numerical approach does not resolve
the dynamic effect of a high phenocryst density on multibubble interactions or on
Figure 3-12: Dependence of the steady-state shape of conduit-filling slugs on Re. All computations are based on a spherical initial condition and $\Pi_5 = 0.7$. At finite Re, a dimple forms at the rear of the slug visible on all three interfaces. As Re increases from left to right, the steady-state width of the slug increases and the magmatic films separating interfaces and conduit walls are thinned out. Shear stresses will intensify as the magmatic films thin out and eventually lead to the tearing-off of small droplets similar to gradual breakup of isolated bubbles (Fig. 3-4B).

coalescence/breakup of individual bubbles, which might very well be substantial.

3.6.3 Non-dimensional conditions for stable slug rise

The CF model is based on a series of laboratory experiments [125, 126] in which the magma chamber is represented as a cylindrical tank and the volcanic conduit as a narrow pipe located in the center of the roof. Gas is introduced into the tank from below and accumulates below the flat top, where it coalesces. Eventually the gas layer emptyes into the pipe. Depending on the fluid properties in the tank and on the incoming gas flux, three flow regimes are observed in the conduit: bubbly flow (interpreted as the analogue of passive degassing), spherical bubbles with a characteristic spacing (analogue of normal Strombolian-type eruptions), and slug flow (analogue of Hawaiian-type eruptions). The main assumptions of the CF model are (1) coalescence occurs entirely in the magma chamber (or, more generally, underneath a large roof area in the conduit) and (2) gas slugs rise stably through the conduit. Only the second assumption lends itself to evaluation through our simulations.

In section 3.5.3 we demonstrate that slugs are prone to dynamic instabilities if they are characterized by $\text{Re} \sim O(10)$ or larger (sec. 3.5.3). [301] suggest that the gas slugs causing normal activity at Stromboli are characterized by $\text{Re} \approx 80$. Our
simulations, however, indicate that a slug at Re \( \approx 80 \) would break up catastrophically within seconds after formation (see Fig. 3-11C). The three key factors determining Re are (1) the size of the slug, (2) the width of the conduit, and (3) the magma viscosity. Additional considerations, not included in our simulations, are deviations from the assumed vertical conduit geometry (e.g. a local widening of the conduit) and velocity gradients in an ambient magmatic flow field, both of which are expected to reduce slug stability. At least the latter of these two aspects might be important to consider, because acoustic pressure oscillations during the eruption are thought to be related to vigorous vibrations of the slug interface [300].

In order to stabilize the ascent of a Strombolian slug from the magma chamber to the free surface, we estimate that magma viscosities above \( \mu_f \approx 5 \times 10^4 \) Pa-s would be required throughout the entire conduit. This conflicts not only with petrological observations indicating lower viscosities, at least in the deep conduit [189, 23], but also with acoustic observations [302] and the presumed rise speed of a Strombolian slug (e.g. [104]). Although the incompatibility of slug stability with the presumed low viscosities in the deep conduit could be reconciled by slug formation at shallow depth, for example in a dike located in the upper conduit [186], the disagreement with acoustic data and a presumed rise speed of 10-70 m/s [104] remains.

Since the CF model [125, 126] is based on fluid-dynamical experiments, it is valuable to briefly assess the reasons why slug instability is not observed in the experiments. We suggest that simulations and experiments scale differently because of the small width \( w \) of the laboratory conduit \( w \sim O(\text{cm}) \) as compared to the size of the Strombolian conduit \( w \sim O(\text{m}) \). Therefore, the slugs in the experiment fall well into the stable size range (see Table 3.1 and Figure 3-2), but Strombolian slugs might not. Also, [126] investigated variations in surface tension by a factor 3, but surface-tension forces vary by a factor of about \( 10^4 \) for bubbles in the centimeter as compared to the meter range (eq. 3.13).
3.7 Conclusions

We investigate the interface dynamics of a segregated gas phase in the context of basaltic volcanism. The two physical parameters of gas/basalt systems that may vary by several orders of magnitude are bubble size and magma viscosity. This variability in physical parameters translates into a wide range of relevant non-dimensional regimes. The two most important non-dimensional numbers to consider are Re and Bo, based on which we identify three fluid dynamical regimes (Fig. 3-1). Resolving the detailed bubble dynamics is not equally important in each of the three scaling regimes. In fact, the bubble interactions may typically be neglected in the first regime. However, once bubbles become deformable (Bo > 1) the fluid dynamical interactions between the bubbles begin to play an important role. The observation that deformability enhances coalescence has been investigated in detail in previous studies [170, 171]. An important contribution of our study is the observation that deformability not only enhances coalescence but also breakup (sec. 3.5.2). At finite Re, we observe a balance of breakup and coalescence in our computations, with coalescence dominating at low Re and breakup at large Re.

Our simulations demonstrate that both bubbles and slugs are prone to dynamic instabilities, even in the absence of interactions with other bubbles/slugs. We observe two modes of breakup, gradual and catastrophic. A typical breakup sequence entails a small Rayleigh-Taylor instability forming at the leading surface of the bubble or slug. Surface tension is insufficient to restore the surface if the radius of the gas pocket exceeds $a_{cr}$ (eq. 3.16). Viscous forces, however, tend to stabilize the gas pocket through a combination of damping and lateral transport of the perturbation towards the periphery of the gas volume. The onset of breakup depends on the relative dominance of these processes (sec. 3.3). Interestingly, we find that while bubbles and slugs begin to break apart gradually at approximately the same Re, catastrophic breakup is observed at lower Re for slugs than for bubbles. We suggest that the difference is partly due to the lower rise speed of large slugs as compared to bubbles of the same size and partly due to the more intense shearing of the slug surface near
the conduit wall, which may give rise to Kelvin-Helmholtz instabilities.

The breakup criteria provided here are inevitably underestimates, for the following two reasons: (1) All of our computations are based on spherical initial conditions, which are dynamically the most stable. However, bubbles or slugs with radii representative of the third scaling regime have probably formed through coalescence of smaller bubbles or breakup of an even larger bubble and will generally not be spherical. The fact that we commonly observe complex sequences of coalescence and breakup (Fig. 3-9) in the third scaling regime attests to the additional complexity introduced by distorted bubble shapes. We also note that we observe dynamic instabilities even in the Stokes regime if the initial condition of the bubble or slug is not spherical. (2) We only discuss breakup in a stagnant fluid. Any additional complexities in the flow field such as shearing or turbulence will tend to aid breakup, because they facilitate the formation of destabilizing surface distortions [50]. For Stromboli in particular, the existence of vigorous and possibly turbulent flow is not merely hypothetical [189, 23].

Applied to Stromboli, our simulations suggest that the presence of large stable gas slugs in the conduit requires zero or very low Re independent of whether the RSD or the Cf model is invoked to explain slug formation (sec. 3.5). Since gas slugs at Stromboli are thought to represent gas volumes of several meters in size, unusually high viscosities (i.e. well above $O(10^4)$ Pa-s) would be needed to stabilize the slugs. While viscosities in this range are certainly possible [189], geophysical data indicates that Strombolian slugs are characterized by rapid rise speeds (10-70 m/s) [104] and surface oscillations [301, 302]. This evidence is difficult to reconcile with zero Re. The apparent conflict between dynamic instability and finite-Re flow in Stromboli’s plumbing system might be resolved in various ways including: (1) The gas slugs causing normal Strombolian activity might be significantly smaller than previously thought and characterized by $Re \ll 80$. (2) Either the acoustic signal and/or the eruption itself is caused by a mechanism other than the viscous ascent and burst of a large gas slug. (3) There might be a stabilizing mechanism not accounted for in our computations such as Non-Newtonian rheology or surfactants.
Chapter 4

Slug or plug? A new look at the mechanism of normal activity at Stromboli

4.1 Introduction

Although Stromboli volcano in Italy is best known for its famously episodic 'normal' activity, it exhibits a wide range of eruptive regimes from passive degassing to explosive fire-fountaining. Normal Strombolian activity is defined by [14] as discrete explosive bursts that last a few tens of seconds and eject pyroclasts to a height of 100-200 m. Despite its persistence, the frequency and intensity of normal activity is highly variable ranging from several dozen events per hour to rare periods of quiescence. The idea that eruptive activity at Stromboli is intricately linked to degassing was pioneered by [47] and developed further by [25], who suggested that normal eruptions represent the bursts of large conduit-filling gas bubbles, commonly referred to as slugs, at the upper surface of the magma column (Fig. 4-1). This line of reasoning

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A. Slug model

B. Plug model

Figure 4-1: Comparison of the slug and plug model. A: The slug model assumes that the volcanic conduit is filled with fluid magma (grey) throughout. Each Strombolian eruption is thought to represent the burst of a gas slug of up to 35 m$^3$ [226]. B: Instead of focusing on one vent, the plug model captures the dynamics of the entire crater terrace. It incorporates the dichotomy of Strombolian magma with HP magma residing at shallow and LP magma at large depth. Flow in the LP magma is driven by buoyant ascent of gas bubbles inducing convective flow in the magma. For the first few hundred meters below the free surface, HP magma is crystalline enough to behave as a porous plug at low shear and strain rates.

has been taken up by numerous later studies and has not only become the leading paradigm underlying our thinking about Stromboli but has also been extended to include similar activity at other volcanoes (e.g., [304]).

When the slug model was first devised, the petrological characteristics of the Strombolian plumbing system were essentially unknown. Since then, numerous petrological studies have established the existence of two different types of magma at Stromboli that vary drastically in crystallinity. Highly-porphyritic (HP), water-low magma with 40-60 vol.% phenocrysts and microphenocrysts resides in the upper few hundred meters of the plumbing system and is erupted as scoriae during normal activity. The most abundant mineral phase is plagioclase (\(\sim 65\%\)), followed by clinopyroxene (\(\sim 25\%\)) and olivine (\(\sim 10\%\)) [187, 78]. For a detailed analysis of crystal and bubble
Figure 4-2: Illustration of the rheological transitions with increasing crystal fraction. Estimates of melt strength are computed by viscosity $\times$ strain rate. At zero to low crystal fraction, the aggregate is fully liquid (regime A), where the increase in effective viscosity is given by the Einstein-Roscoe relationship. In the transitional regime, B, it is partly liquid and partly solid. The strength of the aggregate increases rapidly through a power-law (Bingham rheology). Beyond a rheologically critical crystal fraction, the aggregate behaves like a solid body (domain C).

populations in HP magma, please refer to Appendix C. Low-porphyritic (LP), water-rich magma with $< 10$ vol.% phenocrysts originates much deeper and is ejected in the form of pumice only during paroxysms or major eruptions, alongside with scoriae bearing the characteristics of HP magma [81, 230, 187, 23, 78]. Plagioclase, clinopyroxene, and olivine are still the most common mineral phases in LP samples, but their proportions are much more variable than in HP samples [23, 78]. HP magma can be derived from LP magma by degassing-induced crystallization accompanied by limited fractionation [187]. The petrological findings have important ramifications for the interior dynamics of Stromboli volcano, because they reveal that the dynamic behavior of the HP magma at shallow depth is not well approximated by a Newtonian rheology. Both theoretical [242] and experimental [211, 118] studies have concluded
that load-bearing frameworks can start to develop at low crystallinity and material strength increases in a power-law fashion upon further crystallization [212, 308] as illustrated in Fig. 4-2. The material strength of HP magma with 45-60 vol.% crystals is expected to be several orders of magnitude larger than that of LP magma at < 10 vol.% crystals and may be comparable to the material strength of solid bodies [294, 178]. Hence, the drastic contrast in crystallinity between HP and LP magma is associated with a similarly drastic contrast in the rheology of the two magmas. As a consequence, while LP magma should behave like a Newtonian fluid, HP magma should form a plug in Stromboli’s upper plumbing system and deform more like a solid body (Fig. 4-2).
4.2 Plug model of normal Strombolian activity

To estimate the thickness of the plug, we compute the increase in crystallinity with decreasing pressure using MELTS [88, 10]. Based on the shoshonite bulk composition [80] and a temperature of 1115°C, we find that the crystallinity starts increasing rapidly from about 30 MPa (~ 2000 m depth) and reaches the crystallinity representative of HP magma around 10 MPa, which corresponds to 600 - 700 m depth for an assumed magma density of 1500 kg/m³ (Fig. 4-3). This depth range is consistent with prior assessments [106, 150] and provides an upper bound for the thickness of the plug. The actual thickness of the plug is likely less than that. We suggest that only the top portion of the HP magma forms the plug based on the criterion that the crystallinity has to exceed ~ 50 % to fall into the range of the rheologically-critical crystal fraction (Fig. 4-2) which marks the transition point of a crystalline suspension to solid-body behavior. This transition occurs at a thickness of approximately 300 m (~ 5 MPa).

The simplified vertical geometry we assume for the slug model is shown in Fig. 4-1A. HP magma (top) extends from the free surface to approximately 700 m in depth and LP magma (bottom) resides at larger depths. In the first few hundred meters (~ 300 m) below the surface, HP magma forms a porous plug which is permeable only to small bubbles. The horizontal geometry assumed in our model is adapted to fit the elliptical shape of the crater terrace at Stromboli. In contrast to the slug model (Fig. 4-1B), our model does not assume the existence of fixed vents, because mapping of the crater terrace indicates variability in the locations of craters and vents [105, 104]. The present general three-crater morphology, however, can be traced back to at least 1776 [311]. Therefore, we assume that the location and shape of the crater terrace remains largely fixed over time and model the dynamics of the entire crater terrace. One of the goals of this more general view is to understand why normal Strombolian eruptions occur predominantly at the NW and SE craters and not at the central crater - a question not addressed by the slug model.

In our plug model, flow in the LP magma is driven by the buoyant ascent of
gas bubbles consisting primarily of carbon dioxide, which is thought to have been assimilated from a carbonate platform at depth [40, 39]. Buoyancy-driven flow in the LP magma creates a convective cell underneath the plug [13, 75]. The bubble content increases rapidly once the depth of water exsolution is reached, both because of the exsolution itself and because of the associated increase in both viscosity and crystallinity which slows bubble ascent. The buoyancy of the growing gas-rich layer underneath the plug exerts an increasing pressure onto the overlying layer. It is worth noting that it is of no specific relevance in our model whether the accumulating gas forms a foam layer or coalesces into one or several larger gas pockets.

In order to analyze the plug’s response to the homogeneous pressure from below, we model the plug as an elastic body (Fig. 4-4). There is no doubt that this view of the plug is overly simplified. The assumption of elastic deformation will fail not only at the microscopic scale (see Appendix C for an analysis of stress concentration in the vicinity of percolating bubbles), at which the smallest bubbles are still percolating slowly through the pore space, but also for large strains leading up to the failure of the plug when plasticity becomes important. Nonetheless, we argue that even the
simplistic assumption of elastic deformation can explain some of the first-order effects of normal Strombolian activity.

At low to intermediate thicknesses, the equations of linear elasticity inside the three-dimensional elliptical cylinder representative of the Strombolian plug can be solved analytically [162] as detailed in Appendix C. The analytical model assumes symmetry of the stress field with respect to the midplane - an assumption that is no longer valid if the thickness is comparable to or larger than the horizontal extent of the plug. In that case, a numerical treatment of the governing equations becomes inevitable. The numerical procedure used to solve the plug model in the limiting case of large thicknesses is also summarized in Appendix C.

4.3 Results

4.3.1 Failure of the plug

The plug will eventually fail because continuous gas accumulation below it leads to an ever increasing basal pressure. We suggest that failure occurs through a ductile mechanism, as supported by three pieces of evidence. First, both crystals and bubbles are mobile to variable degrees at the microscopic scale depending on their size. Therefore, we expect plastic and/or viscous deformation inside the plug, particularly at the high stresses and strains leading up to failure. Second, while the speed characteristic of normal eruptions (10 – 70 m/s) [47, 225] is very large compared to the viscous rise speeds of bubbles inside the plug, it is slow compared to the speed of crack propagation through brittle material. Third, thin sections of HP magma do not indicate pervasive cracking of crystals suggesting that crack propagation does not proceed intergranularly.

Given that failure occurs in a ductile mode, the locations where we expect failure to occur first are those of maximum shear stress. Experimental verification of the maximum-shear criterion have shown that it applies well to the beginning of plastic yielding in ductile materials and subsequent failure [57]. Using the solution for the
Figure 4-5: Overview of the spatial distribution of maximum shear at different depth intervals inside the plug with semimajor axis $a$, semiminor axis $b$ and moderate thickness $h = 70$ m based on the analytical solution for moderately thick plates (Appendix C). The top panel compares the value of maximum shear at the two boundary points furthest from the center, $(a, 0)$ and $(-a, 0)$, the two boundary points closest to the center, $(0, b)$ and $(0, -b)$ and the center throughout the plug. The bottom panels show the spatial distribution of maximum shear at various depths through color shading and five iso-stress contours. All stresses are nondimensionalized by the pressure applied at the lower surface of the plug.

stress tensor inside the Strombolian plug, we derive the principal stresses and principal orientations through Eigenvalue decomposition. The maximum shear stress is then given by $\tau_{max} = \frac{1}{2}(\sigma_{max} - \sigma_{min})$, where $\sigma_{max}$ and $\sigma_{min}$ are the largest and the smallest principal stress, respectively. The maximum shear stress thus corresponds to the radius of the Mohr circle spanned by these two principal stresses.

An analysis of the spatial distribution of maximum shear stress inside a Strombolian plug of moderate 70 m thickness (Fig. 4-5) shows that the level of maximum shear stress depends primarily on depth. The highest value of maximum shear at any given depth is attained at the lower surface of the plug. We conclude that for a
Strombolian plug of this thickness, plastic yielding and subsequent failure begins at the lower surface of the plug. Fig. 4-5 also demonstrates that at a given depth, the highest level of maximum shear is reached at the end points of the semimajor axis with the exception of the deepest few dozen meters for which the maximum shear is slightly larger at the end points of the semiminor axis.

The spatial distribution of the maximum shear stress changes with increasing thickness. For large thicknesses \( h \approx 300\text{m} \), the highest level of maximum shear is still obtained at the lower surface of the plug. The spatial distribution at a given depth level, however, is increasingly dominated by the side boundaries. Also, the maximum shear stress tends to be slightly higher at the end points of the semiminor axis (see Appendix C). The rapid increase in maximum shear stress along the boundaries is probably not entirely realistic, because the transition from plug to host rock is not discontinuous.

4.3.2 Mechanism of normal eruptions

A simple mass balance comparing the mass ejected during a single normal eruption, which ranges from \(16\text{ kg}\) to \(5990\text{ kg}\) \([47, 25, 227]\) to the total mass of the plug \( M = \pi abh \rho \approx 1.5 \times 10^{10}\text{ kg}\) with density \( \rho = 1500\text{ kg/m}^3\), thickness \( h = 100\text{ m}\) and axes \( a = 140\text{ m}\) and \( b = 75\text{ m}\) (see Fig. 4-1), highlights that the plug not only remains intact between eruptions, but is depleted by a negligible percentage of its mass \(< 10^{-4}\%\) even during the most violent eruptions. Further evidence for the persistence of the plug comes from thermodynamic calculations that indicate a time period of hours to days \([151]\) for generation of HP magma from LP magma. As this is much longer than the typical eruption recurrence time of tens of minutes, inter-eruption crystallization would not be sufficiently fast to replenish the HP magma lost during individual eruptions. Given that observations point to a highly persistent plug in the shallow Strombolian plumbing system, we suggest that normal eruptions are caused by ductile failure within the porous plug. The driving force behind failure is inter-eruptive gas accumulation underneath the plug, which exerts an increasing pressure on the overlying material. An analysis of the stresses inside the plug show
Figure 4-6: Comparison of the increase in integrated maximum shear at the edges of the ellipse (in percent with respect to the center of the ellipse) and the vent locations (black dots) from October 1994 to September 2002 as mapped by [104]. The size of the ellipse is adjusted to coincide with the edge of the crater terrace.

that plastic yielding and subsequent failure initiates at the lower surface of the plug. Bubble clustering would facilitate failure by locally concentrating the applied stresses. In this way, the abundant vesicles inside the plug could play a role similar to microcracks in more classical fracture scenarios. After the onset of failure, strain and shear intensification in the vicinity of the propagating gas-filled crack is sufficient to cause shear thinning and a local transition to a more fluid-like rheology, as illustrated by the fluidal form of many of the ejecta (e.g. [307]). The eruption ends once the overpressure of the accumulated gas-rich layer is released and the crack in the plug closes up under the confining pressure.

By including solid-fluid interactions, the plug model resolves the conflict between a purely fluid-dynamical view of Strombolian eruptions, as suggested by the slug model, and petrological data that indicates exceptionally high crystallinities in the upper portion of the plumbing system. It also offers a promising framework for understanding other observational data sets such as acoustic and seismic recordings. In fact, several previous studies have concluded that a fluid-filled crack best accounts for the seismic and acoustic patterns at Stromboli [47, 46]. It is also worth noting that
Figure 4-7: The gas-driven eruption cycle suggested in the plug model. Continuous gas accumulation underneath the plug exerts an increasing pressure onto the overlying material until the critical pressure for failure is reached. Normal eruptions represent ductile failure of the plug during which the gas-rich layer underneath is partially drained. The buoyancy pressure drops, the eruptions ceases and gas accumulation begins again.

the characteristic very-long-period (VLP) seismic signal on which these conclusions are based originates at a depth of 285-290 m [46]. We suggest that the VLP might be an indication of the actual thickness of the Strombolian plug. If a normal eruption does indeed represent plug failure, it would be consistent for the onset of cracking at the plug’s lower surface to be associated with a seismic signal from that depth. A key requirement for any model of normal Strombolian activity is to offer an explanation for its unusual episodicity. Within the framework of the plug model, the recurrence interval of eruptions is governed by the time it takes for a critical gas overpressure to build up underneath the plug to blow through it (Fig. 4-7). One piece of evidence in support of this explanation is the strong correlation between the recurrence time of the eruptions and the intra-eruptive gas flux (e.g. [51]): the higher the gas flux between eruptions, the shorter the time interval separating eruptions. Taking the intra-eruptive gas flux as a proxy for the gas fluxing through the LP magma, higher
gas fluxes would be expected to lead to shorter recurrence times of the eruptions within the framework of the plug model.

In addition to offering an alternative explanation for the available observational constraints, the plug model could provide a promising framework for shedding some light on previously little understood features of Strombolian activity. For example, normal eruptions occur predominantly at the NW and SE craters, a location preference that seems at odds with the simple slug model. Superimposing the crater locations of normal Strombolian activity onto a depth-average of the maximum shear stress distribution for a plug of intermediate thickness (Fig. 4-6) leads to the conjecture that the far sides of the elliptic crater terrace might be particularly prone to failure. An important caveat is that this specific distribution of maximum shear is characteristic only for plugs of intermediate thickness ($h = 80\text{m}$). The correlation between crater location and maximum shear would thus tend to favor a moderately thick plug, which is at odds with the hypothesis that the VLP could be an indication for the position of the lower surface of the plug.

4.3.3 Conclusion

The slug model has dominated our thinking about normal Strombolian eruptions for several decades. It has been the motivation behind, and the basis for, a vast number of remarkable studies that have advanced our understanding of Stromboli considerably. However, when the slug model was first devised, the petrological characteristics and related rheological properties of the magma erupted during normal activity were poorly understood. Since then, numerous petrological and textural studies have established that the pyroclasts ejected during normal activity consist primarily of crystals (45-60 vol.% ) and vesicles. The mounting empirical evidence that crystals contribute prominently to the dynamics at Stromboli is difficult to reconcile with the purely fluid-dynamical view of the slug model. Since one of the key appeals of the slug model for both modelers and field volcanologists lies in its simplicity, we develop an equally simple alternative model, the plug model, which is based directly on the available petrological evidence. We show that the plug model not only offers an in-
tuitive conceptual framework for understanding previously investigated geophysical
data sets, but also offers the potential of making progress on some of the outstanding
questions regarding eruptive behavior at Stromboli and other hydrous and crystal-rich
mafic volcanic systems.

An important open question regarding the plug model concerns its thickness. If
the VLP signal is taken as an indication for the thickness of the plug, the predicted
locations of plug failure no longer coincide with the observed crater locations. One
potentially important aspect missing in the current setup of the plug model is that
that the crater terrace at Stromboli is not fully symmetric. One of the flanks is
aligned with the Sciara del Fuoco, a partially filled scar generated < 5000 years ago
by the collapse of Stromboli’s NW sector [139]. Preliminary results indicate that if
the boundary conditions of the plug along side the Sciara del Fuoco might not be
fully clamped, predicted and observed crater locations would coincide even for plugs
with large thicknesses. However, a more realistic treatment of the plug boundaries
should also entail a gradual increase in material strength along the boundaries which
will be the subject of future work.
Chapter 5

The possibility of catastrophic magma ocean degassing and implications for the formation of early planetary atmospheres

5.1 Introduction

An important uncertainty in current models for the early evolution of terrestrial planets is the origin and composition of primordial atmospheres. Three primary sources may contribute to planetary atmospheres: capture of nebular gases, early degassing during accretion, and late assimilation of volatiles from cometary impactors. While capture of nebular gases is thought to be critical for gas giants, the mass of terrestrial planets is probably too low to capture and retain nebular gases. Furthermore, nebular gases may have largely dissipated from the inner solar system by the time terrestrial planets have grown to their current sizes. Degassing during accretion is thus a reasonable starting point for modeling early planetary atmospheres on terrestrial-like
planets and exoplanets.

Terrestrial planets are thought to have accreted through runaway growth from a large population of km-sized bodies [317, 37]. During this phase of oligarchic growth, gravitational focusing caused the largest planetesimals to quickly outgrow the rest of the population [140]. It is likely that at least some of these building blocks of the terrestrial planets were of sufficient size to have differentiated early and rapidly [7] due to heat generated by the decay of the short-lived isotope $^{26}$Al. Vesta 4 might be a preserved example of these differentiated protoplanets [331].

The heat provided by accretion and differentiation is sufficient to melt the silicate mantle of a terrestrial planet or planetary embryo wholly or partially (e.g. [324, 243, 309]), creating magma oceans that may span a wide range of depths. The solidification processes in these magma oceans are crucial for constraining the subsequent evolution of the planet. They also create an important link between the properties of the solid mantle and the atmosphere: Depending on the ratio of volatiles retained in the mantle to the volatiles degassed to build the atmosphere, magma oceans with similar starting compositions may lead to planets with dry or wet mantles and substantial or minimal atmospheres. The build-up of an early atmosphere also sensitively affects the heat loss to space and thereby the solidification rate of the magma ocean [182, 4, 325, 1, 3, 66].

A previous study of the linked evolution of magma ocean solidification and atmospheric growth [66] assumes instantaneous degassing of all volatiles in excess of saturation in the liquid portion of the magma ocean. The contribution of this study is to provide a more detailed model of the physical processes determining the onset of degassing. The first step in our model is to identify the size range of bubbles in a magma ocean based on an analysis of bubble nucleation, growth, and breakup. The second step is to identify the conditions under which bubbles in the given size range are able to decouple from the ambient flow field in the magma ocean, rise to the surface and degas. At this stage, we only consider the combined effects of carbon dioxide and water. These two volatiles are the most important ones to consider, because they are thought to be relatively common in the planetary disk and because they are greenhouse gases and will slow the cooling processes inside the magma ocean.
substantially. Other volatile species could be included into our model as long as data on their solubility and diffusivity is available.

The primary goal of our study is to identify which parameters govern the exsolution and subsequent degassing of volatiles. Given the large uncertainties associated with individual parameters, the confidence of quantitative estimates is inevitably limited and the qualitative insights provided here might be more valuable. We devote particular attention to the role of planetary mass on degassing efficiency: The insight that radioactive decay of $^{26}$Al may lead to melting of planetesimals indicates that magma ocean may develop on planetary bodies with very small masses [69]. On the other end of the spectrum, Super Earths with $1 - 30$ Earth’s masses may also have experienced magma oceans [68] raising the question how planetary mass affects degassing properties to first order.

5.2 Model

Our model of bubble dynamics consists of two components. We first analyze bubble nucleation, growth, and breakup at the microscopic scale. Then, we identify the implications of bubble dynamics at the microscopic scale for degassing at the planetary scale. An overview of the variables used in the models is given in Table 5.1.

5.2.1 Bubble dynamics at microscopic scales

The two main goals of investigating bubble dynamics at the microscopic scale are (1) to identify when bubbles nucleate and (2) what their size distribution is likely to be.

Heterogeneous nucleation

A melt that is supersaturated in volatiles exsolves a gas phase to reestablish thermodynamic and chemical equilibrium. The classical theory of homogeneous nucleation posits that nucleation in a pure melt phase requires high energies to form new interfaces (see Appendix D for details). In the more common case in which heterogeneities exist in the melt phase, nucleation is facilitated greatly. In solidifying magma oceans,
Table 5.1: Overview of variables used in the text.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Variable</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_0$</td>
<td>Mean distance between two volatile molecules</td>
</tr>
<tr>
<td>$g$</td>
<td>Gravitational acceleration</td>
</tr>
<tr>
<td>$h$</td>
<td>Depth of the magma ocean</td>
</tr>
<tr>
<td>$k$</td>
<td>Boltzmann constant</td>
</tr>
<tr>
<td>$m_g$</td>
<td>Mass of the gas phase</td>
</tr>
<tr>
<td>$n_0$</td>
<td>Concentration of nucleation sites</td>
</tr>
<tr>
<td>$r$</td>
<td>Bubble radius</td>
</tr>
<tr>
<td>$r_{max}$</td>
<td>Maximum stable bubble radius</td>
</tr>
<tr>
<td>$r^*$</td>
<td>Critical radius</td>
</tr>
<tr>
<td>$t$</td>
<td>Time</td>
</tr>
<tr>
<td>$B_t$</td>
<td>Thermal buoyancy force</td>
</tr>
<tr>
<td>$B_c$</td>
<td>Compositional buoyancy force</td>
</tr>
<tr>
<td>$B_0$</td>
<td>Bond number</td>
</tr>
<tr>
<td>$D$</td>
<td>Diffusion coefficient</td>
</tr>
<tr>
<td>$D_0$</td>
<td>Stokes-Einstein diffusion constant</td>
</tr>
<tr>
<td>$J$</td>
<td>Nucleation rate</td>
</tr>
<tr>
<td>$J_0$</td>
<td>Forefactor factoring into the nucleation rate</td>
</tr>
<tr>
<td>$\Delta F$</td>
<td>Helmholtz free energy</td>
</tr>
<tr>
<td>$\Delta F_{surf}$</td>
<td>Helmholtz free energy of the bubble surface</td>
</tr>
<tr>
<td>$\Delta F_{vol}$</td>
<td>Volumetric Helmholtz free energy</td>
</tr>
<tr>
<td>$\Delta F^*$</td>
<td>Critical Helmholtz free energy (i.e. activation energy)</td>
</tr>
<tr>
<td>$P$</td>
<td>Pressure in the melt</td>
</tr>
<tr>
<td>$P^*$</td>
<td>Internal pressure in the nucleus</td>
</tr>
<tr>
<td>$\Delta P$</td>
<td>Supersaturation pressure</td>
</tr>
<tr>
<td>$\Delta P_{hom}$</td>
<td>Supersaturation pressure of homogeneous nucleation</td>
</tr>
<tr>
<td>$\Delta P_{het}$</td>
<td>Supersaturation pressure of heterogeneous nucleation</td>
</tr>
<tr>
<td>$Pe$</td>
<td>Péclet number</td>
</tr>
<tr>
<td>$T$</td>
<td>Temperature</td>
</tr>
<tr>
<td>$R$</td>
<td>Gas constant</td>
</tr>
<tr>
<td>Re</td>
<td>Reynolds number</td>
</tr>
<tr>
<td>$\Pi$</td>
<td>Nondimensional buoyancy ratio</td>
</tr>
<tr>
<td>$\nu_S$</td>
<td>Stokes settling speed</td>
</tr>
<tr>
<td>$V_{mol}$</td>
<td>Volume of a volatile molecule</td>
</tr>
<tr>
<td>$\Delta Z$</td>
<td>Depth interval corresponding to $\Delta P$</td>
</tr>
</tbody>
</table>
phenocrysts or microlites are probably always present in the melt, even during the very early stages of solidification and serve as sites onto which gas molecules can attach during the nucleation process. The relative ease of heterogeneous as compared to homogeneous nucleation is determined by the surface energy of the crystal-gas as compared to the melt-gas interface (e.g. [26]). If the surface energy of the crystal-gas interface is lower than that of the melt-gas interface, the activation energy \( \Delta F^* \) for nucleation on a crystal face is lower than the energy required for spontaneous nucleation in the melt (see Appendix D) and bubbles are likely to nucleate heterogeneously [262].

An empirical criterion for comparing the two surface energies is the wetting angle \( \theta \) (Fig. 5-1). The larger the wetting angle \( \theta \), the easier it is for the bubble to wet the crystal surface, and the lower the supersaturation pressure required for heterogeneous nucleation. The wetting angle depends on the surface energy of the three interfaces through the relationship

\[
\cos \theta = \frac{\sigma_{gc} - \sigma_{mc}}{\sigma_{gm}},
\]

where the subscript \( c \) denotes the crystalline, \( g \) the gaseous, and \( m \) the melt phase. The surface energy of the crystal-bubble-melt system can be related to the surface
Figure 5-1: The wetting angle $\theta$ is the angle between the crystal face and the tangent to the bubble surface at the point of contact.

Energy of a spherical bubble surrounded by melt through a factor $\psi$ defined as:

$$\psi = \sqrt{\frac{(2 - \cos \theta)(1 + \cos \theta)^2}{4}}$$  \hspace{1cm} (5.2)

implying that the activation energy required for heterogeneous nucleation is lower than that for homogeneous nucleation by $\psi$

$$\Delta F_{\text{het}}^* = \Delta F_{\text{hom}}^* \psi.$$  \hspace{1cm} (5.3)

Based on an extension of the classical theory for homogeneous nucleation to heterogeneous nucleation [26, 197], the supersaturation required for heterogeneous nucleation, $\Delta P_{\text{het}}$, may thus be estimated from that for homogeneous nucleation, $\Delta P_{\text{hom}}$, by multiplying $\Delta P_{\text{hom}}$ with the factor $\sqrt{\psi}$. Figure 5-2 shows how the ratio of supersaturation pressures required for heterogeneous versus homogeneous nucleation depends on the wetting angle of the exsolving gas on the crystals present. Unfortunately, the experimental determination of wetting angles is extremely challenging, partly because visible angles might not represent critical wetting angles [84]. Nonetheless, some observational evidence on wetting angles exists in a terrestrial context [62, 123, 174] and is valuable for the purpose of obtaining an order-of-magnitude estimate of the super-
The supersaturation pressure required for nucleation plays an important role in our modeling and merits a brief clarification: Assuming a purely hydrostatic pressure in the magma, the supersaturation pressure $\Delta P$ may be converted to a depth interval $\Delta Z$. In order for homogeneous nucleation to occur, the melt has to experience a pressure drop of $\Delta P$, or equivalently, ascend by a distance of $\Delta Z$. This implies
that melt has to be saturated in volatiles at depths $Z > \Delta Z$. The level of volatile enrichment required to reach the saturation threshold at these potentially significant depths depends sensitively on the solubility of the volatile. If the solubility increases rapidly with depth, considerable enrichment in volatile may be necessary to reach the saturation limit at large depths (i.e. at several km depth), particularly in small bodies where even moderate pressure drops correspond to large depths.

**Bubble growth**

Generally, bubble growth in magmas can occur through four basic processes: diffusional growth, decompressional growth, bubble coalescence, and Ostwald ripening. The latter two are likely negligible in magma oceans because of vigorous thermal convection limiting the time scale of interaction between bubbles. Ostwald ripening [202] and probably also bubble coalescence are thought to require bubble interaction over a longer time. We will return to the potential role of coalescence again in the next section (sec. 5.2.1); for now, we focus on diffusional and decompressional growth.

The classic theory for the growth of a solitary bubble in an unlimited body of fluid [252] predicts the parabolic growth law

$$r = 2\gamma \sqrt{Dt},$$

(5.4)

where $r$ is the radius, $t$ the time, $D$ the diffusion coefficient, and $\gamma$ the growth rate constant. The growth rate of homogeneously nucleated bubbles $\gamma$ is strongly dependent on supersaturation pressure, with lower supersaturation pressures corresponding to lower growth rates, as also observed in experimental studies of bubble growth (e.g. [174]).

The parabolic nature of the growth law (eq. 5.4) implies that initial bubble growth is rapid. However, if bubbles may no longer be regarded as approximately solitary, their growth is expected to slow substantially. Therefore, apart from the initial volatile content and total pressure drop, bubble growth is ultimately limited by the bubble number density, because it determines how many bubbles a given mass of
volatiles will be divided among \([166, 85, 218, 220, 221]\). The dependence of bubble growth on bubble number density results in significantly smaller bubble sizes than expected theoretically for solitary bubbles \([252, 274]\). For a quantitative estimate of the expected bubble size distribution in a magma ocean please refer to sec. 5.3.2.

**Bubble breakup**

The maximum size a bubble may attain is limited not only by the volatile content, pressure drop, and bubble number density, but also by the dynamic instability of large bubbles. Large bubbles tend to break apart rapidly because the stabilizing effect of surface tension on the bubble surface decreases rapidly with increasing bubble radius. Breakup is delayed in highly viscous fluids \([96]\), but the viscosity of magma oceans is probably not sufficient \([155]\) for this effect to play a major role.

While conceptual models of bubble breakup in turbulent flows exist (e.g. \([113]\)), they require specification of eddy length scales, local shear stress, and/or turbulent energy that are unknown for magma oceans. Instead, we suggest using the Bond or Eötvös number as a first order estimate for the maximum stable size of gas bubbles in magma oceans

\[
Bo = \frac{\Delta \rho g r^2}{\sigma} > 1. \tag{5.5}
\]

The Bond number represents the ratio of body to surface tension forces. More intuitively, it captures the deformability of bubbles where \(Bo > 1\) implies that bubbles are deformable, or equivalently, that surface tension is insufficient to restore the bubbles to sphericity. Independent of the exact mechanism, breakup inevitably requires bubble to be deformable such that surface instabilities can form. Thus, \(Bo > 1\) may be regarded as a prerequisite of breakup implying that the bubble radius

\[
r_{max} > \sqrt{\frac{\sigma}{\Delta \rho g}} \tag{5.6}
\]

provides a lower bound for the maximum stable bubble size. An upper bound may be derived from chapter 3 which concluded that bubbles characterized by \(Bo > 1\) and Reynolds numbers of order 10 or larger (\(Re > O(10)\)) are prone to rapid breakup,
even in stagnant fluids. Since Re is thought to be much larger than \( O(10) \) in magma oceans independent of bubble size, we argue that \( r_{\text{max}} \) is a reasonable overall estimate of the maximum stable bubble size.

It is worth noting that the insight that bubbles in magma oceans are likely characterized by \( Bo < 1 \) also implies that coalescence is probably of little relevance for bubble growth (sec. 5.2.1), because small deformations on the bubble surface impede coalescence [233, 231] and large deformations lead to breakup (eq. 5.6).

### 5.2.2 Degassing at macroscopic scales

In order to take the leap from the microscopic to the macroscopic scale, we identify the conditions under which gas bubbles are able to decouple from the vigorous ambient flow field, rise to the surface and degas.

**Bubble entrainment**

The degree to which bubbles are able to decouple from the ambient flow field determines to what degree degassing and atmosphere formation occurs. The two main factors controlling whether a gas bubble remains entrained in the convection or rises to the surface under its own buoyancy is (1) the bubble radius \( r \), because the rise speed of bubbles increases rapidly with increasing bubble radius and (2) the bubble number density.

For very small bubbles (e.g. bubbles immediately after nucleation), Brownian motion is sufficient to keep them suspended regardless of fluid motion. The critical size beyond which this is no longer the case can be estimated from the Péclet number, which measures the relative importance of the rate of advection to the rate of diffusion.

\[
\text{Pe} = \frac{rv_S}{D_0} = \frac{4\pi \Delta \rho g r^4}{3 kT},
\]

where \( v_S = 2 \Delta \rho g r^2/(9 \mu) \) is the Stokes settling speed and \( D_0 = kT/(6 \pi \mu r) \) the Stokes-Einstin diffusion constant for individual particles. If Pe > 1 gravity overcomes the randomizing effect of Brownian collision and the bubble can decouple from the
stagnant fluid surrounding it. In a vigorous flow field, however, the bubble might remain entrained because its rise speed is still much smaller than the convective velocity.

The competing effects of entrainment versus decoupling have been investigated primarily in the context of crystals [181, 142, 272, 270]. For example, [272] found that crystals with diameters of $10^{-2}$ to $10^{-1}$ cm are likely to remain entrained in magma oceans. The primary drawback associated with applying an analogous rationale to bubble entrainment is that the volume fraction of bubbles is highly localized inside the magma ocean and essentially confined to upwellings at a maximum distance of a few km from the surface (sec. 5.2.1). Once the critical supersaturation for homogeneous nucleation has been exceeded (eq. D.3), the volume fraction of bubbles will increase very rapidly from essentially zero to close to its maximum value. This sudden increase in buoyancy within the upwelling will have important dynamic consequences even if bubbles are small, because it shifts the local force balance between thermal and compositional buoyancy.

Thermal buoyancy drives magma ocean convection initially. The change in magma density is related to pressure and temperature through the isothermal compressibility $\beta$ and the thermal expansion $\alpha$

$$d\rho_m = \rho_m(\beta dP - \alpha dT) \quad \text{(5.8)}$$

or, more simply

$$\Delta \rho_m \approx -\alpha \rho_m \Delta T \quad \text{(5.9)}$$

when setting $dP \approx 0$ to obtain an upper bound estimate for the thermal buoyancy force

$$B_t = -\alpha \rho_m gh \Delta T, \quad \text{(5.10)}$$

where $h$ is the depth of the magma ocean. Note that analogous to previously, the subscripts $g$ and $m$ refer to the magma and gas phase, respectively.
The change in density for a bubble-bearing magma with bubble fraction \( \phi \) is

\[
\Delta \rho_m = \rho_m - \phi \rho_g - (1 - \phi) \rho_m = \phi \rho_m - \phi \rho_g ,
\tag{5.11}
\]

where the pressure-dependent density of the gas phase \( \rho_g \) may be approximated using the ideal gas law yielding

\[
\Delta \rho_m = \phi \left( \rho_m - \frac{m_g P}{RT} \right)
\tag{5.12}
\]

where \( R \) is the gas constant, and \( m_g \) is the mass of the gas phase. Thus, the compositional buoyancy force may be expressed as

\[
B_c = -\phi gh \left( \rho_m - \frac{m_g P}{RT} \right) .
\tag{5.13}
\]

The relative importance of these two contributions to buoyancy is captured in the non-dimensional force ratio

\[
\Pi = \frac{B_t}{B_c} = \frac{\alpha \rho_m \Delta T}{\phi (\rho_m - \frac{P}{RT})} .
\tag{5.14}
\]

We suggest that if \( \Pi < 1 \), degassing will occur even if individual bubble sizes may be too small to decouple from flow based on the rationale by [270], because the volume fraction of bubbles is large enough to cause a local shift from thermal convection to compositional convection. The change to compositionally-driven convection implies that bubble-rich upwellings originating near the depths of bubble formation will dominate the flow field, disrupting the existing pattern of thermal convection, and separated by regions of diffuse downward return flow with low bubble content.

### 5.3 Results

We apply our model to a magma ocean of 1000 km depth as may have existed on terrestrial planets and exoplanets shortly after accretion and differentiation. The bulk composition of the silicate mantle is taken from and represents a typical melt composition for the Earth and Earth-like planets [107]. We assume that the magma
Table 5.2: Supersaturations required for non-zero homogeneous (eq. D.3) and heterogeneous (eq. 5.3) nucleation in a basaltic magma ocean with variable volatile contents. We consider nucleation rates of $J < 1 \text{cm}^{-3} \text{s}^{-1}$ to be negligible. The remaining parameters are $\sigma = 0.3 \text{N/m}$, $\rho_m = 3400 \text{kg/m}^3$, $T = 1100K$, $g = 9.5 \text{m/s}^2$, $V_{H_2O} \approx 11.5 \text{Å}^3$, $V_{CO_2} \approx 4 \text{Å}^3$, $D_{H_2O} = 100 \times 10^{-12} \text{m}^2/\text{s}$ [326], and $D_{CO_2} \approx 13 \times 10^{-12} \text{m}^2/\text{s}$ [315, 326, 313]. In order to take both water and carbon dioxide into account for the computation of the forefactor $J_0$, we take the weighted mean of the parameters characterizing water and carbon dioxide, respectively.

<table>
<thead>
<tr>
<th>H$_2$O content [wt%]</th>
<th>CO$_2$ content [wt%]</th>
<th>Supersaturation (homogeneous) $\Delta P$ [MPa]</th>
<th>Supersaturation (heterogeneous) $\Delta P$ [MPa]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.05</td>
<td>0.01</td>
<td>736</td>
<td>37 - 405</td>
</tr>
<tr>
<td>0.5</td>
<td>0.1</td>
<td>702</td>
<td>35 - 386</td>
</tr>
<tr>
<td>5.0</td>
<td>1</td>
<td>673</td>
<td>34 - 370</td>
</tr>
</tbody>
</table>

ocean is entirely molten initially and has retained a portion of the volatile content of the accreted material equivalent to 0.01 wt % carbon dioxide and 0.05 wt % water.

5.3.1 Early phase of magma ocean solidification

We define the early phase of magma ocean solidification as spanning the time interval from the generation of the magma ocean until the onset of nucleation. The duration of this phase depends primarily on whether nucleation occurs homogeneously or heterogeneously.

The supersaturations for nucleation in basalts tend to be higher than those in rhyolites (e.g. [123]), because of the higher surface energy of gas bubbles in basalt (e.g. [27]). However, while the surface energy of the melt-gas interface is significantly higher in basalts compared to rhyolites, the surface energy of the crystal-gas interface may not be drastically different, because it is not thought to be strongly dependent on the surrounding melt phase. The high surface energy of gas bubbles in basaltic melt should thus increase the relative importance of heterogeneous over homogeneous nucleation in basaltic as compared to rhyolitic melts in agreement with field observations (e.g. [175]). Experimental studies of bubble nucleation in rhyolitic melts
Figure 5-3: Evolution of the volatile content (top) and saturation pressure (bottom) in a 1000-km-deep magma ocean with the fluid composition derived by [107] and initial volatile content 0.05 % water and 0.01 % carbon dioxide. The solubility behavior is computed based on [205]. The grey domain highlights volatile enrichment levels sufficient for heterogeneous nucleation based on the uncertainty interval given in sec. 5.3.1. The inset in the bottom figure illustrates that the supersaturation pressure corresponds to a depth which increases with increasing volatile enrichment (not plotted to scale).
found that while homogeneous nucleation exists [193, 174, 192, 194], heterogeneous nucleation is more common [123, 85, 84, 83]. Combining these experimental findings with the insight that bubbles are more likely to nucleate heterogeneously in basalts as compared to rhyolites, we conclude that heterogeneous nucleation is the dominant mechanism of nucleation in magma oceans.

A necessary condition for heterogeneous nucleation is obviously the presence of crystals, which may act as nucleation sites. But this condition is unlikely to create an impediment, even if crystal settling is thought to be fairly efficient, because (1) only low crystal contents are required ([12] observed that only 5 – 10% microlites in the melt speed up vesiculation of rhyolite by a factor of 10-100 compared to crystal-free rhyolite) and (2) microlites of size $r \leq O(\mu m)$ are probably ubiquitous in the flow because even Brownian motion would be sufficient to keep them suspended (see sec. 5.7). Constraining the supersaturation required for heterogeneous nucleation is
challenging. We rely on experimental evidence for water-dominated bubbles in rhyolitic melt by [174] who report wetting angles in the range of 129° to 135°, and on [123] who observed lower wetting angles (θ > 90°) for a range of different minerals. We will not attempt to distinguish wetting angles for specific minerals in the solidifying magma ocean, because of a lack of experimental data that we could base our estimates on. Experimental findings do indicate, however, that different minerals exhibit a wide range of wetting behavior implying that at least some of the crystallizing minerals in a magma ocean are expected to have medium to high wetting angles. Thus, we define an uncertainty interval of 10° to 135° reflecting our current stage of knowledge about wetting angles of water-dominated bubbles. The lower bound of this uncertainty interval is not consequential as there will be enough mineral phases that trigger nucleation earlier. The upper bound, however, determines the onset of degassing sensitively. In order to obtain a conservative estimate and because the wetting angles of bubbles consisting primarily of carbon dioxide might be slightly higher as compared to water bubbles [314], we assume that the supersaturations required for heterogeneous nucleation could be 5 – 50% that required for homogeneous nucleation (eqs. 5.2 and 5.3). Table 5.2 lists estimates of the supersaturation for homogeneous (eq. D.3) and heterogeneous nucleation (eq. 5.3) in the magma ocean.

During solidification from below, volatiles are continuously enriched in the liquid portion of the magma ocean because they partition preferentially into the melt phase. Initially, volatile saturation is only achieved very close to the surface, but as the volatile content increases, the depth at which the liquid melt is saturated in volatiles moves deeper and deeper. Eventually, the saturation depth reaches depths representative of the supersaturation pressure required for nucleation. Note that since magma ocean dynamics at this stage are almost certainly vigorous and probably turbulent, the magma ocean should be well mixed and volatile content equally distributed with depth.

Figure 5-3 shows the increase in saturation depths computed based on the solubility model of [205] for increasing depth within the magma ocean. The area shaded in grey represents the uncertainty interval of supersaturation pressure required for
heterogeneous nucleation. Two aspects of Figure 5-3 merit further discussion. (1) Despite the substantial uncertainty in the supersaturation required for heterogeneous nucleation, Figure 5-3 demonstrates that nucleation is only possible during the final stages of magma ocean solidification (i.e. \( \sim 80 - 100\% \) solidified). (2) The volatile enrichment required for the onset of nucleation depends sensitively on the solubility behavior of the gas species, in particular on how rapidly solubility increases with depth.

### 5.3.2 Late phase of magma ocean solidification

We define the late phase of magma ocean solidification to span the time interval from the onset of nucleation until solidification is complete. We apply the bubble model developed in sec. 5.2.1 to first identify the size range of bubbles in the magma ocean and then the condition under which degassing occurs (sec. 5.2.2).

At the time of nucleation, the size of the bubbles is given by the critical radius (eq. D.1), which will typically be \( O(\text{nm}) \) in magma oceans. At this size, bubbles are expected to grow very rapidly to \( O(\mu \text{m}) \), probably within less than 1s, because of the parabolic nature of bubble growth (see eq. 5.4). Observed growth rates of bubbles in basalt are typically on the order of \( \beta = O(10^{-4}) \) cm/s [274, 176]. Bubble growth in magma oceans is probably not viscosity limited as is sometimes the case for more silicic magmas in terrestrial contexts (e.g. [274, 291, 292]), because the viscosity of magma oceans is thought to be very low by terrestrial standards [155].

The rapid growth of bubbles to sizes of \( O(\mu \text{m}) \) in combination with the rapid
breakup of very large bubbles ($r \approx 1\text{mm}$) in vigorous flow fields (see sec. 5.2.1) means that the vast majority of the bubbles in the magma ocean will fall into the size range $1\mu\text{m} < r < 1\text{ mm}$ (see Table 5.3). Therefore, individual bubbles might remain too small to decouple from the ambient flow field. An assemblage of bubbles, however, will lower the effective density of the magma and may cause a local shift in the mode of convection from thermally- to compositionally-driven if $H < 1$ (eq. 5.14, sec. 5.2.2). We conclude that out of the two parameters determining the ability of bubbles to decouple from the flow field and degas (i.e. bubble radius and bubble fraction, see sec. 5.2.2), the bubble fraction $\phi$ is more important than the bubble size $r$ in vigorously convecting magma oceans. For a potential magma ocean depth of 1000 km, we estimate that the critical bubble fraction at which a local shift in convection may happen is $\phi \approx 0.03$ (see eq. 5.14) at low pressures ($P < 1$ GPa). This estimate may be converted to a critical bubble number density when assuming a certain bubble size or bubble size distribution. $N$ ranges from $\approx 7\text{ cm}^{-3}$ for bubble
radii of $r = 1 \text{ mm}$ to $N \approx 7 \times 10^6 \text{ cm}^{-3}$ for $r = 10 \mu\text{m}$. These estimates demonstrate that the propensity of bubbly magma to degas depends on both the nucleation rate and the growth period: Very large nucleation rates (Fig. 5-4) lead to large bubble number densities such that even small bubbles ($r < 100 \mu\text{m}$) should be able to degas. Very low nucleation rates on the other hand might not create enough bubbles per volume to cause degassing even if they all achieve maximum size.

Thus, the onset of nucleation at the microscopic scale does not necessarily imply the onset of degassing at the macroscopic scale. Two supersaturation pressures need to be considered when evaluating the capability of a magma ocean to degas: The supersaturation required for nucleation and the supersaturation needed to achieve a nucleation rate sufficient for high enough bubble number densities. For the magma ocean discussed here, we estimate that the nucleation rate must exceed $O(100) \text{ cm}^{-3}\text{s}^{-1}$ to generate a high enough bubble number density such that the critical bubble fraction (eq. 5.14) can be reached after sufficient bubble growth. Figure 5-4 shows an example of the relationship between the supersaturations required for nucleation and degassing representative of intermediate wetting behavior (i.e. $\Delta P_{het} = 30\% \Delta P_{hom}$). In this case, the temporal delay in degassing due to bubble entrainment is small compared to the time it takes the magma ocean to solidify by an additional 1%.

Depending on the assumed supersaturation for nucleation, we expect widespread nucleation events in hot upwellings throughout the magma ocean sometime after $\sim 80\%$ solidification. As long as the supersaturation pressure is insufficient for degassing, the bubbles remain entrained in the ambient flow field and will be resolved in the magma when carried back down to greater depths. Therefore, the magma ocean is further enriched in volatiles during this transient state until it is supersaturated enough for degassing to occur. The initiation of degassing facilitates further degassing, because (1) the presence of bubbles in the flow field obviates a separate nucleation event by allowing volatiles in excess of saturation to diffuse into existing bubbles instead of nucleating new ones and (2) degassing implies a local shift from thermal to compositional convection and as a consequence the flow field should have a more pronounced vertical component which is essential for providing the pressure drop.
Figure 5-6: Overview of the two phases of magma ocean solidification that are pertinent to catastrophic degassing sequences. Left: Nucleation delayed by insufficient supersaturation and bubble breakup create small bubbles that remain entrained and do not degas. Right: Once bubbles have reached a critical size required for degassing, compositional convection becomes dominant at shallow depths. Catastrophic degassing may not happen until > 80% solidification for a 1000-km-deep magma ocean as may have existed on terrestrial planets and exoplanets.

Thus, a sequence of nucleation events would occur in a given upwelling until the inflowing melt from below is no longer supersaturated in volatiles. Given that bubble nucleation and growth happen on time scales that are small compared to the time scale of magma ocean solidification, degassing constitutes an exceptionally rapid and sudden event that we refer to as 'catastrophic' degassing. After experiencing catastrophic degassing, magma ocean solidification will proceed much more slowly because of the insulating effect of the newly formed atmosphere. Fig. 5-6 gives an overview of the two solidification phases for magma oceans that exhibit catastrophic degassing.

5.4 Discussion

5.4.1 Catastrophic degassing of magma oceans

Whether magma oceans degas catastrophically (sec. 6.4) or continuously as assumed in a previous study [66] depends on two factors: (1) the delay in degassing that

144
may result from a finite supersaturation required for nucleation and (2) the delay in degassing that may result from bubble entrainment in the vigorous convective flow field (Fig. 5-4). Assuming a similar nucleation process on both small and large planets, the nucleation delay becomes more important the smaller the mass of the planet. The reason is that even a small pressure drop may translate into a substantial depth in a low gravitational field. If a finite supersaturation pressure is required for nucleation, a substantial enrichment in volatiles is necessary, which effectively limits nucleation to the late stages of solidification. The relationship between magma ocean size and entrainment delay, however, is less straightforward to evaluate. On the one hand, deep magma oceans tend to convect more vigorously than shallow ones and will thus tend to keep bubbles entrained for longer. On the other hand, the convective vigor of the entire magma ocean is less relevant than the flow speed in the upper boundary layer, which depends sensitively on crystal fraction, the potential presence of a conductive lid and other dynamic factors including fluid viscosity. These other factors may very well play a more important role for degassing than the overall depth of the magma ocean.

The possibility that magma oceans may degass catastrophically instead of continuously has important ramifications both for the early atmosphere and for the volatile composition of the solidified mantle:

1. The onset of nucleation at the microscopic scale does not necessarily imply the onset of degassing at the macroscopic scale. For a given magma ocean, the temporal delay between the two depends primarily on the degree of solidification (Fig. 5-3), because volatile enrichment in the magma proceeds much faster towards the end of solidification (see Fig. 5-3). Even in vigorously convecting magma oceans, the delay in degassing due to bubble entrainment is probably very small compared to the time scale of solidification.

2. The onset of catastrophic degassing is determined primarily by the volumetric bubble fraction resulting from nucleation and growth. After a local shift from thermally- to compositionally-driven convection, bubbles in all size ranges will
be swept up to the surface and degas rapidly to form the earliest atmosphere. The duration of catastrophic degassing depends on the convective flow field in the magma ocean. Using potential convective velocities of $O(1)$ m/s [270], we estimate that a catastrophic degassing event could last from several hours up to a few days depending on the degree of solidification upon onset of degassing.

3. The composition of the atmosphere formed by degassing clearly depends on the partitioning behavior of the volatiles involved (e.g. [205]), but possibly even more importantly on the vigor of convection in the magma ocean: The convective velocity determines the time scale of decompression relative to diffusion, which controls degassing efficiency (i.e. the ability to equilibrate melt and vapor phase during bubble growth). The faster the decompression, the less time is available for diffusion which could lead to substantial residual volatiles in the melt [174].

5.4.2 Water hitching its way up to the surface

Water and carbon dioxide play different roles in the degassing process, because of their different solubility behavior at depth and diffusivity. Figure 5-5 contrasts the solubility of each volatile based on [205]. The fact that the solubility of water increases much more rapidly with depth than the solubility of carbon dioxide (Fig. 5-5) implies that much higher levels of volatile enrichment are required to trigger nucleation of water as compared to carbon dioxide bubbles.

The main ramification is that water can only degas efficiently in the presence of another volatile that nucleates more easily. In fact, if a magma ocean contains almost exclusively water, degassing might not occur during the convective phase of magma ocean solidification. In the case of the terrestrial magma ocean discussed above, carbon dioxide fulfills the function of a carrier volatile facilitating degassing. Once carbon dioxide bubbles have nucleated, water diffuses into these bubbles and degasses through them, much like a hitchhiker getting a ride to the surface. After nucleation, water tends to degas more efficiently because the diffusivity of water is
about one order of magnitude larger than that of carbon dioxide [326, 315, 326, 313].

The complementary behavior of water and carbon dioxide may be illustrated through the following thought experiment: Let us consider three hypothetical magma oceans which are identical in all respects except that the first contains primarily water, the second primarily carbon dioxide and the third an equal mix of the two volatiles. The magma ocean that contains both water and carbon dioxide would degas most efficiently, because nucleation is facilitated by carbon dioxide and diffusive growth by water. In addition to having the higher diffusivity, water also tends to increase the diffusivity of carbon dioxide [312]. The magma ocean containing only carbon dioxide would degas but probably to a lesser degree than the magma ocean containing both volatiles, because diffusion proceeds much more slowly. Finally, the magma ocean containing almost exclusively water might not degas through these processes, but only lose some water vapor from a very late-stage crystal mush layer. If degassing does occur, it is particularly violent and rapid because of the high supersaturation.

5.4.3 Extent of early melting might determine the fate of volatiles

An important prediction of our model is that degassing depends not only on the initial volatile content, but also sensitively on the depth of the magma ocean. The main reason is that for a given initial volatile fraction the total mass of volatiles increases with magma ocean volume. Consequently, a shallow magma ocean may never reach the enrichment level required to trigger degassing.

For potential magma oceans with the same initial volatile content (e.g. 0.5 wt. % water and 0.1 wt. % carbon dioxide) but variable depths, the uncertainty in the supersaturation required for heterogeneous degassing (see sec. 5.3.1) translates into uncertainty regarding the minimal initial magma ocean depth required for eventual degassing. At depths of \( \geq 1000 \) km, degassing occurs over the entire uncertainty interval of supersaturations. At intermediate depths (\( \approx 750 \) km), degassing only occurs if the supersaturation required for nucleation falls into the lower 50% percentile
of the distribution of possible supersaturations. At small magma ocean depths ($\approx 250$ km), the magma ocean is not expected to degas during the convective phase of magma ocean solidification unless the supersaturation required for nucleation is approximately zero. An important caveat of these estimates is that they assume a constant gravitational acceleration.

Two magma oceans with comparable initial volatile content but different depths might therefore experience drastically different degassing histories. The consequences for the planetary interior are substantial: the magma ocean that does not degas catastrophically will be characterized by elevated volatile contents during most of its solidification, which translate into higher volatile contents in the nominally anhydrous phases as well as in trapped interstitial liquid. Since even a few parts per million of water or hydroxyl in the rocky interior of an emerging planet lowers its viscosity and melting temperature notably, these differences may have a lasting impact on the later evolution of the planet and the onset of solid-mantle overturn. Our model thus demonstrates why early planetary embryos with a similar initial composition might deviate early in their evolution.

5.4.4 Three end-member cases of degassing

Based on the dynamics of nucleation and entrainment, magma oceans may follow three distinct degassing paths: (1) continuous degassing, (2) catastrophic degassing, and (3) negligible degassing (Fig. 5-7).

First, continuous degassing implies that degassing of volatiles in excess of saturation occurs constantly during the solidification of a magma ocean. This scenario is viable if there is reason to believe that heterogeneous nucleation requires negligible supersaturation (i.e. if the gas phase wets the crystal interface close to perfectly). That might be the case, for example, if Fe-Ti oxides, which are known to greatly facility nucleation of water-rich bubbles [123], are abundant in flow. Alternatively, continuous degassing might arise if the volatile content is high enough to initiate degassing immediately after the formation of the magma ocean and/or if the magma ocean is constantly replenished in volatiles by volatile-rich impactors. A key factor
Figure 5-7: Illustration of the three end-member cases of magma ocean degassing. Note that the wiggly arrows in red represent heat flux and not degassing. The first case (A) represents continuous degassing and gradual atmosphere formation. It applies to magma oceans with extremely high initial volatile contents or alternatively, with a content of crystals that are wetted perfectly by at least one of the dissolved volatiles. The second case (B) represents a degassing history characterized by one or several catastrophic degassing events with little or no degassing happening prior or after. Catastrophic degassing leads to the sudden formation of a substantial atmosphere. In the third case (C), the volatile content is never sufficient to trigger degassing and little atmosphere will form during solidification. The initial magma ocean depth is smaller in this case to reflect that this scenario is more likely for shallow magma oceans.
facilitating high initial volatile contents is a preexisting atmosphere, because volatiles in the magma ocean equilibrate with those in the atmosphere. High partial pressures in the atmosphere may thus translate into high volatile contents in the magma ocean. Magma oceans that degas continuously are characterized by substantial atmospheres and comparatively low solidification speed. These very high volatile scenarios, however, are unlikely for terrestrial planets in our solar system unless they have an unusually thick preexisting atmosphere. They might be more pertinent for Super Earths since very massive planets are more likely to have inherited an atmosphere from accreting protoplanets.

Second, catastrophic degassing is pertinent for planets of intermediate size and relatively low initial volatile contents. We hypothesize that magma oceans on terrestrial planets may have degassed discontinuously through a single (or possibly multiple) catastrophic degassing events. Catastrophic degassing divides the solidification history of the magma ocean into two distinct segments (Fig. 5-6). Compared to discontinuous degassing, magma oceans that exhibit catastrophic degassing are characterized by a less substantial early atmosphere and a higher volatile content in the solidified mantle.

Third, negligible degassing in combination with volatile enrichment in the silicate mantle is a likely scenario for magma oceans on small planetesimals or very shallow magma oceans on larger planets. It may also depend on the relative abundance of certain volatile phases: If the total volatile content – particularly the carbon dioxide content (see sec. 5.4.2) – is insufficient, the solidifying magma ocean might never reach the enrichment level required for degassing. Although volatile enrichment increases rapidly during the very late stages of solidification (e.g. Fig. 5-3), this effect is offset partly by the rapidly decreasing temperature that leads to even higher supersaturations for nucleation (eq. D.3) and by the increasing solid fraction in the solidifying mantle which could halt degassing through fluid-dynamical ascent of gas bubbles. The dynamic consequences of a lack of degassing are (1) high volatile contents in the solidified magma ocean, (2) a minimal atmosphere, and (3) exceptionally rapid time scales of solidification.
5.5 Conclusion

We present a new framework for modeling the degassing of magma oceans. Its main contribution as compared to previous approaches is that we consider bubble nucleation, growth, and breakup at the microscopic scale (sec. 5.2.1). At the macroscopic scale, we suggest that the onset of degassing coincides with a local shift from thermally-driven to compositionally-driven convection (sec. 5.2.2). We apply our model to a hypothetical magma ocean of 1000 km depth and find that degassing may occur catastrophically, dividing the solidification history of a potential terrestrial magma ocean into two distinct segments (Fig. 5-6): During the early phase of magma ocean solidification, heat flux through the surface is very high and solidification from below rapid. Rapid interior cooling in turn makes the time to clement surface conditions rapid, preparing the planetary surface for liquid water. Once the magma ocean is sufficiently enriched in volatiles, a catastrophic degassing event will lead to the sudden formation of an early atmosphere, probably in as little as a few hours or days. Its insulating effects lower the heat flux through the surface and diminish the solidification speed.

Numerous parameters determine the degassing history of a magma ocean. The three most important parameters are the initial volatile content, the depth of the magma ocean, and the gravitational field. In terms of volatile content, carbon dioxide (or a different carrier volatile, see sec. 5.4.2) is of particular importance for facilitating nucleation. The insight that the magma ocean depth plays an important role points to one process by which terrestrial planets could begin with different internal volatile budgets.

Small bodies with a low gravitational field are more likely to experience significant volatile enrichment instead of degassing during a magma ocean phase than large bodies. In addition, the wetting behavior of the volatiles on the mineral phases crystallizing in the magma is of crucial importance, because it determines how much volatile enrichment is required before nucleation becomes possible. Unfortunately, little experimental data is available to constrain the supersaturation pressure required
for nucleation exactly and we are thus led to assume a wide uncertainty interval (sec. 5.3.1). Finally, surface tension is worth mentioning. Gas bubbles in low-silicate melts are thought to have fairly high surface tension (e.g. [135]), but if there is reason to think that the surface tension would be significantly lower for a given volatile or melt composition, degassing would occur earlier.
Chapter 6

Direct numerical simulations of solid-fluid coupling in crystalline suspensions

6.1 Introduction

Countless problems in the Earth sciences involve the dynamic interaction between solid bodies and viscous flow. In selected cases, one of the two phases dominates the behavior of the ensemble and the effect of the other can be incorporated in a simplified manner. Examples in which the liquid phase dominates include the rheology of molten magma with low crystal fraction, where the presence of crystals can be accounted for by defining an increased effective viscosity through the Einstein-Roscoe relation [63, 229]. Conversely, an example in which the solid phase dominates is the deformation of partially molten rock with a limited percentage of melt, which can be treated through a poroelastic approximation considering only the elevated pore pressure due to the presence of the fluid, but neglecting more complex aspects such as a flow field in the fluid phase.
These two examples highlight that we are well equipped to deal with the two end-member cases of the solidification process, i.e. the early stages in which the aggregate is largely molten and the final stages in which it is mostly solid. The greatest challenge is posed by the intermediate stages in which both the solid and the liquid phase contribute significantly to the dynamics of the system. The goal of this chapter is to develop a computational methodology capable of capturing the complex solid-fluid interactions at this intermediate stage and to do so from first principles.

Numerical schemes that resolve the physics of the problem without relying on approximate drag formulas or prescribed settling speeds are often referred to as 'direct'. Here, we formulate a tool for direct simulations of solid-fluid coupling in crystalline suspensions. The added challenges in devising a method for direct numerical simulations of solid-fluid suspensions, as opposed to pure fluid or purely solid systems, are three-fold. First, two sets of governing equations, those describing fluid and those describing solid motion, need to be solved. Second, the solid and fluid phases are fully coupled, meaning that the motion of the solid bodies induces a flow field in the fluid and that a flow field in the fluid will cause the solid bodies to move. Third, the time and length scales determining motion in the fluid as compared to the solid might be drastically different. The latter is particularly problematic in many geophysical applications: While the crystallized mineral phases are typically on the order of only μm to mm, the flow in the fluid occurs on the scale of tens or hundreds of km, for example, if convection occurs in large magma chambers, lava lakes, or magma oceans, which might span planetary scales.

The drastic separation of scales by several orders of magnitude requires a decision on the part of the modeler as to which scale to focus on. If the dynamic behavior at small scales is well understood, it can incorporated into large-scale simulations through scaling laws, approximate drag formulas or prescribed settling speeds (e.g. [115, 116, 238, 305]). In most cases, however, the multiphase-flow dynamics arising from the interaction of one or several fluid and solid phases is too complex and too variable to be captured in a simple scaling relationship. Direct numerical simulations that are able to resolve the relevant details allow expanding the reach of numerical
modeling to these types of problems. That being said, the added numerical sophistication of fully resolving the solid-fluid interactions at the scale of the interface, typically in the sub-meter range, may come at the price of not capturing all processes contributing to the dynamics at the very large scale. This limitation warrants a brief discussion of the merits of direct approaches to solid-fluid coupling in geophysical systems.

The main advantage of direct numerical simulations is that they provide insights into the dynamics of a multiphase system from first principles. Thus, they are particularly advantageous for complex flow problems, for which it is usually not possible to specify drag and lift forces a priori. Numerous examples of multiphase processes in Earth science fall into this category, ranging from the fluidization of sedimentary beds to the variable rheology of sea ice and the settling of metal droplets in a liquid silicate magma ocean in the form of metal rain at finite Reynolds number [236]. Direct numerical simulations of solid-fluid coupling also provide insights into how and why the properties of the immersed solid bodies and the ambient fluid determine their dynamic interaction. For example, the presence of plagioclase in magmatic flow is thought to be an important factor for the onset of non-linear rheological effects, because of the high aspect ratio of the crystals [211, 118, 242]. The different behavior of various mineral phases in a given ambient magmatic flow field is also crucial for determining the conditions under which fractional as opposed to batch crystallization occurs – a fundamental question in petrology and magmatic processes. Therefore, direct simulations allow modelers to take advantage of observational data at small scales, such as crystal-size distributions derived from thin section analysis, and explore its ramifications for large-scale dynamics.

We develop a method for direct simulations of solid-fluid coupling in an isothermal system at zero and finite Reynolds number. Our main focus is suspensions involving moderately to highly viscous fluids, but our approach could be easily modified for less viscous systems. The fluids solvers in both the zero- and the finite-Reynolds-number regime rely on a two-step projection scheme: In the first step, we solve the multiple-phase Navier-Stokes or Stokes equation in both domains. In the second step, we
Figure 6-1: Computational domain for the simplified case of a single sphere sinking in viscous fluid. $\Omega$ describes the entire computational domain including both solid and fluid phases and $\partial \Omega$ its boundaries. $P$ is the portion of the domain occupied by a single or multiple particles and $\partial P$ is the solid-fluid interface.

Project the velocity field in the solid domain onto a rigid-body motion by forcing the deformation-rate tensor in the solid domain to be zero. This procedure is also used to enforce the no-slip boundary condition on the solid-fluid interface. We carefully validate and benchmark our approach in two and three dimensions to ensure that we accurately reproduce analytical and laboratory results for the settling speed as well as drag and lift forces.
6.2 Governing equations

The governing equation in the fluid domain of the solid-fluid mixture is Navier-Stokes

\[ \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} = -\frac{1}{\rho_f} \nabla p + \frac{\mu_f}{\rho_f} \nabla^2 \mathbf{v} + \mathbf{g} \]  (6.1)

together with the incompressibility constraint

\[ \nabla \cdot \mathbf{v} = 0, \]  (6.2)

where \(\rho_f\) is the density of the fluid, \(\mu_f\) the viscosity, \(\mathbf{v}\) the velocity field, \(p\) the pressure, \(t\) the time, and \(\mathbf{g}\) the gravitational acceleration.

The motion of the solid bodies is determined by Newton’s laws of rigid-body motion

\[ \frac{M_p}{dt} \mathbf{V}_p = \mathbf{F}_p + M_p \mathbf{g}, \]  (6.3)
\[ \frac{d(\mathbf{I}_p \cdot \omega_p)}{dt} = \mathbf{T}_p, \]  (6.4)
\[ \frac{dX_p}{dt} = \mathbf{v}_p \]  (6.5)

where \(M_p\) is the mass of the particle, \(\mathbf{V}_p\) the velocity of its center of mass, \(X_p\) the position of the center of mass, \(\mathbf{I}_p\) the particle’s moment of inertia tensor, and \(\omega_p\) the angular velocity of the particle. Furthermore, \(\mathbf{F}_p\) and \(\mathbf{T}_p\) represent the hydrodynamic force and torque exerted onto the particle by the surrounding fluid. Defining \(\mathbf{r}\) as the relative position inside the solid body relative to the center of rotation and translation, the velocity field inside the solid body \(\omega_p\) is given by

\[ \mathbf{v}_p = \mathbf{V}_p + \omega_p \times \mathbf{r}. \]  (6.6)

Finally, an important difference between solid-fluid coupling problems as compared to fluid-fluid systems is that the solid-fluid interface \((\partial P)\) is no-slip while fluid-fluid interfaces tend to be free-slip.
We non-dimensionalize the Navier-Stokes equation (eq. 6.1) by defining

\[ x = \frac{dx'}{u_0}, \quad v = u_0 v', \quad t = \frac{d}{u_0} t', \quad p = \frac{\rho d^2}{\mu}, \quad \rho = \rho_f \rho', \quad \mu = \mu_f \mu', \]  

(6.7)

where \( u_0 \) denotes the characteristic speed and \( d \) the characteristic length scale. Substituting these characteristic quantities into equation 6.1, rearranging, and dropping the primes yields the non-dimensional Navier-Stokes equation

\[ \frac{\partial v}{\partial t} + (v \cdot \nabla)v = -\frac{1}{\rho(x)} \nabla p + \frac{1}{Re} \nabla^2 v + \frac{1}{Fr} z \]  

(6.8)

where \( z \) denotes the unit vector in vertical direction, \( Re = \rho_f u_0 d/\mu_f \) denotes the Reynolds number, i.e. the ratio of inertia to viscous forces, and \( Fr = u_0^2 / gd \) denotes the Froude number, i.e. the ratio of inertia to gravity. The boundary condition and incompressibility constraint are non-dimensionalized accordingly.

In complex multiphase systems it is not always possible to specify a single characteristic speed. More commonly, the flow in the fluid and the motion of the solid bodies will be determined by two different speeds. In that case, it is necessary to define two sets of non-dimensional numbers, the particle Reynolds number \( Re_p \) and Froude number \( Fr_p \), where \( u_0 \) captures the speed of motion in the solid phase, and a fluid Reynolds and Froude number \( Re_f \) and \( Fr_f \) based on the flow speed in the fluid.

### 6.3 Numerical method

Significant effort has been devoted over the recent years to the development of robust numerical methodologies for the direct numerical simulation of solid-fluid coupling. Most approaches fall into two categories: (1) Arbitrary-Lagrangian-Eulerian techniques relying on unstructured meshes which are usually fitted around the solid body [122, 120, 130, 121] and (2) Distributed-Lagrange-Multiplier methods operating on fixed grids that typically incorporate the presence of the solid body through a fictitious-domain approach [90, 209, 207, 208, 91, 257, 9]. Alternative approaches include Immersed-Boundary methods [165, 190], extended Lattice-Boltzmann methods
hybrids of Lattice-Boltzmann and Distributed-Lagrange-Multipliers [73] as well as spectral approaches limited to solid bodies with spherical shapes [328].

The key difference between Arbitrary-Lagrangian-Eulerian and Distributed-Lagrange-Multiplier methods is that the former use moving body-fitted meshes while the latter operate on a fixed grid. The choice of grid entails a payoff between accuracy and efficiency. While body-fitted simulations provide accurate solutions at the solid-fluid interface, they suffer from the complexity of moving meshes, the interpolations required when switching meshes and the mathematical difficulty associated with the mesh regeneration. Particularly in 3D, the computational cost and memory requirements are substantial.

Approaches relying on Distributed-Lagrange-Multipliers on the other hand operate on a fixed grid and thus eliminate the need for remeshing or moving the mesh. In the vicinity of the solid-fluid interface, however, they tend to have a lower order of convergence as compared to state-of-the-art ALE codes. Nevertheless, modern fixed-grid schemes provide a compelling alternative, particularly for 3D applications, and accurate implementations are known to reach comparable accuracy as ALE approaches [9].

### 6.3.1 Mathematical formulation

Our implementation is based on the Distributed-Lagrange-Multiplier approach. The basic idea behind these types of methods is to treat the entire computational domain as a fluid and add a rigidity constrain to enforce rigid-body motion in the solid domain. Considering a computational domain with both fluid and solid phases (Fig. 6-1), we solve the Navier-Stokes or Stokes equation not only in the fluid $\Omega \setminus P$ but in the entire domain $\Omega$. The flow inside the solid domain is projected onto a rigid body motion using a field of Lagrange multipliers. Several ways of defining the rigidity constraint have been proposed [90, 209, 207, 91, 299]. We adopt the formulation by [209] which requires that the deformation-rate tensor be zero

$$
\dot{\mathbf{D}} = \frac{1}{2} [\nabla \mathbf{v} + (\nabla \mathbf{v})^T] = 0 \quad \text{in } P,
$$

(6.9)
because it reduces the number of variables in the coupled system of equations.

The incompressibility constraint in the fluid (eq. 6.2) is a scalar constraint at each point in the computational domain $\Omega$. It therefore gives rise to a scalar field of Lagrange multipliers in $\Omega$, the pressure. In contrast, the rigidity constraint (eq. 6.9) represents a vector constraint and thus gives rise to a vector field in $P$, which we will refer to as the rigid-body force $f_{RB}$. It acts only in the solid domain and ensures that no deformation of the rigid body occurs. Since $\hat{D} = 0$ implies incompressibility, the equation of motion in the entire computational domain $\Omega$ can now be rephrased as

$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} = -\frac{1}{\rho(x)} \nabla p + \frac{\mu}{\rho(x)} \nabla^2 \mathbf{v} + \mathbf{g} + f_{RB} \quad \text{in } \Omega \quad \text{and} \quad (6.10)$$
$$\nabla \cdot \mathbf{v} = 0 \quad \text{in } \Omega, \quad (6.11)$$

where $f_{RB}$ is non-zero only in the solid domain and the density differs for the solid and fluid phases

$$\rho(x) = \begin{cases} 
\rho_p & \text{in } P \\
\rho_f & \text{in } \Omega \setminus P. 
\end{cases} \quad (6.12)$$

We stress that the viscosity in eq. 6.10 is constant and given by the Newtonian viscosity of the fluid. The rigidity constraint supersedes the definition of a viscosity in the solid domain.

The correct velocity field in the particle domain can be represented as the superposition of translational and angular velocities (eq. 6.6). Since the linear and angular momenta need to be conserved during the projection onto rigid-body motion, the translation and angular velocity components can be determined from

$$M_p \mathbf{V} = \int_P \rho_p \mathbf{v}^* \, dV \quad (6.13)$$
$$\hat{I}_p \omega = \int_P \mathbf{r} \times \rho_p \mathbf{v}^* \, dV, \quad (6.14)$$

where $M_p$ is the mass of the particle, $\hat{I}_p$ the moment of inertia tensor, and $\mathbf{v}^*$ the velocity field prior to the projection. Throughout, we use the asterisk to denote auxiliary variables that are updated in a subsequent projection.
Summarizing, the solution of the extended equation of motion (eqs. 6.10) subject to the two constraints of incompressibility (eq. 6.11) and vanishing deformation-rate tensor in the solid domain (eq. 6.9) corresponds to the following basic sequence of computational steps:

1. Solve the extended equations of motion (eq. 6.10) subject to incompressibility (eq. 6.11) inside the entire computational domain $\Omega$ by using the correct densities for the fluid and solid phase, but constant fluid viscosity.

2. Compute linear (eq. 6.13) and angular momentum (eq. 6.14) inside the solid body.

3. Project the fluid motion onto a rigid-body motion based on eq. 6.9.

4. Advect the solid-fluid interfaces.

### 6.3.2 Navier-Stokes solver

The projection step onto rigid-body motion is analogous to the treatment of the incompressibility constraint in the projection method [45]. It is thus natural to combine the two yielding a direct solver without the need to iterate. We use finite differences on a staggered grid to solve the extended Navier Stokes equation based on this extended projection method with an implicit diffusion step:

\[
\begin{align*}
\frac{v^* \! - \! v^n}{\Delta t} &= \frac{1}{\text{Fr}} g - (v^n \cdot \nabla) v^n \quad \text{in } \Omega \quad \text{(6.15)} \\
\frac{v^{**} \! - \! v^*}{\Delta t} &= \frac{1}{\text{Re}} \nabla^2 v^{**} \quad \text{in } \Omega \quad \text{(6.16)} \\
\nabla \cdot \left[ \frac{1}{\rho(x)} \nabla p^{**} \right] &= \frac{1}{\Delta t} \nabla v^{**} \quad \text{in } \Omega \quad \text{(6.17)} \\
\frac{v^{***} \! - \! v^{**}}{\Delta t} &= \frac{1}{\rho(x)} \nabla p^{**} \quad \text{in } \Omega \quad \text{(6.18)} \\
v_p^{n+1} &= \frac{1}{M_p} \int_P \rho_p v^{***} dV + \left( \frac{1}{I_p} \int_P \mathbf{r} \times \rho_p v^{***} dV \right) \times \mathbf{r} \quad \text{in } P \quad \text{(6.19)} \\
v_f^{n+1} &= v^{***} \quad \text{in } \Omega \setminus P, \quad \text{(6.20)}
\end{align*}
\]
where \( v^*, v^{**}, \) and \( v^{***} \) represent auxiliary values that are updated by the various projection steps. The non-linear term is discretized through a backward-Euler and the diffusion term through a Crank-Nicholson scheme.

### 6.3.3 Computation of the linear and angular momenta

Previous implementations of Distributed-Lagrange-Multiplier methods approximate the integrals for linear and angular momentum of the solids (eqs. 6.13 and 6.14) by dividing the body into small cubes referred to as material volumes (e.g. [9, 257, 207]). The solid-interface is thus represented by a stair-stepped boundary resulting in an error in both the total mass of the solid body and in the fluid flow close to the interface. In order to limit these errors, a large number of material volumes are required per particle, adding unnecessary computational expense. In addition, any property defined at the material volumes needs to be projected onto the background grid through interpolation.

We have developed a different quadrature scheme to improve accuracy in the vicinity of the interface. Analogous to the quadrature based on material volumes, we discretize the integrals (eqs. 6.13 and 6.14) by introducing the solid-volume fraction \( \phi \), which represents the volume occupied by the solid phase in a given grid cell

\[
\phi = \frac{V_s}{\Delta x \Delta y \Delta z}.
\] (6.21)

Using the solid-volume fraction, the integrals for linear and angular momentum may be reformulated and approximated as

\[
V = \frac{\rho_p}{M_p} \int_P \phi v^* dx = \frac{\rho_p}{M_p} \sum_{i,j,k} \phi_{i,j,k} v^*_{i,j,k},
\] (6.22)

\[
\omega_p = \frac{1}{I_p} \int_P \phi \tau \times \rho_p v^* dx = \frac{1}{I_p} \sum_{i,j,k} \phi_{i,j,k} r_{i,j,k} \times \rho_p v^*_{i,j,k},
\] (6.23)

where the summation extends over all grid cells \((i, j, k)\).

By basing the discretization of the momentum integrals (eqs. 6.13 on the solid-
volume fraction, the problem of integrating the velocity field is reduced to integrating the volume of intersection of the solid body and a given grid cell. For spheres and cubes, this volume may be determined analytically. We have derived analytical solutions for the volume of a sphere or rectangular cuboid in the region $x \leq a, y \leq b, z \leq c$. The volume occupied by the solid phase in a given grid cell can then be reconstructed very accurately by evaluating these integration formulas for each of the grid cell’s corners. The three main advantages of the approach we are suggesting are (1) the greater accuracy afforded by an integration relying on analytical solutions, (2) the gain in computational efficiency and (3) the ability to compute the solid-volume fraction for each of the three velocity grids without needing to interpolate while still spending $< 1\%$ of the computational time on quadrature in 3D.

6.3.4 Collision forces

The mechanism of particle collisions in flow fields spans a wide spectrum ranging from fully elastic collisions under conditions of negligible fluid resistance to an asymptotically slow approach of particles that do not deform or rebound in highly viscous fluids. In between these two limiting cases, a portion of the kinetic energy of the particles will be dissipated by fluid forces and internal solid friction and the rest will be transformed into energy of deformation. The mode of collision therefore depends on the relative importance of inertia to viscous forces as captured by the impact Stokes number

$$\text{St} = \frac{\rho_p u_0 d}{9 \mu_f} \quad (6.24)$$

and a dimensionless measure of elasticity defined by

$$\epsilon = \frac{4 \theta \mu u_0 d^{3/2}}{x_0^{5/2}} \quad (6.25)$$

[56]. The parameter $\theta$ is given by

$$\theta = \frac{1 - \nu_1^2}{\pi E_1} + \frac{1 - \nu_2^2}{\pi E_2}, \quad (6.26)$$
Figure 6-2: Comparison of the wake behind a fixed cylinder at Re = 26 as observed experimentally (top) by [284] and computed numerically (bottom). The green arrow highlights the position of the second stagnation point in both cases.

where \( \nu_i \) is the Poisson’s ratio for particle \( i \), \( E_i \) is the Young’s modulus for particle \( i \) and \( x_0 \) is the distance between the particles before deformation begins [56]. For both non-dimensional numbers, the characteristic speed \( u_0 \) is the relative approach speed of the colliding particles.

The solid components in many types of natural suspensions, such as sediment transport in rivers, volcanic ash in eruptive plumes, or crystals settling in magma chambers, are characterized by \( \epsilon < 1 \) reflecting the strength of the rock matrix of which they consist. For example, \( \epsilon \) for crystals settling in basaltic magma will typically be in the range of \( 10^{-2} - 10^{-5} \) (for mm - cm sized crystals with Poisson’s ratio \( \nu = 0.2 \),
Youngs modulus $E = 7 \times 10^{10}$ Pa, magma viscosity $\mu = 100$ Pa s, $x_0 = 0.01d$ and collision velocity $u_0 = 0.1u_S$ where $u_S$ is the Stokes settling velocity).

Several studies have studied collisions in the viscous limit in recent years and have established that St is the pertinent non-dimensional parameter for determining the collision mode [56, 54]. Even for deformable particles ($\epsilon > 1$), the rebound velocity is still determined primarily by St not $\epsilon$ [131]. For $\text{St}<10$, no rebound occurs [92, 131, 93] because the kinetic energy of the collision is dissipated in the fluid. For $\text{St}>500$, the coefficient of restitution approaches that for a dry collision. St spans a wide range in natural systems, but will probably rarely exceed 500 in fluid suspensions since $\text{St}<\text{Re}$. This simple scaling analysis highlights collisions in crystalline suspensions are typically represented by the viscous case $\epsilon \ll 1$ and St $\ll 500$. Theoretical analyses of this regime indicate that the lubrication forces become singular as the distance between two smooth particles approaches zero and hence prevents them from touching (e.g. [54]). In practice, however, numerical simulations can generally not afford the computational cost of fully resolving the flow in the infinitesimally thin film between colliding particles. As a remedy, a repelling force representative of the collision may be activated once the distance between two particles falls below a critical value dependent on grid resolution. While several implementations for collision forces have been suggested, we follow the approach by [91] owing to its simplicity and to the fact that it is applicable both at St $< 10$ and St $> 10$. However, the stiffness parameter needs to be adjusted such that rebound is limited to St $> 10$ to avoid spurious rebounds while not being so low that particles overlap [121]. For more details see Appendix E.

6.4 Results

We conduct several benchmark studies to evaluate the accuracy of our proposed method in comparison to both other numerical computations and experimental measurements.
Figure 6-3: Instantaneous out-of-plane vorticity over a fixed cylinder at three different Reynolds numbers showing Von-Kármán-vortex shedding.
Table 6.1: Mean drag coefficient $C_D$ for flow over a circular cylinder at different Reynolds numbers based on the simulations in Fig. 6-5.

<table>
<thead>
<tr>
<th>Study</th>
<th>$Re_T = 40$</th>
<th>$Re_T = 100$</th>
<th>$Re_T = 300$</th>
<th>$Re_T = 1000$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Present scheme</td>
<td>1.54</td>
<td>1.36</td>
<td>1.39</td>
<td>1.52</td>
</tr>
<tr>
<td>[9]</td>
<td>1.54</td>
<td>1.36</td>
<td>1.41</td>
<td>1.50</td>
</tr>
<tr>
<td>[190]</td>
<td>1.53</td>
<td>1.35</td>
<td>1.36</td>
<td>1.45</td>
</tr>
<tr>
<td>[177]</td>
<td>1.52</td>
<td>1.36</td>
<td>1.28</td>
<td>-</td>
</tr>
<tr>
<td>[110]</td>
<td>1.54</td>
<td>1.35</td>
<td>1.37</td>
<td>1.51</td>
</tr>
</tbody>
</table>

Table 6.2: Strouhal numbers for flow over a fixed cylinder at different Reynolds numbers based on the simulations in Fig. 6-3.

<table>
<thead>
<tr>
<th>Study</th>
<th>$Re_T = 100$</th>
<th>$Re_T = 300$</th>
<th>$Re_T = 1000$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Present scheme</td>
<td>0.174</td>
<td>0.214</td>
<td>0.239</td>
</tr>
<tr>
<td>[9]</td>
<td>0.165</td>
<td>0.212</td>
<td>0.238</td>
</tr>
<tr>
<td>[190]</td>
<td>0.165</td>
<td>0.210</td>
<td>0.231</td>
</tr>
<tr>
<td>[319]</td>
<td>0.176</td>
<td>0.205</td>
<td>-</td>
</tr>
</tbody>
</table>

6.4.1 Flow over a circular cylinder

Flow past a circular cylinder has become the gold standard for assessing the fidelity of numerical techniques for solid-fluid interaction. All our computations for flow over fixed cylinders are two-dimensional. On the inflow boundary we define a constant velocity $U_{inf}$. The boundary condition on the opposite side is convective outflow defined by

$$\frac{\partial \mathbf{v}}{\partial t} + U_{inf} \frac{\partial \mathbf{v}}{\mathbf{n}} = 0,$$

(6.27)

where $\mathbf{n}$ is the normal vector [200]. On the side walls, we impose a free-slip condition $\partial \mathbf{v}/\partial \mathbf{n} = 0$. In evaluating the rigidity constraint, the linear and angular momenta of the cylinder are set to zero. Even at low Re ($Re > 5$), the flow around a circular cylinder separates from the surface of the body and forms a twin vortex in the near wake [284]. We compare the computed size of the twin vortices with the experimental observations by [284]. Fig. 6-2A shows the photograph of the wake behind a circular cylinder at $Re = 26$ [284] and Fig. 6-2B the corresponding computation. The numeri-
Figure 6-4: Convergence test for the drag on a fixed circular cylinder at \( \text{Re} = 40 \). We investigate the convergence of the viscous \( C_v \) and the pressure contribution \( C_p \) to the drag on the cylinder’s surface separately (see eq. 6.28 and [110]). Despite using a second-order fluid solver, the convergence at the fluid-solid interface is only first order.

Numerical results were computed based on a fixed grid with aspect ratio \( 15d \times 30d \), where \( d \) is the diameter of the cylinder, and a grid resolution of \( 800 \times 1600 \). Both the position of the stagnation point and the non-dimensional recirculation length, \( s/d \approx 1.17 \) agree very well for experiment and simulation. Upon increasing \( \text{Re} \), the twin-vortex configuration becomes unstable to perturbations and forms a Von-Kármán vortex sheet at approximately \( \text{Re} > 49 \) (see [320] and references therein). We reproduce periodic vortex shedding over a wide range of \( \text{Re} \) (Fig. 6-3). In order to limit wall effects at low \( \text{Re} \) and maximize resolution at high \( \text{Re} \), the size of the computational domains varies from \( 15d \times 30d \) (Fig. 6-3A and B) to \( 12.5d \times 25d \) (Fig. 6-3C) with a grid resolution of \( 800 \times 1600 \) in all three cases. We compute drag and lift per unit length of the cylinder for various \( \text{Re} \) by evaluating the hydrodynamic forces in \( \mathbf{x} \) and \( \mathbf{y} \) direction

\[
F_D = \int_S (-p + 2\mu_f u_x)n_x + \mu_f (u_y + v_x)n_y \, dS \quad (6.28)
\]

\[
F_L = \int_S \mu_f (u_y + v_x)n_x + (-p + 2\mu_f v_y)n_y \, dS , \quad (6.29)
\]
Figure 6-5: Temporal evolution of drag and lift coefficients for flow over a circular cylinder at four different Reynolds numbers. The grid resolution in all four cases is $800 \times 1600$.

where $S$ is the cylinder cross-section, and normalizing by the dynamic pressure $\frac{1}{2} \rho_f U_{\infty}^2$. The drag and lift coefficients per unit length are thus

$$C_D = \frac{2F_D}{\rho_f U_{\infty}^2 d}$$  \hspace{1cm} (6.30)

$$C_L = \frac{2F_L}{\rho_f U_{\infty}^2 d}$$  \hspace{1cm} (6.31)

Comparing both the frequency of vortex shedding $f$ as captured by the Strouhal number, $St = f d / U_{\infty}$ (Table 6.2) and the mean drag and lift in steady state (Table 6.1), we find very close agreement with prior estimates. We have performed detailed convergence tests for flow over circular cylinders; an example at $Re = 40$ is given in Fig. 6-4.
Figure 6-6: Instantaneous out-of-plane vorticity over a square cylinder at three different rotation angles and Re = 410 showing Von-Kármán-vortex shedding.
Figure 6-7: Temporal evolution of drag and lift coefficients for flow over a square cylinder at \( Re = 500 \). Contrary to the case of a circular cylinder, both drag and lift exhibit period doubling as previously observed by [266].

6.4.2 Flow over a square cylinder

The wakes behind square cylinders exhibit similar instabilities as the wakes behind circular cylinders including the formation of twin vortices and vortex shedding. The two main additional complications are the presence of sharp corners and the dependence of drag, lift and Strouhal number on the cylinder's orientation with respect to the incident flow field. Consequently, the structure of the wake behind a square cylinder depends on \( Re \) and cylinder orientation in a different way than for a circular cylinder and shows some features not observed in the circular case such as force fluctuations and period doubling [266]. Our computations of the flow over square cylinders are set up analogous to those for circular cylinders (see sec. 6.4.1). In Fig. 6-6 we reproduce the well-known finding that square cylinders, similar to circular cylinders, give rise to a Von-Kármán vortex sheet in their wake at intermediate \( Re \) [198, 265, 266, 61]. We are also able to reproduce period doubling in the temporal evolution of drag and lift during vortex shedding (see Fig. 6-7). Period doubling at relatively low \( Re \) is of interest, because it is one possible indication for a transition to turbulence in a fluid
Table 6.3: Mean drag coefficient $C_D$ for flow over a square cylinder.

<table>
<thead>
<tr>
<th>Study</th>
<th>$\alpha = 0^\circ$</th>
<th>$Re_f = 200$</th>
<th>$Re_f = 250$</th>
<th>$Re_f = 500$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Present scheme</td>
<td>0</td>
<td>-</td>
<td>1.48</td>
<td>1.87</td>
</tr>
<tr>
<td>[266]</td>
<td>0</td>
<td>-</td>
<td>1.49</td>
<td>1.89</td>
</tr>
<tr>
<td>Present scheme</td>
<td>30</td>
<td>1.91</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>[265]</td>
<td>30</td>
<td>1.91</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

Experimental investigations of the drag on a square cylinder at low to moderate $Re$ are scarce and often limited to low to moderate aspect ratios which complicates the comparison with 2D numerical results [198, 199, 267]. We thus resort to compare the mean drag observed in our computation with previous numerical results [265, 266] in table 6.3 and find satisfactory agreement.

### 6.4.3 Sedimentation of a single sphere

As a 3D benchmark we consider the sedimentation of a single solid sphere in a rectangular tank of viscous fluid (e.g. Fig 6-1). An important consideration in comparing numerical simulations and experimental measurements is the blocking ratio $\beta$ of the settling sphere, which is defined as

$$\beta = \frac{d}{L},$$

(6.32)

where $d$ is the diameter of the sphere and $L$ the length of the tank or computational domain, respectively. Our simulations are based on a blocking ratio of $\beta = 1/3$. In order to account for wall effects, we employ the graphical correction method developed by [74] based on a comprehensive analysis of available experimental data. An example computation of a single settling sphere at $Re = 95$ is shown in Fig. 6-8. The sphere approaches the bottom of the tank without bouncing in agreement with the asymptotically slow approach expected in this non-dimensional regime (sec. 6.3.4).

We compute the drag coefficient on the sphere from the equilibrium settling speed $U$.
Figure 6-8: Solid sphere sinking in viscous fluid at $Re_b = 90$. The computational domain is $3d \times 3d \times 9d$ and the resolution is $41 \times 41 \times 121$. The local speed of the flow field is represented in colour and the contours of the stream function are shown in white. The colouring of the sphere itself indicates its speed at a given time.
using the relationship

\[ C_D = \frac{8F_D}{\rho_f U^2 \pi d^2}, \]  

(6.33)

where

\[ F_D = \frac{\pi}{6} d^3 (\rho_p - \rho_f) g \]  

(6.34)

and compare our results with the empirical relationship by [50] over a wide range of \( \text{Re}_p \) in Fig. 6-9. We observe a good agreement between predicted and expected drag values. The domain size for the computations varies from \( 3d \times 3d \times 9d \) at lower \( \text{Re}_p \) to \( 3d \times 3d \times 12d \) at higher \( \text{Re}_p \). Accordingly, the resolution is increased from \( 51 \times 51 \times 151 \) to \( 51 \times 51 \times 201 \).

### 6.4.4 Sedimentation of two interacting spheres

As a test of our code in the presence of multiple particles, we consider the interaction between two settling spheres known as drafting, kissing and tumbling [77]. This nonlinear mechanism occurs only at finite Re, when the leading particle creates a wake of low pressure in which the trailing particle is caught (Fig. 6-10). As a consequence,
the trailing particle experiences lower drag and hence falls faster than the leading one. This stage of the interaction is called drafting. The increased settling speed of the trailing particle impels a kissing contact with the leading particle. During the kissing stage, the two spheres form a long body with the center line approximately aligned with the flow direction. This constellation is unstable to perturbations in a Newtonian fluid and hence the particles tumble and drift apart.

Contrary to the benchmark computations discussed so far (sec. 6.4.1-6.4.3), the collision behavior of two settling spheres should not be considered as an independent validation of our code. Rather, it is needed to adjust the collision parameters such that the experimentally observed and theoretically expected collision mode for the respective St can be reproduced (see sec. 6.3.4). Fig. 6-10 shows an example of a particle collision at St≈120 during which the colliding spheres rebound as expected in this non-dimensional regime [54]. The collision also closely resembles previous numerical studies (e.g [90, 209]. For an example of particle collisions at St<10 during which the particles roll by each other without rebound, please refer to Appendix E.
6.5 Conclusion

Countless problems in the Earth sciences involve the dynamic interaction between solid bodies and viscous flow, many in the context of melting or solidification. While we are well equipped to deal with the end-member cases of predominantly liquid or solid systems, the intermediate regime in which both solid and liquid components contribute significantly to the dynamics of the aggregate remains challenging to model and is consequently little explored. The contribution of this study is to extend our modeling capabilities from the entirely fluid regime to fluid systems that contain a non-negligible volume fraction of solid bodies.

We present a numerical scheme for the direct numerical simulation of solid-fluid coupling in crystalline suspensions. The hydrodynamic forces on the surfaces of the solid bodies are fully resolved, obviating the use of approximate formulas for drag, lift or settling speed. This more general approach is particularly advantageous for quantifying the dynamic interaction between solid bodies, the effect of crystal geometry on settling behavior, and the onset of non-linear rheologies at low to intermediate crystal fraction.

Our numerical approach relies on a fictitious-domain approach in which the entire computational domain is treated as a fluid and the equations of solid-body motion in the crystalline domain are enforced through distributed Lagrange multipliers (DLMs). The main advantage of the DLM methodology is that it adds a minimal overhead of < 1\% for the computations presented in this chapter to the expense of the fluid solver. As compared to previous DLM approaches of solid-fluid coupling, our implementation relies on an analytic quadrature scheme for cuboids and spheres that enhances accuracy, reduces computational expense and obviates the need to interpolate. We validate our code through several benchmarks in both 2D and 3D.
Chapter 7

When crystals collide: Constraints on the fate of terrestrial planets during magma ocean solidification

7.1 Introduction

The terrestrial planets of our solar system vary notably in their basic properties ranging from core size to the prevalence of volcanism and from the presumed convective pattern in the mantle to the composition of the atmosphere. These differences present a puzzle from the standpoint of planetary evolution, because all the terrestrial planets are thought to have accreted within the inner solar system, implying a basic similarity in composition [35, 36]. Given that differences in the starting compositions are unlikely to account for the differences observed today, the question arises when the evolutionary paths of the terrestrial planets started to deviate. A potential branching point in the evolution of terrestrial planets is the formation of a magma ocean on the planetary surface. The heat provided by accretion and core formation is sufficient to wholly or partially melt the silicate mantle of an emerging planet (e.g.

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177
Table 7.1: Order-of-magnitude estimates for the key non-dimensional parameters characterizing flow in magma oceans.

<table>
<thead>
<tr>
<th>Nondimensional parameter</th>
<th>Symbol</th>
<th>Definition</th>
<th>Magma ocean</th>
</tr>
</thead>
<tbody>
<tr>
<td>Prandtl number</td>
<td>Pr</td>
<td>$\frac{\mu_f}{\mu_f \alpha} \Delta T h^3$</td>
<td>$10^1 - 10^5$</td>
</tr>
<tr>
<td>Rayleigh number</td>
<td>Ra</td>
<td>$\frac{\rho_f g \alpha \Delta T h^3}{\mu_f}$</td>
<td>$10^{22} - 10^{27}$</td>
</tr>
<tr>
<td>Fluid Reynolds number</td>
<td>Re_f</td>
<td>$\frac{\mu_f}{\rho_f \nu_f h}$</td>
<td>$10^8 - 10^{14}$</td>
</tr>
<tr>
<td>Particle Reynolds number</td>
<td>Re_p</td>
<td>$\frac{\mu_f}{\rho_p \nu_p}$</td>
<td>$10^{-2} - 10^2$</td>
</tr>
</tbody>
</table>

Table 7.2: Approximate physical parameters for a theoretical magma ocean.

<table>
<thead>
<tr>
<th>Physical parameter</th>
<th>Symbol</th>
<th>Unit</th>
<th>Magma ocean</th>
</tr>
</thead>
<tbody>
<tr>
<td>Characteristic length</td>
<td>$h$</td>
<td>m</td>
<td>$10^6$</td>
</tr>
<tr>
<td>Characteristic velocity</td>
<td>$v$</td>
<td>m/s</td>
<td>0.1 - 100</td>
</tr>
<tr>
<td>Settling velocity</td>
<td>$v$</td>
<td>m/s</td>
<td>$10^{-4} - 10^{-1}$</td>
</tr>
<tr>
<td>Fluid density</td>
<td>$\rho_f$</td>
<td>kg/m$^3$</td>
<td>3500</td>
</tr>
<tr>
<td>Particle density</td>
<td>$\rho_p$</td>
<td>kg/m$^3$</td>
<td>2500 - 3800</td>
</tr>
<tr>
<td>Particle radius</td>
<td>$r$</td>
<td>m</td>
<td>0.01 - 0.001</td>
</tr>
<tr>
<td>Gravitational acceleration</td>
<td>$g$</td>
<td>m/s$^2$</td>
<td>1 - 10</td>
</tr>
<tr>
<td>Fluid viscosity</td>
<td>$\mu_f$</td>
<td>Pa s</td>
<td>0.01 - 0.1</td>
</tr>
<tr>
<td>Effective fluid viscosity</td>
<td>$\mu_{eff}$</td>
<td>Pa s</td>
<td>0.1 - 1000</td>
</tr>
<tr>
<td>Thermal diffusivity</td>
<td>$\kappa$</td>
<td>m$^2$/s</td>
<td>$10^{-6}$</td>
</tr>
<tr>
<td>Thermal expansivity</td>
<td>$\alpha$</td>
<td>$/^{\circ}$</td>
<td>$3 \cdot 10^5$</td>
</tr>
<tr>
<td>Temperature range</td>
<td>$\Delta T$</td>
<td>$/^{\circ}$</td>
<td>1000</td>
</tr>
</tbody>
</table>

[324, 243, 309]). The solidification processes of these magma oceans are highly complex and highly dependent on planetary properties such as planetary mass [290, 65] and the density of a potential primordial atmosphere [182, 4, 325, 1, 3]. Two magma oceans may therefore yield solidified mantles with very different properties even if the initial bulk composition of the fluid magma is similar. Since even slight differences in the density stratification or volatile content of the solidified mantle influence the later fate of the planet sensitively [65, 66], studies of magma ocean solidification provide a promising starting point for understanding when and how the characteristics of today’s terrestrial planets began to emerge. One of the biggest uncertainties in constraining the properties of the silicate mantle resulting from magma ocean solid-
Figure 7-1: Convective regimes in a solidifying magma ocean. At the planetary scale flow is driven by thermal convection. Flow is turbulent for most of the depth range of the magma ocean except for a boundary layer at the bottom where flow is rapid but non-turbulent. The conductive boundary layer is not visualized. The degree to which crystals can settle out of suspension in the steady-flow regime at the bottom of the magma oceans depends on the local fluid-dynamical conditions and is therefore dominated by compositional convection at the microscopic scale.

fractionation is whether fractional or batch crystallization dominates. This controversy is partly fuelled by observational evidence which supports significant fractionation and flotation of anorthositic phases for a lunar magma ocean [309, 259], but does not indicate strong chemical stratification of the Earth’s mantle [224, 286, 269]. Furthermore, there is evidence from terrestrial magma flows that anorthosites may cluster into polycrystalline aggregates called glomerocrysts instead of fractionating efficiently [213, 127]. These varied pieces of evidence raise the question what crystal settling depends on and whether efficient crystal settling might be limited to certain fluid-dynamical regimes. Over the last decades, important progress has been made in evaluating the stability of crystalline suspensions for magma oceans [290, 270, 269]. A primary focus of these studies has been to identify a critical size above which crystals decouple from the ambient flow and settle or float. The idea that sedimentation is governed primarily by crystal size is appealing because the competition between convective and settling speed determine the net motion of individual crystals. There are,
however, other factors that control the suspension dynamics including the presence of boundaries along which convective velocities are zero [181], the influence exerted by a finite solid fraction on convection and turbulence [142], and the competition between thermal and compositional buoyancy in suspensions with variable density [237, 115].

The goal of this study is to gain insights into the differentiation histories of magma oceans by investigating the fluid-dynamical conditions that govern crystal settling or flotation. We apply our insights to presumed magma oceans on Vesta and the Moon. We do not consider thermodynamic processes or phase changes at this stage. Our approach complements earlier efforts [290, 270] by focusing specifically on non-dilute suspensions for which the dynamic interactions between individual crystals begins to play an important role. In order to identify the different parameters that facilitate or impede crystal settling, we use direct numerical simulations at the scale of individual crystals. While this choice of length scale requires simplifying assumptions regarding the properties of the ambient flow field (see sec. 7.2), it allows for a detailed insights into the fluid-dynamical processes governing crystal settling. The numerical methodology used was developed and benchmarked in chapter 6.

7.2 Model

Heat and mass transfer in a magma ocean is fundamentally different to a solid mantle. The low viscosity of the melt [155] in combination with the drastic temperature contrast between the top and the bottom of the magma ocean lead to very vigorous convection that resemble atmospheric circulation more than solid-mantle flow [290, 1, 2, 3, 271]. Table 7.1 gives an overview of the most relevant non-dimensional numbers that characterize flow in magma oceans. These estimates are based on the physical parameters listed in table 7.2. The exceptionally high Rayleigh and Reynolds numbers indicate turbulent convection over a wide depth range [261], which is expected to result in an adiabatic variation of temperature with depth and a compositionally well mixed liquid.

Mixing-length theory indicates that even at high Ra, a vigorously convecting sys-
tem can be divided into three flow regimes [143, 34, 290, 276]: In the immediate vicinity of a solid boundary, heat transfer is conductive and flow is creeping. At least during the early stages of magma ocean solidification when $Re$ is very high, this conductive boundary layer is probably negligibly small and, in the absence of a conductive lid, restricted to the bottom boundary of the magma ocean. The conductive boundary layer borders on a typically much wider region of rapid but non-turbulent flow. Heat in this region is transferred primarily by convection. Finally, at great distances from the solid boundaries, flow is fully turbulent and dominated by inertial effects. Since the $Ra$ in magma oceans is thought to be very large (see table 7.1) the turbulent regimes extends over a wide depth range. As solidification proceeds, the conductive boundary layer and the regime characterized by non-turbulent flow grow at the expense of the inertial zone and become dynamically increasingly important, particularly in the presence of a conductive lid which slows heat loss and thus convective vigor.

The solidification of magma oceans is thought to proceed from the bottom up, because the adiabat first intersects the liquidus at the bottom of the mantle. The depth range over which crystal settling is most important is constrained by three depths; (1) the depth representing the solidification front of the cumulate pile within which differential crystal motion is too restricted for settling, (2) the depth at which the adiabat intersects the liquidus above which crystals might not be stable over the time scale of sedimentation or flotation and (3) the depth at which the convective flow field becomes fully turbulent and thus spatially variable which may annihilate differential crystal motion. It is thus likely that crystal settling occurs predominantly within the non-turbulent flow regime (Fig. 7-1). Several different scaling relationships have been suggested to estimate the relative thicknesses of the three different flow regimes (see [261] for an overview). For the purposes of this study, the only important aspect common to all of these scaling analyses is that the thickness of the non-turbulent boundary layer is much larger than the size of individual crystals.

Motivated by experimental studies that have highlighted the importance of crystal sedimentation and flotation along boundaries [181], we focus our investigation of crys-
tal settling on the non-turbulent zone above the conductive boundary layer (Fig 7-1). Our work complements previous studies of the crystal-settling problem [290, 270] by resolving the dynamics of crystalline suspensions at the length scale of individual crystals (Fig. 7-1) using direct numerical simulations. These types of computational methods fully resolve the physics of a given problem without relying on approximate drag formulas, simplified interaction, or prescribed settling speeds that are commonly used in more traditional approaches. The main advantage of direct numerical simulations is thus that they provide insights into the dynamics of a multiphase system from first principles. This is particularly advantageous for complex flow problems such as crystalline suspensions in magma oceans, for which it is challenging to specify the drag and lift exerted by the flow field, the dynamic interaction between crystals, and the effect of the crystals on the ambient flow field a priori. All of our simulations are based on the methodology developed and benchmarked in chapter 6.

At the planetary scale, flow in magma oceans is driven by thermal convection. At the scale of individual crystals, the temperature differential is negligible and the dynamics of crystalline suspensions is governed by the Navier-Stokes equation

\[
\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} = -\frac{1}{\rho_f} \nabla p + \frac{\mu_f}{\rho_f} \nabla^2 \mathbf{v} + \mathbf{g}
\] (7.1)

together with the incompressibility constraint

\[
\nabla \cdot \mathbf{v} = 0,
\] (7.2)

where \( \rho_f \) is the density of the fluid, \( \mu_f \) the viscosity, \( \mathbf{v} \) the velocity field, \( p \) the pressure, \( t \) the time, and \( \mathbf{g} \) the gravitational acceleration. The motion of each crystal is determined by Newton's laws of rigid-body motion

\[
\frac{M_p d(V_p)}{dt} = \mathbf{F}_p + M_p \mathbf{g},
\] (7.3)

\[
\frac{d(I_p \cdot \omega_p)}{dt} = \mathbf{T}_p,
\] (7.4)

\[
\frac{dX_p}{dt} = \mathbf{v}_p
\] (7.5)
Figure 7-2: Body centered cubic (bcc) particle array consisting of spheres with radius \( r \). In this staggered setup, the smallest gap between particles is given by \( g \). The side length of the cell is given by \( a \); a reasonable proxy for a typical separation distance of the crystals.

Table 7.3: Overview of different types of suspensions grouped according to the crystal fraction and the corresponding non-dimensional gap between crystals as defined in Fig. 7-2.

<table>
<thead>
<tr>
<th>Crystal fraction ( \phi )</th>
<th>Non-dimensional gap ( g )</th>
<th>Suspension type</th>
</tr>
</thead>
<tbody>
<tr>
<td>&lt; 0.3 %</td>
<td>&gt; 5</td>
<td>Very dilute suspension</td>
</tr>
<tr>
<td>( \sim 0.5 - 5 % )</td>
<td>( \sim 1.4 - 4 )</td>
<td>Dilute suspension</td>
</tr>
<tr>
<td>&gt; 8 %</td>
<td>&lt; 1</td>
<td>Dense suspension</td>
</tr>
</tbody>
</table>

where \( M_p \) is the mass of the particle, \( \mathbf{V}_p \) the velocity of its center of mass, \( \mathbf{X}_p \) the position of the center of mass, \( \mathbf{I}_p \) the particle’s moment of inertia tensor, \( \mathbf{\omega}_p \) the angular velocity of the particle, and \( \mathbf{F}_p \) and \( \mathbf{T}_p \) the hydrodynamic force and torque exerted onto the particle by the surrounding fluid. The interfaces between solid and fluid phases exhibit no slip (Fig. 7-1). The existence of an ambient flow field is captured in our simulations by specifying inflow and outflow along the boundaries such that mass is preserved. Since the size of our computational domains are typically only on the order of a few mm or cm, we assume that the inflowing velocity field is approximately uniform. The outflow is determined self-consistently from the flow field inside the domain [200] in order to capture the effect of the presence of crystals on the
down-wind flow field. In our simulations, we only investigate the vertical component of the ambient flow field. While most realistic flow fields would of course have a velocity component in all three spatial directions, only the vertical flow component opposes the body forces of the crystals directly and thereby determines the ability of the flow field to keep crystals entrained.

Settling in crystalline suspensions is bound to entail collisions between crystals. The physical nature of these collisions depends on the relative importance of inertia to viscous forces as captured by the impact Stokes number

\[
St = \frac{\rho g u_0 \tau}{9 \mu_f} \tag{7.6}
\]

and a dimensionless measure of elasticity defined by

\[
\epsilon = \frac{4 \theta \mu u_0 \tau^{3/2}}{x_0^{5/2}} \tag{7.7}
\]

[56]. The parameter \( \theta \) is given by

\[
\theta = \frac{1 - \nu_1^2}{\pi E_1} + \frac{1 - \nu_2^2}{\pi E_2}, \tag{7.8}
\]

where \( \nu_i \) is the Poisson’s ratio for particle \( i \), \( E_i \) is the Young’s modulus for particle \( i \) and \( x_0 \) is the distance between the particles before deformation begins [56]. For both non-dimensional numbers, the characteristic speed \( u_0 \) is the relative approach speed of the colliding particles. For crystalline suspensions in magma oceans, \( \epsilon \ll 1 \) and \( 0 < St < 100 \) implying that crystal rebound is not uncommon for fast moving crystals [56]. Since it is not feasible to resolve the flow in the infinitesimally thin film between colliding particles, we activate a repelling force representative of a collision once the distance between two crystals falls below a critical value dependent on grid resolution as suggested by [91]. See chapter 6 and Appendix E for a more detailed discussion of crystal collisions.
7.3 Results

Based on the crystal fraction, we distinguish between three types of suspensions, very dilute suspensions in which the interaction between neighboring crystals is negligible, dilute suspensions in which crystal interact but the average separation distance of crystals is large enough for settling crystals to pass by, and dense suspension in which crystals are in close contact during flow (e.g. Table 7.3). Here, we only investigate crystal settling in very-dilute and dilute suspensions containing mineral phases of variable density and size. We do not model settling in dense suspensions, because the solid fraction is so high that they require separate treatment through continuum or granular-flow approaches.

For equisized crystals, it is straightforward to identify the range of crystal fractions over which a suspension could be regarded as very dilute, dilute or dense (Fig. 7-2). Considering a body-centered-cubic arranged array of spherical crystals with radius \( r \) submerged in a fluid, the total volume \( a^3 \) of the array contains the volume of two spheres and hence the volume fraction is

\[
\phi = \frac{8}{3} \pi \left( \frac{r}{a} \right)^3 .
\]
Table 7.3 gives an overview of the relationship between crystal fraction and the minimum gap between crystals $g$ non-dimensionalized by the crystal diameter for a homogeneous crystal-size distribution. The limiting case of very dilute suspensions (defined as $g > 5$) is restricted to extremely low crystal fractions ($< 0.3\%$). Even the case of a dilute suspension, which we define as suspensions with $g > 1$ such that there is enough space in between crystals to allow a settling crystal to pass through, requires crystal fractions below $5\%$.

### 7.3.1 Very dilute suspensions

The simplest scenario for investigating the settling behavior of crystals in a magma ocean is the limiting case of very low crystal fraction. If the crystal fraction is low enough for the mean distance between crystals to be much larger than the size of the crystals, the interactions between crystals can be neglected. This simplification reduces a multi-body problem to a single-body problem. Although crystal settling in very-dilute suspensions is probably of limited practical relevance in magma oceans because of the extremely low crystal fractions required, it is useful to consider this case for comparison purposes.

The settling velocity of individual crystals is determined by the balance between the body forces of the crystal and the hydrodynamic forces exerted onto the crystal by the ambient flow field. It is common to distinguish between the vertical component of the hydrodynamic force (drag) and the horizontal components of the hydrodynamic force (lift). Lift acts perpendicular to the crystals’ body force and is of secondary importance for keeping crystals entrained, at least in the very dilute limit. In a stagnant fluid, it is well known that the drag experienced by a spherical crystal during settling depends sensitively on $Re_p$ as illustrated in Fig. 7-3. For comparison purposes, we also extend Stokes law into the finite $Re_p$ domain. Assuming Stokes drag for crystals settling in a magma ocean underestimates the drag experienced by the crystals and thereby underestimates the potential of the flow field to keep crystals entrained in flow.

In the Stokes regime ($Re_h = 0$), the drag depends only on the relative speed of
Figure 7-4: Simultaneous settling of 30 identical crystals with $\text{Re}_p \approx 80$ in a linear flow field at times $0.6s$, $1.05s$, $1.65s$, $2.25s$, $3.9s$ and $4.5s$. The influx speed is set to the equilibrium settling speed of an isolated crystal in stagnant fluid. Since the presence of other crystals increases the drag experienced by each single crystal, the crystals tend to drift backwards over time. The color shading represents the average local flow speed normalized by the influx speed and the white contour lines represent the out-of-plane vorticity. The computations was done at a grid resolution of $800 \times 1600$. 
crystal and ambient fluid, as captured through $\text{Re}_p$, not on the absolute speed of either crystal or ambient fluid. At finite $\text{Re}_\text{f}$, however, the standard drag curve (Fig. 7-3) applies strictly only if the ambient flow field is steady and uniform. At $\text{Re}_\text{f} \gg 0$, the mean drag may depend non-linearly on the relative velocity and increases with increasing turbulence intensity even if $\text{Re}_p \approx 0$ [185, 11]. While we do observe slightly elevated mean drag in the presence of vigorous flow fields, the total effect of the nonlinearity is small ($< 10\%$) for $\text{Re}_f < 1000$ in agreement with a previous study [11]. Since the flow in the bottom boundary layer of a magma ocean is presumably not turbulent (Fig. 7-1) we conclude that it is reasonable to use the standard drag curves (Fig. 7-3) as first-order approximations for the mean drag experienced by settling crystals in a magma ocean.

### 7.3.2 Dilute suspensions of equisized crystals

Since the crystal fraction required to neglect crystal interactions is extremely small (Table 7.3), crystal interactions will generally play an important role in the dynamics of crystalline suspensions. As a first step to gaining a better understanding of the nature and effects of these interactions, we start by investigating dilute suspensions with a homogeneous crystal-size distribution.

In all simulations in this section, the influx speed at the bottom of the box is set to the settling speed of an isolated crystal inside the given computational domain. 7-4 illustrates how the presence of other crystals alters settling behavior in the case of 30 identical spheres arranged in staggered rows of crystals spaced at $a \approx 10r$. (A) Soon after the onset of the simulations, low-pressure and low-velocity wakes form behind the crystals. Once the length of the wake becomes comparable to the spacing of the crystals, the draft associated with the wakes becomes noticeable (B) and crystals begin to align (C). The approximately linear alignments of crystals into several extended wakes (C) are dynamically unstable due to the rapid flow in the mostly fluid channels in between and tend to break up soon after formation (D). Once the flow field has fully evolved, the spatial distribution of crystals is dominated by small clusters of crystals that distribute more or less randomly throughout the
domain (E, F). The tendency of crystals to cluster into multiples, sometimes referred to as V and multiples, has been predicted theoretically [297, 298]. Most of the spheres in Fig. 7-4 tend to drift back slightly as compared to their initial position. At the given crystal fraction, this drift is associated primarily with the finite time it takes the crystals to reach their equilibrium settling speed.

The evolution of the drag and lift forces exerted onto the individual crystals reflects the different stages of the establishment of a realistic distribution of crystals in the domain (see Fig. 7-5). At the given crystal fraction, however, the mean drag and lift force deviate little from their value in the very dilute limit, apparently because the reduction in drag due to drafting is approximately balanced by the increase in drag due to clustering. This indicates that as the crystal fraction increases above the very-dilute limit, the main effect of crystal interactions is to significantly increase the standard deviation of the drag and lift force distribution while altering the mean very little (Fig. 7-5). The increase in the standard deviation of the lift experienced by individual crystals by up to a factor of 100 is particularly noteworthy, because it entails a rapidly increasing probability of crystal collisions.
Figure 7-6: Simultaneous settling of 5 heavy crystals ($Re_p \approx 120$) amidst 30 light crystals ($Re_p \approx 80$) in a linear flow field at times 0.38s, 0.9s, 1.5s, 2.25s, 3.75s and 4.5s. The influx speed is set to the equilibrium settling speed of an isolated grey crystal akin to Fig. 7-4. The color shading represents the average local flow speed normalized by the influx speed and the white contour lines represent the out-of-plane vorticity. The computations was done at a grid resolution of $800 \times 1600$. 
As long as crystal interactions do not lead to a significant increase in the mean drag (e.g. Fig. 7-4), crystal settling is very efficient in the sense that fractionation may happen on the time scale of seconds. Fig. 7-6 shows the example of five heavy crystals at the same crystal fraction as Fig. 7-4. Since $\text{Re}_p$ is larger for the heavy crystals than for the light ones, the mean drag they experience is lower (Fig. 7-7). Therefore, although the density difference between the two crystal types is only approximately 6%, the mean settling velocity of the heavy crystals is $\approx 18\%$ higher than for the light crystals. Since drag decays more rapidly with $\text{Re}_p$ in 3D than in 2D (Fig. 7-3), this effect should be even more pronounced in a 3D computation than in the 2D example shown in Fig. 7-6.

Once the crystal fraction increases beyond the relatively moderate crystal fractions discussed so far (Fig. 7-4 and 7-6), the efficiency of crystal settling decreases rapidly primarily due to the increased frequency and duration of crystal collisions. Fig. 7-8 compares the temporal evolution of the average linear momentum in vertical direction $\bar{U}_y$ for two different initial separation distances $a = 10r$ and $a = 7.5r$. Immediately after the onset of the computations, the two curves separate as a reflection of drag

![Figure 7-7: Temporal evolution of the drag (top) and lift (bottom) force for the 30 grey crystals (blue and green, respectively) and the 5 black crystals (red) as shown in Fig. 7-6) normalized by the drag and lift force of a single sphere in the very dilute limit.](image)
increasing with crystal fraction. The contrast in average settling speed, however, remains limited since the difference in crystal fraction is only $\approx 1\%$. As the simulation proceeds, the average vertical moments diverge more and more rapidly, because of the increased frequency of crystal collisions which transfers momentum from the heavy spheres to the light ones. We find that for a homogeneous crystal-size distribution the slowing effect of crystal collisions thwarts the drag effect for crystal fractions of $\approx 2\%$ or higher.

Our simulations indicate that crystal collisions are both more frequent and more energetic if multiple mineral phases with differing densities and sizes are present. Comparing the mean settling of five heavy crystals in a suspension in which they are surrounded by a light mineral phase (Fig. 7-6) with a mono-crystalline suspension, we find that the mean settling speed in a mono-crystalline suspension is significantly higher. We observe the largest difference in settling speeds for a bi-crystalline as compared to a mono-crystalline suspension if the bi-crystalline suspension consists of an approximately equal share of buoyant and heavy crystals. In this limiting case, the
Figure 7-9: Two simulations of 30 spheres with equal density but variable size. In both cases, the influx is identical to Figs. 7-4 and 7-6 and the total crystal fraction is identical to Fig. 7-4 to within 0.001%. Contrary to the case of a homogeneous crystal-size distribution, the crystals begin to segregate immediately. Run A (snapshots are taken at times 0.38 (A1), 1.50 (A2), 3.00 (A3), and 4.51 (A4)) is characterized by a smaller deviation in crystal sizes and therefore separation of the crystals is slower than in case B (snapshots are taken at times 0.38 (B1), 1.13 (B2), 3.00 (B3), and 4.13 (B4)). The computations was done at a grid resolution of $800 \times 1600$.

The averaging effect of frequent crystal collisions may result in negligible net motion of the suspended crystals. The presence of a second mineral phase will therefore generally decrease settling efficiency, particularly if the second mineral phase is buoyant and makes up a large portion of the crystal population.

Summarizing, we find that there are two dynamic regimes governing crystal sedimentation in dilute suspensions with homogeneous crystal-size distributions. In the first regime, crystal settling is dominated by the balance between drag and body
force, analogous to the very dilute limit. Crystal settling is very efficient, primarily due to the decrease in drag with increasing $Re_p$, but this regime is limited to very low crystal fractions of $\approx 2\%$ or lower. In the second regime, the mean settling of the crystals is dominated primarily by crystal collisions. Evidently, drag still plays an important role, but the overall decrease in settling speed is no longer fully accounted for by an increase in drag. Instead, frequent and extended crystal collisions transfer energy from fast to both slow moving crystals and to the fluid itself. The averaging effect of crystal collisions will tend to decrease settling speeds and may do so dramatically in the presence of both buoyant and heavy crystals. The transition from the drag-dominated to the collision-dominated regime is continuous. As a rough guideline, we observe in our simulations that crystal collisions tend to dominate the drag effect for crystal fractions of $>2\%$ and above.

7.3.3 Dilute suspensions with heterogeneous crystal-size distributions

The size distribution of crystals in magmatic systems is determined by the time variations of nucleation and growth and by the dynamics of the magmatic system itself [33, 112, 180]. For magma oceans, the crystallization history of entrained mineral phases is probably characterized by a complex sequence of nucleation and dissolution events as the flow transports crystals from depth upwards and back. Therefore, the crystal sizes likely deviate substantially from the homogeneous distribution discussed previously. When plotting the logarithm of the crystal number $\ln(n)$ over the size of the crystal $r$, the crystal-size distributions of lava lakes and sills are often linear or close to linear [33, 111, 180]. While the crystal-size distributions in magma oceans are probably more variable than that, a linear crystal-size distribution in the above sense provides a reasonable starting point. We will later address possible ramifications of an even more skewed crystal-size distribution. In the simulations presented in this section, the sizes of the crystals are obtained by random sampling of a linear crystal-size distribution for which the minimum size is set to $4\Delta x$, where $\Delta x$ is the spatial
Figure 7-10: Illustration of the entrainment of a small dense crystal (black) in the wake of a large and less dense crystal (grey). The settling of the large crystal dominates the local flow field sufficiently to divert the small crystal without colliding with it. The snapshots are details from the computation shown in Fig. 7-11.

resolutions of the computational grid, and the mean is set to the radius used previously in the simulations for homogeneous crystal-size distributions (sec. 7.3.2). The position of the crystals is assigned randomly on a staggered grid as used previously for homogeneous crystal-size distributions.

Fig. 7-9 shows two cases of simultaneous settling of 30 spheres with the same crystal fraction and the same ambient influx as Fig. 7-4. Although the crystal sizes for run A and B differ, they represent the same crystal-size distribution. Two aspects of Fig. 7-9 in comparison to Fig. 7-4 merit further discussion. First, variably-sized crystals disperse rapidly based on their size in homogeneous flow fields. Second, variably-sized crystals do not tend to cluster and collide to the degree that equisized crystals do. Evidently, the second effect is partly a consequence of the first as the separation of
crystals expands the portion of the spatial domain occupied by crystals. However, the variable settling speed of the crystals contributes to making collisions both rarer and shorter. Collisions become less frequent because slow moving crystals tend to get entrained in the wake of fast moving crystal instead of colliding as exemplified in Fig. 7-10. Also, the interim clusters that do form tend to break up more rapidly than in the case of a homogeneous crystal-size distribution, because of the crystals’ differences in settling speed and shape. In order to compare crystal settling in suspensions with variably sized as opposed to equisized crystals, we construct a scenario comparable to Fig. 7-6: In Fig. 7-11, 5 heavy crystals ($\text{Re}_p \approx 120$) settle simultaneously amidst 30 light crystals with the same density as in Fig. 7-6 but variable radius. Again, we observe that the suspensions disperses very quickly. However, the dispersion is driven primarily by size and not by density. The larger crystals located in the right half of the domain settle rapidly (Fig. 7-11 A,B) and divert the ambient flow field to the left of the domain, where the crystals now experience larger than average inflow (C-F). As a consequence, the 3 black crystals in the left half propagate vertically upwards while the 2 black crystals in the right half of the domain are entrained in the flow generated by the large crystals and propagate vertically downwards (C-F). The mean settling speed of the black crystals in Fig. 7-11 is notably less than in Fig. 7-6.

Clearly, the initial position and sizes of the surrounding crystals introduce a stochastic element into the settling dynamics of heavy crystals in suspensions with heterogeneous crystal-size distributions that was absent in the case of homogeneous crystal-size distributions. For different draws of sizes and positions, the mean settling speed of the heavy crystals exceeds that observed for a homogeneous crystal-size distribution. A large mean settling speed, however, does not necessarily entail separation of heavy crystals from light crystals for heterogeneous size distributions. In all of our computations, we find that for a reasonable density contrasts between the mineral phases the size effect trumps the density effect. This finding is not unexpected theoretically. The variation in radii tends to be much larger (commonly up to a factor of 10) than the density contrasts between various mineral phases (typically somewhere between 1 and 1.3). In addition, the rise speed depends more sensitively on radius
Figure 7-11: Simultaneous settling of 5 heavy crystals ($Re_p \approx 120$) amidst 30 light crystals with a linear crystal-size distribution in a linear flow field at times 0.38s, 0.90s, 1.50s, 2.25s, 3.00s, and 3.75s. The influx speed is identical to Fig. 7-4 and 7-6. The color shading represents the average local flow speed normalized by the influx speed and the white contour lines represent the out-of-plane vorticity. The computations was done at a grid resolution of $800 \times 1600$. 

197
than on density contrast. In the Stokes regime, for example, the rise speed increases linearly with the density contrast but quadratically with the radius. Summarizing, we still observe two regimes in the settling dynamics of heterogeneously-sized crystals, similar to the case of homogeneous crystal-size distributions. The transition from drag-dominated settling to collision-dominated settling, however, occurs at much higher crystal fractions than the $\approx 2\%$ observed in the homogeneous case. In fact, we can no longer identify a 'critical' crystal fraction above which collisions typically dominate. Instead, both the frequency and the duration of the collisions is dependent on the variability in crystal size. In the limiting case of very small variability, collisions are frequent and extended and the settling dynamics approaches that of a homogeneous crystal-size distribution. In the other extreme, in which most of the total crystal fraction is due to a single crystal surrounded by a large number of extremely small crystals, the settling dynamics is well represented by the settling of a single crystal in a Newtonian fluid with an effective viscosity that captures the
presence of the small crystals. Despite a high total crystal fraction, collisions play no significant dynamic role in the latter case due to entrainment of the small crystals in the flow field of the settling crystal. Another key finding is that the settling speed in poly-crystalline suspension is determined primarily by crystal sizes and not by the density contrast. Most efficient separation of different mineral phases occurs if size and density are correlated such that the heavy crystals are relatively large and the light crystals are relatively small. If the opposite is true, crystal settling might still be efficient but the density stratification in the resulting cumulate pile would be inverted, i.e. the light crystals would settle out first simply because they are larger.

7.4 Discussion

Previous studies have argued that crystal settling occurs predominantly during the late stages of solidification after cooling has slowed down thermal convection [1, 268, 269]. Here, we offer an alternative view. Our numerical simulations indicate that the settling speed of crystals depends very sensitively on the overall crystal fraction and the crystal-size distributions of the entrained mineral phases. This important role of crystal collisions suggests that settling would be more efficient at the beginning of solidification than towards the end when the crystal fraction is already very high. However, other factors such as the presence of a conductive lid or the relative slope of adiabat, liquidus and solidus clearly affect the dynamics as well. We discuss the interplay of the numerous factors controlling crystal settling for several specific examples of magma oceans that are presumed to have existed on Vesta and the Moon.

7.4.1 Vesta: Skewed crystal-size distributions may facilitate early crystal settling

The asteroid Vesta 4 is currently the best example of a differentiated protoplanet. It is thought to represent a surviving member of a large number of macroscale bodies in the
early solar system that assembled into the terrestrial planets (see [318] and references therein). Constraints on the compositional stratification and igneous differentiation of Vesta stem primarily from the howardite-eucrite-diogenite (HED) meteorites that are believed to have been excavated from the south pole basin on Vesta [288] and transported to Earth by Vestoids [24].

Diogenites are typically coarse-grained orthopyroxenite cumulates, however in recent years a subset of olivine-rich diogenites has also been identified. Eucrites display both cumulate and non-cumulate textures and are mostly composed of pyroxene, pigeonite, and plagioclase. Howardites appear to represent brecciated mixtures of eucrites and diogenites, indicating a potential common origin of eucrites and diogenites. But the compositional variations of eucrites and diogenites have been difficult to reconcile with a single-stage igneous process [279, 15, 132].

The homogeneity in the oxygen-isotope content of HEDs is consistent with a large-scale melting event [97] and has led to the hypothesis of a magma ocean on Vesta, facilitated by the heat released from the radioactive decay of $^{26}$Al and core formation [222, 223]. However, the petrogenesis of eucrites and diogenites in a magma ocean scenario and the relative importance of fractional versus batch crystallization in particular remain controversial [15, 99, 223, 100]. While most of the discussion has focused on petrological characteristics, our simulations may provide some insights into the fluid-dynamics constraints of crystal fractionation during the various stages of magma ocean solidification on Vesta.

The small size of Vesta creates significant physical differences in the dynamics of crystal settling during magma ocean solidification from those of larger planets. Over the small pressure range ($\approx 0.06$ GPa) in Vesta’s mantle, solidus, liquidus, and adiabat are approximately parallel (Fig. 7-12). Crystallization will therefore occur throughout the entire depth range of the magma ocean. Another ramification of Vesta’s small size is a low gravitational acceleration of approximately $g = 0.32$ m/s$^2$ [141].

Based on the bulk composition of Righter and Drake [223], olivine is expected to be the sole crystallizing phase for a significant portion of magma ocean solidification
on Vesta [15, 99]. Nucleation occurs throughout the entire depth range of the magma ocean (Fig. 7-12) and crystals are dynamically mixed through turbulent flow that extends to all but the deepest few kilometers. It is thus likely that the crystal-size distribution of olivine in a small control volume is representative of numerous nucleation events all over the magma ocean which may increase size variability drastically [180] over the linear crystal-size distribution resulting from a single nucleation event (Fig. 7-13).

The early stages of magma ocean solidification (0 – 20 %) on Vesta thus likely represent the scenario of a crystalline suspension with a very skewed crystal-size distribution. Our simulations indicate that this is the limiting case in which crystal settling is most efficient at finite crystal fraction (see sec. 7.3.3), implying that settling occurs on the time scale of seconds. Given a high efficiency of crystal settling, the local crystal fraction in the non-turbulent boundary layer should remain relatively low even as the magma ocean approaches 50% solidification.

At ≈ 53% solidification, continued cooling of the magma ocean is thought to involve orthopyroxene alone [144]. Our computations indicate that the presence of a second mineral phase reduces settling efficiency, because of the increased frequency of collisions that transfer energy from the heavy to the light crystals. The presence of the relatively light olivine in suspension should therefore reduce the mean settling speed of the heavy orthopyroxene significantly. However, the phase of simultaneous crystallization of both mineral phases appears to be limited. If that is true, orthopyroxene might still be able to settle efficiently once olivine is largely removed from suspension, but the settling speed might be considerably slower than the early olivine settling due to the increasing crystal fraction.

As solidification continues, other mineral phases with variable densities and sizes including clinopyroxene, plagioclase and Fe-Ti-Cr oxides begin to crystallize. We expect that crystal settling in a fluid-dynamical sense will largely cease at this stage. The high overall crystal fraction limits differential motion of crystals. In addition, frequent and extended collisions between crystals will tend to average out differences in settling speeds between different mineral phases, leaving a crystal mush in which
individual crystals move with roughly similar speeds irrespective of their density.

Summarizing, our simulations indicate that crystal settling could be very efficient during the early stages of magma ocean solidification when olivine is the sole crystallizing phase. Since crystal settling is most efficient in mono-crystalline suspensions (sec. 7.3.2), the settling efficiency will drop once orthopyroxene starts crystallizing but settling may not be suppressed entirely if the time of simultaneous crystallization of orthopyroxene and olivine is limited. As solidification proceeds further, crystal settling through fluid-dynamical processes will largely come to a halt, creating a dense crystal mush that overturns through large scale Rayleigh-Taylor instabilities. This late cumulate overturn could reshuffle the initial layering of the solidified mantle and transport olivine and orthopyroxene cumulates closer to the surface where they might provide the source region for diogenites and olivine-diogenites.

7.4.2 The Moon: The possibility of crystal settling during the late stages of solidification

The finding that crystal settling during the late stages of magma ocean solidification is hindered significantly by the high overall crystal fraction of the suspension and the presence of several different mineral phases with variable densities and crystal-size distributions is relevant not only for Vesta but also for the Moon. The Moon is the celestial body for which a magma ocean was first suggested [263, 324] and also the one for which the observational evidence supporting the existence of a magma ocean is most compelling [259].

The "smoking-gun" evidence for a lunar magma ocean is the anorthositic lithology in the lunar crust, which is thought to have formed by plagioclase flotation in a magma ocean (e.g. [273, 287]). A lunar magma ocean also provides an appealing framework for relating the mare basalts to the sinking and accumulation of more dense and mafic silicates in the Moon’s mantle [109, 214] and for suggesting a possible origin of the widespread, uniformly distributed, incompatible-element-rich and isotopically uniform material referred to as KREEP (Potassium, Rare Earth Elements, Phospho-
rous) [310]. A puzzling aspect of the formation of the lunar crust is that plagioclase only appears in the crystallization sequence during the late stages of solidification, i.e. once the magma ocean is approximately 70–80% solidified [264]. Additional evidence in support of high degrees of crystallization prior to plagioclase flotation comes from the trace-element characteristics of the ferroan anorthosites [203]. The petrological data thus points convincingly to late-stage fractionation, which is difficult to reconcile with the physical constraints on crystal settling discussed in sec. 7.3. We will thus briefly address factors that could facilitate crystal settling during the very late stages of magma ocean solidification.

The early stages of magma ocean solidification on the Moon are probably dynamically similar to other small bodies like Vesta in the following three aspects. (1) The adiabat for the Moon falls between liquidus and solidus for the entire depth range of the lunar mantle (Fig. 7-12) implying the possibility of highly skewed crystal-size distributions (Fig. 7-13). (2) The convective flow is turbulent and rapid (on the order of 1 m/s) throughout the vast majority of the depth range (Ra ≈ 10^{27} and Pa ≈ 30), except for the deepest few hundred meters (initially ≈ 0.5 km) in which flow is slower (on the order of 10^{-1} m/s) and non-turbulent. These estimates are based on \( \rho_f = 3600 \text{ kg/m}^3 \) [60], \( g = 1.6 \text{ m/s}^2 \) [141], \( h = 1000 \text{ km}, \Delta T = 600^\circ \text{ km} \), and the remaining parameters as in Table 7.2. (3) Olivine is the sole crystallizing phase during the early phase of solidification, which facilitates very efficient crystal settling initially.

Estimates for the point at which orthopyroxene begins crystallizing vary between 15-40 % solidification [264, 67]. It is also not clear whether orthopyroxene would be the sole crystallizing phase during any period of solidification. For the purpose of evaluating the likelihood of crystal settling, the fraction at which olivine and orthopyroxene crystallize could be important. In our simulations, we observe that crystal collisions will tend to average out differences in settling speed and thereby hinder segregation of heavy from light mineral phases. The continued presence of olivine in the suspension could therefore lead to significantly lower rates of orthopyroxene segregation as compared to the case in which only orthopyroxene would be present.
Figure 7-13: Relationship of the crystal-size distribution slope to the time variation in nucleation rate [180]. The top row (A) describes a single nucleation event and the middle row (B) a sequence of two nucleation events leading to a kinked crystal-size distribution. The bottom row (C) represents the hypothesized origin of skewed crystal-size distributions in solidifying magma oceans due to numerous nucleation events that are closely spaced in time.
Reduced settling efficiency at this intermediary stage might have ramifications for the late stages of solidification: Less crystal settling early on implies higher crystal fractions in suspension and thereby decreasing settling rates later on. This feedback implies that efficient crystal settling during the late stages of solidification requires exceptionally efficient crystal settling throughout the entire early to intermediate solidification history. A scenario in which a late period of efficient crystal settling succeeds an early period of inefficient crystal settling requires a significant secondary melting event that reduces the crystal fraction of the suspension.

The late crystallization sequence in a lunar magma ocean is dominated by anorthosite (~50%) together with olivine and pyroxene [264, 67]. The suspension will thus entail a 50%/50% mixture of both buoyant and heavy phases. Based on our simulations, suspensions with approximately equal shares of buoyant and heavy phases represent the case of least efficient crystal settling (sec. 7.3), because crystal collisions are particularly frequent and intense and the opposing directions of crystal settling may average out to a negligible net motion of the crystals. Thus, we conclude that plagioclase flotation probably requires fairly low crystal fractions at which crystal collisions are not yet as frequent. This finding makes it even more difficult to explain plagioclase flotation at a very late stage in the solidification history of the lunar magma ocean.

This conundrum begs the question whether other factors may facilitate settling. We suggest three possibilities. First, our simulations indicate that size trumps density in determining crystal segregation in heterogeneous suspensions (sec. 7.3.3). In other words, the separation of plagioclase from the pyroxene and olivine phases is facilitated if the different mineral phases also have a different mean sizes. Experimental investigations of the relative sizes of plagioclase in comparison to diopside indicate that plagioclase might be up to an order of magnitude smaller than diopside at rapid cooling rates (see [59, 32, 268] for an overview of experimental data). A possible caveat is that this data refers to rapid cooling rates and it is not clear whether the investigated cooling rates are representative of magma oceans. If the heavy pyroxene phases like diopside would indeed be an order of magnitude larger on average than
plagioclase, crystal settling would be significantly more efficient than if the mean sizes were approximately equal (sec. 7.3.3 and Fig. 7-10).

Second, the existence of a conductive lid on the surface of the magma ocean drastically reduces heat flux and thereby the vigor of the convective flow field; possibly to the degree that the zone of turbulent flow might vanish. However, the existence of a stable conductive lid seems to require the flotation of plagioclase and invoking a conductive lid to explain plagioclase flotation creates a "chicken-and-egg" problem. Prior to the flotation of plagioclase, a conductive lid is unlikely because the mafic phases that may form by quenching at the surface of the magma ocean are heavy with respect to the fluid and will therefore sink. While the constant quenching and sinking may form an effective partial lid, the heat flux within this lid would probably not be governed by conduction and it is unlikely that this type of temporary lid would suffice to suppress turbulence in the fluid portion of the magma ocean. An alternative explanation was put forth by [161] suggesting that due to rapid heat loss through the surface of magma ocean, plagioclase might have become a liquidus phase in the upper boundary layer much earlier than in the rest of the magma ocean. This mechanism could lead to the formation of a protocrust prior to 60% crystallization and may thus facilitate crystal settling significantly.

Third, there is the likelihood of a significant heating event prior to the onset of plagioclase crystallization. If plagioclase is indeed an order of magnitude smaller than simultaneously crystallizing pyroxene phases, crystal settling might be very efficient as long as the crystal fraction is low enough to reduce the probability of crystal collisions and the crystal-size distribution sufficiently skewed. A single or a sequence of melting events could keep the crystal fraction low enough for crystal settling, but it is unclear how the heat required for melting could be delivered to the early Moon. Melting triggered by impactors is one possible scenario. Another contributing factor could be tidal heating. [188] investigate the coupled thermal and orbital history of the Moon and find that large orbital eccentricities may lead to significant heating in the conductive lid. While heating in the mantle was not explicitly considered in the model, impulses of tidal heating could contribute to a reduction in the suspended crystal

206
fraction. The model does indicate, however, that tidal heating slows solidification
to the degree that that cumulate mantle overturn proceeded before the dregs of the
magma ocean solidified, adding another big heat input during this critical flotation
period. Finally, it is worth mentioning that crystal collisions themselves create some
heat through viscous dissipation.

Summarizing, we expect that crystal settling is very efficient during the early
stages of magma ocean solidification, favoring a scenario in which fractional crys-
tallization dominates the early evolution of the lunar magma ocean. The onset of
orthopyroxene crystallization is likely to gradually reduce the efficiency of crystal
settling, which is associated with a continuous increase of the crystal fraction in sus-
pension. The late crystallization sequence on the Moon represents the scenario of a
crystalline suspension with approximately equal shares of buoyant and heavy crys-
tals implying exceptionally inefficient crystal settling unless aided by external factors.
Factors that facilitate settling include early anorthosite flotation [161] and the pos-
sibility that plagioclase has smaller mean sizes than the simultaneously crystallizing
pyroxene phases [268]. Nonetheless, we suggest that one or a sequence of significant
melting events may be required to delay the otherwise inevitable batch solidification
at the high-crystal end of magma ocean solidification. It is not unlikely that im-
pactors and tidal heating in combination with the onset of cumulate mantle overturn
generate enough melting to significantly lower the crystal fraction suspended in the
liquid portion of the magma ocean and allow for plagioclase flotation.

7.4.3 Conclusions

Motivated by the goal of constraining the igneous differentiation of magma oceans
during solidification, we investigate the fluid-dynamical conditions of crystal settling
and flotation using direct numerical simulations. A lot of discussion has been devoted
to the critical size required for crystal settling in a magma ocean [290, 270, 269].
Our simulations do not confirm that mean crystal size is the decisive parameter for
evaluating settling behavior. Instead, we find that the crystal-size distribution and
the overall crystal fraction may play an even more important role. For example, our
simulations indicate that crystal settling is facilitated greatly by skewed as compared to homogeneous crystal-size distributions, even if the mean size of the skewed is much smaller than that of the homogeneous crystal-size distribution (sec. 7.3).

However, since our study does not address crystal settling in the turbulent portion of the magma oceans, it is not directly comparable but rather complementary to most previous studies of crystal settling [290, 270, 269]. In our model, the majority of crystal settling is assumed to occur in the non-turbulent boundary layers of the magma oceans as also observed in the laboratory [181]. This view of crystal settling implies that the overall crystal fraction is the rate-limiting factor for crystal settling and thus favors efficient crystal settling during the early stages of magma ocean solidification instead of during the final stretches [1, 268, 269].

Our simulations also indicate that the dynamics of crystal settling is intricately linked to the geochemical evolution of a magma ocean. For the examples of Vesta and the Moon, we find that the low crystal fraction is not the only factor facilitating crystal settling early on. Another important aspect is that olivine will be the sole crystallizing phase, which increases settling efficiency significantly (sec. 7.3.2). Once mineral phases with a different density or mean size become part of the crystallization sequence, we expect settling speeds to drop notably, because crystal collisions increasingly transfer kinetic energy from slow to fast crystals and to the fluid. The averaging effect of crystal collisions is most relevant for suspension containing buoyant and heavy phases in approximately equal shares as mean settling speeds may drop to approximately zero in this case. This finding indicates that plagioclase flotation in a lunar magma ocean might require very low crystal fractions at which crystal collisions are still relatively inefficient (sec. 7.4.2).

The degree to which mineral phases with different densities may separate through flotation and settling depends primarily on the relative sizes of the various mineral phases and only to second order on the density (sec. 7.3.3). Maximum settling efficiency is achieved only if density and size are correlated, such that fast crystals are also large and slow crystals also small. This case may be pertinent for plagioclase flotation on the Moon (sec. 7.4.2). If the reverse is true and density and size are in-
versely correlated, it is possible that crystal settling may lead to an unstable density stratification in the cumulate pile. It is worth noting that even very small differences in size (on the order of a few \%) may have a significant dynamic effect, because settling speed depends quadratically on size but only linearly on density difference.

A general ramification of the strong effect of crystal collisions on settling speeds is that decreases in the efficiency of crystal settling are difficult to reverse dynamically. The reason is that a period of inefficient crystal settling will lead to an increase in the suspended crystal fraction that thereby hinder crystal settling later on. That does not necessarily mean that efficient fractionation may not occur late during solidification, but it may require a significant melting event to reduce crystal fractions to a level at which differential motion of crystals is possible. This raises the question whether planets that are thought to be characterized by high degrees of fractionation may have experienced a sequence of relatively smaller magma oceans instead of one whole-mantle magma ocean. We hypothesize that this might be the case for the Moon.
Appendix A

Supplement for chapter 2

A.1 Abbreviated derivation of the jump conditions

We briefly summarize the derivation of the jump conditions for pressure (eq. 2.12) and stresses (eq. 2.13) closely following the discussion in [133].

As discussed in section 2.2, the jump conditions of an interface moving with the local fluid velocity are given by

\[
\begin{bmatrix}
n \\
t_1 \\
t_2
\end{bmatrix}
(pI - \tau)n^T = \begin{bmatrix}
\sigma \\
\kappa \\
0
\end{bmatrix},
\]

(A.1)

where the square brackets denote the jump across the interface. Using the definition of the stress tensor

\[
\tau = \mu \begin{pmatrix}
\nabla u \\
\nabla v \\
\nabla w
\end{pmatrix} + \mu \begin{pmatrix}
\nabla u^T \\
\nabla v \\
\nabla w
\end{pmatrix}
\]

(A.2)
in eq. A.1 yields

\[
\left[
\begin{array}{c}
p \\
0 \\
0
\end{array}
\right] - \mu \left( \begin{array}{c} n \\ t_1 \\ t_2 \end{array} \right) \left( \begin{array}{c} \nabla u \cdot n \\ \nabla v \cdot n \\ \nabla w \cdot n \end{array} \right) - \mu \left( \begin{array}{c} \nabla u \cdot t_1 \\ \nabla v \cdot t_1 \\ \nabla w \cdot t_1 \\ \nabla u \cdot t_2 \\ \nabla v \cdot t_2 \\ \nabla w \cdot t_2 \end{array} \right) \cdot n \right] = \left( \begin{array}{c} \sigma \kappa \\ 0 \\ 0 \end{array} \right).
\]  

(Eq. A.3)

Evidently, eq. A.3 can also be written as three separate jump conditions:

\[
[p - 2\mu(\nabla u \cdot n, \nabla v \cdot n, \nabla w \cdot n) \cdot n] = \sigma \kappa \quad (A.4)
\]
\[
[\mu(\nabla u \cdot n, \nabla v \cdot n, \nabla w \cdot n) \cdot t_1 + \mu(\nabla u \cdot t_1, \nabla v \cdot t_1, \nabla w \cdot t_1) \cdot n] = 0 \quad (A.5)
\]
\[
[\mu(\nabla u \cdot n, \nabla v \cdot n, \nabla w \cdot n) \cdot t_2 + \mu(\nabla u \cdot t_2, \nabla v \cdot t_2, \nabla w \cdot t_2) \cdot n] = 0. \quad (A.6)
\]

In viscous flows, the velocities across fluid interfaces are continuous

\[
[u] = [v] = [w] = 0. \quad (A.7)
\]

Furthermore, fluid interfaces cannot support shear stresses implying that the tangential velocity derivatives are continuous as well

\[
[\nabla u \cdot t_1] = [\nabla v \cdot t_1] = [\nabla w \cdot t_1] = 0 \quad (A.8)
\]
\[
[\nabla u \cdot t_2] = [\nabla v \cdot t_2] = [\nabla w \cdot t_2] = 0. \quad (A.9)
\]

Rewriting the incompressibility condition \( \nabla \cdot v = 0 \) as

\[
(\nabla u \cdot n, \nabla v \cdot n, \nabla w \cdot n) \cdot n + (\nabla u \cdot t_1, \nabla v \cdot t_1, \nabla w \cdot t_1) \cdot t_1 \quad (A.10)
\]
\[
+(\nabla u \cdot t_2, \nabla v \cdot t_2, \nabla w \cdot t_2) \cdot t_2 = \nabla \cdot v = 0,
\]  

(A.11)

it follows from eqs. A.8 and A.9 that

\[
[(\nabla u \cdot n, \nabla v \cdot n, \nabla w \cdot n) \cdot n] = 0. \quad (A.12)
\]
Thus, from combining eqs. A.12 and A.4 we obtain

\[
[p] = \sigma \kappa + 2[\mu](\nabla u \cdot \mathbf{n}, \nabla v \cdot \mathbf{n}, \nabla w \cdot \mathbf{n}) \cdot \mathbf{n},
\]  

(A.13)

which is the jump condition for pressure (eq. 2.12) discussed in section 2.3.1 in the paper.

For the derivation of the jump in normal-stresses, eqs. A.5, A.5, A.8, A.9, and A.12 can be compiled to obtain

\[
\begin{pmatrix}
\mathbf{n} \\
\mathbf{t}_1 \\
\mathbf{t}_2
\end{pmatrix}
= [\mu]
\begin{pmatrix}
\nabla u \\
\nabla v \\
\nabla w
\end{pmatrix}
\begin{pmatrix}
\mathbf{n} \\
\mathbf{t}_1 \\
\mathbf{t}_2
\end{pmatrix}
+ [\mu]
\begin{pmatrix}
\nabla u \\
\nabla v \\
\nabla w
\end{pmatrix}
\begin{pmatrix}
0 \\
0 \\
0
\end{pmatrix}
- [\mu]
\begin{pmatrix}
\nabla u \\
\nabla v \\
\nabla w
\end{pmatrix}
\begin{pmatrix}
0 \\
0 \\
0
\end{pmatrix},
\]  

(A.14)

which can be rewritten to yield the expression for the stress-jump used in the paper (eq. 2.13, sec. 2.3.1):

\[
\begin{pmatrix}
\mu u_x \\
\mu v_x \\
\mu w_x
\end{pmatrix}
\begin{pmatrix}
\mu u_y \\
\mu v_y \\
\mu w_y
\end{pmatrix}

= [\mu]
\begin{pmatrix}
\nabla u \\
\nabla v \\
\nabla w
\end{pmatrix}
\begin{pmatrix}
\mathbf{t}_1 \\
\mathbf{t}_1 \\
\mathbf{t}_2
\end{pmatrix}
+ [\mu]
\mathbf{n}^T \mathbf{n}
\begin{pmatrix}
\mathbf{n}^T \mathbf{n} - [\mu]
\end{pmatrix}
\begin{pmatrix}
\nabla u \\
\nabla v \\
\nabla w
\end{pmatrix}
\begin{pmatrix}
\mathbf{t}_1 \\
\mathbf{t}_1 \\
\mathbf{t}_2
\end{pmatrix}
\begin{pmatrix}
\mathbf{n}^T \mathbf{n}
\end{pmatrix}.
\]  

(A.15)

Recasting the jump conditions in this way (eq. A.15) has the advantage that the jumps in the stresses (left hand side of eq. A.15) are reduced to the jump in the viscosity combined with various components of the velocity derivatives which are continuous and can be approximated through finite differences (right hand side of eq. A.15).
A.2 Pressure jump for weak inclusions at extremely large viscosity contrasts

When presenting our results for benchmark problem 2 (sec. 2.5.2), the viscosity contrast is set to \( \Pi_1 = 10^{-3} \) to allow for an easy comparison with previous numerical results by [58]. Our ghost-fluid-type method can also handle viscosity contrasts of numerous orders of magnitude as illustrated in Fig. A-1 for \( \Pi_1 = 10^{-6} \) and \( \Pi_1 = 10^{-10} \). Note that the percentage error in these computations is approximately the same despite the higher viscosity contrast. The reason is the discretization of the jump conditions (eqs. 2.4 and 2.13), where the viscosity jump multiplies the viscous contribution to the jump which is not discontinuous and can thus be discretized without difficulties. In all of these computations, the grid resolution is set to 150 \( \times \) 150 to highlight that the treatment of larger viscosity contrasts does not require higher grid resolutions.

A.3 Convergence tests for benchmark problems 1, 2, and 3

Benchmark problem 1 is targeted specifically at verifying whether the jump conditions at the interface are resolved accurately and at identifying the minimum grid resolution required for that purpose. Although only three points are necessary to build ghost-fluid-type stencils (sec. 2.3.1), this does not guarantee convergence. We note that a convergence proof for ghost-fluid methods exists [159], but for practical purposes it is often a concern whether the required resolution can be reached given available computational resources. Fig. A-2 shows that although the magnitude of the jump is approximated correctly at all grid sizes, resolving the circular shape of the bubble requires a minimum of \( \approx 15 \) grid points in both x- and y-direction inside of the bubble. This is an encouraging result, since resolutions in this range are feasible even in three dimensions. Although the jump conditions in benchmark problem 2
Figure A-1: Numerical (left) and analytical (middle) solution for the pressure field for benchmark problem 2. The viscosity contrast between inclusion and surrounding matrix is 6 (top row) and 10 (bottom row) orders of magnitude. The right panels shows the percentage error for both computations. The grid resolution is $150 \times 150$ in both cases.
Figure A-2: Convergence test for benchmark problem 3. Shown are the numerical solutions for the pressure jump due to surface tension at the interface between a viscous drop and the surrounding fluid at grid resolutions 21 x 21 (left), 31 x 31 (center), and 41 x 41 (right). Each dot represents one grid point. Although the jump as such is resolved sharply without artificial smoothing at all of these resolutions, a minimum of ≈ 15 grid points in both the x- and y-direction are required inside of the drop to resolve its spherical shape.

are more challenging to resolve numerically than the surface-tension-related jump in pressure in benchmark problem 1, we observe that the pressure jump is captured sharply and without spurious oscillations even at very low resolution (Fig. A-3). The additional challenge as compared to benchmark problem 1, is to accurately resolve the magnitude of the jump which could be computed accurately even at minimal grid resolutions for benchmark problem 1. Fig. A-3 shows two example computations at a grid resolution of 20 x 20 and 80 x 80. The percentage error in estimating the maximum pressure jump is 19 % and 8%, respectively.

The dynamics of benchmark problem 3 are not dominated by the jump conditions. Thus, it serves primarily as a verification for the computation of the rise speed of the instability and the advection of the interface. In addition to the convergence test for grid resolution, we also performed a convergence test for the required temporal resolution (Fig. A-4). We observe that the calculation is well converged for grid sizes exceeding 100 x 110 and incremental time steps of Δt ≤ 25Δx. In order to quantify the accumulation of numerical error – an important concern in dynamic problems – we plot the mass fluctuations in the buoyant phase in Fig. A-5. Although we observe notable fluctuations, particularly towards the end of the computation, these fluctuations remain < 1% error, indicating that the numerical solution is still reliable.
Figure A-3: Convergence test for benchmark problem 2. The viscosity contrast is $\eta_1 = 10^{-3}$ as discussed in the paper, sec. 2.5.2. The shown grid resolutions are $20 \times 20$ (top) and $80 \times 80$ (bottom). In both cases, we contrast numerical (left) and analytical solution (right). The comparison shows that the additional challenge of benchmark problem 2 as compared to benchmark problem 1 lies in fully resolve the magnitude of the pressure jump, for which high resolution is required.
A lack of convergence is easiest to identify during the phases of rapid rise of an instability. We illustrate this for the rise of the secondary instability on the right side of the box at time $t=1000$ and four different grid sizes: $60 \times 66$, $80 \times 88$, $100 \times 110$, and $120 \times 132$. We observe convergence for grid sizes above $100 \times 110$. Right: Convergence test for the isothermal and isoviscous Rayleigh-Taylor instability, benchmark problem 3. Analogous to Fig. S7, we illustrate this convergence test for the rise of the secondary instability at time $t=1000$. The four interfaces were computed based on the time steps: $\Delta t = 180 \Delta x$, $\Delta t = 90 \Delta x$, $\Delta t = 45 \Delta x$, and $\Delta t = 25 \Delta x$. We observe convergence for time steps $\Delta t \leq 25 \Delta x$.

A.4 Possible biases related to iterative reinitialization techniques

Iterative reinitialization relies on a fundamentally different approach to coupling the fluid and the interface solver than the one adopted in our method (sec. 2.3.3). Instead of constructing an extension velocity function, the physical velocity field is used to advect the level set function (eq. 2.22). As a consequence, the normalization of the level set function needs to be restored continuously - a procedure known as re-initialization. The need to re-initialize was first noted by [41]. The approach most
Figure A-5: Illustration of the accumulation of numerical error over time reflected in mass fluctuations. The plot shows the mass of the buoyant phase as a percentage of its initial mass. This plot compares to a similar plot presented by Schmalzl and Loddoch, [2003]. We note that fluctuations $< 1\%$ are not unexpected in complex fluid dynamical simulations. Overall, the mass conservation is satisfactory.

commonly used to accomplish re-initialization was developed by [282] drawing on prior work by [234]. The idea is to iteratively find a solution to the so-called re-initialization equation

\[
\frac{\partial \phi}{\partial \tau} + \text{sign}(\phi_0)(1 - |\nabla \phi|) = 0, \tag{A.16}
\]

where $\tau$ is the pseudo-time and $\text{sign}(\phi_0)$ the signum function referring to $\phi_0 = \phi(\tau = 0)$. We refer to $\tau$ as a pseudo-time scale, because it does not correspond to an actual time scale in the physical problem. Unfortunately, the iterative solution to the re-initialization is known to be prone to spurious mass loss and artificial front repositioning (e.g. [5], [256], [281], [43], [134]). We implemented the iterative re-initialization procedure by [282] to test its performance for the isothermal Rayleigh-Taylor instability (benchmark problem 3) and indeed observed both substantial mass loss and significant variations in the final position of the interface. Fig. A-6 illustrates our findings. The instability on the left (Fig. A-6A) is computed based on the extension velocity approach adopted in this paper. The other two (Fig. A-6 B and C) are both
Figure A-6: Illustration of the potential bias introduced through an iterative reinitialization procedure. The left figure (A) shows the isothermal and isoviscous Rayleigh-Taylor instability at t=1500 computed with extension velocities. The other two figures (B) and (C) are based on an iterative reinitialization procedure, but different parameters are used in the iteration. For case (B) a single reinitialization iteration is performed at each computational time step $\Delta t$ and $\Delta \tau = 0.9 \Delta x$ is used in the numerical solution of equation A.16. For case (C) 20 iterative reinitialization steps were taken at each physical time step $\Delta t$ with $\Delta \tau = 0.9 \Delta x/20$. All computations were performed on a $120 \times 132$ grid.

Based on the iterative reinitialization by [282], but reinitialize more (C) or less (B) frequently and use different iterative parameters to solve equation A.16. This comparison highlights that while it is certainly possible to obtain the 'correct' interface based on iterative reinitialization (Fig. A-6B), the accuracy of the solution depends sensitively on the details of the reinitialization procedure and the resulting biases can be substantial. Since iterative reinitialization is still commonly used (e.g. [98, 28], it is important to be aware of these potential problems.

### A.5 Subgrid features

In section 2.6.2, we discuss the role of subgrid features in the context of comparing the level set method to tracer approaches. We consider a certain feature of the interface to be subgrid, if the length scale associated with it is smaller than the resolution afforded by the fluid solver. An example is shown in Fig. A-7. Plotted is the numerical solution of the isothermal and isoviscous Rayleigh-Taylor instability
Figure A-7: The Rayleigh-Taylor instability as computed by the HS-tracer method at time $t=1500$. The equations of motion for this simulation were solved on an $81 \times 81$ grid. The right panel is a zoom onto the peak located left of the descending instability. Each blue dot represents one particle and the grid represents a rough estimate of the scale at which the flow field is approximated correctly.

at $t=1500$ computed by the tracer-based finite-difference method by Schmeling. For the numerical details please refer to [296]. The descending instability in the center is accompanied by a thin tentacle, which is observed to various degrees in all of the explicit interface representation techniques (i.e. both tracer computations and, to a much smaller degree, also for the marker chains).

In the computation shown in Fig. A-7, the Stokes equation is solved on a structured finite-difference grid of size $81 \times 81$. To visualize the resolution afforded by this choice of grid size, we overlay the thin tentacles located to the right of the descending instability on a grid of approximately that size. The length scale at which the Stokes equation is approximated numerically is given by the size of these grid cells. Evidently, the thickness of the tentacle falls well below the resolution limit of the fluid solver. In this case, it becomes a non-trivial challenge to accurately solve the equations of motion.
Appendix B

Supplement for chapter 3

B.1 Projection Method

The basic idea of the projection method for solving the Navier-Stokes equation is to introduce a temporary velocity field, \( \mathbf{v}^* \), representing the best initial prediction, which gets corrected in a subsequent step to ensure incompressibility. Thus, the incompressible Navier-Stokes equation is discretized as a series of three equations which are solved sequentially

\[
\frac{\mathbf{v}^* - \mathbf{v}^n}{\Delta t} + (\mathbf{v}^n \cdot \nabla)\mathbf{v}^n = \frac{1}{\rho(\phi)} \nabla \cdot \left[ \mu(\phi)(\nabla \mathbf{v}^n + (\nabla \mathbf{v}^n)^T) \right] + \mathbf{g} \tag{B.1}
\]

\[
\nabla \cdot \left[ \frac{1}{\rho(\phi)} \nabla p_{n+1} \right] = \frac{1}{\Delta t} \nabla \mathbf{v}^* \tag{B.2}
\]

\[
\frac{\mathbf{v}^{n+1} - \mathbf{v}^*}{\Delta t} = -\frac{1}{\rho(\phi)} \nabla p_{n+1}. \tag{B.3}
\]

Clearly, the predicted velocity field (eq. B.1), \( \mathbf{v}^* \), will not generally fulfill the incompressibility constraint. This requirement is enforced through the second equation (B.2), the pressure correction, which solves for the pressure field at the next time step \( p_{n+1} \) and is derived from the incompressibility condition for the velocity field \( \mathbf{v}^{n+1} \).

In the last step (eq. B.3), the pressure obtained from equation B.2 is used to correct \( \mathbf{v}^* \), yielding the correct velocity field, \( \mathbf{v}^{n+1} \). Two aspects of the described three-step projection (eqs. B.1-B.3) merit further discussion: (1) The jump conditions (eq. 3.5)
Figure B-1: Dependence of the breakup time $t_B$ on bubble radius $a$ for large bubbles. In order to evaluate the dependence of $t_B$, the computation is dimensional with the same parameters as in Fig. 3-6: $\rho_f = 3500 \text{ kg/m}^3$, $\rho_g = 1.226 \text{ kg/m}^3$, $g = 9.81 \text{ m/s}^2$, $\sigma = 0.3 \text{ N/m}$, $\mu_f = 10 \text{ Pa-s}$, and $\mu_g = 10^{-5} \text{ Pa-s}$. The breakup time is expressed in percent of the initial breakup time at $a = 5.4 \text{ cm}$. The numerical data are no longer compatible with the simple scaling relationship $t_B \sim a^3$ (eq. 3.20), which is not unexpected, given the wide fluid dynamical range it spans.

need to be accounted for in the discretization of the viscous term in B.1, the solution of the Poisson (eq. B.2), and the application of the velocity correction (B.3). Please refer to Appendix A or to [133, 157] for a description of the implementation of the jump conditions. (2) The continuous spatial derivatives in eqs. B.1-B.3 are computed as finite differences on a staggered grid, yielding a second-order approximation. For the matrix inversions, we mostly use the Biconjugate gradients stabilized method with an incomplete LU-decomposition as preconditioner. We note that, although the matrix is symmetric, we observe that the Biconjugate gradients stabilized method yields robust convergence.
B.2 Dependence of breakup time on bubble radii for large bubbles

In section 3.5.1 we investigate the dynamic instability of isolated gas bubbles. Based on scaling arguments, we expect that the breakup time, $t_B$, scales with the radius of the bubbles as $t_B \sim a^3$. While this behavior is compatible with our numerical experiments for bubbles with barely unstable radii (Fig. 3-6), it no longer holds at larger bubble radii. In fact, we observe that the breakup time decreases for very large bubbles, as shown in Fig. B-1. We note that the range of bubble radii spans a wide range of Re and it is not unexpected that not the entire range is adequately described by a scaling relationship as simple as eq. 3.20.

B.3 Resolution restriction for breakup induced by multibubble interactions

As discussed in section 3.5.2, it is challenging to reproduce the sequences of breakup and coalescence observed in two dimensions (e.g. Fig. 3-9) in three dimensions. The key problem is that the mode of interaction (i.e. coalescence, breakup or passing) depends sensitively on the fluid dynamics in the thin magmatic film separating the two bubbles, which we cannot accurately resolve in three dimensions on a fixed grid. Fig. B-2 illustrates the resolution requirements in two dimensions. It shows three computations which are identical in all non-dimensional parameters except for the vertical separation distance which varies from $\Pi_3 = 1.3$ (top), $\Pi_3 = 1.16$ (middle), to $\Pi_3 = 1.4$ (bottom). Clearly, the mode of interaction depends very sensitively on the initial separation distance of the bubbles $\Pi_3$. In three dimensions and in the absence of an adaptive grid, it is challenging to resolve these minimal variations in the initial separation distance. An additional concern is that we define coalescence to occur if two bubbles approach each other by less than the grid size (sec. 3.4.1). For high enough resolutions in two dimensions, a coalescence criterion of this type is warranted.
Figure B-2: Dependence of multibubble interactions on the initial vertical separation distance. The three simulations show two bubbles passing (top), breaking up (middle), and coalescing (bottom) as a consequence of increasing the non-dimensional vertical distance $H_3 = 1.16$ (top), $H_3 = 1.3$ (middle), and $H_3 = 1.4$ (bottom). The other non-dimensional numbers are identical for the three simulations: $Re \approx 5$, $Fr \approx 0.2$, $We \approx 70$, $H_1 = 10^{-6}$, $H_2 = 1.43$, and $H_4 = 2$. Snapshots are taken at non-dimensional times $t = 0$, $1.5$, $3.0$, $4.5$, and $6.0$. All three computations were performed with a grid resolution of $100 \times 200$. 
by observational data [136]. For the lower resolution achievable in three dimensions, it might be more problematic. Therefore, we expect three dimensions computations to be more reliable in identifying if two bubbles do not coalesce and included only that case in the paper (Fig. 3-8).

B.4 Convergence tests

We performed detailed convergence tests for the computations presented in this paper. The two dimensions computations converge to the degree expected for interface problems at finite Re. This statement merits a brief explanation: If the motion of the interface is driven by instabilities that evolve self-consistently at the interface (e.g. a Rayleigh-Taylor or Kelvin-Helmholtz instability), computations with different grid spacings will inevitably deviate over time. The primary reason is the dispersive nature of the growth rate of interface instabilities (Fig. 3-2) in combination with the fact that each computation will at best resolve wavelengths \( \lambda > 2\Delta x \) where \( \Delta x \) is the grid resolution because of aliasing. In the Stokes regime, this effect is less of a concern, because of the quasi-stationarity of the flow field (i.e. the equations of motion are solved from scratch at each computational time step). At finite Re, however, the flow field depends sensitively on its value during previous time steps and thus deviations in the long-term evolution are expected. We note that this effect should be distinguished from the accumulation of purely numerical error, which is, of course, an additional concern.

Our convergence tests demonstrate that:

1. The initial rise speed of the bubble prior to breakup is computed accurately even at comparatively low resolution (Figs. B-3-B-6). It deviates by less than 1% for grid resolutions larger than \( 80 \times 160 \).

2. The number and sizes of bubbles generated during catastrophic breakup depends sensitively on the resolution afforded by a given computation (as should be expected based on the aliasing reasoning above), but the time at which it
occurs and the basic sequence are robust for resolutions above approximately 80 × 160, as evident from Figs. B-3-B-4.

3. The number and sizes of bubbles generated during gradual breakup depend less on grid resolution than in the case of catastrophic breakup, probably because the surface instabilities relevant for gradual breakup span a narrower range of wavelengths and are thus easier to resolve (Figs. B-5-B-6).

In three dimensions, we are unable to perform a similarly detailed convergence test due to limitations in available computational resources. The highest resolution reached in our three dimensions computations is comparable to the lowest resolution included in the convergence test for two dimensions. This implies that the time until catastrophic breakup and the size and number of bubbles generated during breakup might tend to be underestimated in three dimensions, because the surface instabilities causing the breakup are not resolved at a sufficiently small spatial scale. In analogy to the two dimensions case, we expect gradual breakup sequences should be more reliable, although we have not been able to verify this presumption quantitatively due to limitations in computational resources.

Figure B-3: Convergence test for the catastrophic breakup of an isolated gas bubble (compares to Fig. 3-4C). Shown are four computations at differing resolutions 40×80, 80×160, 160×320, and 320×640.
Figure B-4: Convergence test for the catastrophic breakup of a conduit-filling gas slug (compares to Fig. 3-11C). Shown are four computations at differing resolutions 40×80, 80×160, 160×320, and 320×640.

Figure B-5: Convergence test for the gradual breakup of an isolated gas bubble (compares to Fig. 3-4B). Shown are four computations at differing resolutions 40×80, 80×160, 160×320, and 320×640.
Figure B-6: Convergence test for the gradual breakup of a conduit-filling gas slug (compares to Fig. 3-11A). Shown are four computations at differing resolutions 40×80, 80×160, 160×320, and 320×640.
Appendix C

Supplement for chapter 4

C.1 Bubble and crystal populations in HP magma

Bubble and crystal shapes and sizes in magma can be studied by image analysis of thin sections of volcanic ejecta. Tephra from Stromboli’s HP magma is usually heterogeneous but very crystal and vesicle rich. Figure C-1 shows a thin section of an HP tephra clast erupted on 19 July 2007. Bubbles are white (void space), crystals are green and gray, and glass is brown. Bubbles in the center are often larger than those in the rims of the clasts because quenching is less rapid in the center, allowing more pronounced syn-eruptive expansion and coalescence. Cumulative bubble and crystal size distributions are shown for different areas around the edge (where bubble expansion is taken to be minimal). Bubble size is calculated from area $A_b$ (measured on the thin section scan) as $2A_b/\pi$. Crystal size is calculated from area $A_c$ as $A_c$.

It can be seen that 1) bubble and crystal sizes are similar, 2) there are many bubbles present in the pore space and 3) small bubbles (< 0.3 mm diameter) are most abundant. These observations indicate that lots of small bubbles are percolating through the pore space between the crystals in the HP plug. While the presence of crystals always increases the effective viscosity of a crystal-bearing fluid, the rheological effect of bubbles depends on their deformability as captured by the capillary number $[278, 169, 240, 160], Ca = \mu v / \sigma$, where $\mu$ is the viscosity of the magma, $v$ the characteristic speed and $\sigma$ the surface tension parameter. At Stromboli, most bubbles
Figure C-1: Thin-section analysis of Stromboli's HP magma.
are small, with capillary numbers \( Ca \ll 1 \) [19]. Thin sections (e.g. Fig. C-1) confirm the theoretical expectation that \( Ca \ll 1 \). Although some of the larger vesicles are deformed, there is no evidence of the type of bubble shapes expected for shear flow [239]. Instead, most larger vesicles appear to be deformed by the presence or relative motion of nearby crystals (see Figure C-1), highlighting that bubbles may be part of a load-bearing framework. The insight that \( Ca \ll 1 \) implies that the rheological effect of the bubbles in HP magma can be approximated by that of solid spheres including a corrective term that accounts for the viscosity contrast [285, 82, 103]. Therefore, the bubbles effectively increase the solid fraction of the aggregate providing further evidence in support of the solidity of the plug.

C.2 Analytic solution for the stresses in an elliptic plate of moderate thickness with clamped edges

In a body in equilibrium the components of stress satisfy the following equations at every point in the body

\[
\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} + \frac{\partial \sigma_{xz}}{\partial z} = 0, 
\]

\[
\frac{\partial \sigma_{xy}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} + \frac{\partial \sigma_{yz}}{\partial z} = 0, 
\]

\[
\frac{\partial \sigma_{xz}}{\partial x} + \frac{\partial \sigma_{yz}}{\partial y} + \frac{\partial \sigma_{zz}}{\partial z} = 0. 
\]

Under the action of these stresses the body is strained and displaced from its initial configuration. For an isotropic body obeying Hooke’s law, the linear relationships
between stresses and strains leads to the additional constraints [163]:

\[
\begin{align*}
\nabla^2 \sigma_{xx} &= -\frac{1}{1 + \nu} \frac{\partial^2 \Theta}{\partial x^2} \\
\nabla^2 \sigma_{yy} &= -\frac{1}{1 + \nu} \frac{\partial^2 \Theta}{\partial y^2} \\
\nabla^2 \sigma_{zz} &= -\frac{1}{1 + \nu} \frac{\partial^2 \Theta}{\partial z^2} \\
\nabla^2 \sigma_{yz} &= -\frac{1}{1 + \nu} \frac{\partial^2 \Theta}{\partial y \partial z} \\
\nabla^2 \sigma_{xz} &= -\frac{1}{1 + \nu} \frac{\partial^2 \Theta}{\partial x \partial z} \\
\nabla^2 \sigma_{xy} &= -\frac{1}{1 + \nu} \frac{\partial^2 \Theta}{\partial x \partial y},
\end{align*}
\]

where \( \nu \) is the Poisson’s ratio and \( \Theta \) is the harmonic function

\[
\Theta = \sigma_{xx} + \sigma_{yy} + \sigma_{zz}. \tag{C.10}
\]

Additionally, the boundary conditions require that the lower face \( z = -h \) is subjected to uniform pressure \( p \) and that the upper face \( z = h \) is free of traction, implying that

\[
\begin{align*}
\sigma_{zz} &= p \quad \text{at} \quad z = -h, \tag{C.11} \\
\sigma_{zz} &= 0 \quad \text{at} \quad z = h, \tag{C.12} \\
\frac{\partial \sigma_{zz}}{\partial z} &= 0 \quad \text{at} \quad z = -h. \tag{C.13}
\end{align*}
\]

We assume that the edge of the plate is fixed in a way that no inclination of the tangent plane to the middle surface to the initial middle plane is possible at a point on the edge. This mode of fixing the edge translates into

\[
\begin{align*}
u_{el} &= 0, \tag{C.14} \\
v_{el} &= 0, \tag{C.15} \\
w_{el} &= 0, \tag{C.16} \\
\frac{\partial w_{el}}{\partial n} &= 0, \tag{C.17}
\end{align*}
\]
where \((u_{el}, v_{el}, w_{el})\) denotes the displacement vector at the edge and \(n\) denotes the direction normal to the edge line.

We solve equations C.1-C.17 analytically for an elliptic plate with semimajor axis \(a\), semiminor axis \(b\) and thickness \(2h\) (see Fig. 4-4) using the methodology by [162]. We find

\[
\sigma_{zz} = \frac{1}{4} \frac{p}{h^3} (z^3 - 3h^2 z + 2h^3), \tag{C.18}
\]

\[
\sigma_{xz} = \frac{3}{8} \frac{p}{h^3} (h^2 - z^2)x + \frac{9}{8} \frac{p}{h^3} \frac{a^4 - b^4}{3a^4 + 2a^2b^2 + 3b^4} xz^2, \tag{C.19}
\]

\[
\sigma_{yz} = \frac{3}{8} \frac{p}{h^3} (h^2 - z^2)y - \frac{9}{8} \frac{p}{h^3} \frac{a^4 - b^4}{3a^4 + 2a^2b^2 + 3b^4} yz^2, \tag{C.20}
\]

\[
\sigma_{xy} = \frac{3}{2} \frac{p}{h^3} (1 - \nu) \frac{1}{3a^4 + 2a^2b^2 + 3b^4} xyz, \tag{C.21}
\]

\[
\sigma_{xx} = -\frac{1}{2} \frac{p}{h^3} \frac{\nu}{1 - \nu} + \frac{z}{1 + \nu} \theta_1 + \frac{3}{8} \frac{p}{h^3} z(x^2 + y^2 + h^2) \tag{C.22}
\]

\[
- \frac{3}{32} (1 - \nu) \frac{p}{h^3} z(x^2 + 3y^2) - \frac{2 + \nu}{8} \frac{p}{h^3} z^3, \tag{C.23}
\]

\[
\sigma_{yy} = -\frac{1}{2} \frac{p}{h^3} \frac{\nu}{1 - \nu} + \frac{z}{1 + \nu} \theta_1 + \frac{3}{8} \frac{p}{h^3} z(x^2 + y^2 + h^2) \tag{C.24}
\]

\[
- \frac{3}{32} (1 - \nu) \frac{p}{h^3} z(3x^2 + y^2) - \frac{2 + \nu}{8} \frac{p}{h^3} z^3, \tag{C.25}
\]

where

\[
\theta_1 = -\frac{E}{1 - \nu} \left( \frac{\partial^2 w_0}{\partial x^2} + \frac{\partial^2 w_0}{\partial y^2} \right) - \frac{3}{8} \frac{p}{h^3} (1 + \nu)(x^2 + y^2) + \frac{3}{4} \frac{p}{h^3} \frac{1 + \nu}{1 - \nu} \tag{C.26}
\]

\[
\chi'_1 = \frac{E}{1 + \nu} w_0 - \frac{E}{1 + \nu} \theta_1 + \frac{3}{128} \frac{p}{h^3} (1 - \nu)(x^2 + y^2)^2 - \frac{3}{16} \frac{p}{h^2} (x^2 + y^2) \tag{C.27}
\]

\[
\chi' = z\chi'_1 + \frac{2 - \nu}{6(1 + \nu)} z^3 \theta_1. \tag{C.28}
\]

In these expressions, \(E\) is the Young's modulus,

\[
w_0 = -\frac{1}{8} \frac{p}{D} \left( \frac{1 - \frac{x^2}{a^2} - \frac{y^2}{b^2}}{\frac{3}{a^4} + \frac{3}{b^4} + \frac{2}{a^2b^2}} \right)^2 \tag{C.29}
\]
D is the displacement in \( z \)-direction in the middle plane \((z = 0)\), and

\[
D = \frac{2Eh^3}{3(1-\nu^2)} \tag{C.30}
\]

is the flexural rigidity of the plate.

## C.3 Numerical approach for plugs with large thicknesses

We solve the equations of linear elasticity in the displacement formulation (Navier-Cauchy problem) inside the computational domain \( \Omega \). On the boundary, the components of the displacement vector \( \mathbf{u} \) satisfy either Dirichlet conditions, \( \Gamma_D \) (along the clamped edge), or Neumann conditions, \( \Gamma_N \) (along the bottom and top surface of the plug). We are thus seeking a solution to the following system of equations

\[
(A + p)(\nabla \text{div} \mathbf{u})^T + \mu \Delta \mathbf{u} = 0 \text{ in } \Omega \tag{C.31}
\]

\[
(\lambda \text{tr}(\epsilon(\mathbf{u}))I + 2\mu \epsilon(\mathbf{u})) \cdot \mathbf{n} = f \text{ on } \Gamma_N \tag{C.32}
\]

\[
\mathbf{u} = 0 \text{ on } \Gamma_D, \tag{C.33}
\]

where \( \lambda \) and \( \mu \) are the Lamé parameters, \( \mathbf{n} \) is the normal vector, \( \mathbf{f} \) the surface force acting on the lower boundary, and \( \epsilon(\mathbf{u}) = (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)/2 \).

We approximate the weak form of eqs. C.33-C.33 (e.g. [29]) using the standard Galerkin method (e.g. [6]). The mesh is generated using the open source package DistMesh [210]. An example grid is shown in Fig. C-2.

Fig. C-2 shows that the correlation between the locations of maximum shear stress and the observed craters (see Fig. 4-6) is not robust for a thick elliptical plug. If the flank of the plug that is aligned with the Sciara del Fuoco were freely moving, the locations of maximum shear stress shift closer to the crater locations. However, the stresses at the transition point from freely moving to clamped boundary now become extremely large. We conclude that it is probably important to incorporate
spatial variations in material strength to obtain a more realistic model of the stress distribution inside the plug. We will address this extension of the plug model in future research.

C.4 Stress concentration at the microscopic scale

While a purely elastic view of the plug provides a reasonable first-order approximation at the macroscopic scale, the presence of vesicles may play an important role at the microscopic level. Therefore, we perform a separate suite of computations to investigate stress and strain at the microscopic scale. We simplify the microscopic texture of the plug by treating the fluid and crystalline phases as one elastic aggregate with interdispersed vesicles representing the gas phase. Due to the irregular spacing of vesicles, we resort to solving for stress and strain numerically using standard Galerkin and a triangular finite-element mesh in two dimensions. The analytical solutions for the macroscopic stresses provide the boundary conditions for the rectangular microscopic domains considered in our computations. The boundary condition on the bubble interface is zero traction. The two example computations in Figure C-3 demonstrate that bubbles concentrate ambient stresses locally within approximately three times

Figure C-2: Left: Maximum shear stress for a thick elliptical cylinder overlain by the computational grid generated by Distmesh. The stresses are extremely high in the vicinity of the side boundaries. Right: Maximum shear stress for a thick elliptical cylinder with a free-moving side flank.
Figure C-3: Stress concentration around the bubble interface in a purely extensional stress field. The stress is measured in multiples of the applied stress at the boundary $\sigma_{bc}$. The black circles surrounding the bubbles correspond to three times the radius of the bubble and denote the range over which the stress concentration due to the presence of the bubble is appreciable (Saint-Venant’s principle). In panel A, the bubbles are spaced closely enough for substantial stress concentration; in panel B, the bubbles are far enough apart to be negligible on the large scale. The purely compressional case is analogous.

their own radii (Saint-Venant’s principle). Therefore, bubbles cause macroscopically relevant stress concentration only if they cluster together, for example within bubble pathways resulting from gas percolation through the highly crystalline medium (Fig. C-3A) and may be neglected otherwise (Fig. C-3B). Analysis of thin sections indicates that the bubble fraction varies between 15-60 vol.% within HP magma (Fig. C-1) implying that bubbles in highly vesicular domains cluster closely enough to cause substantial stress concentration.
Appendix D

Supplement for chapter 5

D.1 Homogeneous nucleation

In the absence of interfaces facilitating bubble nucleation (heterogeneous nucleation), spontaneous (homogeneous) nucleation requires transient clusters of gas molecules in the melt. According to classical nucleation theory pioneered by [306, 18] and [149], these small clusters form due to local fluctuations in the volatile concentration. The growth of these nuclei is determined by a competition between the lower bulk free energy of the new vapour phase as compared to the supersaturated melt and the energy consumed by forming an interface (Fig. D-1). At a critical size \( r^* \), further addition of volatile molecules leads to a decrease in the energy of the two phase system, spurring spontaneous growth of the now stable nucleus. The critical radius is

\[
r^* = \frac{2\sigma}{P^* - P},
\]

where \( \sigma \) is the surface tension, \( P^* \) the internal pressure in the nucleus and \( P \) the ambient pressure in the melt. The energy required to form the critical nucleus is [114, 149]

\[
\Delta F^* = \frac{16\pi\sigma^3}{3\Delta P^2},
\]

(D.2)
Figure D-1: Illustration of the activation energy for homogeneous nucleation. The blue curve represents the Free Helmholtz energy $\Delta F_{surf}$ required for forming a new interface and the red curve the volumetric gain in Free Helmholtz energy $\Delta F_{vol}$ from the presence of a bubble. The sum of the two contributions is shown in green. An activation energy of $\Delta F^*$ needs to be overcome for spontaneous nucleation to occur.

where $\Delta F^*$ is the Helmholtz free energy and $\Delta P = P^* - P$ the supersaturation pressure. $\Delta F^*$ may be interpreted as the 'activation energy' of the nucleation process (Fig. D-1). During ascent of melt saturated in volatiles, the ambient pressure $P$ decreases hydrostatically while the equilibrium vapour pressure of the melt remains constant, and upon reaching a critical level of supersaturation $\Delta P$ nucleation becomes rapid. The nucleation rate $J$ can be estimated from the approximate expression [114, 123]

$$J = J_0 \exp \left( \frac{-\Delta F^*}{kT} \right) \approx \frac{2n_0^2 V_{mol} D}{a_0} \sqrt{\frac{\sigma}{kT}} \exp \left( \frac{-16\pi \sigma^3}{3kT\Delta P^2} \right), \quad (D.3)$$

where $k$ is the Boltzmann constant, $T$ the temperature, $V_{mol}$ the volume of a volatile molecule in the melt, $D$ the diffusion coefficient of the volatile, $a_0$ the distance between two volatile molecules, and $n_0$ the concentration of nucleation sites which, in the case considered here, corresponds to the concentration of dissolved volatile molecules.
Appendix E

Supplement for chapter 6

E.1 Adjustment of the collision parameters

In our implementation, collisions are modeled through short-range repulsive forces following [91]. While their scheme is appealing for its simplicity, it requires careful adjustment of the stiffness parameters such that the repulsive force is not too weak to prevent overlaps but not so large that it results in spurious rebounds occur in non-dimensional regimes for which they are not expected [121]. The repulsive force \( F_{ij} \) is defined by [91]

\[
F_{ij} = \frac{c_{ij}}{\epsilon} \left( \max \left( 0, -\frac{d_{ij} - r_i - r_j - \xi}{\xi} \right) \right)^2 \frac{G_i G_j}{d_{ij}} \tag{E.1}
\]

where \( \xi \) is the range of the repulsive force, \( c_{ij} \) a scaling factor that has the dimension of a force, \( \epsilon \) the stiffness parameter, \( G_i G_j \) the vector connecting the two centers of mass, \( d_{ij} \) the distance between the particles and \( r_i, r_j \) the position vectors of the particles.

This definition of the repulsive force as in eq. E.1 entails the following four properties:  
1. The repulsive force acts parallel to the vector connecting the two centers of mass \( G_i G_j \).  
2. The repulsive force is zero at large distances \( (d_{ij} \geq r_i + r_j + \xi) \).  
3. Upon contact the repulsive force takes on a finite value given by \( c_{ij}/\epsilon \).  
4. In the intermediate regime, the repulsive force decays rapidly with distance as illustrated in...
Fig. E-1.

The range of the repulsive force $\xi$ is set to $2\Delta x$ where $\Delta x$ is the spatial grid size. Since the collisions are driven by gravity, $c_{ij} = \pi r_i^2 \Delta \rho g$ (2D) and $c_{ij} = 4/3 \pi r_i^3 \Delta \rho g$ (3D), where $\Delta \rho$ is the density difference between the particle and the fluid. Finally, $\epsilon$ captures the mode of the collision. In the limit of collisions in viscous systems, $\epsilon$ is typically set to $\Delta x^2$. We find that this choice of parameter leads to rebound at $St < 5$ and thus correct it down slightly to avoid spurious rebounds.
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247


251


253


257


259


265


