Numerical Study of Fully Nonlinear Water Waves in Three Dimensions

by

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Abstract

Steep, even overturning, three-dimensional waves are ubiquitous in the ocean environment. The understanding and modelling of such waves and their interactions are fundamental to free-surface hydrodynamics and to ocean engineering applications. Due to the complexity of the problem, reliable three-dimensional data are still rare. In this thesis, we extend and generalize the mixed-Eulerian-Lagrangian (MEL) approach of Longuet-Higgins & Crokelet (1976) to full three dimensions. Key to the success of this extension includes our development of (i) a highly efficient and robust high-order boundary-element method based on bi-quadratic isoparametric curvilinear elements; (ii) an effective adaptive quadrature scheme for influence integrals over curvilinear elements; and (iii) solution of the resulting linear equations using a powerful iteration scheme based on GMRES with SSOR preconditioning. Extensive convergence tests are performed for fully-nonlinear problems in three dimensions including those with free surface-body contact lines to validate the accuracy (which is quadratic in the number of unknowns) and efficacy of the method.

One of the main focus of our investigation is the kinematics of three-dimensional plunging breaking waves. To generate such waves, we begin with a plane progressive Stokes wave (wavelength $L$) and apply a three-dimensional surface pressure (transverse wavelength $W$) to raise its energy beyond the maximum for a steady Stokes wave. It is found that the resulting kinematics differ qualitatively depending on the value of $W/L$. For $W/L > \sim 1$, a plunging breaker develops along the center where the initial forcing is maximum, while for sufficiently small $W/L (< \sim 1)$, the resulting plunging wave eventually develops, due to energy focussing, in the region where the applied pressure is minimum. Corresponding to these, the ratio of the maximum transverse to longitudinal velocities is found to depend approximately linearly on $L/W$ (for $W/L \sim 5$), which is a measure of the three dimensionality of the overturning wave. Despite these differences, the partition of kinetic and potential energies of the wave is found to differ insignificantly for differing values of $W/L$ even as a function of time. One of the advantages of the present direct simulation is that entire fields of quantities of interest such as velocity and acceleration can be obtained.

Extensions to include finite water depth and boundary walls are included in the present work. With further developments to model also the presence of a body, the ultimate capability for the simulation of general three-dimensional fully-nonlinear wave-body interactions can be anticipated.

Thesis Supervisor: Dick K.P. Yue
Title: Associate Professor of Ocean Engineering
To my parents and
in memory of my grandmother
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Chapter 1

Introduction

One of the most important and difficult wave phenomena to analyze is that of breaking waves in three dimensions. Wave overturning plays an important role in the process of transfer of horizontal momentum to surface currents and energy dissipation in surface waves. It is also one of the major causes of turbulent flows near the ocean surface. From an ocean engineering point of view, breaking waves induce large hydrodynamic loads on offshore structures and cause a floating body to undergo large amplitude motions. The kinematics of breaking waves is of fundamental importance for the design and safe operation of ships and offshore structures. For example, Norway alone lost 41 fishing or cargo vessels due to environmental loads in rough seas during 1970 to 1977 (Vinje & Brevig, 1980). So far, to the best of our knowledge, breaking waves have been successfully computed only in two dimensions. The kinematics of a truly three-dimensional breaking wave is among the least understood wave phenomena. Because of the dangerous environment, field measurements are usually difficult, whereas wave tank measurements are subject to surface tension and scale effects. The difficulty of a mathematical modeling of breaking waves is due to the large steepness and accelerations near wave-breaking. Weakly nonlinear theories based on perturbations are not applicable because the free surface is multi-valued during overturning.

In the corresponding two-dimensional case, the fully nonlinear wave dynamics has enjoyed remarkable progress since the introduction of the mixed Eulerian-Lagrangian
(MEL) method (Longuet-Higgins & Cokelet, 1976). In the MEL method, the free surface is represented by a set of pre-selected Lagrangian fluid points. At a fixed time moment, the Laplace problem in an Eulerian form is solved and the velocity on the free surface is computed. The free-surface geometry and the Lagrangian potential are updated by integrating the free-surface boundary conditions. The time stepping procedure is then repeated. Important extensions of the MEL approach include (1) breaking waves in finite uniform water depth (Cokelet, 1977) and, the Cauchy integral formulation (Vinje & Brevig, 1980); (2) incorporation of a surface-piercing cylinder in beam seas (Vinje & Brevig, 1981); (3) the treatment of the singularity at the intersection point of the free surface and a body and, implementations of a linear matching boundary for axisymmetric flows (Lin, Newman & Yue, 1984). The first rigorous comparison between the computational results and the experimental data of breaking waves was presented by Dommermuth, Yue, Lin, Rapp, Chan & Melville (1988). The satisfactory agreement with the experimental data establishes the computation method based on the MEL method as a very useful tool for analyzing two-dimensional steep waves. Dommermuth & Yue (1987a) further extended the MEL method to study nonlinear axisymmetric wave-body interaction problems, such as the forced heaving of a floating vertical cylinder or an inverted vertical cone. However, their premise of axisymmetric flows excluded the possibility of bifurcations from the radiating nonlinear ring waves to three-dimensional waves. In an experiment of forced heave oscillations of a sphere, Tatsuno, Inoue & Okabe (1969) observed that the resulting axisymmetric ring waves became three-dimensional circumferential standing waves if the amplitude of the oscillations is increased gradually at a fixed frequency. Even though the phenomenon observed was largely for small scale motions (the largest sphere used in the experiment was 6 cm in diameter) where surface-tension may be dominate, the possibility of three-dimensional bifurcations of a nonlinear gravity ring wave may not be ruled out.

In their simulations of surface and interfacial waves, Baker, Meiron & Orszag (1982) put forward a generalized vortex method (GVM). A dipole distribution with
density $\mu$ was used to represent the interface. By using integration by parts, the complex velocity on the interface can be expressed in the form of the Biot-Savart integral in terms of the equivalent vortex distribution on the interface with its density $\gamma$ equal to the tangential derivative of the dipole density. Substituting the expression into the Bernoulli's equations at both sides of the interface, they obtained an evolution equation for $\mu$ or $\gamma$, which is an integral equation of the second kind. This formulation is similar to a Cauchy integral formulation. It was then shown that the resulting integral equation has a globally convergent Neumann series and, can be efficiently solved by iteration without matrix-inversion. With $N$ being the total number of unknowns of the problem, this method only requires $O(N)$ computer storage and $O(N^2)$ arithmetic operations per time step. The GVM takes advantage of the complex formulation in two dimensions and avoids integrating the second normal derivative of the Green function along the boundary. In three dimensions, it is well known that the free surface can still be represented by a dipole sheet with the dipole density to be determined as the solution of a Fredholm integral equation of the second kind. It is also known that this kind of integral equation can be effectively solved through iterations. However, in computing the velocity components on the free surface, which are the physical quantities of interest in most cases, one must differentiate the expression of dipole potential once, which leads to a difficult boundary integral with a hyper-singular kernel. The evaluation of the velocity at $N$ nodes on the free surface requires $N^2$ calculations of this type of boundary integral. Unlike the two-dimensional case, it is not clear how this boundary integral can be avoided in three dimensions. Even though the induced velocity field due to dipoles may be expressed in terms of an equivalent vorticity distribution and an edge vortex (Hess, 1972), the vorticity distribution is not suitable for the representation of Dirichlet boundaries. Therefore, the extension of the generalized vortex method to three dimensions is not straightforward.

A more general vortex sheet formulation valid for three dimensions was discussed by West, Brueckner & Janda (1987), which requires the evaluation of the three-
dimensional stream function. Thus, it is not suitable for study of three-dimensional free-surface flows. A general discussion of modifying a first-kind integral equation into a second kind integral equation was given by Burton & Miller (1971). For more literature reviews on the two-dimensional nonlinear wave computations, see Cokelet (1977) and Romate (1989).

In comparison with the broad literature available for the two-dimensional breaking wave computations, there are only a few reports considering the solution of the fully nonlinear wave equations in three dimensions. Meiron, Saffman & Yuen (1982) presented results for steady symmetric wave patterns calculated from the exact three-dimensional wave equations. Their results at wave steepness \( ka = 0.2 \) is essentially the superposition of the co-propagating three dimensional disturbances on the plane progressive Stokes wave, which leads to finite amplitude three-dimensional waves. This case was predicted by the theoretical results of Mclean, Ma, Martin, Saffman & Yuen (1981), and was confirmed by the experimental observations reported by Su (1982). Isaacson (1982) used the constant-strength panel method (CPM) to study nonlinear wave forces on a floating body.

Romate (1989, 1990) carried out a systematic investigation on the numerical simulation of nonlinear water waves in three dimensions. He used direct Green's integral formulation for the Laplace problem and a time marching procedure similar to the MEL approach. For the solution of the integral equation at each time step, Romate used a second-order panel method which is very similar to the formulation derived by Hess (1979) for unbounded potential flows in three dimensions. To save computing time, he used the Runge-Kutta (RK) fourth order integrator with a so called frozen geometry per time step, wherein the influence matrix was updated only once each time step and was used for all intermediate stages of the RK scheme. Without assessing the accuracy or stability of this hybrid RK scheme, the simulation was continued using numerical stability criterion derived for the original Runge-Kutta fourth order formula. The simulation of a two-dimensional Stokes wave \((ka \approx 0.26)\) broke down before one wave period. Romate reported that there were rapidly growing short waves
on the primary Stokes wave which caused the numerical break down. These short waves are more likely the saw-tooth type of instabilities rather than his conjecture of cross-waves. Romate (1989) has also studied waves over a bottom topography using his three-dimensional formulation. Unfortunately, the simulation also broke down when the wave steepened.

In the recently finished dissertation by Ölmez (1991), an Eulerian formulation was used to describe double-periodic free-surface flows. The boundary integral equation \( (BIE) \) of the Laplace problem was successfully solved by the constant-strength panel method. After evaluating the vertical component of velocity at each collocation point, the fourth order predictor-corrector formula started with RK fourth order scheme (Longuet-Higgins & Cokelet, 1976) was used to update the vertical position of the collocation point and, the new free-surface position is reconstructed by a bi-cubic spline fit on the double-periodic domain. For a plane Stokes wave simulation of one wave period, the agreement with the results obtained by high order Stokes series was satisfactory up to wave steepness \( ka = 0.3 \), beyond that the discrepancy increases noticeably. Using this scheme, Ölmez was able to evaluate the wave-energy transfer rates for an interacting quartet of \( ka = 0.1 \), which were in good agreement with that of the spectral method (Liu & Yue, 1991). However, the Eulerian formulation is not suitable for the study of breaking waves because it requires that the free surface be single-valued.

The recently developed high order spectral method (Dommermuth & Yue, 1987b; West, Brueckner & Janda, 1987) incorporating the Fast Fourier Transform (FFT) technique has been shown to be very efficient for studying the long-time evolution of periodic nonlinear waves in three dimensions. The spectral method is, however, based on the assumption of weak nonlinearities. The exponential convergence of the perturbation series stalls quickly beyond \( ka = 0.35 \). This gives the practical limitation of the spectral method.

The objective of this dissertation is to study the kinematics of highly nonlinear gravity water waves including overturning in full three-dimensional space. In order
to study breaking waves, the mixed Eulerian-Lagrangian idea is adopted. It is not conceptually difficult to generalize the MEL description of free surface flows to three dimensions. However, to implement the time-domain numerical scheme for three-dimensional fully nonlinear waves, one must confront a long list of practical problems. On the top of this list is the development of an efficient and accurate solution scheme of the Laplace boundary value problem in an arbitrary three-dimensional domain. The accuracy requirement is due to the fact that the solution at one time step will be used to update both the boundary geometry and boundary conditions for the next time step. In view of the complexity of the problem, an analytic solution is out of the question. Generally speaking, a volume discretization method requires much more computer storage than a boundary-integral-equation method (BIEM), thus, the volume discretization method is not very promising for high resolution three-dimensional computations. Assuming a BIE formulation is used for the Laplace problem, will CPM be a good choice for the numerical solution? Based on our preliminary study, we estimate that even for the pure Dirichlet problem of simulations of double-periodic surface waves with a one wavelength by one wavelength domain, CPM requires $O(10^2)$ panels in each direction and a total of $O(10^4)$ or more unknowns to yield an acceptable accuracy for $ka \geq 0.4$. For most time domain studies, the calculation of a dense matrix of this size and its solution at each time level will result in prohibitive computation time and computer storage. More importantly, we found that the error of CPM near the intersection lines of Dirichlet and Neumann boundaries does not even converge (see Section 3.3). For these reasons, it is concluded that CPM is not suitable for studies of three-dimensional mixed Dirichlet/Neumann problems.

The success of this work critically depends upon the development of an accurate and robust computational methods for quantitative simulations of the fully nonlinear free surface flows. For the large scale time-domain study, the solution scheme must also be efficient in terms of implementations. After extensive testing and comparisons, we select and extend a high-order boundary element method (BEM) based on bi-quadratic isoparametric curvilinear elements. The singular integrals over a curved
surface domain are regularized by using the triangular polar-coordinate transformation in the parametric space (Li, Han & Mang, 1985). The isoparametric elements have been most extensively used in the stress analysis of elastic and elastic-plastic solids (see, for instance, Lachat & Watson 1976). Recent examples of its application in frequency-domain potential flow computations may be found in Liu & Lu (1988) and Chau (1989). Liu and Lu used the ordinary polar coordinate transformation to reduce the order of singularities, whereas Chau used the triangular polar-coordinate transformation. In terms of numerical convergence, we found that the two transformations are equally effective. In the works of Liu & Lu and Chau, numerical integrations are evaluated until the results of two successive Gauss quadratures agree with each other within a tolerance. This kind of check may not necessarily insure convergence since the high-order derivatives of the integrands of the boundary integrals may not be smooth enough. Moreover, this type of iterative quadrature requires excessive computation time and is very difficult to vectorize. In this study, we establish the convergence by comparing results with the Romberg scheme and by checking the convergence of the solution of the boundary value problem. An efficient adaptive quadrature scheme has been developed for the elemental integrals which uses a set of three parameters to determine the order of Gauss integrations for a given tolerance. For far field collocation points, effective series expansions can be used to avoid numerical integrations.

The system of linear equations arising from discretizing the BIEs has a full nonsymmetric matrix. Because large number of unknowns are usually required for three-dimensional problems, a direct inversion of the matrix ($O(N^3)$ effort) is impractical. The leading iterative methods for nonsymmetric matrices include GMRES (residual minimization in a Krylov space), CGNR (the conjugate gradient iteration applied to the normal equation) and CGS (a biorthogonalization algorithm adapted from the biconjugate gradient iteration). Nachtigal, Reddy and Trefethen (1990) presented various convergence results of applying these three iterative methods to a set of constructed nonsymmetric matrices. In the present work, we found that the matrix
arising from the mixed BIEs is quite amenable to the GMRES iterative scheme (Saad & Schultz, 1986) and, the iterations can be accelerated by using a symmetric successive overrelaxation (SSOR) preconditioner (Nachtigal & Trefethen, 1990, private communication).

In addition to accuracy and efficiency, the treatment of the weak singularities at the intersection lines of a free surface (Dirichlet boundary) and a wall (Neumann boundary) is also considered. In two dimensions, with a complex potential formulation, Lin (1984) successfully resolved the difficulty by specifying the complex potential at the intersection point. This approach was extended to handle the intersection line in the axisymmetric flows by Dommermuth & Yue (1987a). In our two-dimensional case study, we found that the velocity components at the intersection lines can be accurately calculated by a finite difference formula. In three dimensions, the velocity at the intersection lines can be computed either by the isoparametric finite difference scheme (PFD) (see Section 4.8) using the solved potential on the adjacent Neumann boundary or by directly using the solved normal derivative of potential on the free surface. At a given time step, the results from the two computations agree with each other quite well.

The present extensive convergence studies demonstrate that for Kellogg-regular surfaces (Kellogg, 1929), both the maximum and arithmetic average error of our quadratic BEM (QBEM) exhibit quadratic convergence with the number of unknowns, whereas the convergence of CPM is linear. If boundary surface at Dirichlet/Neumann intersection line is only $C^0$-continuous where the normal derivative of the potential is discontinuous, the quadratic convergence of the QBEM is preserved with minor degradation at the intersections, while the maximum error due to CPM diverges. With further complications such as irregular grids and extrapolations, Ölmmez (1991) showed that the error at the intersection can be reduced provided the wave does not break.

In order to advance Lagrangian points, the accuracy of the solved velocity field becomes crucial. For computations of the velocity components on the highly distorted
three-dimensional free surface during overturning, a simple parametric finite difference scheme is devised. The derivatives of all geometric and physical variables are expressed in terms of their derivatives in the parametric space, which is then evaluated by a finite difference formula. This scheme is equivalent to a high order polynomial fit centered at each nodal point on the boundary. Thus, it is more accurate and efficient in comparison with the bi-cubic spline based method, which corresponds to the third order polynomial fit.

For the time integration of the nonlinear free-surface conditions, the fourth order Adams-Bashforth-Moulton integrator is used with the fourth order Runge-Kutta scheme as the starting procedure (Longuet-Higgins & Cokelet, 1976). Following Chan (1975), the size of time step is dynamically selected such that no Lagrangian particle moves more than a fraction of the minimum distance between any two adjacent fluid points.

Because the nonlinear wave equations being solved is non-dissipative, the evaluated free surface in three dimensions eventually will suffer from high wave-number instabilities as have been experienced by almost all two-dimensional simulations of steep waves. To remove the instabilities, Longuet-Higgins & Cokelet (1976) used a Chebyshev smoothing formula (Hamming, 1973). Dommermuth & Yue (1987a, 1988) argued that the cause of the high wave-number instabilities is the concentration of Lagrangian particles in the regions of high curvatures. To reduce the highest wave number, they adopted a regriidding algorithm similar to that used by Fink & Soh (1974). Nevertheless, they found that the smoothing is still necessary after regriidding. Taking advantages of the double-periodic problem and equally spaced control points in the Eulerian formulation, Ölmez (1991) incorporated FFT technique to filter out the high wave-number instabilities. This technique, however, is not applicable in the present study because the Lagrangian points are not necessarily equal-spaced. Based on our test computations, we found that a simple alternating-direction application of the Chebyshev smoothing formula will effectively remove the high wave-number instabilities.
Numerical simulations using the present method on a double periodic, steady Stokes wave of finite amplitude up to several wave periods show excellent agreement with the semi-analytic solutions calculated from Stokes series. The method is then applied to study the unsteady uni-directional progressive waves after applying an initial surface pressure. The results from the present study agree well with the two-dimensional results reported by (Longuet-Higgins & Cokelet, 1976). Subsequently, we select a progressive Stokes wave train and applied a initial three-dimensional surface forcing to raise its local energy density beyond the maximum for a steady Stokes wave. The transverse variation of the surface forcing is a cosine function. The magnitude of the three-dimensional forcing is selected such that at the center of the domain, the corresponding two- and three-dimensional forcing have the same local distribution for the convenience of comparison. After the initial surface forcing is removed at dimensionless time \( t = \pi \), the waves propagate freely. In the corresponding runs using two- or three-dimensional surface forcing, all controlling criteria and smoothing procedures are kept the same. The resulting unsteady wave develops into an overturning wave. By varying the wavelength of the transverse modulation of the surface forcing, some unique features of the breaking waves in three dimensions has been found.

One advantage of the present method is that the entire surface distributions of velocity and acceleration of breaking waves in both two and three dimensions can be computed. It has been found that in both two and three dimensions, the evaluated velocities develop small oscillations during the overturning process. When the normal acceleration of a Lagrangian particle exceeds the gravitational acceleration in a direction into the water, Taylor instability often causes simulations to break down. In Chapter 5, extensive numerical results before the onset of Taylor instability are presented for periodic breaking waves in deep water with extensions to the finite water depth. Further extension to computations of fully nonlinear waves inside a general three-dimensional wave tank is presented in Chapter 6. Future improvements and applications of the method are discussed in Chapter 7.
Chapter 2

Mathematical Formulations

In this chapter, we outline the underlying assumptions, basic equations and boundary conditions for the evolution of fully nonlinear gravity water waves including overturning in three dimensions. The initial-boundary value problem is formulated for the general problem of fully nonlinear free-surface flows with arbitrary bottom topography without the restriction of a single-valued free surface. For the numerical solution of the breaking wave problem, the computational domain must be finite. Thus, an open boundary condition should be invoked at the artificial closure to allow waves to pass through. All existing techniques on the open boundary condition are for two-dimensional or axisymmetric problems (e.g. Baker et al, 1982, Lin et al, 1984). In three dimensions, further research on this issue is necessary. Since our prime interest in this dissertation is the kinematics of breaking waves in three dimensions, we focus on two classes of wave problem: waves with spatial periodicity and waves inside a general wave tank. For the solution of the IBVP, the mixed Eulerian-Lagrangian method (Longuet-Higgins & Cokelet, 1976) is generalized to three dimensions. The three-dimensional Laplace problem at each time step is solved by a BIE formulation. For completeness, the important facts of the boundary integral-equation reformulation are listed in Section 2.2. The solution procedure of the problem is also selected. For the numerical solution of the resulting integral equations, a weighted residual consideration is given in Section 2.3.
2.1 The initial-boundary value problem

Consider an inviscid and incompressible free-surface flow starting from rest in three dimensions. Assuming the motion is subject to conservative forces only, from Kelvin's theorem the motion is irrotational for all subsequent times. We choose an orthogonal reference frame fixed on the earth with its origin at the undisturbed water level, \( z \) and \( y \) being the two horizontal directions, and \( z \) the vertical direction, positive upward. All variables are nondimensionalized such that the density of water \( \rho \) and acceleration due to gravity \( g \) are both unity. In general, the motion is time dependent. The flow can be described by a harmonic function (velocity potential) \( \phi(\mathbf{x}, t) \), with \( \mathbf{x} \) being the spatial position.

Assume \( D \) is a simply-connected fluid domain, not necessarily bounded, and \( \phi \in C^2(D) \). The governing equation of the flow is the Laplace equation, viz.

\[
\nabla^2 \phi(\mathbf{x}, t) = 0, \quad \mathbf{x} \in D,
\]

with \( D \subset \mathbb{R}^3 \). The boundary of \( D \), define it as \( S \), is assumed to be a Liapunov surface\(^1\) (Günter, 1967). Hence, from the harmonic function theory, it is possible to determine \( \phi \) throughout \( D \) in terms of suitably prescribed boundary data on \( S \). For the problems concerned in this study, we assume that

\[
S = S_D \cup S_N,
\]

where a Dirichlet boundary condition is prescribed on \( S_D \) and a Neumann boundary condition is posed on \( S_N \).

On the free surface \( S_f \subset S_D \), Bernoulli's equation gives the dynamic boundary condition, viz.

\[
\frac{D\phi}{Dt} = \frac{1}{2} |\nabla \phi|^2 - z - p_f, \quad \mathbf{x} \in S_f,
\]

---

\(^1\)Roughly speaking a Liapunov surface is a smooth surface possessing a unique tangent plane and normal, but not necessarily a curvature, at each point. It is less general than a Kellogg regular surface (Kellogg, 1929).
where \( D/Dt = \partial/\partial t + \nabla \phi \cdot \nabla \) is the material differentiation following a Lagrangian particle, and \( p_f \) is the surface pressure distribution. The kinematic boundary condition is
\[
\frac{D \mathbf{x}}{D t} = \nabla \phi, \quad \mathbf{x} \in S_f. \tag{2.4}
\]
This vector equation gives the kinematical evolution equation for the free surface profile.

On the other physical boundary surfaces (\( \subset S_N \)), the normal velocity of the flow and that of the surfaces must also be the same, viz.
\[
\phi_n(\mathbf{x}, t) = U(\mathbf{x}, t), \quad U \in C^0(S_N), \tag{2.5}
\]
where \( \phi_n = \nabla \phi \cdot \mathbf{n} \) and \( U = \mathbf{U} \cdot \mathbf{n} \). \( \mathbf{U} \) is the velocity of the surface. The positive direction of a normal vector \( \mathbf{n} \) on the boundary surfaces is defined pointing out of the fluid domain. Hereafter, the subscript \( n \) denotes the normal derivative, unless otherwise stated. On a fixed physical boundary such as a bottom or a wall, function \( U \) vanishes. On a moving boundary such as a wave maker, function \( U \) is prescribed. If a floating body is present, the problem will be more involved since the function \( U \) must be determined as part of the solution.

Other auxiliary conditions may be also needed to ensure the existence and uniqueness of the solution of the free-surface flow problem. For instance, if infinitely deep water is considered, a far field condition must be imposed to ensure the solution to the problem is regular, viz.
\[
\phi(\mathbf{x}) = \mathcal{O}(|\mathbf{x}|^{-1}), \tag{2.6}
\]
\[
\nabla \phi(\mathbf{x}) = \mathcal{O}(|\mathbf{x}|^{-2}), \tag{2.7}
\]
as \( |\mathbf{x}| \to \infty \), for all times.

By virtue of mass conservation, the boundary values of \( \phi_n \) must satisfy the com-
patibility (Gauss) condition

$$\int\int_{S} \phi_n(\omega, t) dS = 0.$$  \hspace{1cm} (2.8)

For the mixed Dirichlet/Neumann problem, equation (2.8) provides a check on the accuracy of the solution. For a periodic Dirichlet problem, where the Green function does not satisfy the far field conditions (2.6) and (2.7), this integral equation gives a necessary constraint for the solution.

The corresponding initial conditions may be written as

$$\phi(\omega, 0) = f_0(\omega), \quad \omega \in S_D, \quad f_0 \in C^0(S_D),$$  \hspace{1cm} (2.9)

$$\phi_n(\omega, 0) = g_0(\omega), \quad \omega \in S_N, \quad g_0 \in C^0(S_N),$$  \hspace{1cm} (2.10)

with $f_0$ and $g_0$ given. As part of the initial conditions, the initial geometry of the free surface must also be specified.

To simulate the three dimensional free surface flows in the time domain, we adopt the MEL approach (Longuet-Higgins & Crokelet, 1976) to update the free surface positions. After all velocity components on $S$ are accurately evaluated, (2.4) may be integrated to give the new geometry of the free surface at time $t + \Delta t$ and, (2.3) may be integrated for the new potential value $\phi(\omega, t + \Delta t)$ on $S_f(t + \Delta t)$. Then, the entire process can be repeated. Two key issues in the process are the accurate solution of the Laplace problem and the evaluation of $\nabla \phi$, which will be addressed subsequently in Chapter 4.

Once the initial conditions are given, the Laplace boundary value problem can be solved for $\phi_n$ over $S_D$ and for $\phi$ over $S_N$. The fundamental existence and uniqueness theorems corresponding to different types of problems in potential theory have been well-established (see, for instance, Kellogg, 1929, Courant & Hilbert, 1962, and Jaswon & Symm, 1977). For the mixed Dirichlet/Neumann problems, the existence and uniqueness of the solution for given continuous boundary data has been proven by Tsuji (1959).
2.2 Boundary integral equation reformulation

The most time consuming step in a MEL approach of the initial-boundary value problem is the solution of the Laplace problem at each time step, which can be transformed into boundary integral equations (BIE). In this section, we shall summarize the relevant facts of the BIE formulation. To proceed, it is convenient to introduce the free-space Green function

\[ G(\mathbf{x}, \mathbf{\xi}) = \frac{1}{r} = \frac{1}{|\mathbf{x} - \mathbf{\xi}|}, \quad (2.11) \]

where \( r = |\mathbf{x} - \mathbf{\xi}| = [(x - \zeta)^2 + (y - \eta)^2 + (z - \zeta)^2]^{1/2} \). Formally, \( G \) is the solution of the Poisson equation

\[ \nabla^2 G(\mathbf{x}, \mathbf{\xi}) = -4\pi \delta(\mathbf{x} - \mathbf{\xi}), \quad \mathbf{x}, \mathbf{\xi} \in D, \quad (2.12) \]

where \( \delta(\mathbf{x} - \mathbf{\xi}) \) is the Dirac delta function, which is essentially an infinite impulse at \( \mathbf{x} = \mathbf{\xi} \), and zero elsewhere. Function \( G \) is the harmonic function of \( \mathbf{x} \), except at \( \mathbf{x} = \mathbf{\xi} \). It satisfies the far field conditions (2.6) and (2.7).

The harmonic function \( \phi \) may be represented by its boundary data. From Green's second identity, we have

\[ 4\pi \phi(\mathbf{x}) + \iint_S [\phi(\mathbf{\xi})G_n(\mathbf{x}, \mathbf{\xi}) - \phi_n(\mathbf{\xi})G(\mathbf{x}, \mathbf{\xi})] dS(\mathbf{\xi}) = 0. \quad (2.13) \]

where the finite part of an integral (Hadamard 1923) is assumed if the kernel is singular. This convention will be used hereafter in this dissertation. The direction of \( n \) is the outward normal at \( \mathbf{\xi} \). Equation (2.13) represents the harmonic function \( \phi \) as the superposition of a source and a dipole distribution over \( S \). This equation provides the fundamental link between harmonic function theory and potential theory.

Taking the limit \( \mathbf{x} \to S \), (2.13) provides a compatibility constraint for \( \phi \) and \( \phi_n \) over \( S \). More importantly, it gives the boundary integral equation reformulation for the Laplace boundary value problem in the last section. In particular, for \( \mathbf{x} \in S_D \),
we have

\[
\iint_{S_N} \phi(\xi)G_n(\omega, \xi) dS(\xi) - \iint_{S_D} \phi_n(\xi)G(\omega, \xi) dS(\xi) = \\
-\alpha(\omega)\phi(\omega) - \iint_{S_D} \phi(\xi)G_n(\omega, \xi) dS(\xi) + \iint_{S_N} \phi_n(\xi)G(\omega, \xi) dS(\xi)
\]

(2.14)

and for \( \omega \in S_N \),

\[
\alpha(\omega)\phi(\omega) + \iint_{S_N} \phi(\xi)G_n(\omega, \xi) dS(\xi) - \iint_{S_D} \phi_n(\xi)G(\omega, \xi) dS(\xi) = \\
-\iint_{S_D} \phi(\xi)G_n(\omega, \xi) dS(\xi) + \iint_{S_N} \phi_n(\xi)G(\omega, \xi) dS(\xi),
\]

(2.15)

where \( \alpha(\omega) \) is the interior solid angle at \( \omega \in S \). If \( S \) has a unique tangent plane at \( \xi, \alpha = 2\pi \). Equation (2.14) is a Fredholm integral equation of the first kind, coupled with equation (2.15), a Fredholm integral equation of the second kind. The kernel functions \( G \) and \( G_n \) are weakly singular at \( \omega = \xi \). It can be shown that the order of both singularities over a \( C^2 \)-continuous surface is \( O(r^{-1}) \) (see Appendix A for the proof). Therefore, both \( G \) and \( G_n \) are integrable. In both equations above, the time dependence is implicit.

Instead of solving the Laplace equation in \( D \), we seek solutions of the integral equation (2.14) and (2.15), which are subject to the boundary conditions defined in the last section. The advantages of working with the boundary integral equations are twofold. First, the BIE formulation directly solves for the boundary values of \( \phi \) (on \( S_N \)) and \( \phi_n \) (on \( S_D \)), which are precisely what are of prime interest. Thus, the BIE formulation is more efficient than solving the Laplace equation in \( D \subset \mathcal{R}^3 \). Secondly, while the restriction to Liapunov surfaces is necessary for formulation of the Laplace problem via potential theory, it may be relaxed to the more general Kellogg regular surfaces by directly utilizing the BIEs, which are based on the theory of harmonic functions (Jaswon & Symm, 1977). Indeed, in the discretized form of integral equations (2.14) and (2.15), the boundary surfaces are approximated by a set of smooth surface elements. The relaxed restriction allows edges or corners to be
included. Of course, sharp edges or cusps must be avoided or the solution may not be unique, as pointed out by Lebesgue (1913) and Jaswon & Symm (1977) (If an object with sharp edge such as a hydrofoil is involved, the Kutta-Joukowski condition must be imposed).

By definition, the interior solid angle $\alpha$ is equal to the area of the projection of $S$ onto a unit sphere centered at $\varpi$, and the evaluation of $\alpha$ in (2.14) and (2.15) is in general cumbersome. However, it can be simplified by using the physical argument that a uniform potential applied over a closed body produces no flux (Brebbia, Telles & Wrobel, 1984). This argument is applicable even if the region $D$ is unbounded, wherein a far field closure is included. Considering a constant potential $\phi = c$ in (2.14) and (2.15), we have

$$\alpha(\varpi) = -\iint_S G_n(\varpi, \xi)dS(\xi). \quad (2.16)$$

Physically, this equation reflects mass conservation in the region enclosed by $S$ and a unit sphere centered at $\varpi$. This relation will be used throughout this study for evaluating $\alpha$. As we shall see, the surface integral in (2.16) can be obtained directly from the influence coefficients without additional work.

Finally, if values of $\phi$ or its derivatives in $D$ are of interest, (2.13) may be used for the evaluation. For the acceleration field on the free surface, we may directly differentiate (2.4) with respect to time, although it is more economical to apply a finite difference scheme to the time history of velocities of each Lagrangian point as seen in Chapter 5.
2.3 Method of weighted residuals

Consider solving a boundary integral equation denoted by

\[ \mathcal{L}\Psi - f = 0, \quad (2.17) \]

where \( \mathcal{L} \) is an integral operator. The exact solution \( \Psi \) may be approximated by a set of linearly independent, complete sequence of functions \( N_j(\varpi) \) such that

\[ \Psi \approx \psi = \sum_{j=1}^{n} \beta_j N_j, \quad (2.18) \]

where \( \beta_j \) are the unknown coefficients which may be determined by minimizing the residual of the approximation with respect to a set of weighting functions \( w_j(\varpi) \), viz.

\[ \iint_S R w_j dS = \iint_S [\mathcal{L}\psi - f] w_j dS = 0, \quad j = 1, 2, ..., n, \quad (2.19) \]

which gives \( n \) equations for \( \beta_j \), subject to boundary conditions. The method of weighted residuals can also be applied to partial differential operators to derive BIEs. In particular, the BIEs in the last section may also be obtained via a weighted residual formulation for the Dirichlet/Neumann problem using the Green function (2.11) as the weighting function (Brebbia, Telles & Wrobel, 1984).

Based on the weighted residual consideration, the numerical solution schemes for the three-dimensional BIEs can be roughly classified into two categories: Galerkin or collocation methods, which correspond to \( w_j(\varpi) = N_j(\varpi) \) or \( w_j(\varpi) = \delta(\varpi - \xi) \), respectively. With different choices of interpolation functions \( N_j(\varpi) \), a numerical method is called a global method, if \( N_j(\varpi) \) are globally defined smooth functions over \( S \); or a local method, if \( N_j(\varpi) \) are piecewise smooth on subregions of \( S \). The boundary element methods\(^2\) (BEM) usually refer to the collocation method with

\(^2\)The BEM formulation which directly solve for \( \phi \) or \( \phi_n \) is called the direct BEM; if source or dipole distributions are used in the formulation, the BEM which solves for the strength of singularities is called the indirect BEM.
piecewise smooth approximations. Obviously, the piecewise smooth approximating functions offer much more flexibility in handling various boundary surface $S$ and boundary conditions than the globally defined ones. Therefore, we choose the direct boundary element method for the numerical solutions of the integral equation (2.14) and (2.15).

Suppose that the boundary surface $S_D$ and $S_N$ are divided into two sets of piecewise smooth elements

$$S_D = \bigcup_{j=1}^{N^1_e} E_j$$  \hspace{1cm} (2.20)

and

$$S_N = \bigcup_{j=1}^{N^2_e} E_j$$ \hspace{1cm} (2.21)

where $E_j$ is a generic element and $N_e = N^1_e + N^2_e$ is the total number of elements. The discretized BIEs can then be written as

$$\sum_{j=1}^{N^2_e} I_d - \sum_{j=1}^{N^1_e} I_s = -\alpha(\varpi)\phi(\varpi) - \sum_{j=1}^{N^1_e} I_d + \sum_{j=1}^{N^2_e} I_s, \hspace{1cm} \varpi \in S_D,$$  \hspace{1cm} (2.22)

and

$$\alpha(\varpi)\phi(\varpi) + \sum_{j=1}^{N^2_e} I_d - \sum_{j=1}^{N^1_e} I_s = \sum_{j=1}^{N^2_e} I_s - \sum_{j=1}^{N^1_e} I_d, \hspace{1cm} \varpi \in S_N,$$ \hspace{1cm} (2.23)

where the elemental integrals are defined by

$$I_s = \iint_{E_j} \phi_n(\xi)G(\varpi, \xi)dS(\xi)$$ \hspace{1cm} (2.24)

and

$$I_d = \iint_{E_j} \phi(\xi)G_n(\varpi, \xi)dS(\xi).$$ \hspace{1cm} (2.25)

where the finite part of a singular integral is assumed if $\varpi \in E_j$. Note there is no approximation in the discretized forms of the BIEs. The type of elements and the degree of local approximating functions will be selected based on the results of feasibility studies in the next chapter.
Chapter 3

Feasibility Studies

3.1 Introduction

Ever since the pioneering works by Hess & Smith (1962), Jaswon (1963) and Symm (1963), the boundary element method\(^1\) has been firmly established as an indispensable method for analyses of potential problems. The BEM with point collocations has been preferred by many analysts in solving three-dimensional potential problems. In spite of this, most of the mathematical analyses on BEM are devoted to the Galerkin methods with smooth boundaries. Much less is known about the convergence properties of the collocation methods with piecewise smooth approximations. The few existing theoretical analyses of collocation methods are for the second kind integral equation over a smooth boundary (Wendland, 1985). Another analysis of the collocation method with piecewise quadratic triangular elements was given by Atkinson (1985). No analysis about the collocation method for the first kind or the mixed first/second kind BIEs in three dimensions is found in our literature survey. A recent comprehensive review on the BIE methods for solving the three-dimensional Laplace equation is presented by Atkinson (1990).

\(^1\)Both boundary element method and panel method belong to the same family of local methods for BIEs. Even though the collocation locations may be chosen differently, they are essentially the same method under two different names. Hence, the two names are interchangeable.
The mixed Dirichlet/Neumann problem described in Chapter 2 can be formulated entirely as the second-kind Fredholm integral equations (Burton & Miller, 1971, Baker et al, 1982), for which there exist efficient iterative solution schemes. However, the difficulty associated with the evaluation of boundary integrals with the hyper-singular kernel overshadows the advantage of the second-kind BIE formulation. Largely because of this reason, the attempt along this line is not pursued presently.

The feasibility of high-resolution simulation of three-dimensional transient waves in time domain depends on how successful the following two key issues are addressed in the implementation: (1) the efficient iterative solution of the BIEs; (2) selection of the orders of approximation for both geometric and physical quantities in the three-dimensional wave problems. These two issues are considered in the next two sections respectively.

3.2 Iterative solutions for the mixed BIEs

For two-dimensional or axisymmetric problems with less than 1000 unknowns, the resulting linear systems are usually solved by Gauss elimination (e.g. Dommermuth & Yue, 1988). However, for the large scale computation of three-dimensional highly nonlinear waves in time domain, solving the system of linear equations with $O(10^4)$ unknowns for a few primary wave periods is anticipated. A direct inversion or inefficient iteration of such a large, dense matrix for $O(10^2)$ time steps is prohibitively time consuming even for modern supercomputers. In the closely related work carried out by Romate (1990), the Conjugate-Gradient-Squared (CGS) iterative scheme was used for solving the system of linear equations. Since there is no well-established theoretical framework for the iterative solution of the linear systems arising from solving mixed BIEs, our primary interest here is to find an iterative algorithm and a preconditioner that can effectively solve the resulting system of linear equations.

One of the most convenient ways to investigate the feasibility of iterative solution for the mixed BIEs is to use the BIE formulation to solve the Laplace problem in
a simpler two-dimensional domain. For the present purpose, we consider a two-dimensional region which is prescribed with Airy wave potential. Then, we define a two-dimensional rectangular domain with a wavy top boundary (see Figure 3-1). Strictly speaking, the linear wave potential is defined only beneath the undisturbed water surface \( z \leq 0 \). For our purpose, we analytically extend its definition to \( z > 0 \). We shall solve the Laplace problem inside the wave-tank-like domain with Dirichlet boundary condition specified on the wavy top and Neumann conditions on the rest of the boundaries. Since the linear potential is the exact solution of this ‘created’ boundary value problem and all boundary geometries are prescribed, we can analytically calculate any quantities of interest. For example, on the Dirichlet boundary we specify the exact potential on the prescribed boundary. After solving the problem, the error on the Dirichlet boundary is obtained by comparing the solution against the analytically calculated normal flux. Similarly, we obtain the error on the rest of boundaries. This test problem allows us to investigate the properties of the matrix arising from the mixed BIE formulation with any boundary geometry. For now, no time marching procedure is introduced.

The mathematical formulation of the two-dimensional problem can be easily ob-
tained by replacing the boundary surface integrals in the mixed BIE (2.14) and (2.15) with boundary line integrals. The definition of the solid angle in these two equations has to be changed to the included angle between two tangential rays starting at the collocation point :math:`x`. The two-dimensional Green function in this case is given by

\[ G(x, \xi) = \ln |x - \xi| \]

(3.1)

with \( x = (x, z) \).

For simplicity, we solve the two dimensional problem by the BEM based on linear isoparametric elements. Taking advantage of linear elements, all elemental integrals are evaluated in closed forms. The detailed formulae are listed in Appendix B.

For solution of the dense, nonsymmetric system of linear equations \( Ax = b \), we select the recently developed generalized minimum residual (GMRES) algorithm (Saad & Schultz, 1986), which minimizes the residual in the Krylov space at every iteration. Unlike the conjugate gradient method for symmetric matrices whose convergence rate can be defined in terms of the condition number of the matrix, the corresponding result for GMRES is not precisely defined. Nachtigal, Reddy and Trefethen (1990) gives three bounds which correspond to GMRES algorithm applied to a normal matrix, diagonalizable matrix and far from normal matrix, respectively. In practice, the convergence rate of GMRES is determined principally by the pseudo-eigenvalues of the matrix (Trefethen, 1990). The \( \epsilon \)-pseudo-eigenvalues of matrix \( A \) can be defined as follows: all points \( z \in C \) which are the eigenvalues of some perturbed matrix \( A + E \) with \( \|E\| \leq \epsilon \), or equivalently, all those points \( z \in C \) with \( \|(zI - A)^{-1}\| \geq \epsilon^{-1} \), where \( I \) is the identity matrix. (See Trefethen, 1990).

Numerical experiments indicate that the present linear system is quite amenable to GMRES iterations. Figure 3-2 summarizes the number of iterations required for different \( N \) for a given boundary geometry. Table3.1 shows the effects on iterations for different geometries with fixed spatial resolution. From these results, it is easy to see that for \( N < 1000 \) the number of iterations varies in proportion to \( N^{1/3} \). For
Figure 3-2: Results from the test computations for the problem defined in Figure 3-1 with $l/d = 2\pi/\pi$, $a = 0.1$ and $\kappa = 1$. GMRES algorithm applied to solve the equations (with tolerance $10^{-7}$). $N$ is the total number of unknowns. Here + and * denote the data obtained from the Green's and Cauchy integral formulations, respectively.
<table>
<thead>
<tr>
<th>$ka$</th>
<th>$N$</th>
<th>$n_{it}$</th>
<th>SD</th>
<th>$\kappa(A)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>120</td>
<td>43</td>
<td>3</td>
<td>0.1658 $10^3$</td>
</tr>
<tr>
<td>0.2</td>
<td>240</td>
<td>57</td>
<td>3</td>
<td>0.3456 $10^3$</td>
</tr>
<tr>
<td>0.4</td>
<td>480</td>
<td>72</td>
<td>2</td>
<td>0.7489 $10^3$</td>
</tr>
<tr>
<td>0.8</td>
<td>960</td>
<td>89</td>
<td>1</td>
<td>0.1448 $10^4$</td>
</tr>
<tr>
<td>1.6</td>
<td>1920</td>
<td>111</td>
<td>1</td>
<td>0.2926 $10^4$</td>
</tr>
</tbody>
</table>

Table 3.1: GMRES algorithm applied to problems with different wave steepness $ka$. The number of elements per wave length is kept at 40. $N$ is the size of the linear system, $n_{it}$ is the number of iterations when the residuals are reduced by a factor of $10^{-7}$, SD is the significant digits of the numerical solutions compared with the analytic calculations. $\kappa(A)$ is the condition number of matrix $A$, evaluated by a standard LINPACK routine ($l_1$-norm is used).

$N > 1000$, the number of iterations grows much slower. In contrast, GMRES algorithm is much more efficient for linear systems from the Cauchy integral formulation. This reflects the well-known result that the matrix of the Cauchy integral formulation, which corresponds to the second-kind BIE, is diagonally dominant and better conditioned.

The next step is to find out whether the GMRES iteration can be accelerated by introducing some preconditioning to the linear system. Generally speaking, a preconditioner $P$ is a scaling matrix which improves the conditioning of the original matrix $A$ such that the convergence of iterations for

$$P^{-1}Ax = P^{-1}b$$  \hspace{1cm} (3.2)

is faster than that of $Ax = b$. Of course, $P$ can also be applied to the right to give

$$AP^{-1}y = b$$  \hspace{1cm} (3.3)

which is to be solved for $y$, and the solution of the original system is given by $x = P^{-1}y$. Since the properties of matrix is usually problem dependent, there are few general purpose preconditioners available. (For a well-conditioned matrix such as that...
arising from a second-kind BIE, it virtually does not require any preconditioning). The “best” preconditioner is of course $A^{-1}$. The rule of thumb is to choose the matrix $P$ which is easy to construct and is a good approximation to $A^{-1}$. Vavasis (1990) has suggested a class of preconditioners for matrices arising from BIE methods. The underlying logic is quite simple: find a submatrix $\tilde{A}$ with dimension $l$ centered for each diagonal element and use all those $\tilde{A}^{-1}$ to form $P$. His examples show that the preconditioner constructed that way is quite effective for the BIE from interior Dirichlet problems.

In the present work, we tested two preconditioning matrices: diagonal preconditioner (Golub & Van Loan, 1989)

$$ P = D $$

(3.4)

and symmetric successive overrelaxation (SSOR) preconditioner (Nachtigal & Trefethen, 1990)

$$ P = (I + \omega L)D^{-1}(I + \omega U), $$

(3.5)

where $D$, $U$, $L$ denote, respectively, the diagonal, upper- and lower-triangular sub-matrix of $A$. The parameter $\omega$ ($\omega \in [0,1]$) must be chosen with some tests. When applied to the same runs as in Table 3-1 (with $\omega = 0.5$), the GMRES iterations are approximately reduced by a factor of two using diagonal preconditioner and, by a factor of five using the SSOR preconditioner, respectively. Based on these results, we choose GMRES with SSOR preconditioner as our solver for the system of linear equations.

After the exercise above, two meaningful problems are considered: (1) the uniform flow past a circle; (2) wave oscillations inside a two-dimensional wave tank for given initial conditions. For the first problem, we specify the exact velocity potential on part of the circle and solve for its normal derivative. On the rest of the circle we reverse the knowns and unknowns. For the wave oscillations, the free surface is posed as the Dirichlet boundary, the rest are Neumann boundaries. Both problems are studied using Green’s integral formulation. For the conciseness of the presentation,
we shall summarize the results for the second problem only, because it is more closely related to our extension to the three-dimensional problem.

The mixed Dirichlet/Neumann problem solver developed earlier in this section is used for the solution at each time step. The normal vector at each node on the free surface is determined using a cubic spline fit through all points on the free surface. For simplicity, the initial conditions are selected as follows

\[ \phi(x, z, 0) = 0, \quad \text{on } z = a \cos\left(\frac{x}{l}\right), \quad x \in [0, l], \]  

(3.6)

with water depth \( d = l/2 \).

Since there is no known analytical solution to the fully nonlinear wave oscillation problem, we validate our solutions against converged results obtained by the Cauchy integral formulation. For wave oscillations \((a = 0.1; 0.2)\) up to several cycles, the number of iteration (with tolerance \(10^{-7}\)) at different time step (different geometry) changes within only a few iterations. For larger initial amplitudes, the wave breaks after reflecting from the wall. Remarkabley, the GMRES iterations continue to converge until the local curvature of free surface is too large, after which the simulation is stopped because the solution becomes unreliable.
At the intersection point of a free surface and a wall, there exists a well-known logarithmic singularity (Kravtchenko, 1954 and Roberts, 1987). For the two-dimensional problem, Lin (1984) demonstrated that for the complex potential formulation, the computational difficulty associated with this weak singularity can be removed by specifying both velocity potential (from the Dirichlet condition on the free surface) and the stream function (from the Neumann boundary condition). In the present study, we enforce the continuity of the velocity potential at the intersection since it is a scalar function and, let its normal derivative on the free surface be unknown. For the dipole type boundary integrals, we introduce dual-status for the nodes at the intersection: the integral on the Dirichlet boundary contributes to the influence matrix A; for integral on the adjacent Neumann boundary contributes to the right hand side vector b. See Figure 3-3 for details.

Due to the limited accuracy of the linear isoparametric elements, the solved normal velocity at two intersection points are not as accurate as the solution on interior nodes. As a result, we found that the free surface position at the intersection can be more accurately updated using the tangential velocity calculated from a one-sided finite difference formula utilizing the solved velocity potential on the wall. We postulated that if the accuracy of the solution at the intersections may be improved, the velocity there may be computed directly from the boundary data on the free surface. This turns out is the case after a more accurate BEM is developed for the three-dimensional problems. Since our primary interest is to investigate the breaking waves in three dimensions, we did not revisit the two-dimensional problem considered in this section.

3.3 Selecting the boundary elements

One of the issues of utmost importance in BEM analysis is the selection of particular boundary elements and the appropriate approximation functions within each element. Since there is no guideline available from theoretical analyses of collocation methods applied to the mixed BIEs, the selection of elements is mostly based on empirical re-
Figure 3-4: Errors due to CPM for solving the exterior mixed Dirichlet/Neumann problem on a sphere. Solid line and * denote arithmetically averaged and maximum relative errors, respectively.

Results. Many applications with piecewise plane geometry approximation and piecewise constant singularity density (CPM) have been very successful in solving Neumann problems such as potential flow past an arbitrary body (Hess, 1964, 1972), and weakly nonlinear water wave problems (Ölmez, 1991). However, for high resolution computations, CPM often requires excessive number of elements (unknowns). For example, consider a uniform flow \( (U = 1) \) past a unit sphere. Assume the onset flow is in negative \( z \) direction. The exact solution to this problem is given by

\[ \phi = x/2, \quad \phi_n = x. \]  

(3.7)

The sphere is discretized into boundary elements by equally dividing the two spherical angular coordinates\(^2\). The fore-hemisphere in the direction of onset flow is prescribed.

\(^2\)The spherical coordinate is defined by \( z = r \cos \theta, y = r \sin \theta \cos \varphi, y = r \sin \theta \sin \varphi. \)
with exact $\phi$ and $\alpha$ is prescribed with exact $\phi_n$. It takes over 2000 elements to reduce the maximum error to half percent as seen in Figure 3-4.

To further investigate CPM's convergence rate when applied to a mixed Dirichlet-Neumann problem wherein the boundary surface at the intersection lines is only $C^0$-continuous, we consider solving a prescribed mixed problem inside a unit cube. For the convenience of checking accuracy of numerical solutions, we assume the field function is given by

$$\phi = ae^{kz} \sin(k_x x + k_y y), \quad k = \sqrt{k_x^2 + k_y^2}, \quad (3.8)$$

and $\phi_n = \nabla \phi \cdot n$, where $n$ is the normal vector of the prescribed boundary surface. The top surface of the cube coincides with plane $z = 0$, where exact $\phi$ is imposed. On the other five facets, $\phi_n$ is imposed. All six facets of the cube are discretized into square elements. For definiteness, let $k_x = k_y = 2\pi$. After solving the mixed problem inside the cube, we compare numerical solutions with the exact quantities and normalize the absolute error by $a$.

The arithmetically averaged and maximum normalized errors for a set of systematically refined grids are shown in Figure 3-5. The four cases in Figure 3-5 correspond to discretizations of 16, 81, 144 and 256 elements on each facet. The error distributions on the Dirichlet boundary for all four cases are quite non-uniform, which is marked by large values at the intersection edges and smaller values away from the edges. The large error at the intersection line is due to the piecewise constant-density approximation since the geometry (flat surface) is accounted for exactly when CPM is used. As we shall see in the next chapter, the errors at the intersection line are convergent when a higher order approximation is used.

The similar error distribution due to CPM has been observed by Ölmez (1991). In his time-domain simulation of weakly nonlinear water waves with Eulerian formulation, irregular grids and extrapolations on the vertical sides were found useful to reduce the large edge error. In the present study with MEL formulation, however,
Figure 3-5: Errors due to CPM for solving the mixed Dirichlet/Neumann problem inside a unit cube. Dashed line and * denote the averaged and maximum absolute errors on Dirichlet boundary; solid line and + corresponds to the averaged and maximum absolute errors on Neumann boundary.

The usefulness of this type of ad hoc remedy is limited because the accuracy of extrapolations at the waterline of steep waves with a side wall is unreliable. Therefore, it is clear now that a more accurate and robust numerical method is needed for solving the mixed Dirichlet/Neumann problem.

For the collocation method applied to the second kind integral equations, Hess (1975, 1979) carried out an analysis based on small curvature expansions in two and three dimensions to arrive at consistent approximations of geometry and functions for a higher order BEM with center collocation. All variables were expanded in local series expansions in terms of curvatures. All elemental integrals were expanded into a series of integrals over the projected domain in the tangent plane at the collocation point. By collecting quantities of the same order, he concluded that the approximation used for dipole density function should be one order higher than that of source density.
function and, the approximation used for geometry should be one order higher than those used for density functions. For uniform flow past an ellipsoid or a circular nacelle, Hess shows that results obtained by using the second order panel method, which included the second order terms in the local expansion in terms of curvature, are more accurate than those of CPM.

The advantage of the second order panel method is that all panel integrals can be evaluated in closed forms. However, in general, the projected integral domains still have curved edges. In order to avoid numerical integration of the singular integrals, the edges of the projected integral domains were further approximated by the straight lines connecting the vertices. In a similar analysis derived by Romate (1989) using the small curvature expansions in both physical and parametric space, the error due to the edge approximation was found to be second order in the expansions, but the straight edge approximation was again employed. This perhaps is one reason for the break down in the numerical simulations of water waves carried out by Romate (1989). Another disadvantage of the second-order panel method is that there is no continuity ensured at the interfaces of elements. All derivatives of source or dipole (vorticity) density function are calculated by a finite difference scheme involving adjacent panels. In particular, both Hess and Romate use the centered finite difference formula based on arc length, which is calculated by a least-square fit. If lifting effects are included, dipole or vorticity distributions were used. More results using this kind of approach for aerodynamic problems are given by Johnson & Rubbert (1975).

In the present study, it is desirable to collocate at the edges of an element in order to handle the weak singularities at the intersection lines (see Section 4.7 and Chapter 7). Secondly, for the convenience of velocity calculations, curvilinear quadrilateral elements are preferred. Since (2.13) can also be obtained from a weighted residual statement (Brebbia, 1980), we may consider the BEM as a special finite element method (FEM) applied to the curved surface domain. Along this line, we may 'borrow' some existing results from the finite element analysis as our guidelines. The following conclusion is given by Huebner & Thornton (1982) for FEM:
Suppose the integrand of the integrals in the element equations contain derivatives up to the \((k+1)\)-th order. Then, to have rigorous assurance of convergence as element size decreases, we must satisfy the following requirements.

1. Compatibility requirement: At element interfaces we must have \(C^k\) continuity.

2. Completeness requirement: Within an element we must have \(C^{k+1}\) continuity.

These requirements are derived for integrals with regular kernels. Thus, they may be regarded as necessary requirements for the elements to be used for the singular integrals in our BIEs. Since the integrands in (2.14) and (2.15) contain up to the first derivatives of \(G\), we need at least \(C^0\)-continuity at the interfaces and \(C^1\)-continuity within the elements.

To improve the accuracy of the linear isoparametric elements used in Section 3.2, we first looked into the super-parametric curvilinear quadrilateral elements\(^3\) with four corner nodes. The \(x, y, z\) coordinates of each node are mapped into the parametric coordinates \((s, t)\), wherein a bi-cubic spline fit is introduced for interpolations. viz.

\[
(x, y, z) = \mathbf{a}(s, t) = \sum_{m=0}^{3} \sum_{n=0}^{3} (X, Y, Z)_{mn} s^m t^n, \tag{3.9}
\]

where \(X, Y\) and \(Z\) are \(4 \times 4\) coefficient matrices. The Jacobian associated with this transform is given by

\[
J(s, t) = \left[ \left( \frac{\partial(x, y)}{\partial(s, t)} \right)^2 + \left( \frac{\partial(y, z)}{\partial(s, t)} \right)^2 + \left( \frac{\partial(z, x)}{\partial(s, t)} \right)^2 \right]^{1/2} \tag{3.10}
\]

with

\[
\frac{\partial(x, y)}{\partial(s, t)} = \frac{\partial x}{\partial s} \frac{\partial y}{\partial t} - \frac{\partial x}{\partial t} \frac{\partial y}{\partial s} \tag{3.11}
\]

---

\(^3\)If the order of approximation for geometry is higher than that for the field function, it is called super-parametric element. If the same order of approximations is used for both geometry and field function, it is called isoparametric element; if higher order approximation is used for field function, it is called sub-parametric element.
and the other two terms of the Jacobian can be defined similarly. The density functions $\phi$ and $\phi_n$ are approximated by bilinear interpolation functions in $(s, t)$ space, viz.

$$ (\phi, \phi_n) = \sum_{i=0}^{1} \sum_{j=0}^{1} (\phi, \phi_n)_{ij} s^i t^j, \tag{3.12} $$

where $(\phi, \phi_n)_{ij}$ are the nodal values of $\phi$ and $\phi_n$. Hence, the aforementioned necessary requirements are satisfied. The normal of the boundary surface is uniquely defined everywhere on $S$.

The elemental integrals can be evaluated by substituting the above approximations into (2.24) and (2.25). For the non-singular elemental integrals, a multipole expansion method can be used for the evaluations. When the distance from the collocation point to the element is comparable to the characteristic dimension of the element, numerical integration with domain partitions is more effective. The difficulty arises from the evaluation of the self-influence function (the influence at a point which is inside the integral domain).

Without loss of generality, consider a collocation at the node which is the local origin $s = 0, t = 0$. Collocation at the other three nodes of the element may be achieved through an appropriate translation and rotation of the coordinates. Substituting (3.9) into $r = |\mathbf{r} - \xi|$, we obtain a polynomial expansion for $r$,

$$ r^2 = as^2 + 2bst + ct^2 + h(s, t) \tag{3.13} $$

with

$$ \begin{align*}
    a &= X_{10}^2 + Y_{10}^2 + Z_{10}^2 \\
    b &= X_{10}X_{01} + Y_{10}Y_{01} + Z_{10}Z_{01} \\
    c &= X_{01}^2 + Y_{01}^2 + Z_{01}^2
\end{align*} \tag{3.14} $$

where the function $h(s, t)$ contains all the higher degree monomials. Note that no constant or linear terms are present here. This is because both $\mathbf{r}$ and $\xi$ share the common local origin. There are three cases to be considered separately.
1. If $a = 0$, which implies $b = 0$, then

$$ r^2 = ct^2 + h(s, t). \quad (3.15) $$

In this case, the Jacobian $J(0,0) = 0$. Thus, the integrands in both (2.24) and (2.25) are regular.

2. If $a > 0$, we introduce another transformation

$$(s,t) = (p - bq/a, q), \quad (3.16)$$

thus,

$$ r^2 = ap^2 + (c - b^2/a)q^2 + h(s, t). \quad (3.17) $$

The Jacobian of the transformation (3.16) is $J_2 = 1$. The behaviour of leading terms of $r$ in both $(x, y, z)$ space and $(s, t)$ space should be the same if the mapping is not degenerate. Since $r$ is non-negative, we have $(c - b^2/a) \geq 0$. If $c - b^2/a = 0$, we have

$$ r^2 = \left[\sqrt{as} + \sqrt{ct}\right]^2 + h(s, t). \quad (3.18) $$

Thus, the integrands have an Cauchy singularity at $(0,0)$. After some algebra, one can show that $J(0,0)$ vanishes as $r \to 0$. Hence, the integrands are again regular.

3. This case is the same as case 2 above except that $c - b^2/a > 0$. Let

$$(u,v) = (p\sqrt{a}, q\sqrt{c - b^2/a}) \quad (3.19)$$

then

$$ r^2 = u^2 + v^2 + h(s(u, v), t(u, v)). \quad (3.20) $$

The Jacobian of this transformation is $J_3 = (ac - b^2)^{-1/2}$. In $(u,v)$ space, the
Singularity of \( r \) appears in its simplest form.

It is this third case that we have a singular integral, which is of course integrable. To evaluate the singular boundary integrals, we subtract out the leading singular term after the integrals are mapped into the \((u, v)\) space. Recall the assumption that the singular point is at \( \xi_0 \), which corresponds to \((s = 0, t = 0)\). For the source type integrals, we have

\[
I_s = \int \int_{E_s} \phi_n(\xi) G(\xi, \varpi) dS(\xi)
= \int \int_{E_s} \frac{\phi_n(\xi(s, t))}{|\varpi(s, t) - \xi(s, t)|} J(s, t) ds dt
= \int_{u_1}^{u_2} dv \int_{u_1}^{u_2} du \frac{\phi_n(\xi(s(u, v), t(u, v))) J(s(u, v), t(u, v))}{\sqrt{(u^2 + v^2 + h(s(u, v), t(u, v))(ac - b^2)}} \tag{3.21}
\]

where \( J \) is the Jacobian (3.10) and, the Jacobians of transformation (3.16) and (3.19) has been included in the last integral. The limits of the last double integral is defined by

\[
\begin{align*}
  v_1 &= 0, \\
  v_2 &= \sqrt{c - b^2/a}
\end{align*} \tag{3.22}
\]

and

\[
\begin{align*}
  u_1 &= bv/\sqrt{ac - b^2}, \\
  u_2 &= \sqrt{a} + bv/\sqrt{ac - b^2}.
\end{align*} \tag{3.23}
\]

We define an auxiliary function

\[
F(u, v) = \frac{\phi_n(\xi(s(u, v), t(u, v))) J(s(u, v), t(u, v))}{\sqrt{(ac - b^2)(1 + H(u, v))}} \tag{3.24}
\]

with

\[
H(u, v) = h(s(u, v), t(u, v))/(u^2 + v^2). \tag{3.25}
\]

Recall that the function \( h \) contains all monomials of \( s \) and \( t \) with degrees greater than 2. Function \( H \) must be regular at \((0, 0)\) or the behaviour of the singularity \( r \) will be changed. The latter is not possible since the transformations (3.16) and (3.19) are
linear. Hence, function $F$ is regular everywhere and has a Taylor expansion at $(0,0)$. To subtract out the singularity, we may write

$$I_s = \iint_{E_j(u,v)} \frac{F(u,v) - F_0}{\sqrt{u^2 + v^2}} dudv + F_0 \iint_{E_j(u,v)} \frac{1}{\sqrt{u^2 + v^2}} dudv$$

(3.26)

where $E_j(u,v)$ denotes the image domain of the element in parametric space $(u,v)$ as given by (3.22) and (3.23), and the subscript 0 denotes that the quantities are evaluated at $(0,0)$. The integrand of the first integral in (3.26) has been regularized. For the second integral, analytic integration (Newman, 1986) is applicable. Of course, in principle, more terms from the Taylor expansion of $F$ can be subtracted out. The dipole type of singular integrals (2.25) can be treated in a similar manner since the singularity of a dipole kernel is the same as that of the source (see Appendix A). For simplicity, we shall omit the details here.

To investigate the convergence rate of the super-parametric element, a computer program is implemented. The influence function at an arbitrary point in three-dimensional space due to a prescribed density function is evaluated for given surfaces such as a sphere or a given wave surface. The grid is systematically refined to study the convergence. The results are compared with those obtained by using a CPM routine based on the same grid. Figure 3-6 shows typical results for a prescribed surface defined by

$$z = a \sin(x + y), \quad \text{where } (x, y) \in [0, 2\pi] \text{ and } a = 0.3.$$  

(3.27)

The harmonic function used is given by

$$\begin{align*}
\phi &= ae^x \sin(x + y), \\
\phi_n &= ae^x \cos(x + y).
\end{align*}$$

(3.28)

The convergent numerical results obtained by systematically refining the grid are used
Figure 3-6: Convergence studies of influence function evaluation using superparametric elements and constant-strength elements. (a) far field influence at (3, 4, 5); (b) self-influence at (0, 0, 0). (see text for explanations).
as the "exact" solution and compared with results obtained by using other grids. In Figure 3-6 the solid and dashed lines denote, respectively, errors in the influence functions due to dipoles and sources, evaluated by constant-strength elements. The * and + denote, respectively, errors in the influence functions due to dipoles and sources, evaluated by super-parametric elements. N is the total number of unknowns.

The comparison in Figure 3-6 indicates that the super-parametric elements and constant-strength elements have virtually the same convergence rate\(^4\). Even though the super-parametric element has slightly improved accuracy, its computational cost is much higher than that of the simpler element. We infer that the accuracy of the super-parametric element is dominated by errors introduced by the bilinear approximation of the density functions. Another numerical experiment using the bilinear interpolation based on a natural coordinate of area in \((s,t)\) space is also found to be unsuccessful. To improve the accuracy, a higher order interpolation function must be used for density functions. An obvious approach is to use the bi-cubic spline fit for both the geometry and density functions, which leads to a \(C^1\)-continuous bi-cubic spline element. This type of method has been used in aerodynamic computations (Roberts & Rundle, 1972, and Sytsma, Hewitt & Rubbert, 1979), but the computational burden is very high. These results convinced us to use simpler interpolation functions rather than the bi-cubic splines. Therefore, we choose to use the bi-quadratic isoparametric curvilinear elements. The nine-node element is preferred for the convenience of velocity calculations. This is described in Chapter 4.

\(^4\)The failure of convergence of the dipole influence due to CPM at the origin is because the constant-strength element is not suitable for evaluating self-influence at the vertex of an element.
Chapter 4

Numerical Formulation and Implementations

4.1 Introduction

An observation on all BEMs regardless the type of elements used is that the major portion of the computation time is spent on constructing the influence matrix and vector. This is because the computation of the matrix and vector of the linear system $Ax = b$ requires $N^2$ evaluations of the elemental integrals, whereas to solve it iteratively, each iteration only requires $O(N^2)$ floating point operations (one multiplication and one addition). Thus, the key to efficient numerical solution for the BIEs lies in the efficient computation of elemental integrals.

There is, however, an exception to the aforementioned observation. That is the recently devised adaptive multipole method (AMM), which does not require the influence matrix to be constructed explicitly (Rokhlin, 1985). Since most of the iterative solution schemes is essentially a process of reducing the residual $r_n = b - Ax_n$, only the matrix-vector product $Ax_n$ is required at each iteration (not the matrix itself). By using this insight, multipole methods can be incorporated into the iterative schemes to reduce the operation count of the product $Ax_n$ to $O(N)$. The AMM evaluates the near field influence directly and, expands the far field influence into Taylor se-
eries. Significantly, Rokhlin points out that for a given tolerance, the Taylor series can be truncated according to analytical expressions of error bounds such that the final solution has the required accuracy. After the domain is partitioned into a $l$-level ($l$ depends on the tolerance) hierarchical data structure, the adaptations of multipole methods into the iterations is accomplished by shifting and combining the expansions of all far-field influences to form expansion of the total far-field influences for each node. It has been shown that this adaptation can be achieved with $O(N)$ efforts and computer storage. The most significant feature of the AMM compared with a classical iterative algorithm for BIEs is that the far-field influence is evaluated collectively rather than individually. The original idea was developed in the adaptive multipole method for the second-kind integral equation in a two dimensional complex plane (Rokhlin, 1985). By using the spherical harmonic expansions, the approach was extended to the simulation of $N$-particle interactions in three dimensions by Greengard & Rokhlin (1987) and Zhao (1987). Zhao has also developed a parallel implementation of the algorithm which requires $O(\log N)$ efforts on the Connection Machine. Typically, for a required accuracy of $10^{-4}$ for three-dimensional potential fields, AMM will outperform a direct algorithm when there are more than 1,000 unknowns. For the parallel implementation, the AMM has a speedup factor of 10 for $N = 1,000$ and a speedup factor of 100 for $N = 10,000$ (Zhao, 1987). An application of AMM to two-dimensional free-surface flows was given by Korsmeyer (1990).

It must be pointed out that AMM as a rapid algorithm is problem dependent. It is merely an intelligent implementation of multipole methods for existing Laplace solvers. The further extension of AMM to three-dimensional potential flows such as the present breaking-wave simulation depends on the success of resolving the fundamental issues about solutions of the mixed BIEs such as accuracy, convergence and treatment of possible singular solutions. It must also be noted that the implementation of AMM in this case is difficult because the influence functions to be evaluated is much more complex than the $1/r$ potential of the $N$-particle problem.

In this chapter, our goals are to develop an efficient BIE solver for the mixed
Dirichlet/Neumann problem at a given time step and to develop an accurate algorithm for the evaluation of velocity components on the free surface. In particular, four major tasks are to be accomplished:

1. defining admissible grids, efficient evaluations of the elemental integrals based on nine-node bi-quadratic isoparametric elements;

2. convergence studies of the quadratic boundary element method (QBEM);

3. accurate evaluations of the velocity vectors on an arbitrary surface;

4. developing an effective algorithm for doubly periodic problems.

Finally, the time stepping procedure and accuracy checks are described. Efficiency without sacrificing accuracy is the central theme of the present numerical implementations.

4.2 Admissible grids and polynomial approximations

In the analysis of boundary elements, we are often required to obtain an approximate representation of a field function $\Phi$ which is only known at a set of discrete nodal points, say $\varphi_i, i = 1, 2, \cdots, I$. Here $\Phi$ includes both the physical and geometrical variables. In particular, we have $\Phi \in (x, y, z, \phi, \phi_n)$. Polynomials are usually preferred for the approximations. The nodal points are the sampling points which can be selected by analysts. Empirically, we know that the nodes should be selected to avoid severely distorted elements. But, what constitutes an admissible element? This difficult question is usually avoided in the literature of boundary elements by showing convergent results for some empirically selected grids. In the present study of free-surface flows, the grid points are subject to motion. Thus, it is necessary to have some criteria for checking the admissibility of the grid at each time step.
Without loss of generality, we define orthogonal parametric coordinates \((s,t)\) for a generic element and map the domain of the element to a square in \((s,t)\) space: \(s \in [-1,1], t \in [-1,1]\). Suppose \(\Phi(s,t)\) is continuous within the element. Its Taylor expansion at the origin \((0,0)\) can be written as

\[
\Phi(s,t) = \Phi_0 + s\Phi_{s,0} + t\Phi_{t,0} + st\Phi_{st,0} + s^2\frac{\Phi_{ss,0}}{2} + t^2\frac{\Phi_{tt,0}}{2} + \\
\frac{s^2t\Phi_{sst,0}}{2} + \frac{st^2\Phi_{s,0}}{2} + \cdots + \frac{s^2t^2\Phi_{s,t,0}}{4} + \cdots (4.1)
\]

where subscripts \(s\) and \(t\) denote the partial derivatives with respect to \(s\) and \(t\) respectively. The subscript 0 denotes the value at \((0,0)\). Since the Taylor expansion for a continuous function is unique, the admissible polynomial approximation of \(\Phi(s,t)\) must correspond to a truncated Taylor series. Given a set of discrete nodal values \(\{\Phi_i\}\) within an element, the partial derivatives in \((4.1)\) may be evaluated by finite difference formulae in terms of the nodal values. Recall \((s,t) \in [-1,1]\). In order to obtain the convergent series expansion of \(\Phi\), the coefficients of the series should also be convergent. Therefore, we obtain the following criterion for iso-parametric elements:

**Definition 1** A numerical grid is admissible if the polynomial representations for all field variables within each element is the truncated convergent series expansions of form \((4.1)\).

Even though this statement is not precise, it allows us to accept or reject a grid based on some computed quantities (the convergence of coefficients of approximation polynomials) rather than based on inspections.

Usually the polynomial representation of \(\Phi\) is indirectly defined by selecting a set of elemental interpolation functions. Here, we will consider the polynomial approximation from a general perspective without specifying the interpolation functions. In order for the polynomial approximation to be useful, its form should remain invariant after a linear transformation of the coordinates. In other words, the polynomials should possess geometric isotropy (Huebner & Thornton, 1982). This turns out to
Figure 4-1: A generic nine-node curvilinear element $E_j$ and its image in parametric space $E_j(s,t): s \in [-1,1], t \in [-1,1]$.

be the most important feature of the polynomials which dictates the selection of interpolation functions. For geometric isotropy, the number of nodes in both $s$ and $t$ direction within an element must be the same. For given $m$ nodal values in each direction within an element, the approximation can be a polynomial in terms of $s$ and $t$ of degree $m - 1$ or less. The question is then what kind of finite difference scheme is optimal in terms of accuracy for computing the coefficients of the polynomial. Intuitively, the optimal choice must be the finite difference formulae which give uniform truncation errors for all coefficients. As shall be seen, this is true for the most popular elements such as Lagrangian elements (which use Lagrangian interpolation functions) and 'serendipity' elements (which have no interior nodes).

4.3 The influence functions

We now restrict our attention to the computation of the elemental integrals. Recall that the boundary surface $S = S_D \cup S_N$ has been discretized into a set of $N_e = N_e^1 + N_e^2$ elements. For each element, all variables of interest $(x, y, z, \phi, \phi_n)$ are defined on nine nodes including the four vertices. The basic idea of bi-quadratic isoparametric interpolation is quite simple: map all variables into a parametric space $(s, t)$ and use a two-dimensional Lagrangian polynomial for interpolations. In the parametric space, the domain of integration is defined as a square $E_j(s,t)$; see Figure 4-1 for the definitions.
Let $\Phi$ signify a variable from the set of $(x, y, z, \phi, \phi_n)$. The value of $\Phi$ at a point on the element surface is defined in terms of its nine nodal values and Lagrangian interpolation functions, viz.

$$\Phi(s, t) = \sum_{m=1}^{9} N_m(s, t)\Phi_m$$

(4.2)

with $\Phi_m$ the $m$-th nodal value of $\Phi$. Let the $m$-th nodal location in the parametric space be $(s_m, t_m)$. The nine interpolation functions can be written explicitly as

$$\begin{cases} 
N_m(s, t) = \frac{1}{4}s(s + s_m)t(t + t_m) & m = 1, 3, 5, 7, \\
N_m(s, t) = \frac{1}{2}(1 - t_m^2 s^2 - s_m^2 t^2)[t_m t (1 + t_m t) + s_m s (1 + s_m s)] & m = 2, 4, 6, 8, \\
N_9(s, t) = (1 - s^2)(1 - t^2) &
\end{cases}$$

(4.3)

Substituting (4.3) into (4.2), we obtain the polynomial representation of $\Phi$ as

$$\Phi(s, t) = a_{00} + a_{10} s + a_{01} t + a_{11} st + a_{20} s^2 + a_{02} t^2 + a_{21} s^2 t + a_{12} s t^2 + a_{22} s^2 t^2$$

$$= \sum_{m,n=0}^{M} a_{mn}s^m t^n \quad (s, t) \in E_j(s, t)$$

(4.4)

where $M = 2$ and

$$\begin{align*}
& a_{00} = \Phi_9 \\
& a_{10} = \frac{1}{2}(\Phi_4 - \Phi_8) \\
& a_{01} = \frac{1}{2}(\Phi_6 - \Phi_2) \\
& a_{11} = \frac{1}{4}[(\Phi_5 - \Phi_7) - (\Phi_3 - \Phi_1)] \\
& a_{20} = \frac{1}{2}(\Phi_4 - 2\Phi_9 + \Phi_8) \\
& a_{02} = \frac{1}{2}(\Phi_6 - 2\Phi_9 + \Phi_2) \\
& a_{21} = \frac{1}{4}[(\Phi_5 - 2\Phi_6 + \Phi_7) - (\Phi_3 - 2\Phi_2 + \Phi_1)] \\
& a_{12} = \frac{1}{4}[(\Phi_5 - 2\Phi_4 + \Phi_3) - (\Phi_7 - 2\Phi_8 + \Phi_1)] \\
& a_{22} = \frac{1}{4}[(\Phi_3 - 2\Phi_2 + \Phi_1) - 2(\Phi_4 - 2\Phi_9 + \Phi_8) + (\Phi_5 - 2\Phi_6 + \Phi_7)]
\end{align*}$$

(4.5)

Since the polynomial representation of $\Phi$ is "symmetric" with respect to $s$ and $t$ (i.e. 61
its form is invariant by exchanging $s$ and $t$), its geometric isotropy is preserved. By comparing the polynomial representation of $\Phi$ with the Taylor expansion in (4.1), it is clear that the coefficient of each monomial is the second order finite difference approximation for the corresponding partial derivative in the Taylor series. This insight is useful in computing the gradient of the potential.

It is easy to show that the coefficients of the polynomial of the 'serendipity' (eight-node) element also correspond to the second-order finite difference approximations to the corresponding coefficients of the first eight terms in (4.1). For the bilinear interpolation, the coefficients of the polynomial corresponds to the first-order finite difference formulae for the first four derivatives in (4.1). See Appendix C for details.

Let the total number of nodal points on $S$ be $N$ (the exact relation between $N$ and total number of elements $N_e$ depends on the specific configuration/discretization of $S$). The type of unknowns ($\phi$ or $\phi_n$) at each node depends on the type of boundaries (Dirichlet/Neumann) on which the node is located. In order to determine these $N$ unknowns, we collocate at $N$ nodes to obtain $N$ equations as have been decided in the last chapter. The vector $r$ from a point on the interpolated element surface to the $i$-th global collocation point $x_i$ is then given by

$$r = (x_i - x, \ y_i - y, \ z_i - z)$$
$$= (x_i - \sum_{m=1}^{9} N_m x_m, \ y_i - \sum_{m=1}^{9} N_m y_m, \ z_i - \sum_{m=1}^{9} N_m z_m) \quad (4.6)$$

with its magnitude $r = |r|$. The normal vector of the interpolated element surface can be defined by

$$n = \frac{x_s \times x_t}{|x_s \times x_t|}. \quad (4.7)$$

Let $x_s \times x_t = (j_1, j_2, j_3)$, we have

$$\begin{cases} 
  j_1 = y_s z_t - y_t z_s, \\
  j_2 = z_s x_t - z_t x_s, \\
  j_3 = z_s y_t - z_t y_s. 
\end{cases} \quad (4.8)$$
By comparing (3.11) with (4.8), the Jacobian can be written as

\[ J(s, t) = \sqrt{j_1^2 + j_2^2 + j_3^2}. \]  

(4.9)

This expression can also be obtained by the relation of the differential area between physical space and parametric space.

Substituting the interpolations introduced above into integral (2.24) and (2.25), we obtain the approximated elemental integrals as

\[ I_{s,i} = \sum_{m=1}^{g} \phi_m S_m^{(j)}(x_i), \]  

(4.10)

\[ I_{d,i} = \sum_{m=1}^{g} \phi_{n,m} D_m^{(j)}(x_i) \]  

(4.11)

where \( S_m^{(j)}(x_i) \) and \( D_m^{(j)}(x_i) \) are the elemental influence functions associated with the \( m \)-th node at \( x_i \) due to source and dipole distributions on a generic element \( E_j \), respectively. Specifically, we have

\[ S_m^{(j)}(x_i) = \int_{E_j(s,t)} \frac{N_m(s,t)J(s,t)}{r(s,t)} dsdt \]  

(4.12)

\[ D_m^{(j)}(x_i) = \int_{E_j(s,t)} -\frac{\mathbf{H} \cdot \mathbf{r}}{r^3(s,t)} N_m(s,t)J(s,t) dsdt \]  

(4.13)

where \( E_j(s,t) \) is the domain of integration in the \((s, t)\) space as defined in Figure 4-1 and \( J(s,t) \) is the Jacobian in (4.9). Again, if \( x_i \in E_j \), \( S_m^{(j)} \) and \( D_m^{(j)} \) is the finite part of the integral.

As the result of the above approximation, the discretized BIEs (2.22) and (2.23) can now be written as the standard system of linear equations,

\[ Ax = b \]  

(4.14)

where the influence matrix \( A \) is a \( N \times N \) matrix, \( b \) is a \( N \)-vector. The \( i \)-th linear equation corresponds to the collocation at \( x_i \). Each element of the matrix \( A_{ij} \) is equal
to the superpositions of the influence functions associated with the \( j \)-th global node.

To be consistent with the approximations introduced above, the interior solid angle at a nodal point (2.16) can be expressed as

\[
\alpha(\mathbf{x}_i) = -\sum_{j=1}^{N} D_{ij}^{(d)}, \quad \text{for } i = 1, 2, \ldots, N, \tag{4.15}
\]

with \( D^{(d)} \) the influence matrix due to dipole type of singularities.

In the next two sections, our attention is focused on the efficient evaluations of the elemental influence functions (4.12) and (4.13) based on bi-quadratic isoparametric Lagrangian interpolation functions. We will develop the algorithms for the elemental integrals involving the free space Green function and its normal derivative.

### 4.4 Multipole method for far field influences

For the far field influence, both multipole methods and direct numerical integrations are applicable. In this section, we present the closed form integrals based on multipole expansions for the far field influence functions.

Since the interpolation functions \( N_j \) defined by (4.3) consists of polynomials in two variables up to degree \( M = 2 \), we consider the integrals of the following two canonical forms:

\[
P_{kt} = \int \int_{E_j(s, t)} \frac{J(s, t)}{r(s, t)} s^k t^l ds dt, \tag{4.16}
\]

\[
Q_{kt} = \int \int_{E_j(s, t)} \frac{[j_1(x_i - x) + j_2(y_i - y) + j_3(z_i - z)]}{r^3(s, t)} s^k t^l ds dt. \tag{4.17}
\]

The objective here is to expand the kernel functions in (4.16) and (4.17) into series expansions by using the polynomial representations for the field variables. To do so, it is convenient to introduce the following recursion formula which is modified from the truncated version given by Newman (1991).
Consider a polynomial of the form (4.4), for any integer power \( k \), we define,

\[
\hat{\Phi}^k = \sum_{m,n=0}^{M_p} a_{mn}^{(k)} s^m t^n, \quad \text{for } (s,t) \in E_i(s,t),
\]

(4.18)

where

\[
a_{mn}^{(k)} = \sum_{i=0}^{m} \sum_{j=0}^{n} a_{ij}^{(1)} a_{m-i,n-j}^{(k-1)}
\]

(4.19)

with \( a_{ij}^{(1)} \equiv a_{ij} \). The resulting series is truncated at \( M_p \geq M \). If \( k = 0 \), this recursion relation is still defined with \( a_{ij}^{(0)} = \delta_{i,0} \delta_{j,0} \) where \( \delta_{i,j} \) is the Kroenecker delta function. If \( k = -1 \), the coefficients of the relation (4.18) are given by

\[
a_{mn}^{(-1)} = \begin{cases} 
1/a_{00} & \text{if } m = n = 0, \\
-\sum_{i=0}^{m} \sum_{j=0}^{n} a_{ij} a_{m-i,n-j}^{(-1)}/a_{00} & \text{if } (m + n) > 0,
\end{cases}
\]

(4.20)

where the prime on the lower limits denotes that the term \((i = j = 0)\) is omitted. If \( k = 1/2 \), the coefficients of the relation (4.18) can be written as

\[
a_{mn}^{(1/2)} = \begin{cases} 
\sqrt{a_{00}} & \text{if } m = n = 0, \\
\frac{1}{2a_{00}^{(1/2)}} \left[ a_{mn} - \sum_{i=0}^{m} \sum_{j=0}^{n} a_{ij}^{(1/2)} a_{m-i,n-j}^{(1/2)} \right] & \text{if } (m + n) > 0,
\end{cases}
\]

(4.21)

where the primes on the lower and upper limits denote that the term \((i = j = 0)\) and \((i = m, j = n)\) are omitted.

In order to expand the normal vector and the Jacobian into series in terms of \( s \) and \( t \), we also need to differentiate expansions of the form (4.4), that is,

\[
\frac{\partial \hat{\Phi}}{\partial s} = \sum_{m=0}^{M-1} \sum_{n=0}^{M} b_{mn} s^m t^n
\]

(4.22)

where \( b_{mn} = (m + 1)a_{m+1,n} \). Similarly,

\[
\frac{\partial \hat{\Phi}}{\partial t} = \sum_{m=0}^{M} \sum_{n=0}^{M-1} c_{m,n} s^m t^n
\]

(4.23)
where \( c_{mn} = (n + 1)a_{m,n+1} \). In practice, it is convenient to extend the polynomials so that they all have the same degree \( M \) by letting \( a_{mn} = 0 \) for \( m, n > M - 1 \).

Let \( P_1 \) and \( P_2 \) be two polynomials of form (4.4). \( P_1 \) has coefficients \( U_{mn} \) with degree \( M_1 \) and \( P_2 \) has coefficients \( V_{mn} \) with degree \( M_2 \). The product \( P_1P_2 \) is a polynomial of degree \( M_1 + M_2 \), viz.

\[
P_3 = P_1P_2 = \sum_{m,n=0}^{M_1+M_2} W_{mn} s^m t^n \tag{4.24}
\]

where

\[
W_{mn} = \sum_{i=0}^{m} \sum_{j=0}^{n} U_{ij} V_{m-i,n-j}. \tag{4.25}
\]

Let the coefficients of polynomial representations of \( \varphi \) be \( X_{mn} = (X_{mn}, Y_{mn}, Z_{mn}) \), respectively. The derivatives of \( \varphi \) can be readily evaluated by relation (4.22) and (4.23). That is,

\[
\varphi_s = \sum_{m,n=0}^{M} X_{mn}^{(s)} s^m t^n \tag{4.26}
\]

where \( X_{mn}^{(s)} = (m+1)X_{m+1,n} \) and the upper limit of the summation has been extended. Similarly, the coefficients of expansion for other derivatives can be obtained by

\[
X_{mn}^{(t)} = (n+1)X_{m,n+1}. \tag{4.27}
\]

Therefore, the components of the normal vector (4.8) can be readily evaluated by relation (4.24) and the derivatives of expansions. Truncating the final polynomials up to degree \( M_p \geq M \), we have

\[
j_l = \sum_{m,n=0}^{M_p} J_{l,mn} s^m t^n \tag{4.28}
\]

where \( l = 1, 2, 3 \) and

\[
J_{1,mn} = \sum_{i=0}^{m} \sum_{j=0}^{n} (Y_{ij}^{(s)} Z_{m-i,n-j}^{(t)} - Y_{ij}^{(t)} Z_{m-i,n-j}^{(s)}), \tag{4.29}
\]
\begin{align*}
J_{2, mn} &= \sum_{i=0}^{m} \sum_{j=0}^{n} (Z_{ij}^{(t)} X_{m-i, n-j}^{(t)} - Z_{ij}^{(t)} X_{m-i, n-j}^{(s)}), \\
J_{3, mn} &= \sum_{i=0}^{m} \sum_{j=0}^{n} (X_{ij}^{(t)} Y_{m-i, n-j}^{(t)} - X_{ij}^{(t)} Y_{m-i, n-j}^{(s)}).
\end{align*}

(4.30)\hspace{1cm} (4.31)

The magnitude of the normal can then be evaluated by (4.18) with \( k = 2 \) and (4.21).
In view of relation (4.9), we have

\[ j^2 = \sum_{m,n=0}^{M_p} J_{mn}^{(2)} \delta^m t^n \]

(4.32)

where

\[ J_{mn}^{(2)} = \sum_{i=0}^{m} \sum_{j=0}^{n} \sum_{l=1}^{3} J_{l,ij} J_{l,ij}. \]

(4.33)

The coefficients of \( J \) can be obtained by taking the square-root of (4.32). From relation (4.21), we have

\[ J = \sum_{m,n=0}^{M_p} J_{mn} \delta^m t^n \]

(4.34)

with

\[ J_{mn} = \begin{cases} 
\sqrt{J_{00}^{(2)}} & \text{if } m = n = 0, \\
\frac{1}{2J_{00}} \left[ J_{mn}^{(2)} - \sum_{i=0}^{m} \sum_{j=0}^{n} J_{ij} J_{m-i, n-j} \right] & \text{if } (m + n) > 0.
\end{cases} \]

(4.35)

Assume the field point \( x_i \) is sufficiently far from the element considered. The coefficients of polynomial representation of the vector \( r = x_i - x \) can be written as

\[ r = \sum_{m,n=0}^{M_p} r_{mn} \delta^m t^n \]

(4.36)

where

\[ r_{mn} = (r_{1, mn}, r_{2, mn}, r_{3, mn}) = \begin{cases} 
x_i - x_{00} & \text{if } m = n = 0, \\
-x_{mn} & \text{otherwise}.
\end{cases} \]

(4.37)

To calculate the coefficients of the expansion for \( r \), we first write down the coefficients
of the expansion for $r^2$,

$$R_{mn}^{(2)} = \begin{cases} 
\sum_{k=1}^{3} (r_{k,0,0})^2 & \text{if } m = n = 0, \\
\sum_{i=0}^{m} \sum_{j=0}^{n} \sum_{k=1}^{3} r_{k,i,j} r_{k,m-i,n-j} & \text{otherwise.}
\end{cases} \quad (4.38)$$

Then, the coefficient of the expansions for $r$ can be readily obtained from relation (4.21). That is,

$$R_{mn} = \begin{cases} 
\sqrt{R_{00}^{(2)}} & \text{if } m = n = 0, \\
\frac{1}{2R_{00}} \left[ R_{mn}^{(2)} - \sum_{i=0}^{m} \sum_{j=0}^{n} R_{ij} R_{m-i,n-j} \right] & \text{if } (m+n) > 0.
\end{cases} \quad (4.39)$$

The coefficients of the expansion for $r^{-1}$ can be obtained from relation (4.20) and (4.39), viz.

$$R_{mn}^{(-1)} = \begin{cases} 
1/R_{00} & \text{if } m = n = 0, \\
-\sum_{i=0}^{m} \sum_{j=0}^{n} R_{ij} R_{m-i,n-j}/R_{00} & \text{if } (m+n) > 0.
\end{cases} \quad (4.40)$$

To expand the normal derivative of the Green function, we need to expand $r^{-3}$, which can be obtained by relation $r^{-3} = r^{-2} r^{-1}$. The coefficients of the expansion for $r^{-2}$ can be obtained from (4.38) using relation (4.20), viz.

$$R_{mn}^{(-2)} = \begin{cases} 
1/R_{00}^{(2)} & \text{if } m = n = 0, \\
-\sum_{i=0}^{m} \sum_{j=0}^{n} R_{ij}^{(2)} R_{m-i,n-j}/R_{00}^{(2)} & \text{if } (m+n) > 0.
\end{cases} \quad (4.41)$$

Thus, the coefficients of the expansion for $r^{-3}$ can be written as

$$R_{mn}^{(-3)} = \begin{cases} 
1/(R_{00}^{(2)} R_{00}) & \text{if } m = n = 0, \\
-\sum_{i=0}^{m} \sum_{j=0}^{n} R_{ij}^{(-2)} R_{m-i,n-j}^{(-1)} & \text{if } (m+n) > 0.
\end{cases} \quad (4.42)$$
From (4.28), (4.36) and (4.24), we have

$$[j_1(x_i - x) + j_2(y_i - y) + j_3(z_i - z)] = \sum_{m,n=0}^{M_p} \chi_{mn}s^m t^n$$

(4.43)

with

$$\chi_{mn} = \sum_{i=0}^{m} \sum_{j=0}^{n} \sum_{l=1}^{3} J_{ij} r_{l,m-i,n-j}. \quad (4.44)$$

Substituting (4.34) and (4.40) into (4.16), the canonical integral (4.16) can then
be written as

$$P_{kl} = \sum_{i,j=0}^{M_p} R_{ij}^{(-1)} \sum_{u,v=0}^{M_p} J_{uv} \int_{-1}^{1} \int_{-1}^{1} s^{u+i+k} t^{v+j+l} ds dt \quad (4.45)$$

$$= \sum_{i,j=0}^{M_p} R_{ij}^{(-1)} \sum_{u,v=0}^{M_p} J_{uv} S_{u+i+k} S_{v+j+l} \quad (4.46)$$

where

$$S_n = \int_{-1}^{1} \tau^n d\tau = \begin{cases} \frac{2}{n + 1}, & \text{if } n = 0, 2, 4, \cdots \\ 0, & \text{otherwise.} \end{cases} \quad (4.47)$$

Similarly, from (4.43) and (4.42), the canonical integral (4.17) can be expressed as

$$Q_{kl} = \sum_{i,j=0}^{M_p} \chi_{ij} \sum_{u,v=0}^{M_p} R_{uv}^{(-3)} S_{u+i+k} S_{v+j+l} \quad (4.48)$$

where $S_k$ has been defined in (4.47).

Therefore, the desired multipole expansions for the elemental influence functions
can be obtained from the sequence $\{P_{mn}\}$ and $\{Q_{mn}\}$ according to (4.3), (4.12) and
(4.13). For example, if $m = 1, 3, 5, 7,$

$$N_m(s,t) = \frac{1}{4} s(s + s_m) t(t + t_m)$$

$$= \frac{1}{4} (s_m s t_m t + s_m s t^2 + s^2 t_m t + s^2 t^2). \quad (4.49)$$
The influence function associated with these nodes can be obtained by

\[ S_m^{(j)} = \frac{1}{4} [s_m t_m P_{11} + s_m P_{12} + t_m P_{21} + P_{22}], \quad (4.50) \]

\[ D_m^{(j)} = \frac{1}{4} [s_m t_m Q_{11} + s_m Q_{12} + t_m Q_{21} + Q_{22}]. \quad (4.51) \]

Similarly, all influence functions \( S_m^{(j)} \) and \( D_m^{(j)}(m = 1, 2, \ldots, 9) \) can be readily computed.

### 4.4.1 Remarks

For a required accuracy, an important question which stems from the multipole expansion formulation is how many terms should be kept in the intermediate expansions of \( r^{-1} \), \( J \) and \( n \) etc. so that the final multipole expansions are valid for field points as close to the element as possible. A common practice in using the expansions is to keep the resulting intermediate polynomials with the same degree as the original polynomial (e.g. Newman, 1991a,b). By keeping \( (M_p = M = 2) \), we find that the multipole expansion method gives 3 significant digits (SD) accuracy for field point \( \omega_i \) which is approximately at a distance greater than 1.5\( d_e \) away from the element, where \( d_e \) is the characteristic dimension of the element. This result is similar to that observed in a two-dimensional analysis by Newman (1991a). It is important to point out that this accuracy is obtained by considering a "not very distorted element" such as part of a sphere, whose polynomial representations for all field variables have rapidly decreasing coefficients. As the curvature of the element surface increases, the rate of convergence of the expansion decreases. For an oblique second order Stokes wave of \( ka = 0.3 \) with 20 elements per wave length, it is found that the field points should be at least 6\( d_e \) away from the element in order to obtain 3 SD accuracy in the evaluated influence functions. By keeping more terms in the intermediate expansions \( (M_p \leq 10) \), we can obtain the same accuracy for field points approximately up to 1.0\( d_e \) away from the element with the same grid. Obviously, a dynamic determination of the appropriate \( M_p \) is desirable. Owing to the complexity of the problem, the
present attempt along this line indicates that it is too time consuming.

The present test computations show that the multipole method described above (with fixed $M_p$) is in general more efficient than numerical quadratures on a scalar computer. However, its implementation on a vector-processor such as Cray Y-MP cannot fully exploit the CPU's capability. Specifically, the coefficients of the multipole expansions are most conveniently programmed using nested do-loops which cannot be effectively vectorized. Therefore, we develop a vectorizable adaptive numerical quadrature for all collocation locations in the next section. This technique is used in all our numerical computations.

4.5 Adaptive numerical integrations

In this section, we develop the adaptive numerical integration algorithm for evaluating the influence functions in (4.12) and (4.13).

If a field point is located outside the domain of the element, the kernel functions in (4.12) and (4.13) are regular. Hence, a standard Gauss-Legendre quadrature can be used for the evaluations. When the field point coincides with one of the elemental nodes, the kernels contain a $1/r$ type of singularity. The singularities can be regularized by introducing a coordinate transformation, after which the influence functions can be evaluated by Gauss-Legendre quadratures. This approach has been commonly adopted in applications of boundary element methods, see for examples, Lachat & Watson (1976), Li, Han & Mang (1985), Liu & Lu (1988) and Chau (1989). Although the convergence of Gauss-Legendre quadrature applied to the integration of a continuous function over a finite region is guaranteed (Hildebrand, 1987), it usually takes excessive quadrature points to obtain convergent results for integration over a curved surface. An adaptive numerical quadrature has been sought by a number of analysts. For the frequency domain analysis of a free-surface flow, Chau (1989) simply increased the order of Gauss-Legendre quadrature until the results of two successive orders of the quadrature agreed within a given tolerance. This "brute-force"
The application of Gauss-Legendre quadrature may result in false convergence if the integrand does not possess smooth high-order derivatives. In particular, the regularized kernel contains a $\frac{\partial^6}{\partial s^6}$ type of indeterminacy at the singular point (see Section 4.5.2). As the order of quadrature increases, quadrature points will inevitably approach this singular point. Furthermore, applications of this type of iterative quadratures for all field points and elements would require an excessive number of evaluations of the integrands and become uneconomical.

To reduce the order of Gauss-Legendre quadrature when a field point is close to the element, it is useful to subdivide the element into a set of subregions wherein the quadrature is used. The upper bound of the error for the $k$-th order Gauss-Legendre quadrature applied to a function in two variables can be deduced from the error bound of single integrals (e.g. Dahlquist & Björck, 1974), viz.

$$E_k = \sum_{i=1}^{2} \frac{C}{(2k_i)!(2^{2k_i} \partial F)}$$

where $C$ is a constant and, $k_i, i = 1, 2$ correspond to the orders of quadrature used for the double integral. Owing to the complicated integrands, it would be uneconomical to calculate the error bound directly. In order to determine the order of the quadrature $k_i$ for each element, Lachat & Watson (1976) introduced the following simplifications to estimate the expression in (4.52):

1. the Jacobian $J(s,t)$ is assumed to be constant and equal to its value at the origin of the local parametric coordinates.

2. the truncation error of $1/r$ is considered and, it is assumed to be a constant within the element.

Based on these assumptions, a formula for $k_i$ can be written as

$$(2k_i + 1)\alpha^{2k_i} \leq K$$

(4.53)
with

\[ \alpha = \frac{S_{\xi_i}}{2r_{\text{min}}}, \quad S_{\xi_i} = \sqrt{x_{\xi_i}^2 + y_{\xi_i}^2 + z_{\xi_i}^2} \]  \hspace{1cm} (4.54)

where \( \xi_1 \equiv s; \xi_2 \equiv t \) and \( r_{\text{min}} \) is the minimum distance from the field point to the element. Lachat & Watson showed that the application of this procedure to three-dimensional parabolic elements was successful. Another approach along this line was presented by Doblaré (1984), who also reviewed different schemes for the numerical integrations over boundary elements. It must be noted that the premises used above are valid only for not very distorted elements. In the present simulation of breaking waves, large curvatures near wave crests or the overturning jet are anticipated. To see the limitation of (4.53), preliminary computations are carried out using progressive plane Stokes waves \((ka = 0.4)\). The evaluated influence functions are compared with those obtained from Romberg scheme with a tolerance of \(10^{-4}\). After the convergence criteria are met, we substitute the \( k_i \) and \( \alpha_i \) into the left hand side of (4.53). If (4.53) is applicable, the value of \((2k_i + 1)\alpha^{2k_i}\) should fall into a narrow range. However, it is found that the value varies from \(10^0\) to \(10^{-6}\) depending on the curvature of the element surface. This test clearly indicates that the simplifications for obtaining (4.53) are not appropriate in this case. Therefore, an alternative approach is needed and is developed here for a general curvilinear boundary surface.

An efficient adaptive algorithm is described in the following two sections for far field- and self-influence respectively. The convergence of the quadrature is established by comparing results against the convergent results of the Romberg scheme. Because it is difficult to regrid free surface when it starts to overturn, several issues on the robustness of the algorithm such as the accuracy of elemental influence functions with high “aspect ratios” and a triangle element treated as a degenerate quadrilateral are also considered.
Figure 4-2: Definitions of $r_{\text{min}}$ and $l_i, i = 1, 2, 3, 4$. The field point is located at $(x, y, z)$.

### 4.5.1 Evaluation of far and near field influences

Assume that the field point is outside the integral domain. The integrands in both (4.12) and (4.13) are continuous functions. Hence, Gauss-Legendre quadrature can be used for the integration of influence functions. In order to reduce the order of the quadrature when the field point is near the element, the integral domain is subdivided. Suppose the number of subdivisions in $s$ and $t$ directions are $m_1$ and $m_2$ respectively. The double integrals in (4.12) and (4.13) can be evaluated by the following formula:

$$
\int \int_{E_j(s,t)} F(s,t) ds dt \approx \frac{1}{m_1 m_2} \sum_{k=1}^{m_1} \sum_{l=1}^{m_2} \sum_{i=1}^{\nu(k,l)} \sum_{j=1}^{\nu(h,l)} w_i^{(v)} w_j^{(v)} F(s_i^{(v)}, t_j^{(v)})
$$

(4.55)

where $\nu = \nu(k, l)$ is the order of the Gauss-Legendre quadrature in subelement $E_j^{(k,l)}$. $F(s, t)$ represents the integrand in (4.12) or (4.13). For simplicity, equal number of quadrature points are used in both $s$ and $t$ directions.

After extensive numerical experiments, we select the following three simple parameters for determining the order of the Gauss-Legendre quadrature:

1. $p_1 = r_{\text{min}}^2$: $r_{\text{min}}$ is the minimum distance from the field point to one of the nodes of the element (see Figure 4-2).

2. $p_2$: the cosine of the greatest perspective angle viewed from the field point
Figure 4-3: Definitions of the lengths $a, b, c$ and $p_2 = \cos \theta/ab$. The field point is located at $(x, y, z)$. For the same element, the perspective angle $\theta$ changes as shown in (a) the closest node is 4 and in (b) the closest node is 3.

Towards the element, which is estimated by

$$p_2 = \frac{\cos \theta}{ab} = \frac{a^2 + b^2 - c^2}{2a^2b^2} \quad (4.56)$$

where the perspective angle $\theta$ and lengths $a, b, c$ are defined in Figure 4-3.

3. $p_3$: an estimated "aspect ratio" of the element, which is defined by

$$p_3 = \sqrt{(l_1^2 + l_4^2)/(l_2^2 + l_3^2)} \quad (4.57)$$

where $l_i, \quad i = 1, 2, 3, 4$ are the distance between four vertices as defined in Figure 4-2.

Several study cases using Stokes waves with various steepness and uniform flow past a sphere are analyzed and compared with results obtained from Romberg quadrature to estimate the required order of Gauss-Legendre quadrature. For definiteness, we describe the adaptive numerical quadrature for evaluating influence functions with an accuracy of $0.5 \times 10^{-4}$.

The computation for $p_1$ is straightforward. For a given time moment, the grid is fixed. Thus $l_i \quad (i = 1, 2, 3, 4)$ and $p_3$ need to be evaluated only once at each time step and can be used for all field points. For a given element, most collocation points are
located at a distance greater than its character dimension away from the element, i.e. $p_1 > 1$. In this case, the order of quadrature is determined by

$$
\nu = \begin{cases} 
2, & \text{if } p_1 > 144, \\
3, & \text{if } 16 < p_1 \leq 144, \\
4, & \text{if } 4 < p_1 \leq 16, \\
5, & \text{if } 1 < p_1 \leq 4.
\end{cases} \tag{4.58}
$$

No subdivision is needed.

$p_2$ needs to be evaluated only if $p_1 \leq 1$. Since $\theta \in [0, \pi]$, $p_2 \in [-1, 1]$, we first determine the local nodal number which is the closest to the field point $z_i$ (this information has been stored when $p_1$ is calculated), then the maximum dimension $c$ of the element viewed at $z_i$ is defined as the maximum distance between any two nodes observed at $z_i$. The possibility that the distance between two points on the element surface other than nodes may be greater than the calculated $c$ is not important because $p_2$ is meant to be an estimate. In fact, if this is true, the grid is usually too coarse (not admissible based on Definition 1 in Section 4.2).

If $p_2 < 0.5$, the domain of the element is subdivided into $m_1 \times m_2$ subregions. The subdivision is made so that the “aspect ratio” of subelements can be close to unity. One way of doing this is given below

$$
\begin{cases} 
m_1 = \text{int}[2p_3], & m_2 = 2, \\
m_1 = 2, & m_2 = \text{int}[2p_3],
\end{cases} \quad \text{if } p_3 > 1; \quad \text{if } p_3 < 1, \tag{4.59}
$$

where $\text{int}[p]$ denotes the integer part of $p$. Note that $p_3$ is also used to determine the parametric direction in which the element is elongated. To be consistent with the notation in (4.55), the subelements are denoted by $E^{(k,l)}_{j}$ where $k \in [1, m_1]$ and $l \in [1, m_2]$. Let the node which is the closest to the field point be $n_s$ and, denote
Figure 4-4: Subdivisions of the domain of an element when a field point \((x, y, z)\) is nearby. Here the domain is divided into 6 subelements. \(n_*\) is node 4.

those subelements which include \(n_*\) by a set \(E_j^{*}\), then

\[
\nu = \begin{cases} 
5, & \text{if } E_j^{(k,l)} \in E_j^{*}, \\
4, & \text{otherwise}
\end{cases}
\]  

(4.60)

The subdivision is illustrated in Figure 4-4.

If \(p_2 \geq 0.5\), no subdivision is needed. The order of quadrature can be determined by

\[
\nu = \text{int}[(0.0083p_2 - 0.0036)p_2 - 0.7119)p_2 + 7.90]
\]  

(4.61)

with maximum \(\nu = 8\) for all \(p_2\). The adaptive algorithm described above is summarized in Section 4.6 along with the algorithm for evaluating the self-influences described in the next section.

### 4.5.2 Evaluation of self-influences

Since we collocate at nodal points, the self-influences at nodes of the element are considered in this section. If the potential or its gradient at an arbitrary point on the boundary surface is needed, the generalization of the algorithm developed here is straightforward. The only complication is that the parametric location \((s, t)\) for given \((x, y, z)\) has to be solved for.

Even though there are special quadratures for integrating singular integrals with a \(1/r\) type of kernel (e.g. Cristescu & Loubignac 1978, and Pina, Fernandes & Brebbia,
we prefer to analytically remove the $1/r$ singularity from the integrands in (4.12) and (4.13) for robustness.

It is well-known that in the parametric space $(s,t)$ both ordinary polar coordinate and the degenerate triangle mapping (also called triangle polar coordinate transformation) can be used to reduce the order of a $r^{-k}$ type of singularities by one. This technique has been most widely used in the analysis of elastostatics and plasticity (e.g. Lachat & Watson 1976, and Li, Han & Mang 1985). Recent applications of the regularization techniques for potential flow computations in frequency-domain can be found in Liu & Lu (1988) and Chau (1989). The detailed descriptions of the ordinary polar coordinate transformation for the ‘serendipity’ elements can be found in Lachat & Watson (1976) and Liu & Lu (1988), whereas the formulation of the degenerate triangle mapping is presented by Li, Han & Mang (1985). Zhang & Xu (1989) have given a class of general mapping for $r^{-k}$ type of singularities, which contains the degenerate triangle mapping as a special case.

To evaluate the singular elemental integrals in the present study, both coordinate transformations are implemented and, the resulting integrals are evaluated by standard Gauss-Legendre quadrature. In terms of the convergence of quadratures, it is found that the two transformations are equally effective. In fact, it can be shown analytically that for the double integrals the transformed quadrature points differ only in one parametric direction. For the convenience of domain subdivision, the degenerate triangle mapping is selected in the present computations.

Consider a plane triangular domain $T$ in three dimensions with three vertices located at $V_1(x_1)$, $V_2(x_2)$ and $V_3(x_3)$. Suppose an integrand $F$ has an $1/r$ type of singularity at $V_1$. The degenerate triangle mapping is defined by

$$
\mathbf{x} = (1 - \rho_1)\mathbf{x}_1 + \rho_1(1 - \rho_2)\mathbf{x}_2 + \rho_1\rho_2\mathbf{x}_3
$$

(4.62)

where $\rho_1$ and $\rho_2$ are the triangle polar coordinates. The image of the triangle domain in $(\rho_1, \rho_2)$ space $T'$ is a unit square. The images of the vertices $V_i$s are denoted by $V'_i$.
Figure 4-5: The degenerate triangle mapping maps the triangular domain $T$ into a unit square $T'$.

respectively. The singular point $V_1$ corresponds to the side $\overline{V''_1V'_1}$ of $T'$. Figure 4-5 illustrates the mapping.

Recall a curvilinear element $E_j$ is approximated by the isoparametric interpolation (4.4) over the square domain $E_j(s,t)$ as shown in Figure 4-1. If the self-influence at one of the nodes which define the element is considered, the parametric integral domain $E_j(s,t)$ can be triangularized so that every triangle has one and only one vertex which coincides with the singular point. The possible triangulation is illustrated in Figure 4-6. Then, each triangle domain can be mapped into a square by relation (4.62) with $s$ and $t$ replacing $x$ and $y$ respectively. The advantage of this mapping is that the $1/r$ type of singularity can be analytically removed from the expressions of the integrands in $(\rho_1, \rho_2)$.

Let the collocation point be node $k$ ($k = 1, 2, \cdots, 9$). The properties of the mapping (4.62) has been described by Li, Han & Mang (1985) and Zhang & Xu (1989). From those properties, it can be shown that after introducing mapping (4.62), the interpolation functions in (4.3) can be expressed as

$$N_m = \begin{cases} 
1 + \rho_1 H_m(\rho_1, \rho_2) & \text{if } m = k \\
\rho_1 H_m(\rho_1, \rho_2) & \text{if } m \neq k
\end{cases}$$  

(4.63)

where $m = 1, 2, \cdots, 9$ and auxiliary functions $H_m$ are nonzero at $\rho_1 = 0$. Substituting
Figure 4-6: Triangulation of the integral domain $E_j(s,t)$ for collocation (a) at corners ($\kappa = 2$); (b) at side nodes ($\kappa = 3$); (c) at the center ($\kappa = 4$).

(4.63) into (4.36), we have

$$x_h - x = x_i - \sum_{m=1}^{9} N_m x_m = -\rho_1 \sum_{m=1}^{9} H_m x_m = \rho_1 X(\rho_1, \rho_2).$$  \hspace{1cm} (4.64)

Similarly, we have

$$y_h - y = \rho_1 Y(\rho_1, \rho_2),$$ \hspace{1cm} (4.65)

$$z_h - z = \rho_1 Z(\rho_1, \rho_2)$$ \hspace{1cm} (4.66)

with

$$X(\rho_1, \rho_2) = -\sum_{m=1}^{9} H_m x_m.$$ \hspace{1cm} (4.67)

Therefore, the distance from an arbitrary point $\mathbf{x}(s,t)$ on the interpolated element surface to the singular point $\mathbf{x}_h$ can be expressed by

$$r = \rho_1 R(\rho_1, \rho_2)$$ \hspace{1cm} (4.68)

where

$$R(\rho_1, \rho_2) = \sqrt{X^2(\rho_1, \rho_2) + Y^2(\rho_1, \rho_2) + Z^2(\rho_1, \rho_2)}.$$ \hspace{1cm} (4.69)
The components of the normal vector of the element (4.8) can be written as
\[ j_i = j_i(s(\rho_1, \rho_2), t(\rho_1, \rho_2)), \quad i = 1, 2, 3. \] (4.70)

The differential area can be written as
\[ dS = J(s(\rho_1, \rho_2), t(\rho_1, \rho_2)) ds(\rho_1, \rho_2) dt(\rho_1, \rho_2) \]
\[ = J(\rho_1, \rho_2) J_\mu(\rho_1, \rho_2) d\rho_1 d\rho_2 \] (4.71)

where \( J \) is the Jacobian defined in (4.9) and
\[ J_\mu = 2 \rho_1 A_\mu \] (4.72)

with \( A_\mu \) the area of the \( \mu \)-th triangle in \((s, t)\). See Figure 4-6 for the triangulation.

Finally, substituting the results above into the influence function in (4.12), we have
\[ S_m^{(j)} = \frac{1}{2} \sum_{\mu=1}^{\kappa} \int_0^1 \int_0^1 \frac{N_m(\rho_1, \rho_2) J(\rho_1, \rho_2) A_\mu}{R(\rho_1, \rho_2)} d\rho_1 d\rho_2 \] (4.73)

where \( m = 1, 2, \ldots, 9 \) and the number of triangles \( \kappa \in [2, 3, 4] \) correspond to collocation on a corner node, side node or center node, respectively. Similarly, if \( m \neq k \), we can rewrite (4.13) as
\[ D_m^{(j)} = \frac{1}{2} \sum_{\mu=1}^{\kappa} \int_0^1 \int_0^1 \frac{K(\rho_1, \rho_2)}{R_\mu(\rho_1, \rho_2)} H_m(\rho_1, \rho_2) J(\rho_1, \rho_2) A_\mu d\rho_1 d\rho_2 \] (4.74)

and if \( m = k \), it becomes
\[ D_m^{(j)} = \frac{1}{2} \sum_{\mu=1}^{\kappa} \int_0^1 \int_0^1 \frac{K(\rho_1, \rho_2)}{\rho_1 R_\mu(\rho_1, \rho_2)} [1 + \rho_1 H_m(\rho_1, \rho_2)] J(\rho_1, \rho_2) A_\mu d\rho_1 d\rho_2 \] (4.75)

with function \( K(\rho_1, \rho_2) = j_1 X(\rho_1, \rho_2) + j_2 Y(\rho_1, \rho_2) + j_3 Z(\rho_1, \rho_2) \). The integrand in (4.75) has a \( \delta_0 \) type indeterminacy as \( \rho_1 \to 0 \). The expressions for this integrand in terms of \( \rho_1 \) and \( \rho_2 \) are lengthy and there are 24 different cases to be considered!
Figure 4.7: Sub-triangulation of \( E_j(s,t) \) for collocation (a) at corner nodes; (b) at side nodes. Note that \( p_2 \) is computed in the physical space, but sub-triangulation is done in \((s,t)\) space for simplicity.

Fortunately, these integrals are not needed because they will be cancelled exactly by the same terms in the expression for solid angles (4.15).

Since the integrands in (4.73) and (4.74) are regular functions, Gauss-Legendre quadrature can be used with a linear mapping \( \rho_i = (\tau_i + 1)/2, \tau_i \in [-1,1], i = 1,2 \).

A numerical detail worth mentioning here is that for the same accuracy the order of quadrature required for integrating \( D_m^{(j)} \) is always higher than that for \( S_m^{(j)} \). This is not surprising because the integrand in \( D_m^{(j)} \) is more complex. To reduce the order of quadrature and thus reduce the requirement for the smooth high order derivatives of the integrand for \( D_m^{(j)} \), we further subdivide the triangles in \((s,t)\) space and then treat the resulting sub-triangles with the same degenerate triangle mapping.

Define the included angle at the singular point of the triangle subdomain in the physical space by \( \theta \) (see Figure 4.7). This angle can be estimated in the same manner as that for \( p_2 \) defined by (4.56). These \( p_2 \) parameters need be evaluated only once for a given grid. If \( p_2 < 0.15 \), the triangle is further subdivided. The number of this sub-triangulation is adaptively determined by

\[
m_3 = \text{int}[2p_2].
\]  

(4.76)

With this sub-triangulation, the fourth order quadrature for each sub-triangle suffices
to give the required accuracy of $3.5 \times 10^{-4}$. Figure 4-7 illustrates this idea for two special cases. This sub-triangulation greatly enhances the robustness of the present adaptive algorithm for elements with aspect ratio $p_3 \leq 30$.

If $p_2 \geq 0.15$, no sub-triangulation is necessary. The order of quadrature can be determined by

$$
\nu = \text{int}[((6.059p_3 - 5.768)p_2 - 4.711)p_2 + 9.629]
$$

(4.77)

with maximum $\nu = 8$ for all $p_2$.

When three nodes on one side of the quadrilateral coincides, a seven-node curvilinear triangle element results. The isoparametric interpolation is still defined in this case. Numerical results for influence functions compared with those obtained by the regular six-node quadratic curvilinear triangle element confirm that the present adaptive algorithm can still be used without loss of accuracy.

### 4.6 The vectorized algorithm

The present Laplace solver using the BEM based on bi-quadratic isoparametric elements is completed by adding an iterative solution scheme for the resulting system of linear equations (time stepping will be introduced in Section 4.10). Based on the feasibility studies in Chapter 3, the GMRES iterative solver with SSOR preconditioner is preferred. The original program was developed on a workstation computer and was highly modularized. With three-dimensional high resolution computations in mind, it is necessary to take advantage of modern fast vector-processors such as Cray computers. The vectorized implementation of the present adaptive algorithm is summarized in Table 4.1. The SSOR preconditioned GMRES algorithm is also vectorized. Table 4.2 compares the performance of the sequential program with that of vectorized one. The data in Table 4.2 are from a test run of Chapter 6, which simulates wave sloshing inside a three-dimensional wave tank. The number of unknowns used was $N = 550$. The CPU time is an averaged quantity over several time steps.
(1) Discretize all boundary surfaces into quadrilaterals, setup connectivity matrix for elements, identify the boundary condition imposed on each element.

(2) for each element, compute and store $l_i$ ($i = 1, 2, 3, 4$), $p_2$ and $p_2$ for self-influence.

(3) for $j$-th element ($j = 1, 2, \ldots, N_e$) do begin
for $i$-th field point ($i = 1, 2, \ldots, N$) do begin
if $p_1 > 1$ then,
determine $\nu$ by (4.58), sort $x_i$ according to $\nu$ for collective evaluation;
else if $p_1 > 0$ then,
compute $p_2$,
if $p_2 < 0.5$ then,
subdivide $E_j$, determine $m_i$ and $\nu$ by (4.59) and (4.60);
else,
compute $\nu$ by (4.61),
end if.
else,
triangularize $E_j$;
if $p_2 < 0.15$ then,
sub-triangularization according to (4.76),
else,
no sub-triangularization, $\nu$ given by (4.77),
end if.
compute self-influence functions,
end if.
end do.
compute far field influences collectively for sorted $x_i$;
assemble the influence of the $j$-th element into the global matrix and vector;
end do.

(4) impose boundary conditions, matrix condensation.

(5) solve the linear system by GMRES scheme with SSOR preconditioner.

(6) velocity computation, postprocessing.

Table 4.1: The vectorized algorithm for Laplace problems.
<table>
<thead>
<tr>
<th>Implementation</th>
<th>CPU (sec.)</th>
<th>$\beta$</th>
<th>MFLOPS</th>
<th>Work</th>
</tr>
</thead>
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<tr>
<td>sequential</td>
<td>37.5</td>
<td>$0.122 \times 10^{-3}$</td>
<td>13.8</td>
<td>517.5</td>
</tr>
<tr>
<td>vectorized</td>
<td>2.0</td>
<td>$0.661 \times 10^{-6}$</td>
<td>81.1</td>
<td>162.2</td>
</tr>
</tbody>
</table>

Table 4.2: Averaged overall performance of the present Laplace solver.

The vectorized algorithm achieved a speedup in time of 19 for a reasonably large $N$. Since the effort of the present Laplace solver is quadratically proportional to $N$, the CPU time can be expressed as $\beta N^2$, where $\beta$ is an estimate of the constant coefficient. From Table 4-2 of Ölmez (1991), the vectorized CPM takes 6 seconds on a Cray-2 supercomputer\(^1\) to solve a three-dimensional Laplace problem with $N = 1325$, which translates to $\beta = 0.342 \times 10^{-5}$. Suppose the CPM's performance is unchanged on a Cray Y-MP. Based on these bench marks, for solving the same Laplace problem with the same number of unknowns, CPM requires less efforts than those required by the present method, but gives less accuracy. Considering the improved accuracy (see the convergence studies below), the present numerical method is very “cost effective”.

The MFLOPS (Million floating point operations per second) rate is a measure of the efficiency of the program\(^2\). MFLOPS rate of 81 reflects that the code is reasonably optimized. The floating point workload is defined as the product of CPU time and the MFLOPS rate. Notice the vectorized algorithm also reduces the workload by a factor of 3, which means that if the examples had been run on a scalar machine, there would have been only a speedup of 3. (Test runs on a workstation confirmed this prediction. The savings are apparently from reduced overhead of subroutine calls).

In average, approximately 90% of the CPU time of the vectorized code is used for computing the influence functions. Since computations of influence functions can be carried out concurrently, multi-tasking on a multi-processor computer may be used to reduce the total CPU time by a factor in proportion to the number of CPUs used. However, on a multi-user time-sharing supercomputer, multi-tasking is very

\(^1\)The Cray-2 has a per processor speed of 88 MFLOPS versus the YM-P's 333 MFLOPS.

\(^2\)According to the guideline of Pittsburgh Supercomputing Center, a MFLOPS rate above 20 is acceptable.
difficult to implement. Another possibility of accelerating the algorithm is, of course, to parallelize it to use massively parallel-processors such as a Connection Machine. Unlike the vectorization, parallel-processing is computer-system dependent, which will effect the portability of the program. Therefore, further improvement of the vectorized algorithm in this direction is not pursued presently.

4.7 Convergence studies

To study the convergence properties of the present Laplace solver, we again considered the problem of uniform flow past a sphere. As has been mentioned in Section 3.3, we assume the onset flow is in negative \( z \) direction, and both the speed of the flow and the radius of the sphere are unity. The exact solution of this problem is given in (3.7). The exterior Neumann problem and mixed Dirichlet/Neumann problem are solved by the present Laplace solver. For the Neumann problem, we assume the far field potential is zero for the uniqueness of the solution. For the mixed problem, the fore-hemisphere \((x > 0)\) is again posed as the Neumann boundary and the aft is Dirichlet boundary.

For comparison, we solve aforementioned two problems by using the present bi-quadratic boundary element method (QBEM) and also by using CPM (with the same grids). The numerical results of the convergence studies are shown in Figure 4-8 and 4-9. The relative error is defined as the absolute error normalized by the magnitude of the field function, which is 0.5 for \( \phi \) and 1 for \( \phi_n \). As shown in Figure 4-8, for the exterior Neumann problem the rate of convergence of QBEM is quadratic, whereas the convergence of CPM is linear. As has been pointed out by many analysts (e.g. Hess 1975, and Wagner 1987), CPM enjoys a favorable error cancellation mechanism when applied to solve a Neumann problem with convex boundary surfaces. In spite of this, the present numerical results clearly indicate that QBEM is more accurate than the CPM for the same number of unknowns \( N \). To be specific, suppose an accuracy of \( 10^{-3} \) for the solution is required. From the maximum error curves in Figure 4-8,
Figure 4-8: Convergence studies of QBEM and CPM for solving the exterior Neumann problem on a unit sphere. $N$ is the total number of unknowns. The solid line and * denote (arithmetically) averaged and maximum relative errors due to QBEM, whereas dashed line and + corresponds to (arithmetically) averaged and maximum relative errors due to CPM, respectively.
Figure 4-9: Convergence studies of QBEM and CPM for solving the exterior mixed Dirichlet/Neumann problem on a unit sphere. Legends are defined in Figure 4-8.

we estimate the required number of unknowns $N \approx 150$ if QBEM is used, $N \approx 2000$ if CPM is used. From the coefficient $\beta$ evaluated for both methods in the last section, we get

$$
\frac{CPU_c}{CPU_q} = \frac{\beta_c}{\beta_q} \left( \frac{N_c}{N_q} \right)^2
= \frac{0.342}{0.661} \left( \frac{2000}{150} \right)^2
\approx 92.0
$$

(4.78)

where subscripts $q$ and $c$ designate the quantities for QBEM and CPM respectively. Hence, for an accuracy of $10^{-3}$, the vectorized QBEM is over 90 times more efficient than the vectorized CPM.

As seen in Figure 4-9, for the mixed Dirichlet/Neumann problem, the quadratic convergence of the present method is preserved, whereas the maximum error due to
Figure 4-10: Definition of coordinates for the prescribed three-dimensional Laplace problem in a rectangular domain.

CPM converges noticeably slower (also see Figure 3-4). For \( N \approx 500 \), the maximum error due to QBEM is \( \mathcal{O}(10^{-4}) \), whereas that due to CPM is \( \mathcal{O}(10^{-2}) \). Another advantage of QBEM is that its error is more evenly distributed than that of CPM, which is reflected in a much smaller difference between the maximum and averaged errors.

In Section 3.3, it has been shown that the errors due to CPM does not converge when boundary surface does not possess a continuous derivative across the Dirichlet/Neumann intersection line. To further investigate the convergence features of the QBEM for solving an interior mixed Dirichlet/Neumann problem, we study the prescribed problem which is the three-dimensional analogue of the two-dimensional prescribed problem studied in Section 3.2.

We choose the velocity potential corresponding to the solution of linearized wave equations in three dimensions as the harmonic field function and define a three-dimensional rectangular domain with a prescribed wavy top surface (see Figure 4-10).
Again, we analytically extend the definition of $\phi$ to $z > 0$, viz.

$$\phi = \frac{a \omega}{k} e^{kz} \sin(k_x x + k_y y)$$  \hspace{1cm} (4.79)

with

$$k = \sqrt{k_x^2 + k_y^2}, \quad \omega = \sqrt{gk}, \quad g = 1.$$  \hspace{1cm} (4.80)

The "free surface" is prescribed by

$$\zeta = a \cos(k_x x + k_y y)$$  \hspace{1cm} (4.81)

The prescribed boundary value problem mimics the problem to be solved at a fixed time moment of the nonlinear waves inside a rectangular tank. Since the exact solution of this prescribed problem and all boundary geometries are known, we can analytically calculate all quantities of interest. On the wavy top surface we specify the exact potential $\phi$. On the rest of the boundary, we prescribe the exact normal flux $\phi_n$. After solving the problem, the error on the Dirichlet boundary is obtained by comparing the solution against the analytically calculated normal flux. The error on the Neumann boundaries is obtained by comparing the solved $\phi$ with that prescribed potential in (4.79). All errors are normalized by the magnitudes of the field variables. As shown in Figure 4-11, the slopes of all error curves are greater than unity, which indicates the convergence rate is greater than linear. The maximum error on the Dirichlet boundary usually appears near the edges. Another calculation using CPM again gives non-convergent errors just like that in Figure 3-5, which is not surprising.
Figure 4-11: Convergence studies of QBEM for solving the interior mixed Dirichlet/Neumann problem on a prescribed rectangular domain. \( N \) is the total number of unknowns. Here * and the dashed line denote the maximum and arithmetically averaged relative error on Dirichlet boundary; and + and the solid line denote the maximum and averaged relative error on Neumann boundary respectively.
4.8 Computation of the velocity on an arbitrary surface

To study the kinematics of breaking waves, the accurate evaluation of the velocity components at the collocation points on the free surface is essential. In this section, our attention is focused on the development of an accurate algorithm for computing the velocities based on the nodal positions and nodal values of \( \phi \) and \( \phi_n \).

Consider a general smooth surface \( F : F(x,y,z) \in \mathbb{R}^3 \) described by an array of collocation points at \( \mathbf{w}_u, (u = 0,1,2,\ldots; v = 0,1,2,\ldots, V) \), where \( U, V \) are integers. The surface \( F \) is not necessarily single-valued in terms of \( x, y, z \). By using the subscripts \( u \) and \( v \) as the curvilinear coordinates, \( \mathbf{w} = \mathbf{w}(u,v) \) are always uniquely defined. At nodal points, \((u,v)\) correspond to integers. The normal vector of \( F \) can therefore be defined at each node by

\[
\mathbf{n}(u,v) = \frac{\mathbf{w}_u \times \mathbf{w}_v}{|\mathbf{w}_u \times \mathbf{w}_v|} \tag{4.82}
\]

with \( n = (n_x, n_y, n_z) \). Here, \( \mathbf{w}(u,v) \) is a global isoparametric representation of the surface \( F \), whereas relation (4.4) is from the isoparametric representation within an element. We can also represent the field variables in the same fashion, that is, \( \phi = \phi(u,v) \) and \( \phi_n = \phi_n(u,v) \). Thus, all derivatives with respective to \( u \) and \( v \) are also defined. Using chain rule differentiation and the definition of normal velocity, We can then write the following relations:

\[
\begin{align*}
\phi_u &= \phi_x x_u + \phi_y y_u + \phi_z z_u, \\
\phi_v &= \phi_x x_v + \phi_y y_v + \phi_z z_v, \\
\phi_n &= \phi_x n_x + \phi_y n_y + \phi_z n_z. \tag{4.83}
\end{align*}
\]

These three linear equations can be readily solved for the gradient of potential. Let
the coefficient matrix be $Q$.

$$Q = \begin{bmatrix} x_u & y_u & z_u \\ x_v & y_v & z_v \\ n_x & n_y & n_z \end{bmatrix}.$$  
(4.84)

Hence, we obtain the following expression

$$\nabla_{xyz} \phi = Q^{-1} \nabla_{uvw} \phi$$  
(4.85)

where $\nabla_{xyz} \phi = (\phi_x, \phi_y, \phi_z)^T$ and $\nabla_{uvw} \phi = (\phi_u, \phi_v, \phi_n)^T$. Therefore, to compute the velocity components at each node, we need to evaluate the normal vector, and the derivatives of all variables with respect to $u$ and $v$.

To have a global representation of $\Phi \in (x, y, z, \phi, \phi_n)$ over the entire surface $F$ in the parametric space $(u, v)$, we may use the bi-cubic spline fit through the nodal points and then differentiate the representation. However, since only the derivatives are needed, we can directly use the local Taylor expansions of the variables at each node. Recall the polynomial representation of $\Phi$ within an nine-node element is a truncated series expansion at the center node with its coefficients approximated by the second-order finite difference (FD) formulae (see equation 4.4. If the partial derivative $\Phi_s$ or $\Phi_z$ at the center node is concerned, we can differentiate the polynomial and evaluate it at $s = t = 0$, which gives the second order FD formula. In general, we can always define a local polynomial representation at a generic node $x_{uv}$ such that it yields exact nodal values at $m \times n$ adjacent nodes around $x_{uv}$. The coefficients of this polynomial must be the finite difference formulae for the corresponding derivative in the local Taylor series. It is easy to see that the local polynomial approximation becomes a global representation as $m \rightarrow U$ and $n \rightarrow V$. In the case of a nine-node Lagrangian element, $m = n = 3$. By varying $m$ and $n$, we may study the accuracy and convergence of this isoparametric finite difference scheme (PFD). The PFD can be shifted so that the node under consideration is centered. This can always be achieved without difficulty for a periodic surface. For the nodes near the edges of
a non-periodic boundary surface, skewed finite difference formulae can be used. To offset the larger truncation error of a skewed formula, higher order formula can be used.

This algorithm allows us to compute the partial derivatives in (4.83) by making use of the existing finite difference schemes in terms of nodal values. It is therefore more efficient than the method which uses the bi-cubic spline fit. For comparison purposes, test computations are carried out using a prescribed surface geometry and field functions, viz.

\[ z = a \cos k(x + y) \quad x \in [0, \pi]; \ y \in [0, \pi] \quad (4.86) \]

and

\[ \phi = ae^{kx} \sin k(x + y). \quad (4.87) \]

\( \phi_n \) and \( n \) are calculated analytically. For the present purposes, these harmonic functions are defined everywhere.

A set of gradually increasing parameter \( ka \) is used. The PFD algorithms with different values of \( m \) and \( n \) are implemented. The accuracy of evaluated velocity components depends on the FD formulae used and the curvatures of the surface as well as the density of the elements. The selection of these parameters for the PFD scheme requires experience. Under most circumstances, if an accuracy of 3 significant digits is required, a FD formula using five or more points is necessary. The numerical results for two different choices of \((m, n)\) are summarized in Table 4.3. In this table, \( PFD_1 \) uses the 5-point FD formulae for all nodes, whereas \( PFD_2 \) uses a 5-point centered FD formula for the interior nodes and the 7-point skewed FD formulae at the edges. The errors are normalized by the magnitude of the field function. The maximum errors usually appear near the edges, where a skewed one-sided FD is used. Typically, the error at the edge is one decade greater than the averaged error of the interior nodes. Note that even though the test problem is doubly-periodic, this advantage is not exploited here since we are interested in the properties of PFD for a
<table>
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<th>24</th>
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<td>0.8</td>
</tr>
<tr>
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<td>$0.2 \times 10^{-2}$</td>
</tr>
<tr>
<td>$PFD_2$</td>
<td>$0.4 \times 10^{-3}$</td>
<td>$0.1 \times 10^{-2}$</td>
</tr>
</tbody>
</table>

Table 4.3: The maximum errors in computed velocities of the prescribed surface with given linear wave potential as the field function. The $PFD_i$s are defined in the text. e.p.w. is the number of elements per wave-length (it is the same in both horizontal directions).

general surface. Had the periodicity been used, the error distributions would have been much more uniform.

An algorithm based on bi-cubic splines is also implemented for comparison purposes. The first order derivatives of the variable at the edges are specified as the boundary conditions for the spline routine, which are computed by the skewed one-sided 6-point FD formula. Numerical computations using the same test cases as above show that the accuracy of $PFD_2$ is comparable with the bi-cubic spline based algorithm using the same discretization. In terms of efficiency, $PFD_2$ has a speed-up of 4 when more than 40 unknowns are used in each horizontal direction.

A comprehensive error analysis of the PFD scheme will enhance our understanding about the usefulness of this method and should be pursued in the future. More numerical results are presented in Chapter 5 with systematic convergence studies using the exact plane Stokes wave potential.

### 4.9 Doubly periodic problems

So far we have described an efficient and accurate numerical method for solutions of various potential problems with quadratic convergence. If a potential flow possesses spatial periodicity, the computation domain can be greatly reduced by using periodic Green functions. For definiteness, consider a free surface flow which is periodic in both $x$ and $y$ directions. We choose a computation domain which is bounded by
periodic boundaries at \( z = 0, L \) and \( y = 0, W \), a free surface on the top and a closure at \( z \to -\infty \).

The doubly-periodic Green function \( G_p(\omega, \xi) \) corresponds physically to the potential at \( \omega \) due to a \( 1/r \) singularity at \( \xi \) and its doubly periodic array of images. Mathematically, the function \( G_p(\omega, \xi) \) is the harmonic function of \( \omega \) inside the computation domain except where \( \omega = \xi \), and satisfies the periodic boundary condition

\[
G_p(x + mL - \xi, y + nW - \eta, z - \zeta) = G_p(x - \xi, y - \eta, z - \zeta).
\]  

(4.88)

Since the image singularity array is symmetric in both \( x \) and \( y \), the flux due to the \( 1/r \) singularity and its images can only have a uniform \( z \) component as \( z \to \pm \infty \). Thus, the function \( G_p \) at far field can be written as

\[
G_p = C_1|z| + o(1) \quad \text{as} \quad |z| \to \infty,
\]  

(4.89)

where \( C_1 \) is a finite constant. Clearly, the function \( G_p \) does not satisfy the far field growth condition (2.6) and (2.7). Therefore, there will be finite contributions from the integration over the far field surface in the Green's integral (2.13).

From the physical interpretation of the doubly-periodic Green function, we may write function \( G_p \) as the following double summation

\[
G_p = \frac{1}{r} + \sum_{m,n=-\infty}^{\infty} \left\{ \left[ (x + mL - \xi)^2 + (y + nW - \eta)^2 + (z - \zeta)^2 \right]^{-1/2} - \left[ (mL)^2 + (nW)^2 \right]^{-1/2} \right\} + C_2
\]  

(4.90)

with \( |m| + |n| > 0 \). The constant \( C_2 \) is required to satisfy the condition (4.89) at infinity. A direct summation of this series is uneconomical due to its very slow convergence. The effective series expansions for the regular part of the doubly-periodic Green function have been given by Newman (1991) and Briet (1991). When the image singularity is situated within a distance of one characteristic dimension of the computation domain away from the singularity, its influence must be subtracted.
out from the expansions in order for the expansions to converge. The influences of these subtracted out singularities and the self-influence are evaluated by the adaptive algorithm presented in Section 4.5.

The original expansions of Newman and Briet are derived for a channel with aspect ratio $L/W \geq 1$. By rotating the two axes in the periodic plane, the expansions can be used for a channel with $L/W < 1$. For our purpose, the expansions are modified so that it can be used for a doubly periodic domain with an arbitrary aspect ratio (practically, $0 < L/W < 20$).

The BIE for double-periodic free surface flows with finite water depth can still be expressed in the form of (2.14) and (2.15). For infinitely deep water, the BIE is given by

$$
\int \int_{S_f} \phi_n G_p dS + \int \int_{S_{\infty}} \phi G_{p,n} dS = -\alpha \phi - \int \int_{S_f} \phi G_{p,n} dS
$$

(4.91)

where $\omega \in S_f$ and $\alpha$ is the solid angle at $\omega$, and the finite part of an integral is assumed if the kernel is singular. The influence functions can still be expressed in the form of (4.12) and (4.13) by substituting $G_p$ for $G$. As mentioned earlier in this section, the function $G_p$ does not decay in the far field. For the present BIE formulation of the free surface flows, we assume, without loss of generality, that the potential $\phi$ in the far field is a constant. Then, the only non-trivial contribution from the boundary integrals at far field is the integral of normal dipoles. Because $\partial G_p / \partial n$ is a constant at infinity, the contribution of the integral to a point on the free surface is also a constant, viz.

$$
\int \int_{S_{\infty}} \phi G_{p,n} dS = C_f(t)
$$

(4.92)

where $C_f$ is a nontrivial constant. For the present computations in the time domain, $C_f$ is a function of time, which must be determined as part of the solution at each time step. Hence, when we use the BIE formulation for a doubly periodic problem, there will be one additional unknown. The Gauss condition (2.8) can be used to provide the additional equation. Therefore, no discretization at the far field closure is necessary.
Because the potential $\phi$ is assumed to be a constant in the far field, $C_f$ does not appear in the additional equation from the Guass condition (2.8). Thus, if the additional equation is added as the last equation of the system of linear equations, the diagonal entry of the last equation is zero. Since most preconditioners including the SSOR technique assume nonzero diagonal elements, the SSOR preconditioned GMRES iterative scheme cannot be directly applied to the resulting matrix. Of course, by re-arranging the sequence of the linear algebraic equations, we may translate the zero entry to an off-diagonal position. However, this modification will inevitably move at least one diagonal element of the original influence matrix to an off-diagonal position. Consequently, numerical experiments indicate that the eigenvalues of the modified matrix are clustered around the origin in the complex plane. This means that the distribution of the approximated eigenvalues of the matrix may cover a region which includes the origin. This is an undesirable feature since the GMRES iteration is sensitive to the pseudo-eigenvalues of the matrix. A simple remedy to the problem is to apply the GMRES iterative scheme to the original influence matrix with the additional equation attached at the end without the SSOR preconditioner.

Another consequence of the unbounded $G_r$ in the far field is that the expression of the interior solid angle (2.16) may need to be modified. For infinitely deep water, we have

$$\alpha = 2\pi - \int_S \phi_n dS$$

(4.93)

where finite part of the singular integral is assumed. For uniform finite water depth or doubly periodic bottom topography, expression (2.16) remains unchanged.

Finally, we mention that the numerical implementation of the evaluation of the influence functions using the doubly periodic Green function are also vectorized. The overall performance of the present numerical algorithm for doubly periodic problems achieves a MFLOPS rate of 121, which indicates the algorithm is efficiently optimized.
4.10 Time integrations and invariants

If the initial condition is given, the QBEM can be applied to simulate the nonlinear wave motion by adding a time-stepping procedure for updating the free surface geometry and potential. In this section, we describe the schemes for time integration and some invariants which can be used to examine the accuracy of the algorithm.

4.10.1 Updating free surface conditions

In a Lagrangian description, the free surface condition (2.3) and (2.4) can be integrated in time to give the free surface geometry and potential at a new time step. Two schemes can be used for this integration. In the original work of Longuet-Higgins & Cokelet (1976), the fourth order Adams-Bashforth-Moulton (ABM4) integrator started by the fourth order Runge-Kutta (RK4) scheme was used for the integration. Dold and Peregrine (1986) introduced another explicit time stepping method based on Taylor expansions in time for both the free surface position and the potential of a Lagrangian particle. In comparison with the ABM4/RK4 integrator, their method has been shown very stable in solving two-dimensional problems. However, to get the coefficients of the Taylor series, they need to solve a succession of Laplace problems for both \( \phi \) and its time derivative \( \phi_t \) at each time step. Furthermore, to achieve high order truncation error, the high order tangential derivatives in the expansions must be retained. These high order tangential derivatives are difficult to evaluate even in two dimensions. For simplicity, we adopt the ABM4/RK4 scheme. ABM4 is a predictor-corrector scheme which requires two solutions of the Laplace problems per time step, whereas RK4 is a multi-stage scheme which requires four solutions of the Laplace problems per time step.

Dommermuth & Yue (1988) have presented a linear stability analysis for the ABM4/RK4 scheme. Their results show that ABM4 is weakly unstable, whereas RK4 is conditionally stable if time step size \( \Delta_t \) and spatial spacing \( \Delta_s \) satisfy the
following condition

\[ \Delta_t^2 \leq \frac{8 \Delta_s}{\pi g}. \]  (4.94)

In addition to this condition, the time step size should also satisfy the Courant condition:

\[ \frac{c \Delta_t}{\Delta_s} < 1 \]  (4.95)

where \( c \) is the phase speed of the wave. In the present study, \( \Delta_s \) is initially selected according to the accuracy consideration. At each time step, the minimum \( \Delta_s \) is computed and \( \Delta_t \) is dynamically selected by satisfying a pre-chosen maximum Courant number \( C_n \):

\[ \Delta_t = C_n \Delta_s \ c \]  (4.96)

with \( 0 < C_n < 1 \). The selected \( \Delta_s \) and \( \Delta_t \) are then substituted into relation (4.94). If it is not satisfied, \( \Delta_t \) will be adjusted accordingly.

### 4.10.2 Checks on accuracy

This problem possesses invariants which can be used to check the global accuracy of the numerical scheme. From mass conservation, the mean water level should be a constant

\[ \bar{z} = \frac{\rho}{S_p} \iint_{S_p} \zeta \, dx \, dy = \text{const}. \]  (4.97)

with \( S_p \) the projected area of \( S \) onto the \( xy \)-plane. \( \zeta \) is the single-valued free surface profile. If the free surface is non-single-valued, we should check the mass conservation directly by computing the total normal flux over \( S \)

\[ \iint_{S} \phi_n(x, t) \, dS = 0. \]  (4.98)

The total kinetic energy can be written as

\[ E_k = \frac{\rho}{2} \iiint_{D} (\nabla \phi)^2 \, dV = \frac{\rho}{2} \iint_{S} \phi \phi_n \, dS \]  (4.99)
where Green’s theorem is used. The total potential energy is given by

\[ E_p = \frac{1}{2} \rho g \iint_{S_t} \zeta^2 c_3 dS \]  \hspace{1cm} (4.100)

where \( c_3 \) is the \( z \)-component of the direction cosine of the normal of \( dS \). If there is no input of energy into the wave system, the total energy \( E = E_k + E_p \) should be invariant. If there is a surface pressure distribution, the power input should be equal to the rate of energy increase in the fluid volume \( D \), viz.

\[ \iint_{S_t} \rho \dot{\phi} \phi_n dS = \frac{d}{dt} \left[ \frac{\rho}{2} \iint_{S_t} \phi \phi_n dS + \frac{1}{2} \rho g \iint_{S_t} \zeta^2 c_3 dS \right]. \]  \hspace{1cm} (4.101)

This time derivative can be easily integrated numerically to yield the total power input and to be compared with the net wave energy increase at each time step. For later numerical studies, all these invariants are computed at each time step and compared against the initial values.
Chapter 5

Numerical Results for Periodic Overturning Waves in 3D

In the previous chapter, we have described an accurate numerical scheme for solving potential flow problems in three dimensions. We have shown that the results of the present method exhibit quadratic convergence for a variety of potential problems including the mixed Dirichlet/Neumann problem with piecewise continuous boundary surfaces. We shall show that this method can also be applied to solve the fully nonlinear wave equations in three dimensions.

In this chapter, we focus on the problems with spatial periodicity in both horizontal directions. We will first establish the numerical convergence of the present method when applied to the nonlinear wave problems. This is shown by carrying out extensive numerical convergence studies using the exact potential functions and profiles of Stokes waves. To reduce the maximum errors, it is found that the grid spacing should be based on local curvatures. The remedy for removing the saw-tooth instability on a three-dimensional free surface is also prescribed. After establishing both spatial and temporal convergence of the present method, we study the overturning of a plane progressive wave using the three-dimensional formulation. By applying three-dimensional surface pressure distributions, we are able to generate three-dimensional overturning waves and to quantify the important kinematics of such waves. Distinct
Figure 5-1: Definition of the coordinate system and the dimensions of the computation domain for a double periodic problem. The origin is situated at the center of the left side periodic boundary. $x \in [0, L]$ and $y \in [-W/2, W/2]$.

characteristics of the breaking waves in three dimensions are uncovered for the first time.

5.1 Application to steady waves

The present numerical method is first tested on the simulation of steady plane progressive waves. Even though the plane wave motion can be described in two dimensions, we solve the problem in full three-dimensional space. The invariance of solutions in the transverse direction of the wave provides a necessary check on the robustness of the scheme. Before carrying out the time domain simulation, we shall investigate the spatial convergence properties of the method by comparing the solutions from systematically refined grids with the known theory. The high wavenumber instability is removed by Chebyshev smoothing.
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</table>

Table 5.1: Convergence check using an oblique Stokes wave as the initial conditions. $\epsilon = ka$ is the wave steepness. Computation domain is defined in the text. $N_w$ denotes the number of unknowns in each horizontal direction. $u$ and $w$ designate the velocity components in $x$ and $z$ directions respectively ($v = u$). $\phi_n$ is the normal velocity. $\bar{e}$ and $e_{max}$ denote the arithmetically averaged and maximum errors in the computed physical quantities, respectively.

### 5.1.1 Curvature based grid and convergence

Assume the free surface flow is periodic in both horizontal directions. We consider a computation domain having one period in each horizontal direction. Figure 5-1 defines the coordinate system and the dimensions of the computation domain for the problem. For now, we assume the water is infinitely deep for simplicity. This problem is essentially an interior Dirichlet problem with far field condition $\phi_n \to 0$ as $z \to -\infty$. The algorithm described in Chapter 4 is used for the solution of the BIEs at each time step. The time integration procedure described in Section 4.10.1 is used for time stepping.

We first consider an oblique Stokes wave propagating along the diagonal direction of a square computation domain with $L = W = \sqrt{2}\lambda$, where $\lambda$ is the wavelength,
<table>
<thead>
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<th>$u$</th>
<th>$w$</th>
<th>$\phi_n$</th>
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Table 5.2: Convergence check using a deep water unidirectional Stokes wave train as the initial condition. The computation domain has one wavelength in $x$ and one-fourth of a wavelength in $y$. Equal-spaced grids are used in this case. $N_w$ is the number of unknowns per wavelength in $x$. The number of unknowns in $y$ is $N_w/4$. Other legends are defined in Table 5.1.

<table>
<thead>
<tr>
<th>$\epsilon$</th>
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<th>$u$</th>
<th>$w$</th>
<th>$\phi_n$</th>
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Table 5.3: Convergence check with a deep water unidirectional Stokes wave train as the initial condition. The computation domain has one wavelength in $x$ and one-fourth of a wavelength in $y$. Curvature controlled grids are used. Other legends are defined in Table 5.2.
see Figure 5.1. Thus, there are two wavelengths along the diagonal. Because of the Stokes drift of the Lagrangian points, the computation domain will not remain a square with straight edges for all time. This does not pose any problems to our algorithm for evaluations of the influence functions with the double periodic Green function because we can always redefine a doubly periodic domain with straight edges centered at each collocation point.

A set of gradually increasing wave steepness $ka \in [0.1, 0.4]$ is selected for test computations. The equal-spaced grid is used in both $x$ and $y$ directions and is systematically refined to study the convergence of the QBEM. As the initial conditions, we specify the wave profile and its potential value from the calculation based on the Stokes series (Schwartz, 1974, and Dommermuth & Yue, 1988). To assess the accuracy of the spatial discretization, we compare the solved velocity components with the known theory. As shown in Table 5.1, the errors in the computed velocity field converges quadratically except for $ka = 0.4$, in which case the maximum error of the solved normal flux stagnated at about 2.3%. Notice that the finest grid for each $ka$ uses a total of 4096 unknowns on the free surface.

To analyze the error distribution, it is convenient to let the Stokes wave propagate along the $x$-axis. The numerical results of systematic test runs are listed in Table 5.2. Figure 5.2 shows a typical error distribution in $x$ of a test run for $N_w = 32$ with equal-spacing in $x$ and $y$. As seen in this figure, the maximum error always occurs near regions where the geometry or field functions have large curvatures. This observation suggests to us that the optimal grid should have a spacing distribution according to the local curvature in order to provide maximum resolution where it is most needed. By using this insight, an algorithm which distributes grid spacing according to local curvatures has been developed. Taking advantage of the two-dimensional motion of Stokes waves, we need only to optimize the grid spacing in the wave direction. This technique involves two steps: first, the local curvatures of the wave profile is calculated using equal-spaced sampling points; second, a functional of the curvature is evaluated and the grid spacings are redistributed according to the local value of the
Figure 5-2: Typical error distribution from equal-spaced grid. Here, the solid line represents the Stokes wave profile with $ka = 0.4$ and wavelength $2\pi$; the dash-dot line represents the potential function $\phi$; the dashed line is the exact normal flux $\phi_n$; + denotes the error in the solved $\phi_n$. 
functional. After some tests, we chose the distribution functional as the square of the curvatures. To evaluate the local curvature, we used the parametric finite difference scheme developed in Section 4.8. The formulation for generating a curvature-based grid is given in Appendix D.

Table 5-3 summarizes the results of the present spatial convergence studies using the curvature based grid. In comparison with the results in Table 5-2, the improved convergence at $ka = 0.4$ is significant. The overall convergence rate is now clearly quadratic for all the wave steepnesses tested. In principle, the concept of a curvature-based grid can be generalized to three dimensions because the curvature for a three-dimensional curve is well-defined. In all the convergence test runs above, the solved $\phi_n$ and evaluated velocity fields are also confirmed to be invariant in the transverse direction of the waves up to the specified accuracy.
Figure 5-3: The saw-tooth instability occurred during the simulation of Stokes wave with $ka = 0.4$ at $t = 1.323T$. The solid line is the exact Stokes wave profile; + represents the solved position of the Lagrangian particles with $N_w = 32$. Curvature based grid is used.

5.1.2 Removal of instabilities

In almost all numerical studies using the MEL method, saw-tooth instabilities were observed. In the original work of Longuet-Higgins & Cokelet (1976), the 5-point Chebyshev smoothing formula was used to remove the instabilities. Dommermuth & Yue (1987a) postulated that a root cause of the instabilities was due to the concentration of Lagrangian particles near the regions of high velocity, so that for a fixed $\Delta_t$ the local Courant condition was violated. Thus, they adopted a regridding algorithm to control the minimum spacing, which redistributes the Lagrangian particles with equal-arclength between them. In their study of the axisymmetric problem, the regridding idea was successful. Nevertheless, the regridding method reduces the resolution in regions of high curvatures such as near the jet of a overturning wave. Thus, for the
simulation of deep-water plunging breakers (Dommermuth & Yue, 1983), they found that a smoothing was necessary near wave breaking. In the dissertation of Ölmez (1991), FFT technique was used to filter out high-wavenumber instabilities by taking advantage of equally spaced grid points in both horizontal directions in his Eulerian formulation.

The saw-tooth instability also occurred near wave crests in the present three-dimensional computations of Stokes waves with \( ka = 0.4 \) (see Figure 5-3). In order to see the effects of numerical error on the saw-tooth instability, we carry out simulations of the Stokes wave \( (ka = 0.4) \) using \( N_w = 32 \) (16 quadratic elements per wave length) and, the maximum Courant numbers for the dynamic time step control are kept at 0.6 and 0.3. If equal-spaced grid points are used, the instability occurs near wave crest at about \( t = 0.6T \), where \( T \) is the wave period. If grid spacing is distributed according to local curvatures, the instability occurred at about \( t = 1.3T \) as shown in Figure 5-3. As we have seen in the convergence studies above, the curvature based grid has a smaller maximum error near the wave crest than the equal-spaced grid. The fact that the onset of saw-tooth instability is delayed when the curvature-based grid is used and the fact that saw-tooth always first occurs near wave crests where numerical errors are near maximum, clearly indicate that the instability is related to the growth of higher modes in numerical errors. The fact that the saw-tooth instability occurred while the maximum Courant numbers are kept at 0.6 and 0.3 in the present computations suggests that the Courant condition may not be a root cause of the instability. On the other hand, the present results support Dommermuth & Yue's (1987a) conjecture that the cause of the saw-tooth instability is numerical rather than physical. In Figure 4-d of Longuet-Higgins & Cokelet (1976), the saw-tooth instability was relatively speaking more evenly distributed along the wave. This shows that their solution scheme has a more evenly distributed error.

In fact, for a non-dissipative nonlinear system such as the fully nonlinear wave equations being solved, harmonics of all frequencies will be present eventually if computation is carried out long enough. This is true regardless what initial condition is
Figure 5-4: Transfer functions of different smoothing formulae. The solid line and dashed line correspond to the 5-point and 7-point Chebyshev smoothing formula, respectively; dash-dotted line corresponds to the 5-point least-square formula. The frequency is in radians.

used. Due to the nonlinearity and the aliasing effect of numerical grids, the Fourier mode with wavelength equal to 2Δ*, grows the fastest if no smoothing/filtering is introduced to remove it.

In the present formulation, because the Lagrangian points are subject to motions and therefore not always equally spaced, a filtering technique using FFT is not the most convenient. In order to remove the saw-tooth instability, we test three smoothing formulae in the parametric space for x, y, z and φ on the free surface. These formulae include the 5-point least-square smoothing formula (Hamming, 1973)

\[
\tilde{y}_j = \frac{1}{35}(-3y_{j-2} + 12y_{j-1} + 17y_j + 12y_{j+1} - 3y_{j+2})
\]  

(5.1)

and the 5-point Chebyshev smoothing formula (Hamming, 1973 and Longuet-Higgins
\[ \bar{y}_j = \frac{1}{16} (-y_{j-2} + 4y_{j-1} + 10y_j + 4y_{j+1} - y_{j+2}) \]  \hspace{1cm} (5.2)

as well as the 7-point Chebyshev smoothing formula (Longuet-Higgins & Cokelet, 1976)

\[ \bar{y}_j = \frac{1}{32} (-y_{j-3} + 9y_{j-1} + 16y_j + 9y_{j+1} - y_{j+3}) \]  \hspace{1cm} (5.3)

For all these smoothing formulae, we apply them in an alternating-direction manner in the \( s \) and \( t \) directions.

The smoothing technique is equivalent to a filtering in the frequency domain. In order to analyze effects of the smoothing formulae, it is useful to obtain their frequency transfer functions. The transfer functions corresponding to equation (5.1) and (5.2) were given by Hamming (1973). For (5.1), the transfer function is

\[ H_1(\omega) = \frac{1}{35} (17 + 24 \cos \omega - 6 \cos 2\omega) \], \hspace{1cm} (5.4)

and for (5.2), the transfer function is

\[ H_2(\omega) = \frac{1}{8} (5 + 4 \cos \omega - \cos 2\omega) \]. \hspace{1cm} (5.5)

Following Hamming (1973), we substitute the Fourier mode \( y_j = e^{i\omega j} \) into (5.3) and obtain its transfer function

\[ H_3(\omega) = \frac{1}{16} (8 + 9 \cos \omega - \cos 3\omega) \]. \hspace{1cm} (5.6)

The effects of these functions on the spectrum are of course given by \( H_j^2, j = 1, 2, 3, \) and the results are plotted in Figure 5-4. From this figure, it is clear that the 5-point least-square formula is not good for filtering out high-frequency harmonics, whereas the 7-point Chebyshev smoothing formula takes out more energy from waves than the 5-point one. Therefore, we choose the 5-point Chebyshev smoothing formula for all
of our three-dimensional computations. By using this smoothing formula every 3 or 6 time steps, we are able to simulate the steady Stokes wave for several wave periods without suffering from the saw-tooth instability. Figure 5-5 compares the computed wave profiles with the steady wave profile calculated from the Stokes series at $t = 2T$ and $t = 3T$. In this test computation, only 16 elements were used per wavelength and the maximum Courant number $C_n$ was kept at 0.8. In order to secure an acceptable accuracy and convergence, these values of the parameters represent a coarse spatial and temporal resolution for the present method. In spite of this, the comparison is still satisfactory. Typically, after each application of smoothing, the change of total wave energy is $\mathcal{O}(10^{-4})$. The results obtained by using smoothing every 3 and every 5 time steps is virtually indistinguishable. We have also carried out similar simulations for oblique Stokes waves. No significant difference from the results above is found.

5.2 Overturning of plane progressive waves

After the numerical convergence studies in the previous sections, we now apply the present numerical method to study unsteady waves. From available two-dimensional results, two kinds of initial conditions are usually used in simulating the wave overturning. The first kind uses the exact solution of a plane progressive Stokes wave as the initial condition and applies an initial surface pressure distribution to raise the wave energy (e.g. Longuet-Higgins & Cokelet, 1976). The second kind uses the linear Airy solution for a sinusoidal wave with large $ka$ as the initial condition (e.g. Cokelet, 1977, Vinje & Brevig, 1980). In the latter case, the linear potential defined for $z \leq 0$ is extended to $z > 0$ and evaluated on the linear wave surface. The difference between the linear initial condition and the exact one can be considered as an initial impulsive pressure distribution on the water surface, which causes the subsequent overturning. Even though the final wave profiles may look plausible, this kind of initial condition is theoretically less sound and experimentally less feasible in comparison with the first kind of initial condition. Therefore, in the present study, we choose to use the
Figure 5-5: Comparison of the computed profiles of a steady wave (denoted by *) and those obtained from Stokes' series (smooth line) with $ka = 0.4$, (a) at $t = 2T$; (b) at $t = 3T$. Using $N_w = 32$, 5-point smoothing every 3 time steps, $C_n = 0.8$. The agreement of the two wave profiles is remarkable.
approach of applying a two- or three-dimensional initial surface forcing to the fundamental plane Stokes waves and let the wave propagate freely afterwards. In this section, we focus on the application of the present method to the plane overturning waves. Since the wave motion is two-dimensional, we can use much fewer elements in the transverse direction than those in the wave direction. Secondly, we may compare results with those of earlier studies on two-dimensional overturning waves.

For the spatial discretization, the grid spacing are distributed according to the local curvatures as described in Section 5.1.1. The maximum value of time step size $\Delta t$ should be selected from the considerations of stability and convergence. In Section 4.10.1, we establish two conditions (4.94) and (4.96) for the selection of $\Delta t$ based on considerations of stability. In general, the condition (4.96) with the Courant number $C_n \in (0,1)$ is more restrictive. Since there is no rigorous theoretical framework for determining the appropriate Courant number, we carry out a numerical convergence study of the present method on the plane overturning waves resulting from the following initial surface pressure distribution

$$p_f = \begin{cases} p_0 \sin t \sin(x - ct) & \text{if } 0 \leq t \leq \pi \\ 0 & \text{if } t > \pi \end{cases} \quad (5.7)$$

where $c$ is the phase speed of the Stokes wave. We choose $p_0 = 0.146$ which corresponds to the fourth case studied by Longuet-Higgins & Cokelet (1976). For the initial condition, we choose a plane Stokes wave with $ka = 0.4$, which is approximately 90% of the theoretical limit for Stokes waves.

In order to study the convergence with respect to smoothing and temporal discretization, we selected three different test cases as listed in Table 5.4. The dimensionless computation domain has one wavelength in $x$ $(2\pi)$ and unity in $y$.

Because of dynamic time stepping, interpolations would have been needed to obtain the results at exactly the same time moment. For simplicity, we select one time step from each case which is the closest to $t = 4.75$ for comparison purposes. As can be seen in Table 5.5, all global invariants are convergent up to two decimal places.
<table>
<thead>
<tr>
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<th>((T/\Delta_t)_{max})</th>
</tr>
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Table 5.4: Study cases for temporal convergence with \( p_0 = 0.146 \). A 5-point Cheby-
shev smoothing formula is used. The second column lists the number of time steps
per smoothing. \( T \) is the wave period of the initial Stokes wave (\( ka = 0.4 \)).

Figure 5-6: Comparison of overturning wave profiles obtained from three test cases
listed in Table 5.4. The dashed line, dash-dotted line and solid line correspond to
cases 1, 2 and 3, respectively, at time \( t \) listed in Table 5.5.
<table>
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</tbody>
</table>

Table 5.5: Comparison of the wave energies and mean water position at approximately $t = 4.75$ for the three study cases. The initial mean water position is $\bar{y} = 0.0624$.

Figure 5-6 shows the comparison of wave profiles at the corresponding times for the three test cases. The agreement among the overturning wave profiles is satisfactory. Although the details of the local overturning wave jets differ few percent, the maximum difference of the computed velocity fields is only approximately 1%. These results depict the accuracy of the present numerical method in terms of resolving the details of the jet.

Figure 5-7 shows the results of accuracy checks as functions of time for Case 3. The energies are all normalized with respect to the total energy of the initial Stokes wave ($ka = 0.4$). The difference between the integrated energy input from the surface pressure distribution and the total energy increase of the wave is less than 1%. After the initial surface pressure distribution is removed at time $t = \pi$, the total energy of the wave indeed remains a constant at least up to two decimal places. The computed mean water position has also achieved the same accuracy. The corresponding results from the other two study cases are graphically indistinguishable from the results shown for Case 3. Because the Gauss condition (2.8) is imposed, the total flux vanishes identically for all times. These results indicate that the convergence for the simulation of overturning waves.

Since our initial condition and surface pressure are comparable with the fourth case studied by Longuet-Higgins & Cokelet (1976), we mention here two comparisons with their results. The height of the overturning wave crest in the present simulation

---

1The initial Stokes wave profile is calculated based on the Stokes series in a reference frame with its origin a distance $\bar{y}$ below the mean water position, where $\bar{y}$ is the mean set-down of the Stokes wave.
Figure 5-7: Normalized energies of the breaking wave and mean water position as functions of time for case 3. The dash-dot line and dotted line correspond to the kinetic and potential energy respectively. The solid line is the total energy. The dashed line is the mean water position, which should be a constant. Also see Table 5.5.
Figure 5-8: Detailed overturning wave crest at $4.6074 \leq t \leq 4.8712$ for case 3 in Table 5.4. Note that at the last time step two Lagrangian points at the tip of the jet have almost coincided with each other on the plot.

is approximately 0.70 as shown in Figure 5-8. From Figure 11 of Longuet-Higgins & Crokelet (1976), the height of the overturning crest is estimated at 0.64 in their reference frame with its origin at the mean water level. Accounting for the mean set-down of 0.0624 for the initial Stokes wave with $ka = 0.4$, the difference of the two computed heights of the overturning wave crest is estimated to be less than or of the order of 1%. The present result for the final total energy density ($E$ divided by area $LW$) is $E/E_{\text{max}} = 1.91$, where $E_{\text{max}} = 0.07403$ is the maximum energy of a Stokes wave. This is in good agreement with the final result of $E/E_{\text{max}} = 1.88$ obtained by Longuet-Higgins & Crokelet (1976).

Figure 5-8 shows close-up profiles for overturning wave in the final stage of breaking. In spite of the concentration of the Lagrangian points near the region of high curvature, the curvature of the overturning jet becomes increasingly large. This thin
wave jet causes difficulties in numerical simulations. For instance, in the final stages of the third simulation above, the smallest distance between two Lagrangian points near the tip of the wave jet is less than $10^{-4}$ before the simulation broke down. When the water surface forms such a thin jet, the collocation points at one side of the jet are so close to the elements on the other side of the jet that errors in numerical quadratures of the influence functions are likely to increase. Moreover, the calculation of surface velocity components is less accurate near the highly curved wave crest, which means the boundary conditions for the next time step are less accurate. More frequent applications of smoothing and/or reduced maximum Courant number is helpful to prolong the simulation time. Another improvement is of course to redistribute the Lagrangian points after some time so that they are not too close to each other. However, an accurate regridding scheme in three dimensions is difficult to implement.

While the high curvature and concentration of Lagrangian points near the overturning wave crests can cause loss of accuracy in computed surface velocities, we find that more often it is another type of instability that causes the computation to break down. By following one Lagrangian point near the tip of the overturning wave crest, we observe that its computed velocity components suffer from the saw-tooth instability at the later stage of overturning. As shown in Figure 5-9, the $u$ component of the velocity reaches its maximum near $t = 4.78$. A saw-tooth instability develops shortly after that. The simulation breaks down because of this instability at about $t = 4.89$. As seen in Figure 5-9, the slopes of the curves corresponding to $u$ and $w$ velocity components are increasing gradually. This clearly indicates that the overturning wave crest is undergoing an increasing acceleration. It is known that when a heavier fluid underneath a lighter fluid is accelerated downward with an acceleration greater than $g$, the interface of the two fluids will develop a Taylor instability (Taylor, 1950 and Yih, 1979). In the present case, the overturning wave crest undergoes a similar acceleration. From this point of view, it is not surprising that the evaluated velocity develops a saw-tooth instabilities since $a_z$ is more than five times greater.
Figure 5-9: Velocity components of a Lagrangian point as the function of time. The point is situated in the upper portion of the concaved side of the overturning wave crest. The solid line and dash-dotted line denote the $u$ and $w$ components respectively. The dashed line denotes the $v$ component, which is identically zero for the plane wave.
than $g$. More results on the instability are to be shown in the next section.

We mention that the convergent results in Figure 5-6 and Table 5.5 are taken approximately at $t = 4.75$ before the onset of the Taylor instability. At that instant, the maximum magnitude of the computed velocity is about twice the phase speed of the initial Stokes wave ($c = 1.0822$ for $ka = 0.4$). The magnitude of acceleration at this moment is about 5.6 times the gravitational acceleration ($g = 1$). These results are in good agreement with the results of earlier studies by Vinje & Brevig (1980), Baker et al (1982), New, McIver & Peregrine (1985) and Dommermuth & Yue (1988).

Finally, we mention that the last two wave profiles in Figure 5-8 correspond to a time moment after the Taylor instability has occurred. In spite of this, these two wave profiles still look reasonably smooth.
5.3 Three dimensional overturning waves

The three-dimensional computations carried out in the previous sections demonstrated that the present numerical method is able to simulate highly nonlinear water waves. We have shown that for steady progressive waves the method gives results in excellent agreement with the semi-analytic solution based on Stokes series for several wave periods. We have also shown that the method gives convergent results for computations of a plane overturning wave after initial surface forcing. In this section, we shall show that the present method is also able to describe accurately the three-dimensional breaking waves.

To generate a three-dimensional overturning wave, we start with a progressive two-dimensional Stokes wave but now apply a three-dimensional surface pressure distribution to raise the energy density beyond the maximum for a steady Stokes wave. As initial conditions, we shall use the same Stokes wave as that used in the convergence study above for the convenience of comparisons. For the initial surface forcing, we introduce a periodic transverse variation to the initial surface pressure distribution of form (5.7). It is assumed that the resulting three-dimensional waves will remain periodic in both horizontal directions. In particular, the following form of the three-dimensional pressure distribution is selected as the initial surface forcing:

\[
p_f = \begin{cases} 
p_0(1 + \cos 2\pi y/W) \sin t \sin(x - ct) & \text{if } 0 \leq t \leq \pi, \\
0 & \text{if } t > \pi.
\end{cases}
\]  

(5.8)

with \(x \in [0, L]\) and \(y \in [-W/2, W/2]\), where \(W\) and \(L\) are respectively the width and length of the computation domain as defined in Figure 5-1. The wavelength of the plane Stokes wave is \(L = 2\pi\). In comparison with its two-dimensional form (5.7), the additional factor provides an cosine envelope to the transverse variation with its maximum at the symmetry plane \(y = 0\) and vanishes at the periodic boundaries at \(y = \pm W/2\). The co-propagating surface pressure is gradually increased from zero at \(t = 0\), reaches its maximum at \(t = \pi/2\) and is gradually decreased to zero at \(t = \pi\).
By selecting $p_0 = 0.073$, the pressure at the center plane has the same longitudinal
distribution as the two-dimensional form (5.7).

Since both the pressure distribution and the initial condition are symmetric with
respect to center plane $y = 0$, we assume the resulting nonlinear wave motion will
be symmetric in $y$ direction. Taking advantage of this symmetry, we only discretize
half of the doubly-periodic domain $y \in [-W/2, 0]$. In order to quantify the three
dimensionality of a overturning wave, computations are performed using the following
three different width (1) $W/L = 3/2$; (2) $W/L = 1$ and (3) $W/L = 1/2$ with $L = 2\pi$.

Based on the results of convergence studies, we use 64 nodal points per wavelength
in the $z$ direction and 48 nodal points per wavelength in the $y$ direction. Because
of the symmetry, we discretize half of the double periodic domain by a $65 \times 25$ grid,
which gives 384 quadratic elements. Including the additional unknown associated
with the integrated influence of the far field, there are a total of 1601 unknowns.
We shall keep the same resolution for all three cases. The initial grid points are
distributed based on the local curvatures using the algorithm developed in Section
5.1.1. The maximum Courant number $C_n = 0.6$ is used initially for dynamic time
step control, and it is reduced to 0.4 after the surface forcing is switched off. The
5-point Chebyshev smoothing is used every 3 time-steps.

The following conventions are used for all three-dimensional plots in this disser-
tation: (1) since the wave is symmetric in $y$, only half of the domain $y \in [-W/2, 0]$ is
plotted. The coordinate system shows the orientation of the three-dimensional plots
and is translated for clarity. (2) The wave travels along the positive $z$ direction. The
intersection line of the free surface and the plane of symmetry ($y = 0$) corresponds to
the edge to the left of the wave direction, whereas the rest three sides of the domain
correspond to the periodic boundaries. (3) The color contour is used to represent the
distribution of a physical quantity such as velocity component $v$ on the free surface
at the corresponding time moment.

\footnote{The first test run using the selected initial conditions with $W = 2\pi$ was performed without assuming symmetry in $y$ to check this assumption. The wave profile up to overturning remains symmetric in $y$.}
5.3.1 For $W/L \geq 1$

Figures 5-10, 5-11 and 5-12 show the three-dimensional wave profiles as a time sequence for $W = 3\pi$. The color contour represents the distribution of velocity component $u$ at the corresponding time moment. The initial condition as shown in Figure 5-10(a) corresponds to the steady plane progressive wave with $ka = 0.4$. As seen from Figures 5-10(b) and 5-10(c), the wave height near the center plane is slowly increasing due to the surface forcing. Because the pressure decreases to zero at the edge of the computational domain ($y = -1.5\pi$), the change of wave height at the edge is small. Thus, the initial plane wave becomes three-dimensional. When the surface forcing is switched off at $t = \pi$, where the wave energy (and wave height) reaches a maximum. Figure 5-10(c) corresponds to the wave profile immediately after the pressure is removed. After that, the three-dimensional wave propagates freely.

From Figure 5-10(b) to Figure 5-12(e), it can be seen that the speed of the wave crest increases gradually from $y = -1.5\pi$ to $y = 0$, which indicates that the wave near the plane of symmetry is the most energetic where the initial surface pressure distribution is maximum. Because the crest near the center plane travels faster, this part of the wave crest plunges forward to overturn. Figure 5-12(f) shows the three-dimensional profile of the breaking wave. Up to $t = 4.8166$, the maximum of velocity $u$ has been tripled from its initial value. We mention that all results presented in this section are before the onset of the Taylor instability.

Figures 5-13(a) to 5-15(f) shows the wave profiles with the distributions of velocity $w$. The time moments of these six figures are the same as those in Figures 5-10 to 5-12. By comparing the $u, w$ velocity distributions at the initial stage with those at the overturning stage, it is apparent that the significant changes in surface velocities are near the wave crest. The ratio of maximum $u$ over maximum $w$ $(u/w)_m$ is increased from the initial value of 1.4 to 3.5 when the wave overturns. These results indicate the energy input from the surface forcing is mostly transformed into horizontal momentum of the wave.

From the time-variation of the $u, w$ velocity distributions in these two sets of
Figure 5-10: Wave profiles and distributions of velocity component $u$ for $W = 3\pi$. Only half of the domain $y \in [-W/2, 0]$ is shown since the wave is symmetric in $y$. The times are included in the figures.
Figure 5-11: As in Figure 5-10, but at different times.
Figure 5-12: As in Figure 5-10, but at different times.
Figure 5-13: As in Figure 5-10, but the contours of velocity component $w$ is plotted.
Figure 5-14: As in Figure 5-13, but at different times.
Figure 5-15: As in Figure 5-13, but at different times.
Figure 5.16: Wave profiles and contours of velocity component $v$ for $W = 3\pi$. 
Figure 5-17: As in Figure 5-16, but at different times.
plots, we can see that the large \( u, w \) values are always in the half of the domain near the center plane. This indicates that the transfer of the high local energy from the center plane to the side is slow up to the point of overturning. This is also reflected in Figures 5-16 and 5-17, which show the wave profiles with the distributions of transverse velocity component \( v \) at times before and after the wave crest overturns. Initially, velocity component \( v \) is zero everywhere. The transverse velocity at the front face of the wave is moving towards the plunger, while \( v \) at the wave crest is moving away from the tip. The region of large negative \( v \) values on the crest increases gradually. The ratio of \((u/v)_m = 20.1\) indicates that the transverse motion is much smaller than the longitudinal one. Because of the symmetry in \( y \), the velocity component \( v \) at the edges \( y = 0 \) and \( y = -1.5\pi \) must vanish as seen in Figures 5-16 and 5-17. This is true for all three cases considered in this study. Hence, the three-dimensional waves considered here correspond to the longitudinally periodic waves (in \( x \)) inside an infinitely deep wave tank with different width. The corresponding results for \( W = 2\pi \) is qualitatively similar to these results for \( W = 3\pi \). This will be evident from the results to be shown later in this section.

5.3.2 For \( W/L = 1/2 \)

Figures 5-18(a) to 5-20(i) shows a sequence of three-dimensional plots of wave profiles with the corresponding distributions of velocity component \( u \) for \( W = \pi \). Figures 5-21(a) to 5-23(i) shows the corresponding sequence of three-dimensional plots of distributions of velocity component \( w \). As can be seen from the plots, from \( t = 0 \) to \( t = 3.0136 \), the wave height near the center plane is increasing due to the surface forcing. The magnitude of \( u \) increases about 30% from its initial value. For the vertical velocity, the positive \( w \) at the crest is also increased by 30%, whereas the negative \( w \) at the trough remains almost unchanged. Like the case for \( W = 3\pi \), the magnitude of \( u \) is tripled when the wave overturns. The ratio of maximum \( u \) to maximum \( w \) increases from 1.4 initially to 3.6 at wave breaking, indicating that the increase of the horizontal momentum by the forcing is again much larger than the increase of other
Figure 5-18: Wave profiles and distributions of velocity component $u$ as a function of time for $W = \pi$. Only half of the domain $y \in [-W/2, 0]$ is shown since the wave is symmetric in $y$. The times are included in the figures.
Figure 5-19: As in Figure 5-18, but at different times.
Figure 5-20: As in Figure 5-18, but at different times.
Figure 5-21: As in Figure 5-18, but distributions of velocity component $w$ are shown as a function of time.
Figure 5-22: As in Figure 5-21, but at different times.
Figure 5-23: As in Figure 5-21, but at different times.
Figure 5-24: As in Figure 5-18, but distributions of velocity component $v$ are shown as a function of time.
Figure 5-25: As in Figure 5-24, but at different times.
Figure 5.26: The wave profile at $t = 3.9900$ and the corresponding distributions of three components of Lagrangian acceleration: (a) $a_x$; (b) $a_y$; (c) $a_z$. 
Figure 5-27: The wave profile at \( t = 5.2009 \) and the corresponding distributions of three components of Lagrangian acceleration: (a) \( a_x \); (b) \( a_y \); (c) \( a_z \).
components. In spite of these similarities, the profiles of the overturning wave with $W = \pi$ are very different from those for $W = 3\pi$. This is evident by comparing the overturning wave profile in Figure 5-20(i) with that in Figure 5-12(f). In comparison with the case for $W = 3\pi$, the transverse energy flux in this case is much greater. This is most noticeable from the $w$ distribution plots from $t = 3.0136$ to $t = 3.9900$. When the surface forcing is applied, the wave near the center plane becomes more energetic as indicated by the greater local wave height and larger $u, w$ values. After the forcing is removed at $t = \pi$, the wave height and $u, w$ velocity near the side section increase rapidly as seen from Figure 5-22(d) to Figure 5-22(f). At $t = 3.9900$ the wave profile looks like a steep plane wave, although the three dimensionality of the $w$ distribution is significant. For $t > 3.9900$, the wave energy is continuously transferred to the side boundary in $y$ as seen from the sequence of distributions of $w$ for $t \geq 3.5057$. The wave profile near the boundary at $y = -0.5\pi$ eventually develops a robust plunging breaker, whereas the wave profile near the center plane only has a nearly vertical crest. This case should be contrasted with the overturning pattern for $W = 3\pi$, in which case the wave near the center plane is constantly more energetic than those near the side boundary and the forward breaking occurred near the center portion of the domain. Recall the only difference between these two study cases is the transverse wavelength of the surface forcing. It is clear that the greater transverse gradient of the wave energy distribution in the case of $W = \pi$ leads to a completely different pattern of three-dimensional overturning. As seen in Figure 5-25 and Figure 5-25, the maximum negative transverse velocity $v$ on the crest for $W = \pi$ is more than three times the value for $W = 3\pi$ case at the overturning stage. In all three-dimensional contour plots of $w$ distributions, the contours are always perpendicular to the periodic boundary and the center plane. This is due to the periodic condition and the symmetric initial forcing in $y$.

Figures 5-28 and 5-29 compare the wave profiles in the plane $y = 0$ (dashed line) with that in the plane $y = -0.5\pi$ (solid line) at the same time moments as those shown in Figures 5-19 to 5-20. Since the wave propagates from left to right in these
Figure 5-28: Wave profiles in the center plane $y = 0$ (dashed line) and at the periodic boundary $y = -0.5\pi$ (solid line) as a function of time. The wave propagates from left to right. Thus, the wave profiles in the plots correspond to (a) $t = 0, 1.0082$ and $2.0176$; (b) $t = 3.0136, 3.5057$. 

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Figure 5-29: As in Figure 5-28, but at different times. (c) $t = 3.9900, 4.5045$; (b) $t = 5.0039, 5.2009$. 

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figures, the profiles at the further right correspond to later times. These plots further illustrates the time-evolution of the three-dimensional overturning wave.

As shown in Figure 5-26(a), the maximum longitudinal acceleration is situated near the boundary \( y = -0.5\pi \), which further indicates that most of the wave energy has been transferred to the side boundary at \( t = 3.9900 \). As seen in Figure 5-26(b) the \( y \) component of the acceleration always has its maximum on the front face of the wave, which indicates the pattern of momentum flux in \( y \). As shown in Figure 5-27, the large acceleration components are all located in the concave side of the overturning wave crest.

Figure 5-30 shows a close-up of wave profiles in the plane of symmetry and periodic boundary for \( W = \pi \). The velocity and acceleration vectors of the Lagrangian points are also plotted. The difference between the profiles in the two extreme sections in this figure clearly indicates that the transverse variation of the wave profiles is quite large. The wave height in the center plane \( (y = 0) \) is about three-quarters of the wave height at the boundary \( (y = \pm 0.5\pi) \). Both velocity and acceleration distributions also indicate that the three-dimensionality of this breaking wave is significant.

Figure 5-31 compares the wave profiles in the center plane for \( W = 3\pi \) and \( W = \pi \) with the two-dimensional results of the convergence study case 3. These three wave profiles correspond to the time moment when the \( u \) component of the breaking waves approximately reaches its maximum. Because the wave profile corresponding to \( W = 2\pi \) is very close to that for \( W = 3\pi \), it is not shown in these plots for clarity. As seen from this figure, the difference between the wave profiles for \( W = \pi \) and the 2D result is large, whereas the center profile of overturning wave of \( W = 3\pi \) is similar to the two-dimensional profile. This indicates that the wave near the center of the periodic domain remains almost two-dimensional.

Similarly, in Figure 5-32, we compare the wave profiles in the boundary sections of the domain for the same waves as in Figure 5-26 with the 2D result. For \( W = 3\pi \), the side wave profile remains very close to the Stokes wave profile in terms of shape, velocity and acceleration distributions. In contrast, the side profile for \( W = \pi \) is
Figure 5-30: Close-up of wave profiles at $t = 5.2009$ at two sections for $W = \pi$ (a) with velocity vectors, (b) with acceleration vectors.
Figure 5-31: Close-up of wave profiles in the center plane compared with 2D results. These three profiles correspond to the time when velocity $u$ of the waves reaches its maximum. For $W = \pi$, $t = 5.2009$; for $W = 3\pi$, $t = 4.8166$ and for 2D case $t = 4.7754$ (a) with velocity vectors, (b) with acceleration vectors, which are normalized by their maximum magnitude respectively. See Table 5.6.
Figure 5-32: As Figure 5-31, but wave profiles in the side sections are compared with the two-dimensional result, (a) with velocity vectors, (b) with acceleration vectors.
\begin{center}
\begin{tabular}{|c|c|c|c|c|c|c|c|}
\hline
$W$ & Time & $\eta_{\min}$ & $\eta_{\max}$ & $H_w$ & $V_{\max}$ & $a_{\max}$ \\
\hline
$\pi$ & 5.2009 & -0.266 & 0.829 & 1.095 & 2.038 & 6.092 \\
$2\pi$ & 5.0038 & -0.265 & 0.774 & 1.039 & 1.958 & 5.673 \\
$3\pi$ & 4.8166 & -0.266 & 0.740 & 1.006 & 1.954 & 5.491 \\
2D & 4.7754 & -0.281 & 0.696 & 0.977 & 2.020 & 5.593 \\
\hline
\end{tabular}
\end{center}

Table 5.6: Comparison of the features of the overturning waves when their horizontal velocity is maximum. $H_w$ is the wave height. $V_{\max}$ and $a_{\max}$ denote the maximum magnitudes of the velocity and acceleration at the given times. The 2D data corresponds to study case 3 in Section 5.2.

clearly a plunging breaker. As we have seen from Figures 5-18 to 5-23, the wave energy for $W = \pi$ has a large transverse transfer rate, which causes the wave to break at the sides. Because of this transverse energy flux, less wave energy is propagated forward. As a result, this overturning wave developed about one-sixth of a wavelength behind the overturning waves for both the 2D and the $W = 3\pi$ case.

Figures 5-33 to 5-35 show the three-dimensional plots of velocity vector distributions for $W = \pi$, $W = 2\pi$ and $W = 3\pi$. All velocity components in these plots are normalized respectively by the maximum magnitudes for the three cases (listed in Table 5.6). From the top view of the plots in these three figures, it is apparent that if $W$ is greater or equal to $L$, the wave motion near the center plane remains two-dimensional in the plane with $y$ equal to constant. If $W < L$, the features of the nonlinear wave motion can be quite different. From Figure refvvb2 and refvvb3, it is evident that the wave motions for $W = 2\pi$ and for $W = 3\pi$ are qualitatively similar. As shown in these three figures, the velocity vectors at the two extreme edges of the computation domain in $y$ ($y = 0, y = -W/2$) are strictly two-dimensional, which confirms that the boundary conditions at these sections are satisfied.

Table 5.6 shows the height of various overturning waves and their maximum magnitude of velocity and acceleration at the given time moment. It should be noted that the times listed in Table 5.6 correspond to when the horizontal velocity is maximum. This does not imply that the acceleration is maximum at the listed times (see below).
Figure 5-33: Three-dimensional vector plots of the velocity distributions for $W = \pi$. (a) the top view (b) perspective view.
Figure 5-34: Three-dimensional vector plots of the velocity distributions for $W = 2\pi$. 
(a) the top view (b) perspective view.
Figure 5.35: Three-dimensional vector plots of the velocity distributions for $W = 3\pi$. (a) the top view (b) perspective view.
Figure 5-36: Three-dimensional vector plots of the acceleration distributions for $W = \pi$. (a) the top view (b) perspective view.
Figure 5-37: Three-dimensional vector plots of the acceleration distributions for $W = 2\pi$. (a) the top view (b) perspective view.
Figure 5-38: Three-dimensional vector plots of the acceleration distributions for $W = 3\pi$. (a) the top view (b) perspective view.
It is interesting to notice that the height of these different breaking waves are comparable. The dimensionless magnitude of velocity is about twice the phase velocity of the initial steady wave \( c = 1.0822 \). The magnitude of the acceleration is as large as 5.5 to 6 times the gravitational acceleration \( g \). As will be seen below, the largest component of acceleration of the overturning wave is in the negative \( z \) direction.

As was shown in Figure 5-9, in the later stage of a overturning wave, the computed velocities suffer from the Taylor instability because of large normal acceleration. In the present computations of three-dimensional overturning waves, we have also computed the velocity time-histories of a few selected Lagrangian points to check the effects of the large normal accelerations. Consider study case \( W = \pi \), for example, three Lagrangian points on the same transverse initial grid line are selected because the magnitude of velocity and acceleration is maximum at \( t = 5.2009 \) at the grid line. This grid line is located on the concave side of the overturning wave crest. Point 1 is the intersection point of this grid line with the side plane \( y = -0.5\pi \), where the velocity magnitude is maximum. Point 2 is the eighth grid point from the side, where the acceleration is maximum. Point 3 is the intersection point of the grid line with the center plane \( y = 0 \).

Figure 5-39 to Figure 5-41 show the time histories of three velocity components of the selected Point 1, 2 and 3. The dashed line in these three sets of figures corresponds to the velocity in the \( y \) direction. The solid line and dash-dot line denote the velocity components \( u \) and \( w \) respectively. Since Point 1 is on the periodic boundary and Point 3 is on the plane of symmetry, their \( v \) velocities vanish identically for all time as seen in Figures 5-39 and 5-41. From Figure 5-40(a), velocity \( v \) of Point 2 starts with a value of zero because the initial plane wave is propagating in \( x \). As the three-dimensional surface forcing is applied, Point 2 starts to drift toward the periodic boundary as marked by the negative \( v \). It then slowly moves toward the center plane as the wave height near the center increases due to forcing. After the surface forcing is removed at \( t = \pi \), \( v \) also starts decreasing. As in Figure 5-40(a), the \( v \) component reaches zero at about \( t = 4.0 \), which is consistent with the wave profile shown in
Figure 5-39: Velocities of Point 1 as functions of time. The solid line denotes the $u$ component, the dash-dot line denote $w$ and the dashed line is for $v$. (b) close-up at the breaking stage. The first large wiggle of $u, w$ curves at $t \approx 5.22$ is due to a large initial time step when the simulation was restarted.
Figure 5-40: Velocities of Point 2 are shown as functions of time. The solid line denotes the $u$ component, the dash-dot line denote $w$ and the dashed line is for $v$. (b) close-up at the breaking stage. Also see caption of Figure 5-39.
Figure 5-41: Velocities of Point 3 as functions of time. The solid line denotes the \( u \) component, the dash-dot line denote \( w \) and the dashed line is for \( v \). (b) close-up at the breaking stage. Also see caption of Figure 5-39.
Figure 5-42: The relative normal accelerations $a_n$ of Point 1, 2 and 3 as functions of time. The dashed line denotes $a_n$ for Point 1; solid line denotes the $a_n$ for Point 2 and the dash-dot line denotes $a_n$ for Point 3.
Figures 5-19(f) and 5-22(f) at \( t = 3.99 \). After that, \( v \) becomes negative marking the transverse momentum flux to the side of the domain until the wave crest near the periodic boundary overturns. From Figure 5-39, Figure 5-40 and Figure 5-41 as well as Figure 5-9, it can be noticed that when velocity \( w \) becomes zero, velocity component \( u \) reaches an extremum. This observation reveals a salient feature of the overturning waves both in two and three dimensions: qualitatively, the time-variations of \( u \) and \( w \) are out of phase.

From these three sets of figures, it is clear that during most of the simulation the free-surface velocity components vary smoothly. After the surface forcing is switched off, the longitudinal acceleration (the slope of the solid line) is much greater than the other two components. Near the final phase of overturning, Point 2 is situated on the concave side of the overturning crest, where the Lagrangian acceleration is the largest at \( t = 5.2009 \) among all Lagrangian points. As shown in Table 5.6, its acceleration at \( t = 5.2009 \) is about six times of \( g \). As we have seen in Section 5.1, large acceleration at the overturning wave crest will destabilize the water surface of the wave jet. Thus, around Point 2 the water surface is the most unstable. From Figure 5-40(b) the enlarged plot of time-variations of velocities for Point 2, all three velocity components develop "wiggles" shortly after \( t = 5.2009 \) (although an oversized initial time step when the simulation is restarted results in the first large wiggle of the velocity curves, the subsequent instability is not induced by the wiggle. As seen in Figure 5-9, when the restarting is smooth, the instability also develops). The oscillations of the velocities clearly marks the onset of Taylor type of instability. As a result, the simulation breaks down at about \( t = 5.3 \). The simulation could have been prolonged by introducing a smoothing scheme to the computed velocities similar to what we do for free surface smoothing. But, when the Taylor instability occurs, a cusp usually develops at the overturning wave crest. The velocity computation at the cusp is not accurate, thus the simulation is not continued.

Taylor (1950) pointed out that when the stratified fluids are accelerated in the same direction as the density gradient (perpendicular to the fluid interface), the fluid
Figure 5-43: The top view of the overturning waves corresponding to (a) $W = \pi$, at $t = 5.2502$; (b) $W = 2\pi$, at $t = 5.0032$; (c) $W = 3\pi$, at $t = 4.9008$. The coordinates have been normalized by the corresponding wave heights: (a) $H_\omega = 1.099$; (b) $H_\omega = 1.039$; (c) $H_\omega = 1.020$. 
Figure 5-44: As in Figure 5-43, but the perspective views of the overturning waves are shown.
Figure 5-45: As in Figure 5-43, but three-dimensional vector plots of free surface velocity distributions are shown.
surface is unstable to disturbance if the acceleration is greater than \( g \). Here, we check the relative normal acceleration \( a_n = (a_x, a_y, a_z + g) \cdot n \) for Points 1, 2 and 3. If the fluid particle is in free fall, its relative normal acceleration is zero. Figure 5-42 shows the time histories of the relative normal accelerations of Points 1, 2 and 3 near the final phase of overturning\(^3\). The relative normal acceleration of Point 2 becomes negative at \( t \approx 5.29 \), when the normal acceleration becomes greater than \( g \). A few time steps later, the rapidly growing Taylor type of instability causes the numerical simulation to break down.

Because the computed velocities oscillate mildly at least in the early stage of the instability development as seen in Figures 5-9 and 5-40, we estimate the Lagrangian acceleration by using the slopes of an averaged velocity curve. The results of using 5 point and 10 point average show good consistency. These results indicate that the magnitude of total acceleration can be as large as \( 10g \) (see Figure 5-42). The computed wave profiles in the early stage of the development of Taylor instability are usually reasonably smooth, as we have seen from the last two wave profiles in Figure 5-8. This is also true for the three-dimensional profiles of breaking waves. Figure 5-43 shows the top view of the late stage overturning waves corresponding to the three cases (\( W/L = 3/2, 1, 1/2 \)) computed in this section. The corresponding three-dimensional perspective views of the overturning waves are shown in Figure 5-44. Figure 5-45 shows the corresponding three-dimensional vector plots of the distributions of Lagrangian velocity. These results are all reasonably acceptable.

From energy conservation, the net increase of wave energy must be equal to the total energy input during forcing. The energy input at a given time can be computed by integrating the product of surface pressure and the surface normal velocity over the free surface. The total energy input is then obtained by integrating the result at each time step with respect to time (i.e. integrating both sides of (4.101)). For the three study cases in this section, the agreement between the net energy increase

\(^3\)The data points corresponds to the large wiggle due to the oversided initial time step of restarting are disregarded.
Figure 5-46: The normalized wave energies as functions of time. KE, PE and TE designate the kinetic, potential and total wave energies for the three-dimensional breaking waves, where the solid line is for $W = \pi$, dashed line for $W = 2\pi$ and dash-dot line for $W = 3\pi$. $z$ denotes the calculated mean water positions, which should be a constant.
and the energy input is within 0.5%. Figure 5-46 shows the time-variation of the normalized kinetic, potential and total wave energies and mean water positions for the three study cases, where the wave energies are normalized by the total energy of the initial Stokes wave $E_0$. After $t = \pi$ when the surface forcing is removed, the total energy is indeed a constant with three significant digits. The mean water position is also a constant up to two decimal places.

In view of the fact that the profiles of the three-dimensional overturning waves for $W < L$ and $W \geq L$ are so different, it is surprising to find out that the time histories of their potential and kinetic energies normalized by $E_0$ are almost the same, respectively. The maximum difference between the energy curves for the three cases is about 0.4%, which suggests that the time variation of the wave energies are linear functions of $W$ at least for the three cases considered. This result reveals the complexity of the three-dimensional overturning waves: for the same time-variation of energies, the pattern of a breaking wave can be totally different as shown in Figures 5-10 to 5-12 and Figures 5-18 to 5-20. Obviously, this property of an overturning wave can not be deduced from a two-dimensional study.

Recall the magnitude of the three-dimensional surface forcing $p_0 = 0.073$ is one half of the two-dimensional forcing in the previous section ($p_0 = 0.146$). If the total energy input of the three-dimensional forcing is a linear function of $W$, the net increase of total wave energy normalized by $E_0$ for the two-dimensional wave in Section 5.2 should be twice that of the three-dimensional waves. Consider $t > \pi$ for example, the value of $(E - E_0)/E_0$ is equal to 0.970 in two dimensions and equal to 0.475 in three dimensions. Their ratio equal to 2.042 seems to confirm the conjecture above. Figure 5-47 shows the comparison of the time-variation of the net increase of wave energy between two and three dimensions (case for $W = \pi$ is plotted to represent 3D waves). The net energy increase corresponding to the nonlinear waves in three dimensions has been multiplied by a factor of two. The agreement is good during the early stage of forcing ($t < \pi$) and shows a small difference for the later stage as expected since one of the wave motion is three-dimensional.
Figure 5-47: Comparison of the normalized total wave energies as functions of time. The solid line represents twice the net energy increase of the 3D wave. The dash-dot line corresponds to the net energy increase of the 2D wave.
Finally, we mention that the effect of the Taylor instability before the break down of the simulation is too small to be detected from these global physical quantities. The simulations are all performed on a Cray Y-MP supercomputer. It takes approximately 60 hours CPU time for the case $W/L = 2$; and approximately 72 CPU hours for the cases $W/L = 1/2$ and $3/2$ because in average the aspect ratio of the elements in these two cases is higher than that in the case $W/L = 2$. About two-thirds of the CPU time are spent for the final one quarter of the simulation time because it is the overturning stage that the surface velocity and acceleration become large.

5.4 Extension to finite water depth

The present method has been generalized to incorporate the effects of finite water depth. Consider a uniform water depth $H$ as defined in Figure 5-1 for simplicity. In this case, the homogeneous Neumann boundary condition is imposed on the bottom surface. After discretizing the bottom and the free surface, we solve for the potential on the bottom and normal flux on the free surface as usual. The formula for the interior solid angle is defined in (2.16) with $S$ including the free surface and bottom. The procedures of time-stepping and global physical quantity calculations remain the same. As an example, we show the results of the three-dimensional computation of a plane overturning wave. As the initial condition, we choose a steady progressive wave with $ka = 0.3$ on water depth $H/\lambda = 0.3$, where $H$ and $\lambda$ correspond to the dimensionless water depth and wavelength. For the initial surface forcing, we choose a variation of (5.7) given by

$$p_f = \begin{cases} p_0 \sin(2\pi t/T) \sin(x - ct) & \text{if } 0 \leq t \leq T/2 \\ 0 & \text{if } t > T/2 \end{cases}$$

where $T$ is the wave period of the initial steady wave. The surface forcing is removed after half of the wave period. The computation domain has a length $2\pi$ in $x$ and unity in $y$. We use 32 quadratic elements in $z$ and 2 elements in $y$. The initial grid
Figure 5-48: A sequence of wave profiles of overturning waves in water of uniform depth. $H/\lambda = 0.3$. See text for definition of the initial surface forcing.

points are again distributed based on curvatures.

Figure 5-48 shows a sequence of overturning wave profiles at various times for $p_0 = 0.300$. In this computation, the maximum Courant number $C_n = 0.8$ is used. The 5-point Chebyshev smoothing is applied every three time steps. The close-up of overturning wave crests is shown in Figure 5-49. From these figures, the wave profiles remain smooth even after the crest develops a cusp at the later stage of overturning. Because of the Taylor instability, the last three wave profiles may be only qualitatively accurate. The computation can not be continued too long after the cusp has developed.

Figure 5-50 shows the conservations of energy and volume for the simulation. The time-variations of kinetic and potential energy are also shown in this figure. All three energy components are normalized by the total energy of the initial steady wave. The total wave energy after the surface forcing is a constant for the first three digits. The
Figure 5-49: Close-up plots of a sequence of overturning wave profiles for $4.6382 \leq t \leq 4.9232$. 
mean water position which reflects the conservation of volume varies less than 0.2% during the entire simulation.

Figure 5-51 compares the features of a deep water overturning wave (case 3 in Section 5.2) with that in finite water depth \((H/\lambda = 0.3)\) at \(t = 4.865\). Because the two initial forcing functions have different time duration and magnitude, the comparison is intended to be qualitative only.

We mention that since waves in finite water depth are considered in this section, the difficulty associated with the unboundedness of \(G_p\) at infinity (see Section 4.9) is no longer present. The additional equation from the Gauss condition is thus not needed. Hence, we use the SSOR preconditioned GMRES solver for the solution of the resulting system of linear equations. Typically, it takes approximately 15 to 20 iterations to converge for an accuracy of \(10^{-5}\).
Figure 5-51: Close-up plot of overturning wave profiles in deep water (denoted by d) and in finite water depth (denoted by f) at $t = 4.865$. 
If we use the same spatial resolution as that used in Section 5.3 for the computation of a three-dimensional overturning wave in finite water depth, the number of unknowns will be doubled. Since the computational cost of the method grows quadratically with the number of unknowns used, it will take approximately 240 to 288 CPU hours on the same computer for the same duration of simulation. In view of the high computational cost, the simulation of three-dimensional finite depth overturning waves is not pursued presently. One way of reducing the wall clock time for the computation is to take advantage of multi-tasking on a multiple CPU vector-processor such as Cray Y-MP.

It should also be noted that because the present Laplace solver uses the piecewise smooth approximation, the method can be directly applied to arbitrary doubly periodic bottom topography. With a larger computation window/domain, the present method can also be used for computations involving an arbitrarily shaped submerged three-dimensional structure.
Chapter 6

3D Wave Sloshing in a Wave Tank

In Chapter 5, we have demonstrated that the present numerical method can be used to describe accurately the doubly periodic overturning waves in three dimensions. In this chapter, we generalize the numerical method to solve the fully nonlinear wave equations inside an arbitrarily shaped three-dimensional domain. For simplicity, we consider the wave sloshing inside a general three-dimensional wave tank for a given initial surface elevation.

As we have seen in the convergence studies in Section 4.7, the present method is convergent for solving the mixed interior Dirichlet/Neumann problem in a general three-dimensional domain. At the intersection line of the free surface (Dirichlet boundary) and a wall (Neumann boundary), we enforce the continuity of potential functions. Like the two-dimensional study case of wave oscillation in Section 3.2, we define dual status for the nodes on the intersection lines. For the nodes on the corner vertices which are the common points of two side walls and the free surface, we introduce triple-status for the points, i.e. there are three different values of $\phi_n$ on the vertex corresponding to the three different boundary surfaces. For the boundary integral on the free surface, the $\phi_n$ is unknown; for the boundary integrals on the other two surfaces (usually Neumann boundaries) $\phi_n$ is given. Therefore, we still end up with the same number of equations and unknowns. The PFD algorithm developed in Section 4.8 can be used to evaluate the velocity components on both the
free surface and the wall/bottom. The boundary condition on the wall is imposed in velocity evaluations to ensure the normal velocity on the wall is zero. It is found that the velocity at the intersection lines can be accurately obtained by the PFD scheme in terms of the solved potential on the adjacent Neumann boundary surfaces or by PFD scheme directly using the solved $\phi_n$ on the free surface. At a given time moment, the results from these two methods agree with each other within 1% for all test computations of wave sloshing.

As a simple application of the present method, we compute the resulting nonlinear motion inside a three-dimensional wave tank subject to an initial surface elevation, which is specified by

$$z = a \cos(k_x x) \sin(k_y y), \quad x \in [0, 1] \text{ and } y \in [0, 1] \quad (6.1)$$

with $a = 0.15$ and $k_x = k_y = \pi$. The definition of the coordinate system is the same as that in Figure 4-10. The initial potential value on the free surface is assigned as zero by assuming the motion starts from stationary. The free surface is discretized into a set of $25 \times 25$ nodal points (i.e. $12 \times 12 = 144$ quadratic elements). The bottom is covered by the same number of elements as the free surface. In vertical direction, 12 segments are used. Thus the four side walls are discretized into $6 \times 12 = 72$ quadratic elements each. In this test computation, the velocities at the intersection lines are evaluated by the PFD using the solved normal velocity. Because of the difficulty of regridding an arbitrary three-dimensional surface, we follow all Lagrangian points on the free surface during the simulation. We may also update the Lagrangian points on the walls if there is any wave overturning along the sides. Since the sloshing wave amplitude is not very large, we adopt an simpler approach: update the Lagrangian points on the free surface and rediscretize the side walls and bottom.

Figures 6-1 and 6-2 show a sequence of free surface profiles at selected time moments. The free surface elevations on the wall $y = -1/2$ as a function of time are shown in Figures 6-3 and 6-4. Different from the prediction of a linear theory, the
Figure 6-1: Three-dimensional plots of the sloshing wave profiles at various times. For the numerical wave tank, we choose $L = W = 1$ and $H = 0.5$. The times are included in the plots.
Figure 6-2: As in Figure 5-52, but at different times.
Figure 6-3: Sloshing wave profiles on the wall $y = -W/2$ as a function of time. (a) $0 \leq t \leq 1.5$; (b) $1.55 \leq t \leq 3.2$. 
free surface profiles do not simply repeat itself, nor is there a time moment at which the free surface is completely flat. These two qualitative conclusions are in good agreement with the results of three-dimensional standing waves with the second order correction (in wave steepness) (Verma & Keller, 1962). From these figures, it can be seen that the resulting steepness of the sloshing wave can be greater than the initial condition. The saw-tooth instability on the free surface does not appear in the present preliminary computation up to two sloshing cycles of the wave. Because wave overturning is not involved, the dynamic time stepping is not necessary. The positions of the intersection lines between the free surface and the walls are also very smooth. Both the wave energy and fluid volume are conserved with an accuracy of 3 significant digits.

To check the convergence of the numerical simulation, we repeated the same computation with $\Delta t = 0.03$. For definiteness, we check the computed positions of three Lagrangian points: two corner points at $x = 0, y = -W/2$ and $x = L, y = -W/2$; the
\begin{center}
\begin{tabular}{|c|c|c|c|}
\hline
$\Delta t$ & Point 1 & Point 2 & Point 3 $(x=0,y,z)$ \\
\hline
0.05 & 0.1660650 & -0.1438406 & (-0.1609606, 0.0602851) \\
0.03 & 0.1660673 & -0.1438305 & (-0.1609600, 0.0602853) \\
\hline
\end{tabular}
\end{center}

Table 6.1: Convergence check on the positions of three Lagrangian points at $t = 4.5$: Point 1 is at $(x, y) = (L, -W/2)$; Point 2 is at $(x, y) = (0, -W/2)$; Point 3 is initially at $(x, y, z) = (0, 0, 0)$.

The third point is initially situated at $(0, 0, 0)$. The time-variations of the positions of the corner points corresponding to the two different temporal discretizations are shown in Figure 6-5. The corresponding comparison of the positions of the third point are shown in Figure 6-6. At $t = 4.50$, the positions of the three points obtained by using two different time-step sizes are listed in Table 6.1. From these convergence checks, it is clear that the numerical method is convergent for computations of the nonlinear wave motion inside a wave tank.

For the problems considered in this section, the Green function $G$ satisfies the far field conditions (2.6) and (2.7). As have been shown in Section 4.7, the resulting system of linear equations is amenable to the SSOR preconditioned GMRES iterative solver. Typically, it takes approximately 15 to 20 iterations to converge for an accuracy of $10^{-5}$. The total CPU time for the sloshing wave simulation (100 time steps, $N = 2306$) is approximately 2.2 hours on a Cray Y-MP. In terms of computation speed, the algorithm for the general wave tank problem is approximately 12 times faster than that for the doubly periodic problem in Chapter 5. This is because the work required for evaluating $G$ is much less than that for $G_p$. Finally, we mention that the requirement of computer storage for the present method is approximately $1.1N^2$. 

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Figure 6-5: The positions of two corner points on the wall of the numerical wave tank as functions of time. * corresponds to the point at \( x = L, y = -W/2 \), + corresponds to the point at \( x = 0, y = -W/2 \). These symbols denote results obtained by using \( \Delta t = 0.05 \). The solid line denotes the results obtained with \( \Delta t = 0.03 \).
Figure 6.6: Convergence check using the position of the Lagrangian point at \( z = y = 0 \). + denotes the results obtained by using \( \Delta t = 0.05 \). The solid line denotes the results obtained with \( \Delta t = 0.03 \).
Figure 6-7: Wave energies and mean water positions as a function of time. TE stands for total wave energy; KE stands for kinetic energy; PE stands for potential energy. z denotes the mean water positions.
Chapter 7

Conclusions and Discussions

The kinematics of three-dimensional highly nonlinear water waves is of fundamental importance to free surface hydrodynamics and its engineering applications. By extending the MEL method to three dimensions, we have now made available an accurate and efficient numerical method for quantifying the kinematics of a three-dimensional fully nonlinear gravity waves including overturning. The key steps to the success may be summarized in the following three aspects.

First, we have developed an accurate and robust Laplace solver in three dimensions using a BEM based on bi-quadratic isoparametric curvilinear elements with an efficient adaptive numerical quadrature scheme. The present algorithm exhibits quadratic convergence rate for a variety of potential problems including interior and exterior mixed Dirichlet/Neumann problems, whereas the classical CPM does not converge for the mixed problem due to numerical discontinuous approximations at the intersection lines.

Secondly, to evaluate free surface velocity components, a general purpose method based on an isoparametric finite-difference (PFD) scheme has been devised. In comparison with a method based on bi-cubic spline fitting, PFD is more efficient and more flexible in handling complex geometries without sacrificing accuracy. Extensive numerical convergence studies show that the accumulative error of the evaluated velocity field also converges quadratically with the number of unknowns if a curvature-based
numerical grid is used.

Thirdly, the resulting system of linear equations from the BIEs is solved by an efficient iterative method based on the GMRES scheme with a SSOR preconditioner. Since the nonlinear wave equations are nondissipative, the evaluated three-dimensional wave profiles will inevitably develop high wavenumber instability which can be removed by applying a Chebyshev smoothing in alternating directions in the parametric space every a few time steps.

Systematic accuracy and convergence checks are performed first using exact Stokes waves of finite-amplitude, and in repeating the two-dimensional overturning wave simulations using an applied surface pressure of Longuet-Higgins & Cokelet (1976) and others. The results are generally in excellent agreement. The present results have shown that the method is able to evaluate the velocity and acceleration fields with an accuracy of a few percent. Thus, the present method is useful for quantitative computations of fully nonlinear free surface flows in three dimensions.

One of the main focus of the present work is the doubly periodic three-dimensional overturning waves in deep water. To generate such an overturning wave, we start with a plane progressive Stokes wave and apply a doubly periodic three-dimensional surface pressure distribution to raise the local energy density beyond the maximum for a steady Stokes wave. To quantify the degree of three-dimensionality of overturning waves, three different values of width-length ratio of the doubly periodic domain are chosen corresponding to $W/L=0.5$, 1 and 1.5. Although the maximum of the forcing pressure for all three cases are along the centerline $y = 0$, the resulting three-dimensional plunging breakers surprisingly develop either at the center ($y \sim 0$) or at the edges ($y \sim \pm W/2$) depending on the value of $W/L$. Equally interesting are the time histories of the kinetic and potential energies, which after normalizing by the width $W$, differ only by a few percent so that the total energies are approximately linear functions of $W$. It is noteworthy, however, that the velocity/acceleration fields and profiles of these three-dimensional overturning waves are otherwise quite different and qualitatively so for $W \geq L$ versus $W < L$. 
It is now clear that shortly after the horizontal velocity of the overturning wave reaches its maximum, the computed velocities near the overhanging wave crest develop a local instability, which is similar to the surface instability due to accelerations in the direction normal to the fluid surface described by Taylor (1950). The instability of velocities always occurs in a small region where the magnitude of acceleration is near maximum. This instability is the major cause of the break down of the numerical simulation. The onset of the Taylor instability can be detected by monitoring the relative acceleration normal to the wave profile. Before the onset of Taylor instability, the maximum magnitude of Lagrangian acceleration is about 5 to 6 times the gravitational acceleration $g$. We suggest that in the future studies of overturning waves using a MEL approach, the smoothness of the time-variation of Lagrangian velocities should be used as one of the criteria of determining whether the numerical solution is acceptable.

The deep water breaking waves including spilling breaker and plunging breaker. The former may be considered as a small scale plunger near a wave crest. The present results show that the evaluated wave profiles are smooth. In reality, it is commonly observed that the surface of an overturning wave crest is usually non-smooth. Particularly, the tip of an overturning wave crest often breaks up into water droplets before its re-entry into the water surface. The present results indicate that a root cause of the phenomena is the Taylor type of instability.

The present method has also been extended to include the effects of a uniform finite water depth. Because QBEM uses piecewise smooth approximations, further extension to incorporate a doubly periodic arbitrary bottom topography is straightforward. The present method has also been extended to study the nonlinear wave motion inside an arbitrarily shaped three-dimensional region such as a wave tank. The velocity on the Dirichlet/Neumann intersection lines can be computed by PFD in terms of either the solved potential on the Neumann boundary or the solved normal flux on the free surface.

For an accuracy of a few percent, the major restriction for the three-dimensional
Table 7.1: The data for wave sloshing case is from a test run in Chapter 6. The estimate for the wave tank problem is for an accuracy $\delta = 1\%$, $\beta_2 = 32$, for the first three wave periods $\gamma = 100$ and for the fourth wave period $\gamma = 200$.

<table>
<thead>
<tr>
<th>cases</th>
<th>$N_x$</th>
<th>$N_y$</th>
<th>$N_z$</th>
<th>$N_T$</th>
<th>CPU(Y-MP hrs.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>wave sloshing</td>
<td>0.5</td>
<td>0.5</td>
<td>0.25</td>
<td>1.5</td>
<td>2.2</td>
</tr>
<tr>
<td>wave tank</td>
<td>4</td>
<td>2</td>
<td>0.5</td>
<td>4</td>
<td>375</td>
</tr>
</tbody>
</table>

wave computations is still the high computational cost. The CPU time of the method can be estimated by $O(N_xN_y + N_xN_z + N_yN_z)^2\beta_2^4N_T\gamma$, where $\beta_2$ is the number of unknowns per wavelength, $N_x$, $N_y$ and $N_z$ are the number of waves in three coordinate directions, $\gamma$ is the number of time steps per wave period and $N_T$ is the number of wave periods in simulation. Table 7.1 gives an estimate of the computational cost for a realistic wave tank problem based on the present results, where we assume wave overturning occur during the fourth wave period. We emphasize that for steep, non-overturning waves, the computation using the present method is inexpensive as seen from the wave sloshing case.

By utilizing multi-tasking or parallelizing the algorithm, we can extend our ability to solve more complex problems involving nonlinear surface waves. The extension of incorporating AMM as reviewed in Section 4.1 will also be rewarding. With further developments to incorporate an open boundary condition and a floating body, the ultimate capability for the simulation of general three-dimensional fully-nonlinear wave-body interactions can be anticipated.
Appendix A

The Singularity of a Dipole Distribution

Locally, all continuous surfaces can be considered single-valued. Without loss of generality, suppose the \( S \in \mathcal{R}^3 \) is a smooth single-valued surface, which can be described by function \( F(\mathbf{x}) = 0 \) for \( \mathbf{x} \in S \). Consider a normal dipole distribution over \( S \) with density \( \mu(\mathbf{x}) \). The potential at a point \( \mathbf{x}_0 \) can be written as

\[
\phi(\mathbf{x}_0) = \int_S \mu \frac{\partial G}{\partial n} dS
\]  
(A.1)

where

\[
\frac{\partial G}{\partial n} = \frac{\partial}{\partial n} \left( \frac{1}{r} \right) = \frac{\mathbf{n} \cdot \mathbf{r}}{r^3}
\]  
(A.2)

where \( G = 1/r \) is the Green function, \( \mathbf{r} = \mathbf{x}_0 - \mathbf{x} \) and \( r = |\mathbf{x}_0 - \mathbf{x}| \). Let the direction cosine of \( \mathbf{r} \) be \((c_1, c_2, c_3)\), thus,

\[
\mathbf{r} = r(c_1 \mathbf{i} + c_2 \mathbf{j} + c_3 \mathbf{k}) = r \mathbf{r}_c
\]  
(A.3)

When \( \mathbf{x}_n \in S \), the kernel contains a singularity at \( \mathbf{x}_0 \). The question is how fast the integrand approaches zero as \( \mathbf{x} \to \mathbf{x}_0 \) or what the order of the singularity is?

Assume \( F \) is \( C^\infty \)-continuous at \( \mathbf{x}_0 \). The Taylor expansion of \( F \) at \( \mathbf{x}_0 \) can be
written as
\[ F(\mathbf{r}) = \sum_{n=0}^{\infty} (-\mathbf{r} \cdot \nabla)^n F|_{\mathbf{r}=\mathbf{a}_0} \quad (A.4) \]

where \(-\mathbf{r} \cdot \nabla\) is a vector notation of the differential operator with
\[ \nabla = \frac{\partial}{\partial x} \mathbf{i} + \frac{\partial}{\partial y} \mathbf{j} + \frac{\partial}{\partial z} \mathbf{k}. \quad (A.5) \]

Symbol \(|\mathbf{r}=\mathbf{a}_0\) denotes that all partial derivatives of \(F\) are evaluated at \(\mathbf{a}_0\) (not \(r\!).

Notice \(F(\mathbf{r}) = F(\mathbf{a}_0) = 0\). From (A.4) and (A.3), we have
\[ (r \cdot \nabla)F|_{\mathbf{r}=\mathbf{a}_0} = \sum_{n=2}^{\infty} (-\mathbf{r} \cdot \nabla)^n F|_{\mathbf{r}=\mathbf{a}_0} = \sum_{n=2}^{\infty} r^n (-\mathbf{r}_c \cdot \nabla)^n F|_{\mathbf{r}=\mathbf{a}_0}. \quad (A.6) \]

From this last expression, it is clear that the leading order of the right hand side is \(r^2\) as \(\mathbf{r} \rightarrow \mathbf{a}_0\).

The normal vector of the surface \(S\) can be expressed by
\[ \mathbf{n} = \frac{\nabla F}{|\nabla F|}. \quad (A.7) \]

From (A.6) and (A.2), we have
\[ \frac{\partial G}{\partial n} = \frac{\mathbf{r} \cdot \mathbf{n}}{r^3} = \sum_{n=2}^{\infty} r^{n-3} \frac{(-\mathbf{r}_c \cdot \nabla)^n F}{|\nabla F|} \bigg|_{\mathbf{r}=\mathbf{a}_0}. \quad (A.8) \]

From the last expression, it is apparent that the order of the singularity of normal dipoles is truly \(r^{-1}\) as \(\mathbf{r} \rightarrow \mathbf{a}_0\). In terms of leading behaviour, this conclusion is true if \(F\) is \(C^1\)-continuous and has finite higher-order derivatives (not necessarily continuous) as seen from (A.6). If the surface \(S\) contains a cusp or sharp corner, the order of the singularity will be greater than one.
Appendix B

2D Influence Functions

The results of the closed form influence functions based on isoparametric linear elements for two-dimensional problems are listed in this appendix.

Consider a generic two-dimensional element with nodes at \( x_j \) and \( x_{j+1} \). The isoparametric interpolation can be defined by

\[
\Phi(s) = \Phi_j(1-s) + \Phi_{j+1}s
\]

(B.1)

where \( \Phi \) represents a geometric or physical variable, and \( s \in [0,1] \) is a parameter.

Let the collocation point be \( p_i = (x_i, y_i) \). The Green function is then given by

\[
G(p_i, q) = \ln |p_i - q| \\
\ln \left\{ [x_i - x_j - (x_{j+1} - x_j)s]^2 + [y_i - y_j - (y_{j+1} - y_j)s]^2 \right\}^{1/2}.
\]

(B.2)

If \( i = j \), i.e. \( (x_i, y_i) = (x_j, y_j) \),

\[
G = \ln(l_j s)
\]

(B.3)

where \( l_j = |x_{j+1} - x_j| \) is the distance between the two nodal points.

If \( i = j + 1 \), i.e. \( (x_i, y_i) = (x_{j+1}, y_{j+1}) \),

\[
G = \ln[l_j(1-s)].
\]

(B.4)
Define
\[
\begin{aligned}
a &= x_i - x_j, \\
b &= x_{j+1} - x_j, \\
c &= y_i - y_j, \\
d &= y_{j+1} - y_j.
\end{aligned}
\]  
(B.5)

Then, \( l_j = (b^2 + d^2)^{1/2} = A^{1/2} \). Furthermore, we have
\[
G = \ln[(a - bs)^2 + (c - ds)^2]^{1/2} \\
= \ln[As^2 - 2Bs + C]^{1/2}
\]  
(B.6)

where
\[
A = b^2 + d^2 = l_j^2; \quad B = ab + cd; \quad C = a^2 + c^2.
\]  
(B.7)

Also,
\[
As^2 - 2Bs + C = A[(s - B/A)^2 + D^2]
\]  
(B.8)

with \( D = (AC - B^2)/A^2 = (ad - cb)^2/A^2 \). Thus, \( D \) is non-negative.

When \( D \) vanishes, we have
\[
\frac{x_i - x_j}{x_{j+1} - x_j} = \frac{y_i - y_j}{y_{j+1} - y_j}
\]  
(B.9)

This result indicates that the collocation point is on the straight line which passes through the two nodes of the element.

For the normal dipoles, we have
\[
G_n(p_i, q) = \nabla G \cdot n = \frac{cb - ad}{l_j(As^2 - 2Bs + C)}.
\]  
(B.10)

For convenience, we denote elements by their first node number. For example, for an element with end node \( j \) and \( j + 1 \), it is called element \( j \). Since we are collocating at nodal points and each node is usually shared by two neighboring elements, it is
convenient to write the influence at \( p_i \) due to node point \( q_j \) as the following summation

\[
I_{ij}^* = I_{ij}^{(s,j)} + I_{ij}^{(s,j-1)} = \int_0^1 G_j l_j (1 - s) ds + \int_0^1 G_{j-1} l_{j-1} s ds. \tag{B.11}
\]

where the subscripts \( j \) and \( j - 1 \) denote the variable is evaluated on element \( j \) or \( j - 1 \) respectively. Similarly, we define the influence of dipoles

\[
I_{ij}^d = I_{ij}^{(d,j)} + I_{ij}^{(d,j-1)} = \int_0^1 G_{n,j} l_j (1 - s) ds + \int_0^1 G_{n,j-1} l_{j-1} s ds. \tag{B.12}
\]

If the boundary is open-ended, one of the two integrals in the above expressions will vanish.

We summarize the integral results as follows

1. If \( D \neq 0 \), we have

\[
I_{ij}^{(s,j)} = \frac{l_j}{2} \ln l_j + \frac{l_j (A - B)}{2A} \left\{ \frac{A - B}{A} \ln \frac{A + C - 2B}{A} + \frac{B}{A} \ln \frac{C}{A} - 2 + 2D \left[ \tan^{-1} \frac{A - B}{AD} - \tan^{-1} \frac{-B}{AD} \right] \right\} - \frac{l_j}{4} \left\{ \frac{A + C - 2B}{A} \ln \frac{A + C - 2B}{A} - \frac{C}{A} \ln \frac{C}{A} + \frac{2B}{A} - 1 \right\}. \tag{B.13}
\]

where \( A, B, C, D \) are defined above, and evaluated for element \( j \).

\[
I_{ij}^{(s,j-1)} = \frac{l_{j-1}}{2} \ln l_{j-1} + \frac{l_{j-1} B}{2A} \left\{ \frac{A - B}{A} \ln \frac{A + C - 2B}{A} + \frac{B}{A} \ln \frac{C}{A} - 2 + 2D \left[ \tan^{-1} \frac{A - B}{AD} - \tan^{-1} \frac{-B}{AD} \right] \right\} + \frac{l_{j-1}}{4} \left\{ \frac{A + C - 2B}{A} \ln \frac{A + C - 2B}{A} + \frac{C}{A} \ln \frac{C}{A} + \frac{2B}{A} - 1 \right\}. \tag{B.14}
\]

where all variables are evaluated for element \( j - 1 \).

\[
I_{ij}^{(d,j)} = \frac{E (A - B)}{AD} \left[ \tan^{-1} \frac{A - B}{AD} - \tan^{-1} \frac{-B}{AD} \right] - \frac{E}{2} \ln \frac{A + C - 2B}{C}. \tag{B.15}
\]
where \( E = (cb - ad)/A \) and all variables are evaluated for element \( j \).

\[
I_{ij}^{(d,j)} = \frac{EB}{AD} \left[ \tan^{-1} \frac{A - B}{AD} \ln \frac{A + C - 2B}{C} \right] + \frac{E}{2} \ln \frac{A + C - 2B}{C}
\]  

(B.16)

where all variables are evaluated for element \( j - 1 \).

2. if \( D = 0 \), the collocation point is situated on the line defined by the two nodes of a element under consideration. If the collocation point does not coincide with any of the two nodes, the influence due to sources can be evaluated by the results presented at above. The formula for dipole influence in this case is given below

\[
I_{ij}^{(d,j)} = -E(1 + A - B) - \frac{E}{2} \ln \frac{A + C - 2B}{C}
\]  

(B.17)

where all variables are evaluated for element \( j \).

\[
I_{ij}^{(d,j-1)} = EB \left( \frac{1}{B - A} - 1 \right) + \frac{E}{2} \ln \frac{A + C - 2B}{C}
\]  

(B.18)

where all variables are evaluated for element \( j - 1 \). \( B = A \) only if the collocation point coincides with one of the two nodes.

For collocating on node \( j \), we have

\[
I_{ij}^{(s,j)} = \frac{l_j}{2} \ln l_j - \frac{3}{4} l_j.
\]  

(B.19)

\[
I_{ij}^{(s,j-1)} = \frac{l_{j-1}}{2} \ln l_{j-1} - \frac{3}{4} l_{j-1}.
\]  

(B.20)

For collocating on node \( j + 1 \), we evaluate \( I_{ij}^{(s,j-1)} \) by the general formula for \( D \neq 0 \). For contribution for element \( j \), we have

\[
I_{ij}^{(s,j)} = \frac{l_j}{2} \ln l_j - \frac{1}{4} l_j.
\]  

(B.21)
For collocating on node $j-1$, we evaluate $I_{ij}^{(*,j)}$ by the general formula for $D \neq 0$. For contribution for element $j-1$, we have

$$I_{ij}^{(*,j-1)} = \frac{l_{j-1}}{2} \ln l_{j-1} - \frac{1}{4} l_{j-1}. \tag{B.22}$$

The self-influence of dipole on the nodes is zero.
Appendix C

Polynomials of the Isoparametric Elements

The coefficients of the parametric polynomial representation for a field function $\Phi$ inside two types of isoparametric element are given in this appendix.

(a) For a bilinear element,

$$\Phi = \sum_{j=1}^{4} N_j \Phi_j$$

with $N_j = (1 + s_j s)(1 + t_j t)/4$. Then

$$\Phi = a_{00} + a_{10} s + a_{01} t + a_{11} st.$$

where

$$a_{00} = \Phi_1$$
$$a_{10} = \Phi_2 - \Phi_1$$
$$a_{01} = \Phi_4 - \Phi_1$$
$$a_{11} = (\Phi_1 - \Phi_2) - (\Phi_4 - \Phi_3).$$

(b) For an 8-node serendipity element, we use the same node numbering convention as in Figure 4-1 without the center node 9.

$$\Phi(s, t) = a_{00} + a_{10} s + a_{01} t + a_{11} s t + a_{20} s^2 + a_{02} t^2 + a_{21} s^2 t + a_{12} s t^2$$
\[ = \sum_{m,n=0}^{2} a_{mn} e^{mt} \]  

\((s, t) \in [-1, 1]\) \hspace{1cm} (C.4)

where the prime on the upper limit of summation denotes that the term \(n = m = 2\) is not included. The coefficients of the polynomial are given by

\[ a_{00} = \frac{1}{2}(\Phi_5 + \Phi_8 + \Phi_7 + \Phi_9) - \frac{1}{4}(\Phi_1 + \Phi_2 + \Phi_3 + \Phi_4) \]
\[ a_{10} = \frac{1}{2}(\Phi_5 - \Phi_7) \]
\[ a_{01} = \frac{1}{2}(\Phi_8 - \Phi_9) \]
\[ a_{11} = \frac{1}{4}[(\Phi_1 - \Phi_4) - (\Phi_2 - \Phi_3)] \]
\[ a_{20} = \frac{1}{4}[(\Phi_1 - 2\Phi_6 + \Phi_2) + (\Phi_4 - 2\Phi_8 + \Phi_3)] \]
\[ a_{02} = \frac{1}{4}[(\Phi_8 - 2\Phi_6 + \Phi_4) + (\Phi_2 - 2\Phi_7 + \Phi_3)] \]
\[ a_{21} = \frac{1}{4}[(\Phi_1 - 2\Phi_6 + \Phi_2) - (\Phi_4 - 2\Phi_8 + \Phi_3)] \]
\[ a_{12} = \frac{1}{4}[(\Phi_1 - 2\Phi_6 + \Phi_4) - (\Phi_2 - 2\Phi_7 + \Phi_3)] \]  

(C.5)
Appendix D

An Algorithm for a Curvature Based Grid

Consider a curve in three dimensions defined parametrically by

$$ \mathbf{x} = \mathbf{x}(t). \quad (D.1) $$

Then its curvature can be written as

$$ F_c(t) = \frac{1}{R_c} = \frac{\sqrt{(y_t z_{tt} - z_t y_{tt})^2 + (z_t x_{tt} - x_t z_{tt})^2 + (x_t y_{tt} - y_t x_{tt})^2}}{(x_t^2 + y_t^2 + z_t^2)^{3/2}} \quad (D.2) $$

where $R_c$ is the radius of the curvature. The subscript $t$ denotes the derivative. To evaluate the local curvature, we use the PFD scheme developed in Section 4.8.

Suppose the curve is single-valued in a local coordinate, call it $t$, with its projected length $L$. We first divide $L$ into $N$ equally spaced segments with $\Delta = L/N$.

We then define a non-negative function

$$ D_j(t) = \Delta[1 - wK_j(t)] \quad (D.3) $$

where $j = 1, 2, \ldots, N + 1$, $K(t)$ is a functional of the curvatures and $w$ is a weighting
function with \( w \in [0, K_{\max}) \). Then, we have

\[
L' = \sum_{j=1}^{N} D_j = \sum_{j=1}^{N} \Delta[1 - wK_j(t)]dt = L(1 - \frac{w}{N} \sum_{j=1}^{N} K_j).
\]  

(D.4)

The local segment length is, then, obtained by normalizing the \( D_j(t) \), viz.

\[
\Delta'_j = \frac{D'_j L}{L'} = \frac{L}{N} \frac{1 - wK_j}{1 - \frac{w}{N} \sum_{j=1}^{N} K_j}.
\]  

(D.5)

Functional \( K(t) \) governs the local density of elements and is called distribution function. For the problem in this work, we choose \( K(t) = F_c^2(t) \). If the curve is two-dimensional in \( x \) and \( y \), we have

\[
F_c^{2D}(t) = \frac{z(t)y(t) - y(t)x(t)}{(z(t)^2 + y(t)^2)^{3/2}}.
\]  

(D.6)
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