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# Pore Fluids and the LGM Ocean Salinity—Reconsidered

Carl Wunsch\*

Department of Earth and Planetary Sciences

Harvard University

Cambridge MA 02138

email: cwunsch@fas.harvard.edu

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## Abstract

Pore fluid chlorinity/salinity data from deep-sea cores related to the salinity maximum of the last glacial maximum (LGM) are analyzed using estimation methods deriving from linear control theory. With conventional diffusion coefficient values and no vertical advection, results show a very strong dependence upon initial conditions at -100 ky. Earlier inferences that the abyssal Southern Ocean was strongly salt-stratified in the LGM with a relatively fresh North Atlantic Ocean are found to be consistent within uncertainties of the salinity determination, which remain of order  $\pm 1$  g/kg. However, an LGM Southern Ocean abyss with an important relative excess of salt is an assumption, one not required by existing core data. None of the present results show statistically significant abyssal salinity values above the global average, and results remain consistent, apart from a general increase owing to diminished sea level, with a more conventional salinity distribution having deep values lower than the global mean. The Southern Ocean core does show a higher salinity than the North Atlantic one on the Bermuda Rise at different water depths. Although much more sophisticated models of the pore-fluid salinity can be used, they will only increase the resulting uncertainties, unless considerably more data can be obtained. Results are consistent with complex regional variations in abyssal salinity during deglaciation, but none are statistically significant.

## 1 Introduction

McDuff (1985) pointed out that pore-waters in deep-sea cores have a maximum chlorinity (salinity) at about 30m depth owing to the sea level reduction during the last glacial period. He

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\*Also, Department of Earth, Atmospheric and Planetary Sciences; Massachusetts Institute of Technology

25 emphasized, however, the basic million-year diffusive time-scale of change in cores of lengths of  
 26 several hundred meters. Schrag and DePaolo (1993) pioneered the interpretation of the data,  
 27 focussing on  $\delta^{18}\text{O}$  in the pore water, and noted that in a diffusion-dominated system, the most  
 28 useful signals would be confined to about the last 20,000 years. Subsequently, Schrag et al.  
 29 (1996, 2002), Adkins et al. (2002), Adkins and Schrag (2003; hereafter denoted AS03) analyzed  
 30 pore water data to infer the ocean abyssal water properties during the last glacial maximum  
 31 (LGM) including chlorinity (interpreted as salinity) and  $\delta^{18}\text{O}_w$ . (The  $w$  subscript is used to  
 32 distinguish the values from  $\delta^{18}\text{O}_c$  in the calcite structures of marine organisms.)

33 The latter authors started with the uncontroversial inference that a reduction in sea level of  
 34 about  $\Delta h = -125$  m in an ocean of mean depth  $h = 3800$  m would increase the oceanic average  
 35 salinity,  $\bar{S}$ , by and amount  $\Delta S$  as,

$$\frac{\Delta S}{\bar{S}} = -\frac{\Delta h}{h} = \frac{125}{3800} \approx 0.03. \quad (1)$$

36 With a modern average salinity of about 34.7 g/kg,  $\Delta S \approx 1.04$  g/kg for a global average LGM  
 37 salinity of about 35.7 g/kg. By calculating the salinity profile as a function of core depth, they  
 38 drew the now widely accepted inference that the abyssal LGM ocean contained relatively more  
 39 salt—with values above the LGM global mean—than it does today. A Southern Ocean core  
 40 produced calculated values exceeding 37 g/kg. (AS03, used a somewhat higher value of 35.85  
 41 g/kg for the LGM mean. The difference is unimportant in what follows.)

42 Those inferences, coupled with analogous temperature estimates from  $\delta^{18}\text{O}_w$  (Schrag et al.,  
 43 2002) that the deep ocean was near freezing, has widespread consequences for the oceanic state,  
 44 carbon storage, deglaciation mechanisms (e.g., Adkins et al., 2005), etc. A salty, very cold,  
 45 Southern Ocean abyss has become a quasi-fact of the subject (e.g., Kobayashi et al., 2015).

46 In the interim, a few other analyses have been published. Insua et al. (2014), analyzed core  
 47 pore-fluid data in the Pacific Ocean and came to roughly similar conclusions. Miller (2014) and  
 48 Miller et al. (2015), using a Monte Carlo method, carried out a form of inversion of the available  
 49 pore water profiles and drew the contradictory inference that the data were inadequate for any  
 50 useful quantitative conclusion about the LGM salinity or  $\delta^{18}\text{O}_w$ .

51 Determining the stratification of the glacial ocean and its physical and dynamical conse-  
 52 quences is where paleo-physical oceanography meets sedimentology and core chemistry; see  
 53 Huybers and Wunsch (2010). The purpose of the present note is to carry out a more generic  
 54 study of the problem of making inferences from one-dimensional time-dependent tracer profiles.  
 55 For maximum simplicity, only chlorinity/salinity data are discussed, with an analysis of  $\delta^{18}\text{O}_w$   
 56 postponed to a second paper. The question being addressed is *whether the chlorinity data alone*  
 57 *determine the ocean salt stratification during the LGM?* The papers already cited can be in-

Core No.	Reference	Location	Water Depth (m)
ODP981	Jansen et al. (1996)	NE Atlantic, Feni Drift/Rockall	2200
ODP1063	Keigwin et al. (1998)	Bermuda Rise	4600
ODP1093	Gersonde et al. (1999)	Southern Ocean, SW Indian Ridge	3600
ODP1123	Carter et al. (1999)	E. of New Zealand, Chatham Rise	3300
ODP1239	Mix et al. (2002)	E. Tropical Pacific, Carnegie Ridge/Panama Basin	1400

Table 1: Cores from which chlorinity/salinity data were used, along with a reference to their initial description in the Ocean Drilling Program (ODP) and with a geographical label. A nominal water depth of the core-top is also listed.

58 interpreted as asking whether, given other knowledge of the LGM, the chlorinity data contradict  
59 their picture of that time?

60 Conventional inverse methods derived from control theory are used: these have a more  
61 intuitive methodology and interpretation relative to those of the more specifically Bayesian  
62 Markov Chain Monte Carlo (MCMC) method of Miller et al. (2015). Although the MCMC  
63 method produces full probability densities for the results, interpretations almost always begin  
64 with the mean and variance, quantities emerging from the more conventional methods. As in  
65 the formal Bayesian approaches, prior knowledge with statements of confidence is both needed  
66 and readily used. (For modern physical oceanographers, parallels exist with understanding the  
67 establishment through time of the “abyssal recipes” formulation of Munk (1966) although the  
68 parameter ranges are far different.) The approaches here are those used by Wunsch (1988) for  
69 oceanic passive tracers and by MacAyeal et al. (1991) to infer temperatures in ice boreholes  
70 (and see MacAyeal, 1995) .

### 71 *Profiles*

72 To set the stage and to provide some context, Fig. 1 shows the positions of the cores discussed  
73 by AS03 plotted on a contour map of modern salinity at 3600 m depth. A bimodal histogram  
74 of those salinity values is shown in Fig. 2. Figs. 3 and 4 display the data available from five  
75 cores whose positions are shown on the chart. Considerable variation is apparent in both space  
76 (latitude and longitude) and time (that is, with water depth and depth in the core).

77 Consider the Southern Ocean core ODP 1093 (see Gersonde et al., 1999, and Figs. 3, 5)  
78 analyzed by AS03 and by Miller et al. (2015). It was this core that displayed the highest  
79 apparent salinity during the LGM and which led to the inference of a strongly salinity-stratified  
80 ocean dominated by Antarctic Bottom Waters. (Its position on top of a major topographic  
81 feature, Fig. 5, raises questions about the one-dimensionality of the core physics, but that

82 problem is not pursued here.) The overall maximum of about 35.7 g/kg perceptible in the core  
 83 is somewhere between 50 and 70 m depth below the core-top and is plausibly a residual of high  
 84 salinity during the LGM (a very large value near 400 m depth is assumed to be an unphysical  
 85 outlier). Initially, only the top 100 m of the measured cores, Fig. 4, will be dealt with here. The  
 86 main questions pertain to the magnitude and timing of the maxima and their interpretations.  
 87 Very great differences exist in the water depths of the cores (Table 1) and the physical regimes  
 88 in which they are located are today very different. Differences amongst the core salinity profiles  
 89 are unresponsive of simple global-scale change.

90 In what follows, only the Atlantic Cores 1063 (about 4500 m water depth) and 1093 (about  
 91 3600 m water depth) will be discussed. Notice (Fig. 4) that the maximum salinity observed in  
 92 Core 1093 in the upper 100 m is at best at, but not above, the estimated oceanic LGM global  
 93 mean salinity maximum of 37.08 g/kg of AS03.

94 In Core 1063, at the northeastern edge of the Bermuda Rise, the apparent maximum occurs  
 95 somewhere in the vicinity of 40 m core depth, with a value of about 35.35 g/kg—above the  
 96 modern water mean—but well-below the LGM mean. Core 1063 was used to infer that the  
 97 deep North Atlantic Ocean had not become as saline as in the Southern Ocean, and hence with  
 98 the results from Core 1093, that the Southern Ocean had an extreme value of abyssal salinity,  
 99 relative to the rest of the LGM ocean. Generally, the salinity of Core 1063 is lower than that of  
 100 1093 except near the core-top where the variability in Core 1093 precludes any simple statement.

101 Inferences from pore water profiles correspond to what in the control literature is known as a  
 102 “terminal constraint” problem (e.g., Luenberger, 1979; Brogan, 1991; Wunsch, 2006—hereafter  
 103 W06): In a physical system, the externally prescribed disturbances are sought that will take the  
 104 system from a given initial state to a known, within error-bars, final state.<sup>1</sup> Here the physical

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<sup>1</sup>A more intuitive analogue of this problem may be helpful, one based upon the terminal control problem for a conventional robotic arm. An arm, with known electromechanical response to an externally imposed set of control signals, has to move from a three dimensional position,  $\xi_0 \pm \Delta\xi_0$ , at time  $t = 0$ , to a final position  $\xi_{t_f} \pm \Delta\xi_f$  at time  $t_f$ . In three-dimensions, there exists an infinite number of pathways between the starting and ending position, excluding only those that are physically impossible (such as a movement over a time-interval physically too short for transit between the two positions). Even if the trajectory is restricted to a straight line, there will normally be an infinite indeterminacy involving speed and acceleration. The control designer “regularizes” the problem by using a figure-of-merit e.g., by demanding the fastest possible movement, or the least energy requiring one, or minimum induced accelerations etc. The designer might know e.g., that the arm must pass close to some known intermediate position  $\xi_i \pm \Delta\xi_i$  and which can greatly reduce the order of the infinity of possible solutions. In the case of the pore fluid, the initial “position” (initial pore fluid value,  $c(z, t_f)$ ), is at best a reasonable guess, and no intermediate values are known. The assumed prior control represents an initial guess at what controlling signals can be sent, e.g., that a voltage is unlikely to exceed some particular value. The “identification” problem would correspond to the situation in which the model or plant describing the reaction of the robotic arm to external signals was partially uncertain and had to be determined by experiment. And perhaps the response would also

105 system is an assumed advection-diffusion one, with the initial state being the salinity profile far in  
 106 the past (perhaps -100,000 y), the terminal state is represented by data from the measured core  
 107 pore-water. The disturbances sought are the abyssal water salinity—providing a time-varying  
 108 boundary condition at the sediment-water interface. Readers familiar with advection-diffusion  
 109 problems will recognize their dependence upon a long list of knowns, including the initial and  
 110 boundary conditions, and the advective flows and diffusion coefficients governing the time-depth  
 111 evolution. In the present case, flows and diffusion coefficients are expected to display structures  
 112 varying in both space (depth in core) and time. In the best situation, only their terminal  
 113 values can be measured in the core. The problem is further compounded by the dependence of  
 114 advection and diffusion on the time history of the solid phase in the sediment containing the  
 115 pore waters. Finally, and a question also ignored here, is whether a handful of core values can  
 116 be used to infer global or regional mean properties (see Figs. 1, 2) with useful accuracy.

117 For the time being, the problem is reduced to a basic skeletal framework to understand its  
 118 behavior under the most favorable conditions.

## 119 2 Models

120 General discussion of pore fluid behavior in sediments can be found in Berner (1980), Boudreau  
 121 (1997), Fowler and Yang (1998), Einsele (2000), Bruna and Chapman (2015) and in the papers  
 122 already cited. Simplifying a complex subject, LGM pore fluid studies reduce the vertical profiles  
 123 to the one-space-dimension governing equation, the canonical model,

$$\frac{\partial c}{\partial t} + w \frac{\partial c}{\partial z} - \frac{\partial}{\partial z} \left( k \frac{\partial c}{\partial z} \right) = 0 \quad (2)$$

124 Here  $k$  is an “effective” diffusivity, and  $w$  is a non-divergent vertical velocity within the core  
 125 fluid relative to the solid phase. Note that if  $\partial k / \partial z \neq 0$ , the diffusion term breaks up into two  
 126 parts, one of which is indistinguishable from an apparent advective term,  $w^* = -\partial k / \partial z$ , so that  
 127 Eq. (2) is,

$$\frac{\partial c}{\partial t} + \left( w - \frac{\partial k}{\partial z} \right) \frac{\partial c}{\partial z} - k \frac{\partial^2 c}{\partial z^2} = 0. \quad (3)$$

128  $k$  depends upon the porosity,  $\phi$ , and the tortuosity,  $\theta$ , of the sediment through relations such as,

$$\theta^2 = \phi^{1-\alpha}, \quad \alpha \approx 1.8, \quad k \propto \phi / \theta^2. \quad (4)$$

129 An upward increasing porosity (Fig. 6 and Eq. 4) produces, an apparent effective  $w^* = -\partial k / \partial z$ .  
 130 The oceanographers’ convention that  $z$  is positive upwards is being adopted, but here the origin is  
 depend upon time, involving the changing mechanical configuration, as occurs for example, in controlling the  
 trajectory of aging spacecraft.

131 at 100m below the sediment-water interface, and where a boundary condition must be imposed.  
132 Experiments (not shown) with  $k$  changing linearly by a factor of two showed little change from  
133 the constant  $k$  values.

134 The core fluid is visualized as being contained in a vertical “pipe,” extending from  $z = 0$  at  
135 the base of the pipe to  $z = h$  at the sediment-water interface. At that interface, it is subject  
136 to a time-dependent boundary condition  $C_h(t) = c(z = h, t)$ ,  $0 \leq t \leq t_f$  representing (here)  
137 the salinity of the abyssal water and whose values through time are sought. The only available  
138 data are the measured profile at  $t = t_f$  over a depth range  $0 \leq z < h(t_f)$  where  $t_f$  is the date  
139 at which a core was drilled.  $h$  is here taken as 100m above the origin. Information about the  
140 initial condition,  $C_0(z) = c(z, t = 0)$ , and the boundary condition at  $z = 0$ , may, depending  
141 upon parameters, be essential.

142 Sediment continues to accumulate and erode over the time history recorded in the core. Thus  
143 the sediment-water interface,  $z = h$ , is time-dependent, and perhaps monotonically increasing.  
144 A somewhat typical sedimentation rate (they vary by more than an order of magnitude) might  
145 be about 5 cm/ky =  $1.6 \times 10^{-12}$  m/s. Following Berner (1980) and Boudreau (1997),  $h$  is fixed  
146 to the moving sediment-water interface, meaning that the solid material directly exposed to the  
147 abyssal salinity would be 5 m displaced from the initial surface at the end of 100,000 y. The  
148 assumption is thus made that while the particulate material is displaced, the *fluid* in contact  
149 with the overlying sea water remains the same. With  $h(t)$  taken as a fixed point, a corresponding  
150 5 m error at the core-base,  $h = 0$ , is incurred, and will be ignored.

151 The canonical model omits a complex set of boundary layers just below and just above  
152 the interface at the sea floor (e.g., Dade et al., 2001; Voermans, 2016), which in principle are  
153 observable at the core top, and which would affect the boundary condition there. These too,  
154 are being ignored.

### 155 *Scale Analysis—Orders of Magnitude*

156 Before doing any specific calculations, obtaining some rough orders of magnitude is helpful.  
157 Although every core is different, the time interval of most interest here is the LGM, taken to end  
158 nominally at  $t = t_f - 20,000$  y =  $t_f - 6.3 \times 10^{11}$  s (20 ky BP) following which deglaciation begins.  
159 For several cores, AS03 estimated  $k \approx 3 \times 10^{-10}$  m<sup>2</sup>/s and Miller (2014) a value of  $k \approx 2 \times 10^{-10}$   
160 m<sup>2</sup>/s. In the purely diffusive limit with  $w \approx 0$ , the  $e$ -folding diffusion time to reach the whole  
161 core depth is  $L^2/k \approx 1.6 \times 10^6$  y, with the latter value of  $k$ . The  $e$ -folding diffusion decay time at  
162 any depth is  $l^2/k$ , where  $l^2$  is the vertical length scale of any disturbance in the profile. For  $l = 10$   
163 m,  $l^2/k \approx 16,000$  y not far from the time interval since the LGM. Depending directly upon the  
164 analytical sensitivities and the space/time scales of interest, a 100 m core can retain a signature  
165 of some disturbances dating back more than 1 million years, consistent with McDuff’s (1985)

Notation	Variable	Definition
Initial Condition	$C_0(z)$	$c(t=0, z)$
Boundary Condition	$C_h(t)$	$c(t, z=0)$
Terminal Condition	$C_{\text{term}}(z)$	$c(t=t_f, z)$

Table 2: Notation used for initial, final and boundary conditions and for algebraic expressions. In the discrete form, two time-steps of the concentration  $c$  make up the state vector,  $x(t)$ , and corresponding imposed conditions, Tildes over variables denote estimates. Matrices are bold upper case letters, column vectors are bold lower-case letters.

166 inference. In the shorter term, and as noted by Schrag et al. (2002), in a purely diffusive system  
 167 the depth and attenuated amplitude of a local maximum represent competing dependencies on  
 168  $k$ , with smaller scale signals not surviving beyond about 20,000 y.

169 Should the vertical velocity,  $w$ , of fluid within the core become significant, additional time  
 170 and space scales emerge—depending upon the sign of  $w$ ; the position and amplitude of maxima  
 171 are then no longer simply related. For  $w > 0$ , a boundary layer familiar from Munk (1966) of  
 172 vertical scale,  $k/w$ , appears with an establishment time of  $k/w^2$ . Should  $w \approx 2 \times 10^{-10}$  m/s= 6  
 173 m/thousand years, the vertical scale is 1 m, with an establishment time of  $5 \times 10^9$  s or about 150  
 174 y. Two Péclet numbers appear, one based upon  $L$ , the other upon  $l$ . If  $w < 0$ , the advection  
 175 time  $L/w$  is relevant and the combined  $k, w$  scales are unimportant.

176 In a number of published results the initial conditions at some time,  $t = 0$  in the core,  
 177  $C_0(z)$ , are simply assumed to be of little influence in the interpretation of the final profile  
 178  $c(z, t = t_f) = C_{\text{term}}(z)$ , with most attention focussed on determining the temporal boundary  
 179 condition control,  $C_h(t)$ . Whether the initial conditions are unimportant (the signal having  
 180 decayed away) or dominant, given the long time scales within the core, will depend upon the  
 181 magnitudes of  $w, k$ , the sign of  $w$ , as well as the core length.

182 In principle,  $w, k$  values can be calculated from the available data and various hypotheses,  
 183 both physical and statistical the—“identification problem.” Introducing further unknowns into  
 184 what will be perceived as an already greatly underconstrained problem, leads necessarily to even  
 185 greater uncertainty in the estimates  $\tilde{C}_h(t), 0 \leq t \leq t_f$ , or of  $\tilde{C}_0(z)$  (see Table 2 for notation;  
 186 tildes are used to denote estimates.) The simplest problem, with known  $k, w$ , produces a lower  
 187 bound uncertainty on the results. Should that lower bound be too large for use, solving the  
 188 nonlinear estimation problem involving  $k, w$  as additional unknowns to be extracted from the  
 189 same limited data would not be justified.

190 *Analytical Reference Solutions*



In the simplest case with  $w = 0$ , and  $k$  constant, a variety of analytical solutions to Eq. (2) is available. These are again useful for understanding the solution structure. As a representative calculation, set  $w = 0$  and  $k = 2 \times 10^{-10} \text{m}^2/\text{s}$  at zero-Péclet number. Let  $C_h(t) = H(t)$ ,  $H(t)$  being the unit step (Heaviside) function, be the upper boundary value, and let  $C_0(z)$  be the initial conditions. Fig. 7 displays the profiles from the analytical solution (Carslaw and Jaeger, 1986, p. 101) calculated as a summation here over 100 terms of a weighted cosine series, as a function of time,

$$c_{anal}^{(1)}(z, t) = 1 + \frac{2}{L} \sum_{n=0}^{\infty} \left\{ \frac{2L(-1)^{n+1}}{(2n+1)\pi} + \int_0^L C_0(z') \cos\left(\frac{(2n+1)\pi z'}{2L}\right) dz' \right\} \times \quad (5)$$

$$e^{-k(2n+1)^2\pi^2 t/4L^2} \cos\left(\frac{(2n+1)\pi z}{2L}\right),$$

191 for a unit amplitude surface boundary condition, zero flux at the bottom, and  $C_0(z) = 0$ . The  
 192 terminal profile is also shown. Weighting,  $\exp(-k(2n+1)^2\pi^2 t/4L^2)$ , connects the dissipation  
 193 rate to the vertical structure present in the solution,<sup>2</sup> and which rapidly removes even moder-  
 194 ately high wavenumber,  $(2n+1)\pi/2L$ , structures whether present in the initial conditions, or  
 195 emanating from the boundary condition (here, with zero initial conditions, only the boundary  
 196 step-function gives rise to high wavenumbers). Fig. 8 shows the decay time to 1% of the initial  
 197 value as a function of vertical scale in the initial conditions or those induced by the boundary  
 198 conditions. Vertical scales shorter than about 12 m will have decayed by 99% after 20,000 years  
 199 and need not be considered with this value of  $k$ .

200 The equivalent solution for zero initial conditions and a periodic surface boundary condition,  
 201  $C_0(t) = \sin(\sigma t)$  is (Carslaw and Jaeger, 1986, p. 105),

$$c_{anal}^{(2)}(z, t) = \left\{ \frac{\cosh 2(\sigma/2k)^{1/2} z - \cos 2(\sigma/2k)^{1/2} z}{\cosh 2(\sigma/2k)^{1/2} L - \cos 2(\sigma/2k)^{1/2} L} \right\}^{1/2} \sin(\sigma t + \varphi) + \quad (6)$$

$$2\pi k \sum_{n=0}^{\infty} \frac{n(-1)^{n+1} \sigma L^2}{k^2 n^4 \pi^4 + \sigma^2 L^4} e^{-kn^2\pi^2 t/L^2} \sin\left(\frac{n\pi z}{L}\right)$$

$$\varphi = \arctan \left\{ \frac{\sinh \left[ (\sigma/2k)^{1/2} z (1+i) \right]}{\sinh \left[ (\sigma/2k)^{1/2} L (1+i) \right]} \right\}$$

202 where here the lower boundary condition is  $c(0) = 0$  and placed at  $z = -500$  m. The first term  
 203 is the steady-state sinusoidal profile, whose amplitude is shown in Fig. 10a as a function of  
 204 depth for varying  $\sigma$  and the above values of  $k, L$ . The second term is the starting transient with

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<sup>2</sup>The scale used above,  $L^2/k$ , describes the lowest wavenumber response.

205 decay times shown in Fig. 10b. If the LGM were regarded as part of a quasi-periodic signal  
206 with the obliquity period of about 40,000 y, the signal would not penetrate much below 50 m.  
207 Even at 100 ky periods, no measurable signal reaches the base of a 100 m core.

208 Analytical solutions also exist for the case  $w \neq 0$ , but are not displayed here (see Wunsch,  
209 2002 for references).

### 210 **3 Representative Model Solutions**

211 An axiom of inverse methods is that full understanding of the forward problem is a necessary  
212 preliminary. In a conventional forward calculation, solutions depend directly and jointly upon  
213 all of:

- 214 (1) The initial conditions,  $C_0(z)$ ,
- 215 (2) The top boundary condition here,  $c(z = h, t) = C_h(t)$
- 216 (3) The bottom boundary condition involving  $c(z = 0, t)$  and/or its derivatives (here always  
217 a no-flux condition)
- 218 (4) Physical parameters,  $w, k$ .

219 Conventionally, these values are all perfectly known with the solution changing if any of  
220 them does.

221 In practice in the present case, only the final state of the solution,  $C_{term}(z) = c(t_f, z)$ ,  
222 is approximately available. The inverse problem involves making inferences about the state,  
223  $c(z, t)$ ,  $0 \leq t \leq t_f$ ,  $0 \leq z \leq h$ , initial and boundary conditions, and the  $w, k$  parameters from  
224 the limited supply of information. Use of prior information (assumptions) with statements of  
225 confidence becomes crucial. If incorrectly formulated, so-called inverse solutions to diffusive  
226 systems can become extremely unstable and demonstrably stable methods are required.

227 AS03 and subsequent authors have suggested that a good prior estimate of the boundary  
228 conditions on all cores consists of making  $C_h^{a\ priori}(t)$  proportional to the best-estimated sea level  
229 curve. Fig. 11 shows the calculated global mean salinity over 120,000 years (Miller, 2014; Miller,  
230 et al., 2015) from a number of sources (their Table 1), and Eq. (1). Between about  $-70,000$  y  
231  $< t - 25,000$  y, values higher than 35 g/kg are estimated owing to the reduction in sea level,  
232 reaching a maximum at a sea level minimum near  $t = -20,000$  y. After that, the deglaciation  
233 leads to an estimated fall.<sup>3</sup>

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<sup>3</sup>Adkins and Schrag (2003) used a considerably more structured estimated sea level curve. But because prior to -20 ky it was based upon measured  $\delta^{18}\text{O}$ , which is one of the tracers under consideration in these cores Miller (2014), Miller et al. (2015) chose to avoid any possibility of circular reasoning. Much of the small scale structure present in the former curve would not survive the diffusive process in the core. Large scale structures are qualitatively the same in both approaches.

234 Thus, following the previous literature, the top boundary condition is, for now, assumed  
235 to be  $C_h^{\text{a priori}}(t)$  and the bottom boundary condition to be one of zero diffusive flux. Initial  
236 conditions are problematic. The purely diffusive numerical calculation and the analytic solutions  
237 both show that disturbances at the surface will not penetrate significantly below about 40 m  
238 depth in 100,000 years. Structures in Figs. 3, 4 below that depth cannot have arisen from  
239 the core surface in the last 100 ky. At least four possibilities suggest themselves: (1) The  
240 structures are simply the noise in the core from measurements (see AS03 for of the technicalities  
241 and difficulties of shipboard measurements) or from processes not yet included in the model  
242 (time-space-dependent  $w, k$ , or clathrate formation, for example). (2) The structures arise from  
243 the memory of the initial conditions. (3) A purely diffusive model is inadequate. (4) The  
244 structures are the result of upward diffusion/advection across the base of the core,  $z = 0$ , noting  
245 in particular that  $\partial C(0)/\partial z$  in general does not vanish. All of these possibilities could be at  
246 work.

247 The simplest interpretation of the solutions discussed by AS03 and others is based on as-  
248 sumption (1): that all structures other than the deep overall maximum represent errors in the  
249 data, and that *only the gross maximum feature must be reproduced*. In contrast, a more agnostic  
250 approach is taken here, in which an attempt is made to understand the extent to which some  
251 or all of the additional core-data features can be regarded as signals. For example, if structures  
252 in the initial conditions can persist in the core, they should be visible at the terminal time.  
253 Some of the published solutions have taken the sensible approach of maximum ignorance, and  
254 set  $C_0(z) = \text{constant}$ , where the constant might be the modern mean salinity. In that situation,  
255 either all of the terminal structure arises from  $C_h(t)$ , and/or non-uniform initial conditions are  
256 nonetheless also required by the terminal data. Another possibility is based upon the description  
257 of the glacial-interglacial cycles as being quasi-periodic, with glaciations recurring at intervals  
258 lying between 80,000 and 120,000 y, leading to a second plausible hypothesis that the initial  
259 condition at  $t = -100$  ky is close to the observed terminal profile of the individual core (Fig. 3).  
260 Except where specifically stated otherwise, this quasi-periodic condition, but with different un-  
261 certainty estimates applied to the initial and terminal data, is used throughout this study. The  
262 initial condition uncertainty is always larger than the terminal one. A similar initial condition  
263 (set at -125 ky) was used by Miller et al. (2015).



277 As a demonstration of the numerical model, let the time-step be  $\Delta t = 4 \times 10^9$  s (127 years),  
 278  $L = 100$  m, and  $\Delta z = 1$  m,  $k = 2 \times 10^{-10}$  m<sup>2</sup>/s,  $w = 0$ , for the Heaviside boundary condition,  
 279  $q(t) = 1, 0 \leq t \leq t_f$  and zero initial condition, with result shown in Fig. 7 and the terminal  
 280 state compared to the analytic solution. Consistent with the scale analysis and the analytic  
 281 solution, the signature of the surface boundary condition has not reached beyond about 50 m  
 282 after 100,000 years.

283 Now consider the quasi-periodic initial condition with the same  $w, k$ . Fig. 9 shows the results  
 284 after 100 ky of forward model integration. The smallest scales present in the initial condition  
 285 have vanished—as expected. However, much of the intermediate and largest structures at the  
 286 terminal time originate with the initial conditions. In contrast, also shown is the state when  
 287  $w = -|k|$ . In that situation, the initial conditions are swept downward, out of the core, before  
 288 the terminal time.

289 When  $w \neq 0$ , qualitative changes in the solutions occur. With  $w > 0$ , confinement of  
 290 disturbances from  $C_h^{\text{a priori}}(t)$  towards the surface is even more marked than for the purely  
 291 diffusive case. When  $w < 0$ , structures in  $C_h(t)$  can be carried much further down into the core  
 292 than otherwise. The magnitude and sign of  $w$  thus become major issues.

## 293 4.2 Inversions/Control Solutions

294 Miller (2014) also discussed the linear time-dependent inverse problem of determining  $u(t)$ ,  
 295 the modification to  $q(t) = C_h^{\text{a priori}}(t)$  and chose to solve it by “Tikhonov regularization.” (Here  
 296 both  $\mathbf{q}$  and  $\mathbf{u}$  are scalars—a special case). Although that method is a useful one for deterministic  
 297 problems, it does not lend itself to a discussion of data and model error, nor of the uncertainties  
 298 of the results owing to noise. Determining a best-solution involves not only the core physical  
 299 properties and time-scales, but also the analytical accuracies, and systematic down-core errors.

Consider the problem of determining  $C_h(t) = q(t) + u(t)$  (that is,  $u(t)$ ) from the terminal  
 values  $\mathbf{x}(t_f)$ , which involves assuming here that  $\mathbf{c}(t_f - 1) = \mathbf{c}(t_f) = C_{term}(z)$ . Now,  $\mathbf{\Gamma} = \mathbf{B}$ ,  
 and  $u(t)$  is sought. Several standard methods exist. One approach is to explicitly write out  
 the full set of simultaneous equations governing the system in space and time, recognizing that  
 the only information about the state vector are its final values,  $\mathbf{x}(t_f)$ , and a guessed initial  
 condition,  $\mathbf{x}(0)$ . In practice, neither will be known perfectly, and a covariance of the error in  
 each is specified, here called  $\mathbf{P}(0)$  and  $\mathbf{R}(t_f)$  respectively. Writing out the full suite of governing

equations, setting  $\Delta t = 1$  for notational simplicity but with no loss of generality,

$$\begin{aligned}
 \mathbf{x}(0) + \mathbf{n}(0) &= \mathbf{C}_0(z) \\
 \mathbf{x}(1) - \mathbf{A}\mathbf{x}(0) - \mathbf{\Gamma}u(0) + \mathbf{n}(1) &= \mathbf{B}q(0) \\
 \mathbf{x}(2) - \mathbf{A}\mathbf{x}(1) - \mathbf{\Gamma}u(1) + \mathbf{n}(2) &= \mathbf{B}q(1) \\
 \mathbf{x}(3) - \mathbf{A}\mathbf{x}(2) - \mathbf{\Gamma}u(2) + \mathbf{n}(3) &= \mathbf{B}q(2) \\
 &\dots \\
 -\mathbf{A}\mathbf{x}(t_f - 1) - \mathbf{\Gamma}u(t_f - 1) + \mathbf{n}(t_f) &= -\mathbf{C}_{\text{term}}(z) + \mathbf{B}q(t_f - 1),
 \end{aligned} \tag{10}$$

300 where all unknowns are on the left of the equals sign, and all known fields are on the right.  
 301 Vectors  $\mathbf{n}(t)$  represent the presence of errors in the starting and ending profiles and their  
 302 propagation through the system. The  $\mathbf{\Gamma}u(t)$  terms are the controls and which, more gener-  
 303 ally, include the model error, but here are specifically accounting only for the uncertainties in  
 304  $\mathbf{B}q(t), q(t) = C_h^{\text{a priori}}(t)$ . Equations (10) are a set of linear simultaneous equations which is,  
 305 however, extremely sparse; unless  $t_f$  or  $N$  become very large, they can be solved by several  
 306 methods for dealing with underdetermined systems. This route is not pursued here, but the ex-  
 307 istence of the set shows that any other method of solution is equivalent to solving it, and which  
 308 can help greatly in the interpretation. The special structures present in the equations permit  
 309 rapid and efficient solution algorithms not requiring explicitly inverting the resulting very large,  
 310 albeit very sparse, matrix (a generalized-inverse would be involved in practice), and which is the  
 311 subject of the next sections.

## 312 5 Lagrange Multipliers-Pontryagin Principle

### 313 5.1 Formulation

One approach uses ordinary least-squares and Lagrange multipliers to impose the model (Eq. 9) with an error represented by the controls, and minimizing the weighted quadratic misfit between the calculated value of  $\mathbf{x}(0)$  and  $\mathbf{x}_0$  and between the calculated  $\mathbf{x}(t_f)$  and  $\mathbf{C}_{\text{term}}$ ,

$$J = (\tilde{\mathbf{x}}(0) - \mathbf{C}_0(z))^T \mathbf{P}(0)^{-1} (\tilde{\mathbf{x}}(0) - \mathbf{C}_0(z)) + (\tilde{\mathbf{x}}(t_f) - \mathbf{C}_{\text{term}})^T \mathbf{R}(t_f)^{-1} (\tilde{\mathbf{x}}(t_f) - \mathbf{C}_{\text{term}}) + \tag{11}$$

$$\sum_{t=0}^{t_f-1} \tilde{\mathbf{u}}(t)^T \mathbf{Q}^{-1} \tilde{\mathbf{u}}(t).$$

314 respectively. Tildes denote estimates, but are sometimes omitted where the context makes clear  
 315 what is being described. The third term renders the problem fully determined as a constrained

316 least-squares problem, by simultaneously minimizing the weighted mean square difference be-  
 317 tween  $u(t)$  and its prior value (here written as zero), and with a result that is a form of the  
 318 “Pontryagin Principle.” The figure of merit in the  $L_2$  norm attempts to minimize the mean  
 319 square deviation of  $u(t)$  from the prior, which as written here is zero, while simultaneously  
 320 minimizing the squared difference from the assumed initial and final conditions in what is just  
 321 a form of least-squares. (Other figures-of-merit such as maximum smoothness can be used. The  
 322 problem can be reformulated too, using different norms such as  $L_1$  or  $L_\infty$ ; see the references.)  
 323 Because the system of equations (10) has a special block structure, a closed form solution can  
 324 be obtained (W06, P. 218+, or the Appendix here) and which makes explicit the relationships  
 325 between the initial and final states, and the control, all of which are subject to modification.

## 326 5.2 Using Lagrange Multipliers

327 With  $w = 0$ , pure diffusion, and the quasi-periodic initial condition taken from Core 1093, an  
 328 integration is started at  $t = -100,000$  y using the  $C_h^{\text{a priori}}(t)$  in Fig. 11 with result shown in Fig.  
 329 9. Although a rough comparability to the core values occurs in the top 10-20m, they diverge  
 330 qualitatively below that depth, both in the large-scale structures and in the high wavenumbers  
 331 apparent in the core data. The first question to be answered is whether it is possible to modify  
 332  $C_h^{\text{a priori}}(t)$  within acceptable limits,  $\pm\sqrt{Q}$  so as to bring the two terminal profiles together  
 333 within estimated error?

334 The second immediate question is whether the smaller scale structures in the core data are  
 335 real structures or noise (issue (1) above)? Assume that they are uncorrelated white noise of RMS  
 336 amplitude approximately 0.1 g/kg, and allowing the control  $u(t)$  to have the possible large RMS  
 337 fluctuation of 1 g/kg. The initial conditions are assumed to have a white noise (in depth) RMS  
 338 error of 1.7 g/kg, the terminal data RMS uncertainty is 0.1 g/kg, and the result is shown in Fig.  
 339 12. Assuming that none of the structures visible in the core data, except the maximum in the  
 340 vicinity of 40m from the core bottom, are just noise, this solution is a qualitatively acceptable  
 341 one. AS03 noted, that their solutions *above* the maximum in depth did not produce a good fit.  
 342 Much of the terminal state here is controlled by the initial conditions, not  $C_h(t)$ , except for the  
 343 last few thousand years in the very upper parts of the core.

344 Introducing  $w > 0$  exacerbates the confinement of the core-top disturbances to the upper  
 345 core placing even more emphasis on the initial conditions.. On the other hand, permitting  
 346  $w < 0$ , here  $w = -|k|$  m/s succeeds in producing a slightly better fit overall (see Fig. 14) and  
 347 increases the sensitivity to  $C_h(t)$  (using the same prior statistics, held fixed throughout this  
 348 paper). The modification required to  $C_h^{\text{a priori}}(t)$  is also shown along with the resulting total  
 349  $q(t) + \tilde{u}(t)$ . This result decreases the maximum salinity estimated to 35.75 g/kg and delays its

350 timing to about -12,000 y, and is followed by a large variability. Notice that the estimated  
 351 maximum salinity again lies *below* the LGM average—implying high salinities elsewhere. This  
 352 solution is also a formally acceptable one, and if taken at face value, moves the salinity maximum  
 353 several thousand years before that in the prior, and still below the LGM mean. The central  
 354 question at the moment is whether any of the variations in  $C_h(t) = q(t) + \tilde{u}(t)$  are significant?  
 355 Further discussion of this result is postponed pending the calculation of its uncertainty.

356 The large negative value of  $w$  or  $w^*$ —required to carry information downward from the  
 357 core top before diffusion erases the observed structures—is counter to the conventional wisdom  
 358 that the appropriate model is nearly purely diffusive. No claim is made that the model here is  
 359 “correct,” only that if the magnitude of  $w$  is much smaller, or that it is positive upwards, then  
 360 the canonical model cannot explain *any* of the pore-water salinity properties below about 20  
 361 m unless they originate in the initial conditions. On the other hand, the physics of fluid-solid  
 362 interaction through hundreds of thousands of years is sufficiently unclear (see the references  
 363 already cited) that ruling out large negative  $w$  is premature, particularly in partially saturated  
 364 cores where the effects of sea level-induced pressure changes of hundreds of meters of water have  
 365 not been accounted for. Violation of any of the other basic assumptions, including especially,  
 366 that of a one-dimensional-space behavior, could render moot the entire discussion.

367 The Lagrange multiplier formalism does permit an affirmative answer to the question of  
 368 whether a model can be fit to the top 100m of the core data within a reasonable error estimate?  
 369 The stable flow of information, nominally “backwards” in time from the terminal state is partic-  
 370 ularly apparent (Eq. A1) via the transposed matrix  $\mathbf{A}^T$  (the “adjoint matrix”). But it neither  
 371 answers the question of whether this model is “correct” (or “valid” in modelling jargon), or if  
 372 the model is nonetheless assumed correct, how uncertain is the estimate,  $\tilde{C}_h(t) = q(t) + \tilde{u}(t)$ ?  
 373 We next turn to this latter question.

## 374 6 Smoothers

375 A great advantage of the Lagrange multiplier approach is that it is computationally very efficient,  
 376 not involving calculation of the uncertainty of  $\tilde{\mathbf{u}}(t)$ , (the adjustment to  $C_h^{\text{a priori}}(t)$ ) nor of  
 377 the intermediate time values of the profiles in  $\tilde{\mathbf{x}}(t)$ . On the other hand, the absence of those  
 378 uncertainties is the greatest weakness of the estimated state and controls in problems such as  
 379 this one. The need to find formal uncertainties leads to the alternative approach based upon  
 380 the idea of “smoothers”, which are recursive estimation methods for calculating the state and  
 381 control vectors using data from a finite time-span. Several different smoothing algorithms exist  
 382 depending upon the particular need. Perhaps the easiest to understand is the so-called RTS



383 (Rauch-Tung-Striebel) algorithm which involves two-passes through the system in time.

384 To start the RTS algorithm, a prediction algorithm known as the Kalman filter is used,  
385 beginning with the initial conditions and their uncertainty, employing the model (Eq. 9) to  
386 predict the state at the next time when more observations become available (perhaps many  
387 time-steps into the future). By weighting the prediction inversely to its uncertainty and the  
388 observations inversely to their errors, a new estimate is made combining the values appropriately,  
389 and determining the covariance matrix of the new combined estimate. With that new estimate,  
390 further predictions are made to times of new data. (Note that the state estimate jumps every  
391 time a new model-data combination is made, meaning that at those times the model evolution  
392 equation fails.) After arriving at the final data time,  $t_f$ , another algorithm is used to step  
393 backwards in time to  $t = 0$ , using the later-arriving data to correct the original predicted and  
394 combined values of  $\mathbf{x}(t)$ , and estimating the control vector  $u(t)$  necessary to render the model  
395 exactly satisfied at *all* time-steps. Uncertainty estimates are required in the calculation for both  
396 state vector and control.

397 Because several covariance matrices are square of the dimension of  $\mathbf{x}(t)$ , for large systems the  
398 computational load can become enormous. Calculating the error covariance matrix of the state  
399 predicted by the Kalman filter is equivalent to running the model  $N^2$  times at every time step,  
400 and which is why true Kalman filters and related smoothers are never used in real atmospheric  
401 or oceanic fluid systems. Nonetheless, in the present context, realistic calculations are feasible  
402 on modest computers. The state vector solution from the Lagrange multiplier method and from  
403 the RTS smoother can be shown to coincide (e.g., W06, P. 216) and the uncertainties may be  
404 of little interest as long as the controlling solution is physically acceptable.<sup>4</sup>

## 405 **6.1 Using the Filter-Smoother**

406 Consider again Core 1093. The Lagrange multiplier method shows that with  $w = 0$  or  $-|k|$ ,  
407 consistency can be found within varying estimated errors between the model and the measured  
408 terminal state. Those solutions, which minimize the square difference from  $C_h^{\text{a priori}}(t)$ , are not  
409 unique, and as in least-squares generally, an infinite number of solutions can exist, albeit with  
410 all others having a larger mean-square. The question to be answered is what the uncertainty of  
411 any particular solution is, given the existence of others? To do so, the filter-smoother algorithm  
412 is now invoked.

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<sup>4</sup>For example, in operating a vehicle such as an aircraft, that a useful control exists may be the only concern, and with its non-uniqueness being of no interest.

413 **6.2 The Filter Step**

414 With the same initial condition and  $C_h^{\text{a priori}}(t)$  as before, the model is run forward, one time  
 415 step of  $4 \times 10^9$ s (127 y), from Eq. (9) as before, but with a slightly different notation,

$$\tilde{\mathbf{x}}(t + \Delta t, -) = \mathbf{A}\tilde{\mathbf{x}}(t, -) + \mathbf{B}q(t) + \mathbf{\Gamma}\tilde{u}(t), \quad (12)$$

416 with the minus sign showing that no data have been used in the model prediction one time-step  
 417 into the future. This prediction based upon the state estimate at the previous time, and  $\mathbf{B}q(t)$   
 418 set by  $C_h^{\text{a priori}}(t)$ . For now,  $\mathbf{\Gamma}\tilde{u} = \mathbf{0}$ . Simple algebra shows that the error covariance (uncertainty)  
 419 of this one-step prediction is,

$$\mathbf{P}(t + \Delta t, -) = \mathbf{A}\mathbf{P}(t)\mathbf{A}^T + \mathbf{\Gamma}\mathbf{Q}\mathbf{\Gamma}^T, \quad (13)$$

420 where the first term arises from errors in the state estimate,  $\tilde{\mathbf{x}}(t)$ , and the term in  $\mathbf{\Gamma}\mathbf{Q}\mathbf{\Gamma}^T$  rep-  
 421 represents the error from the unknown deviation,  $u(t)$ , from  $q(t)$ . The estimated prior covariance  
 422  $\mathbf{Q}$  is here being treated as time-independent, and is also a scalar,  $Q$ . The progression is started  
 423 with the given  $\mathbf{P}(0)$ .  $\mathbf{P}(t + \Delta t, -)$  is the uncertainty at time  $t$  if no data at  $t + \Delta t$  are used,  
 424 and if no data are available then,  $\mathbf{P}(t + \Delta t) = \mathbf{P}(t + \Delta t, -)$ .

425 Let there be a time  $t'$  when measurement of the full profile is available, written for generality  
 426 as,

$$\mathbf{y}(t') = \mathbf{E}\mathbf{x}(t') + \mathbf{n}(t'). \quad (14)$$

427 With a full profile observation,  $\mathbf{E} = \mathbf{I}$ , the identity matrix.  $\mathbf{n}(t')$  is the zero-mean noise in each  
 428 profile measurement, and with error covariance  $\mathbf{R}(t')$ . Evidently, at  $t'$ , two estimates of the state  
 429 vector,  $\mathbf{x}(t')$  can be made:  $\tilde{\mathbf{x}}(t', -)$  from the model prediction, and  $\tilde{\mathbf{x}}_{\text{data}}(t') = \mathbf{E}^+\mathbf{y}(t')$ , where  
 430  $\mathbf{E}^+$  is a generalized-inverse of  $\mathbf{E}$ , but here is the identity,  $\mathbf{I}$ . Their corresponding uncertainties  
 431 are  $\mathbf{P}(t', -)$ , and  $\mathbf{R}(t')$ . The gist of the Kalman filter is to make an improved estimate of  $\tilde{\mathbf{x}}(t')$   
 432 by using the information available in these two (independent) estimates. With a bit of algebra  
 433 (see any of the references), the best new estimate is the weighted average,

$$\tilde{\mathbf{x}}(t') = \tilde{\mathbf{x}}(t', -) + \mathbf{K}(t') [\mathbf{y}(t') - \mathbf{E}\tilde{\mathbf{x}}(t', -)], \quad (15a)$$

$$\mathbf{K}(t') = \mathbf{P}(t', -) \mathbf{E}^T [\mathbf{E}\mathbf{P}(t', -) \mathbf{E}^T + \mathbf{R}(t')]^{-1} \quad (15b)$$

434 and the new combined estimate has an uncertainty covariance matrix,

$$\mathbf{P}(t') = \mathbf{P}(t', -) - \mathbf{K}(t') \mathbf{E}(t') \mathbf{P}(t', -) \quad (16)$$

435 (variant algebraic forms exist). In the absence of data at  $t'$ ,  $\tilde{\mathbf{x}}(t') = \tilde{\mathbf{x}}(t', -)$ ;  $\mathbf{P}(t') = \mathbf{P}(t', -)$   
 436 because no new observational information is available. In this linear problem, Eqs. (13, 16)

437 are independent of the state  $\mathbf{x}(t)$ , and the uncertainties can be determined without calculating  
438  $\tilde{\mathbf{x}}(t)$  (and which is already available from the Lagrange multiplier solution).

439 In the present situation, only one time, the last one, exists where observations are available.  
440 Thus the model is run forward from the assumed initial conditions and two boundary conditions,  
441 making a prediction of  $\tilde{\mathbf{x}}(t' = t_f, -)$ , using the predicted profile from Eq. (12), along with an  
442 estimate of the error of that prediction (Eq. 13). Then from the weighted averaging in Eq. (15),  
443 a final profile is determined that uses both the information in the a priori model and in the data,  
444 paying due regard to their uncertainties.

### 445 6.3 The Smoothing Step

446 The Kalman filter is seen to be an optimal<sup>5</sup> *predictor* and, contrary to widespread misinter-  
447 pretation, is not a general purpose estimator. The intermediate state  $\tilde{\mathbf{x}}(t) = \tilde{\mathbf{x}}(t, -)$ ,  $t < t_f$ ,  
448 is estimated without using any knowledge of the observed terminal profile and so cannot be  
449 the best estimate.  $\tilde{\mathbf{x}}(t)$  does not satisfy the governing equation at the times when the pre-  
450 dicted estimate and that from the data are combined and  $\tilde{\mathbf{u}}(t)$  is not yet known. Thus in this  
451 particular algorithm (others exist, including direct inversion of the set, Eqs. (10)), the filter  
452 step is followed by the RTS algorithm, as written out in the Appendix and in the references.  
453 The calculation steps backward in time from the final, best estimate  $\tilde{\mathbf{x}}(t_f)$  and its uncertainty,  
454  $\mathbf{P}(t_f)$ , comparing the original  $\tilde{\mathbf{x}}(t_f - \Delta t)$  (Eq. 15) and the prediction made from it, with the  
455 improved estimate now available at one time step in the future, which is both  $\tilde{\mathbf{x}}(t_f)$  and its  
456 uncertainty. The RTS algorithm leads to a third, smoothed, estimate,  $\tilde{\mathbf{x}}(t, +)$ , (in addition  
457 to the existing  $\tilde{\mathbf{x}}(t)$ ,  $\tilde{\mathbf{x}}(t, -)$ ) and  $\tilde{\mathbf{u}}(t)$  from the recursion given in the Appendix. The result  
458 includes the uncertainty,  $\mathbf{P}(t, +)$ , of the smoothed state, and  $\mathbf{Q}(t, +)$  for  $\tilde{\mathbf{u}}(t)$ . Together,  $\tilde{\mathbf{x}}(t)$   
459 and  $\tilde{\mathbf{u}}(t)$  satisfy the model at all times. At  $t_f$ , filtered and smoothed estimates are identical.

460 In the present special case, as in many control problems, the major changes in the scalar  $\tilde{u}(t)$   
461 occur near the end, as the terminal data are accounted for. Those data change  $\tilde{\mathbf{x}}(t_f - \Delta t)$  and  
462 its uncertainty, leading to a change in its immediate predecessor,  $\tilde{\mathbf{x}}(t_f - 2\Delta t)$ , etc., commonly  
463 with a loss of amplitude the further the estimate recedes in time from the terminal data.

## 464 7 Results

### 465 7.1 Top 100 m

466 *Core 1093*

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<sup>5</sup>The term “optimal” is only justified if the various statistics are correctly specified.

467 Fig. 12 displays the inferred modification,  $\tilde{u}(t)$  to  $C_h^{\text{a priori}}(t)$  and its standard deviation  
 468  $\sqrt{\tilde{\mathbf{Q}}(t, +)}$ . The terminal state itself is identical to that in Fig. 9 from the Lagrange multiplier  
 469 method. The maximum value of  $C_h(t)$  occurs at -12ky with a value  $35.8 \pm 0.7$ . With an a priori  
 470 uncertainty of  $\mathbf{Q} = (1\text{g/kg})^2$ , the information content of the terminal state alone is unable,  
 471 except near the very end, to much reduce it. If the same calculation is done using  $\mathbf{Q} = (0.1$   
 472  $\text{g/kg})^2$  (not shown) the uncertainties are correspondingly reduced by producing a different  $\tilde{u}(t)$ ,  
 473 but the smaller permissible adjustments to  $C_h^{\text{a priori}}(t)$  increase the terminal misfits. The a priori  
 474 uncertainties are directly determining the accuracy with which  $C_h(t)$  can be inferred from these  
 475 data. A residual  $\tilde{u}(t)$  uncertainty of  $\pm(0.5\text{-}1 \text{ g/kg})^2$  precludes any interesting inference about  
 476 LGM salinity changes.

477 That the general structure of the solution is nearly independent of the prior control is shown  
 478 by Fig. 13 in which the prior was made a uniform value of the mean value of  $C_h^{\text{a priori}}(t)$ . Only  
 479 in the last 20 ky does any structure appear, and it remains below the estimated LGM mean.  
 480 A similar calculation with a very high prior of 37 g/kg (not shown), with  $w = -|k|$ , is *reduced*  
 481 below the LGM mean in the last 20 ky. The inability here to obtain values as high as those found  
 482 by AS03 and others lies in part with the requirement that the near-core-top data should also be  
 483 fit, data that generally require a strong decrease in  $C_h(t)$  in the last tens of thousands of years.  
 484 Should the core-top data be regarded as noise, perhaps the result of unresolved boundary layers  
 485 in the sediment, higher values of  $C_h$  could be obtained, particularly if the initial conditions are  
 486 made uniform, and near-perfect, and so unchangeable by the estimation procedure.

487 Fig. 14 shows the result obtained by choosing the sea level prior, but allowing  $w = -|k|$  m/s  
 488 with the initial conditions nearly completely ineffective in the final state. The fit to the terminal  
 489 state is somewhat improved, but the uncertainties for  $\tilde{u}(t)$  remain  $O(1 \text{ g/kg})$  except at the very  
 490 end.

### 491 *Core 1063*

492 For core 1063, with  $w = 0$  and the same value of  $k$ , the results are shown in Fig. 15. The state  
 493 estimate is generally within the estimated prior uncertainty. Control  $\tilde{u}(t)$  produces the maximum  
 494 at about -20ky, of  $35.55 \pm 0.85 \text{ g/kg}$ , with a value for the total well-below the estimated LGM  
 495 mean, but with an uncertainty encompassing it. The specific estimated maximum lies below  
 496 that for the Southern Ocean core, consistent with the AS03 result, but here both nominally fall  
 497 below the average. Following that maximum, a considerable variation again occurs, but it is  
 498 without statistical significance.

499 The considerable structure in the estimated control (bottom water salinity) that emerges  
 500 during the deglacial period is interesting, if only in its general variations (none of which are

501 statistically significant). During deglaciation, the injection of  $\approx 125$  m of freshwater and the  
 502 shift in the entire ocean volume to the modern lower salinity, along with the major change in  
 503 atmospheric winds and temperatures, must have generated a host of regional circulation and  
 504 salinity shifts and with complicated spatial differences. Differences found here between the two  
 505 cores do not support an hypothesis of any globally uniform shifts in abyssal salinity—although  
 506 they cannot be ruled out.

## 507 Deeper Core Data

508 Using the values of  $k$  above, the purely diffusive system cannot explain disturbances down-core  
 509 deeper than about 50m or from before about -20,000 y. If the possibility that the effective  
 510  $w = -|k|$  is accepted, signals can penetrate from the surface far deeper into the sediments.  
 511 Assume that the deeper structures are signal, and not measurement or geological noise. Then  
 512 the smoother calculation was carried out for Cores 1093 and 1063 using data from -300 m to  
 513 the surface with a start time of  $t = -200$  ky, a 100 ky periodic  $C_h^{\text{a priori}}(t)$ , and with results  
 514 shown in Figs. 17, 18. The Southern Ocean core shows early excursions even exceeding the  
 515 LGM mean at about -38 ky, while the Atlantic Ocean core is consistently below both the prior  
 516 and the LGM mean. Although it is tempting to speculate about what these apparent excursions  
 517 imply—attaching them to events such as the Bølling-Allerød, Heinrich events, etc.—none of  
 518 them is statistically meaningful, and far more data would be needed to render them so.

519 Because the uncertainty,  $\tilde{Q}$ , of the control remains dominated by the prior assumption of  
 520 independent increments in  $u(t)$ , the estimated values  $\tilde{u}(t)$  remain largely uncorrelated. A  
 521 plausible inference is that on the average over the LGM and the deglaciation that the near-  
 522 Bermuda abyssal waters were considerably fresher than those near the Southwest Indian Ridge  
 523 and to that extent supporting previously published inferences, but not the conclusion that the  
 524 salinity in the latter region was above the global-volume mean.

## 525 8 Modifications and Extensions

526 Thus far, the models used have been purely nominal, one-dimensional with constant in space  
 527 and time diffusion and fixed  $w$ , either zero, or  $w = -|k|$ . Neither of these models is likely very  
 528 accurate; both parameters are subject to variations in time and space, including higher space  
 529 dimensions which would permit non-zero values of  $\partial w/\partial z$ . The central difficulty is that using  
 530 some of the information contained in either  $C_0^{\text{a priori}}(t)$ , or in  $C_{\text{term}}(z)$  to find  $w$  or  $k$  *necessarily*  
 531 *further increases* the calculated uncertainty of  $\tilde{u}(t)$ . More measurements with different tracers  
 532 would help, as would a better understanding of the time-depth properties of pore fluids in abyssal

533 cores. More sophisticated use of the prior covariances (functions of depth and time) could also  
534 reduce the uncertainties—but only to the extent that they are accurate.

## 535 9 Summary and Conclusions

536 Reproducing pore-water chlorinity/salinity observations in a deep-sea core involves an intricate  
537 and sensitive tradeoff of assumptions concerning diffusion rates,  $k$ , magnitudes and signs of the  
538 fluid vertical velocity,  $w$ , prior estimates of lower and upper boundary conditions, and in some  
539 cores, the nature of the initial conditions, the one-dimensional behavior of an advection-diffusion  
540 equation and, crucially, strong assumptions about the nature of the recorded noise. Most previ-  
541 ous inferences with  $w = 0$ , which have led to a picture of the abyssal ocean as particularly saline,  
542 have been based essentially on the assumption that only the salinity maximum appearing at  
543 tens of meters from the core-top is signal, and does not originate with the initial conditions. All  
544 remaining structures are supposed noise of unspecific origin.

545 In the more general, approach used here, initial condition structures in a purely diffusive 100  
546 m core can persist for more than 100 ky, greatly complicating the inference that the terminal  
547 data are controlled by the sea level changes of the past 20 ky alone. When observed structures  
548 beyond the gross maximum in salinity are treated as signals related to abyssal water properties,  
549 a statistically acceptable fit can be obtained by permitting a substantial downward fluid flow,  
550  $w < 0$ , and which removes the initial conditions from the system. The abyssal water property  
551 boundary condition (the system “control” in the present context) however, then displays a  
552 complex and rich structure, none of which is statistically distinguishable from the LGM mean  
553 salinity. Terminal time conditions,  $C_{\text{term}}(z)$ , only weakly constrain the time history of the  
554 control,  $C_h(t)$ , insufficient in the two cores analyzed to reduce salinity uncertainties below  
555 about  $\pm 0.5$  g/kg at any time before a few hundred years ago. This inference is consistent with  
556 that of Miller et al. (2015), using the same pore-water data, but a different analysis methodology.

557 That the Southern Hemisphere ocean was heavily salt-stratified in the abyss, with values well  
558 above the LGM mean, remains a not-implausible *assumption* about the last glacial period ocean,  
559 one depending upon the claim that initial conditions have little or no effect at the core terminal  
560 state data or upon other data not used here. If that assumption is take at face value, it raises  
561 the question of what the initial conditions were in practice and why their effects are invisible at  
562  $t_f$ ? With this particular type of core data, reducing the resulting uncertainty requires among  
563 other elements, providing a prior estimate,  $C_h^{\text{a priori}}(t)$ , with smaller levels of uncertainty (better  
564 than 0.1 g/kg), a requirement for which little prospect exists.

565 The uncertainties derived here are all lower bounds, and are based in part upon the assump-

566 tion of perfectly known, simple, core profiles of  $w, k$ . These parameters can, in a formal sense, be  
567 treated as further unknowns as a function of depth and time, but if the information contained  
568 in the terminal chlorinity data is used to estimate their values, the uncertainties of  $\tilde{C}_h(t)$  will  
569 become even larger. No claim is made that the chosen parameters here,  $k = 2 \times 10^{-10} \text{m}^2/\text{s}$ , and  
570  $w = -|k| \text{ m/s}$  are “correct”, merely that they give a reasonable fit to the terminal data. If the  
571 equivalent of  $k$  is measured at the terminal time in the cores (via the porosity and tortuosity)  
572 the measurement errors are necessarily greater than the zero values used here in treating it as  
573 perfectly known. A further generalization estimates the uncertainty covariances as part of the  
574 calculation (“adaptive” filtering and smoothing; see e.g., Anderson and Moore, 1979), but it  
575 again necessarily further increases the estimated state and control vector uncertainties.

576 Of particular use would be pore water properties in regionally distributed cores. It would then  
577 become possible to better understand the background structures (are they regional covarying  
578 signals, or are they noise particular to one core?) and their geography. Such additional data  
579 would be a major step towards expanding the data base to the point where an accurate global  
580 average would become plausible.

581 Numerous interesting questions arise, at least within a theoretical framework. How the  
582 dynamical and kinematical response to an excess of evaporation, leading to formation of the  
583 continental ice sheets would have worked its way through the entire ocean volume, raising the  
584 mean by about 1 g/kg is far from obvious. Equally obscure is how the global volume salinity  
585 mean re-adjusted itself, much more rapidly, to its lower modern value through the excess runoff  
586 in the deglaciation. Complex transient behavior would be expected with time scales exceeding  
587 thousands of years. Amongst many such interesting issues, note that much of the salt in the  
588 modern upper North Atlantic Ocean arises from the highly saline Mediterranean Sea outflow.  
589 Paul et al. (2001) have discussed possibilities for LGM salinity changes there, also from pore  
590 fluid data. Whether any of the world-wide symptoms of these major re-adjustments can be  
591 detected in paleoceanographic data remains a challenging question.

592 To answer the two questions posed in the Introduction: An LGM ocean with greatly inten-  
593 sified salinity in the abyssal Southern Ocean is *not* required by the pore-water chlorinity data  
594 and, such an ocean is not contradicted by the pore water data within the large lower-bound  
595 residual error estimates.

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600 his thinking that the wrong questions were being posed.

## 601 Appendix-Control Algorithms

602 The algorithms for the Lagrange multiplier (or adjoint) solution, and for the filter-smoother are  
 603 written out here for reference purposes; cf. W06.

### 604 *Lagrange Multipliers*

Assume a model (Eq. 9) with a state vector  $\mathbf{x}(t)$ , and a terminal data set,  $\mathbf{x}_d(t_f)$ , having error covariance  $\mathbf{R}(t_f)$ ,  $\tilde{\mathbf{x}}(0)$  is the initial condition with uncertainty  $\mathbf{P}(0)$ , and assuming for notational simplicity that none of  $\mathbf{A}$ ,  $\mathbf{B}$ , or  $\mathbf{\Gamma}$  is time-dependent. The covariance of the control,  $\mathbf{u}(t)$ , is  $\mathbf{Q}(t)$ . Let the objective or cost function be Eq. (11), the model is adjoined (appended) to  $J$  using a set of vector Lagrange multipliers,  $\boldsymbol{\mu}(t)$ . Generating the normal equations by differentiation in ordinary least-squares,  $\boldsymbol{\mu}(t)$  satisfy a time-evolution equation

$$\boldsymbol{\mu}(t-1) = \mathbf{A}^T \boldsymbol{\mu}(t), \quad t = 1, 2, \dots, t_f \quad (\text{A1a})$$

$$\boldsymbol{\mu}(t_f) = \mathbf{R}^{-1} (\tilde{\mathbf{x}}(t_f) - \mathbf{x}_d(t_f)), \quad (\text{A1b})$$

605 time appearing to “run backwards.” The unknown controls are then,

$$\mathbf{u}(t) = -\mathbf{Q}\mathbf{\Gamma}^T \boldsymbol{\mu}(t+1) \quad (\text{A2})$$

606 and

$$\begin{aligned} & \left\{ \mathbf{I} + \mathbf{A}^{(t_f-1)} \mathbf{\Gamma} \mathbf{Q} \mathbf{\Gamma}^T \mathbf{A}^{(t_f-1)T} \mathbf{R}^{-1} \right. \\ & \quad \left. + \mathbf{A}^{(t_f-2)} \mathbf{\Gamma} \mathbf{Q} \mathbf{\Gamma}^T \mathbf{A}^{(t_f-2)T} \mathbf{R}^{-1} + \dots + \mathbf{\Gamma} \mathbf{Q} \mathbf{\Gamma}^T \mathbf{R}^{-1} \right\} \tilde{\mathbf{x}}(t_f) \\ & = \mathbf{A}^{t_f} \tilde{\mathbf{x}}(0) + \left\{ \mathbf{A}^{(t_f-1)} \mathbf{\Gamma} \mathbf{Q} \mathbf{\Gamma}^T \mathbf{A}^{(t_f-1)T} \mathbf{R}^{-1} \right. \\ & \quad \left. + \mathbf{A}^{(t_f-2)} \mathbf{\Gamma} \mathbf{Q} \mathbf{\Gamma}^T \mathbf{A}^{(t_f-2)T} \mathbf{R}^{-1} + \dots + \mathbf{\Gamma} \mathbf{Q} \mathbf{\Gamma}^T \mathbf{R}^{-1} \right\} \mathbf{x}_d. \end{aligned} \quad (\text{A3})$$

607 explicitly relates the estimated terminal state,  $\tilde{\mathbf{x}}(t_f)$ , to the desired one,  $\mathbf{x}_d$ . Eq. (A1a) is then  
 608 solved for  $\boldsymbol{\mu}(t)$ , and the entire state then follows from Eqs. (A2, 9). See W06, p.218+).

### 609 *RTS Smoother*

The RTS smoother uses a Kalman filter in the forwards-in-time direction, with the equations in the main text. In the time-reverse direction, the algorithm is more complicated in appearance because it takes account of the time-correlations in the error estimates that were built up in the



filter sweep. The resulting system, in the notation of W06, p. 208, is,

$$\tilde{\mathbf{x}}(t, +) = \tilde{\mathbf{x}}(t+) \mathbf{L}(t+1) [\tilde{\mathbf{x}}(t+1, +) - \tilde{\mathbf{x}}(t+1, -)], \quad (\text{A4a})$$

$$\mathbf{L}(t+1) = \mathbf{P}(t) \mathbf{A}(t)^T \mathbf{P}(t+1, -)^{-1}, \quad (\text{A4b})$$

$$\tilde{\mathbf{u}}(t+1) = \mathbf{M}(t+1) [\tilde{\mathbf{x}}(t+1, +) - \tilde{\mathbf{x}}(t+1, -)], \quad (\text{A4c})$$

$$\mathbf{M}(t+1) = \mathbf{Q}(t) \mathbf{\Gamma}(t)^T \mathbf{P}(t+1, -)^{-1}, \quad (\text{A4d})$$

$$\mathbf{P}(t, +) = \mathbf{P}(t) + \mathbf{L}(t+1) [\mathbf{P}(t+1, +) - \mathbf{P}(t+1, -)] \mathbf{L}(t+1)^T, \quad (\text{A4e})$$

$$\tilde{\mathbf{Q}}(t, +) = \mathbf{Q}(t) + \mathbf{M}(t+1) [\mathbf{P}(t+1, +) - \mathbf{P}(t+1, -)] \mathbf{M}(t+1)^T, \quad (\text{A4f})$$

$$t = 0, 1, \dots, t_f - 1$$

610

Data do not appear, all information content having been used in the forward sweep.

## References

- 612 Adkins, J.F., Ingersoll, A.P., Pasquero, C., 2005. Rapid climate change and conditional  
613 instability of the glacial deep ocean from the thermobaric effect and geothermal heating. *Quat.*  
614 *Sci. Revs.* 24, 581-594.
- 615 Adkins, J.F., McIntyre, K., Schrag, D.P., 2002. The salinity, temperature, and  $\delta^{18}\text{O}$  of the  
616 glacial deep ocean. *Science* 298, 1769-1773.
- 617 Adkins, J.F., Schrag, D.P., 2003. Reconstructing Last Glacial Maximum bottom water  
618 salinities from deep-sea sediment pore fluid profiles. *Earth Planet. Sc. Letts.* 216, 109-123.
- 619 Anderson, B.D.O., Moore, J.B., 1979. *Optimal Filtering*. Prentice-Hall, Englewood Cliffs,  
620 N. J.
- 621 Berner, R.A., 1980. *Early Diagenesis: A Theoretical Approach*. Princeton University Press,  
622 Princeton, N.J.
- 623 Boudreau, B.P., 1997. *Diagenetic Models And Their Implementation: Modelling Transport*  
624 *And Reactions In Aquatic Sediments*. Springer, Berlin; New York.
- 625 Brogan, W.L., 1991. *Modern Control Theory*, 3rd Ed. Prentice-Hall/Quantum, Englewood  
626 Cliffs, N. J.
- 627 Bruna, M., Chapman, S.J., 2015. Diffusion in Spatially Varying Porous Media. *SIAM J.*  
628 *Appl. Maths* 75, 1648-1674.
- 629 Carslaw, H.S., Jaeger, J.C., 1986. *Conduction of Heat in Solids*. Oxford Un. Press.
- 630 Carter, R.M., McCave, I.N., Richter, C., Carter, L., et al., 1999. *Proc. ODP, Init. Repts.*,  
631 181.
- 632 Dade, W.B., Hogg, A.J., Boudreau, B.P., 2001. Physics of flow above the sediment-water  
633 interface, in: Boudreau, R.D., Jørgensen, B.B. (Eds.), *The Benthic Boundary Layer. Transport*  
634 *Processes and Biogeochemistry*. Oxford University Press, New York.
- 635 Einsele, G., 2000. *Sedimentary Basins: Evolution, Facies, and Sediment Budget*, 2nd, Ed.  
636 Springer, Berlin ; New York.
- 637 Forget, G., Campin, J.-M., Heimbach, P., Hill, C., Ponte, R., Wunsch, C., 2015. ECCO  
638 version 4: an integrated framework for non-linear inverse modeling and global ocean state esti-  
639 mation. *Geosci. Model Dev.* 8, 3071–3104.
- 640 Fowler, A.C., Yang, X.S., 1998. Fast and slow compaction in sedimentary basins. *SIAM J.*  
641 *App. Maths.* 59, 365-385.
- 642 Gersonde, R., Hodell, D.A., Blum, P., et al., 1999. *Proc. ODP, Init. Repts.*, 177
- 643 Huybers, P., Wunsch, C., 2010. Paleophysical oceanography with an emphasis on transport  
644 rates. *Annu. Rev. Mar. Sci.* 2, 1-34.

645 Insua, T.L., Spivack, A.J., Graham, D., D'Hondt, S., Moran, K., 2014. Reconstruction of  
646 Pacific Ocean bottom water salinity during the Last Glacial Maximum. *Geophys. Res. Letts.*  
647 41, 2914-2920.

648 Jansen, E., Raymo, M.E., Blum, P., et al., 1996. *Proc. ODP, Init. Repts.*, 162: College  
649 Station, TX (Ocean Drilling Program), 49–90. doi:10.2973/odp.proc.ir.162.103.1996.

650 Keigwin, L.D., Rio, D., Acton, G.D., et al., 1998. *Proc. ODP, Init. Repts.*, 172: College  
651 Station, TX (Ocean Drilling Program), 251–308. doi:10.2973/odp.proc.ir.172.106.1998.

652 Kobayashi, H., Abe-Ouchi, A., Oka, A., 2015. Role of Southern Ocean stratification in  
653 glacial atmospheric CO<sub>2</sub> reduction evaluated by a three-dimensional ocean general circulation  
654 model. *Paleoceanography* 30, 2015PA002786.

655 Luenberger, D.G., 1979. *Introduction to Dynamic Systems. Theory, Models and Applica-*  
656 *tions.* John Wiley, New York.

657 Macayeal, D., 1995. Challenging an ice-core paleothermometer. *Science* 270, 444-445.

658 Macayeal, D.R., Firestone, J., Waddington, E., 1991. Paleothermometry by control methods.  
659 *J Glaciol* 37, 326-338.

660 McDuff, R.E., 1985. The chemistry of interstitial Waters, Deep-Sea Drilling Project Leg-86.  
661 *Initial Reports of the Deep Sea Drilling Project* 86, 675-687.

662 Miller, M.D., 2014. The Deep Ocean Density Structure at the Last Glacial Maximum. What  
663 Was It and Why? PhD Thesis Cal. Tech., p. 136.

664 Miller, M.D., Simons, M., Adkins, J.F., Minson, S.E., 2015 The information content of pore  
665 fluid  $\delta^{18}\text{O}$  and  $[\text{Cl}^-]$ . *J. Phys. Oc.* 45, 2070-2094.

666 Mix, A., Tiedemann, R., Blum P., 2002. *Initial Reports, Proc. Ocean Drilling Prog.*, 202.

667 Munk, W.H., 1966. Abyssal recipes. *Deep-Sea Res.* 13, 707-730.

668 Paul, H.A., Bernasconi, S.M., Schmid, D.W., McKenzie, J.A., 2001. Oxygen isotopic com-  
669 position of the Mediterranean Sea since the Last Glacial Maximum: constraints from pore water  
670 analyses. *Earth Planet. Sci. Letts.* 192, 1-14.

671 Roache, P.J., 1976. *Computational Fluid Dynamics.* Hermosa, Albuquerque, N.M.

672 Schrag, D.P., Adkins, J.F., McIntyre, K., Alexander, J.L., Hodell, D.A., Charles, C.D.,  
673 McManus, J.F., 2002. The oxygen isotopic composition of seawater during the Last Glacial  
674 Maximum. *Quat. Sci. Revs.* 21, 331-342.

675 Schrag, D.P., Depaolo, D.J., 1993. Determination of delta-o-18 of seawater in the deep ocean  
676 during the last glacial maximum. *Paleoceanog.* 8, 1-6.

677 Schrag, D.P., Hampt, G., Murray, D.W., 1996. Pore fluid constraints on the temperature  
678 and oxygen isotopic composition of the glacial ocean. *Science* 272, 1930-1932.

679 Stengel, R.F., 1986. *Stochastic Optimal Control.* Wiley-Interscience, N. Y.

- 680 Voermans, J., Ghisalberti, M., Ivey, G., 2016. Coherent vortex structures at the sediment-  
681 water-interface, 11th International Symposium on Ecohydraulics, Melbourne, Australia, pp.  
682 unpagged, in press.
- 683 Wunsch, C., 1987. Using transient tracers: The regularization problem. *Tellus*, 39B, 477-492.
- 684 Wunsch, C., 1988. Transient tracers as a problem in control theory. *J. Geophys. Res.*, 93,  
685 8099-8110.
- 686 Wunsch, C., 2002. Oceanic age and transient tracers: Analytical and numerical solutions.  
687 *J. Geophys. Res.*, 107, 304810.1029/2001jc000797.
- 688 Wunsch, C., 2006. *Discrete Inverse and State Estimation Problems: With Geophysical Fluid*  
689 *Applications*. Cambridge University Press, Cambridge ; New York.

690 1. Core positions—white circles— used by Miller et al. (2015), Adkins and Schrag (2003).  
691 Shown on a chart of the modern 20-year average salinity at 3600 m from the ECCO 4 state  
692 estimate (e.g., Forget et al., 2015). The focus of attention here is on the North Atlantic core near  
693 Bermuda and the South Atlantic one southwest of the Cape of Good Hope. A modern average  
694 salinity calculated from these 5 positions might be useful but would not be very accurate. See  
695 Table 1 for descriptive references of each core, and the greatly varying water depths at each site.  
696 In the modern ocean, the North Atlantic at 3600 m is more saline than the Southern Ocean.  
697 The modern full volume average salinity is about 34.7 g/kg. The average value at this depth  
698 today is about 34.75 g/kg (not area weighted) and about 34.74 g/kg when weighted. A suite of  
699 charts for modern salinity and other properties in section and latitude-longitude form is available  
700 in the online WOCE Atlas. Variations are complex and defy a simple verbal description. In  
701 particular note that strong zonal structures in salinity exist in the abyssal Southern Ocean; it  
702 is not zonally homogeneous.

703 2. Histogram of the modern ocean salinity at 3600m as a time average over 20 years from the  
704 ECCO state estimate (Forget et al., 2015). Perhaps the glacial ocean was more homogeneous?  
705 The two modes roughly correspond to North Atlantic Deep Water and Antarctic Bottom Waters.  
706 The probability of an accurate global average from any handful of values is low and note that  
707 the core tops here lie at considerably different water depths (Table 1).

708 3. Salinity, g/kg over the full measured depth in each of the five cores. This paper focusses  
709 on Cores 1063, 1093 plotted as thicker lines. See Table 1 for a reference and geographical label  
710 for each core. Vertical dashed lines are the approximate modern global volume mean salinity,  
711 34.7 g/kg and the approximate LGM value of 35.7 g/kg. and dotted line fragment shows the  
712 LGM maximum value of  $C_h(t)$  estimated for this core by Adkins and Schrag (2003).

713 4. Same as Fig. 3 except expanded to show only the top 100m. The maximum measured  
714 value in core 1093 lies near the estimated LGM mean of 35.7 (vertical dashed line), but does not  
715 exceed it except slightly in short, possibly noise, events. Thick lines are the data from the two  
716 cores analyzed, 1063, 1093. Approximate modern mean salinity of 34.7 g/kg is also shown as a  
717 vertical dashed line. The salinity increase with depth in the much fresher Core 1239 is almost  
718 as large as that appearing in Core 1093. Near surface, the core is either undersampled, or the  
719 data are extremely noisy.

720 5. Location of ODP Core 1093 on the Southwest Indian Ridge. See Gersonde et al. (1999).

721 6. Measured porosity from all five cores. Tortuosity is assumed to follow Eq. (4). In  
722 the present calculations the corresponding diffusivity,  $k$ , is taken to be constant with depth.  
723 Experiments with linear  $k$  produced only slight changes from the solutions with a constant  
724 value.

725 7. Time-depth profile of a numerical solution using a Dufort-Frankel method (Roache, 1976)  
726 (a), and the analytic solution from Carslaw and Jaeger (1986, P. 101) for a zero-initial condition,  
727 (b) for  $w = 0$ ,  $k = 2 \times 10^{-10} \text{m}^2/\text{s}$  in a 100 meter length “core” over a duration of 100,000 years.  
728 Panel (c) shows the terminal profile in the two solutions which are visually indistinguishable.  
729 Time scale zero is at -100 ky BP.

730 8. Time for a particular vertical scale to decay to 1% of its initial value (from Eq. 5).  
731 Horizontal dashed line is at 20 ky.

732 9. (a) Forward solution, with pure diffusion, using the quasi-periodic condition: starting  
733 with the observed Core 1093 at  $t = -100$  ky and forced by  $q(t) = C_h^{\text{a priori}}(t)$ . Much of the  
734 terminal structure originates with the initial conditions, although some small scale-structure is  
735 lost in the terminal-time profile (solid line) in (c). (b) Shows the forward calculation with the  
736 same initial and boundary conditions, except now  $w = -|k|$  m/s. All of the initial condition  
737 data is swept out of the system before the end. (c) Observed terminal data (dashed) and the  
738 two terminal states for  $w = 0$ , and  $w = -|k|$ .

739 10. (a) Amplitude (Eq. 6) of the steady-periodic state component of  $c(z)$  for different forcing  
740 periods using the same value of  $k$ . Short period (“high” frequency) responses rapidly diminish  
741 with depth. A 500 m depth was used because of the dependence on the zero boundary condition  
742 at the core bottom. (b) 99% decay times of the transient element of periodic surface forcing  
743 against vertical scale. Horizontal dashed line is at 20 ky.

744 11. Estimated global mean salinity from the sea level change curve (Miller, 2014, Miller et  
745 al., 2015, from a variety of sources). The direction of the time axis has been converted to the  
746 physics convention from the geological “age”. This curve becomes the prior boundary condition  
747  $C_h^{\text{a priori}}(t)$ . Dashed lines are the estimated volume average modern (lower) and LGM salinities  
748 (upper), the latter the value used by Adkins and Schrag (2003). Here the time scale represents  
749 time before the present.

750 12. (a) Kalman filter solution, Core 1093, pure diffusion ( $w = 0$ ) and the sea level prior.  
751 The filter solution is identical to that shown from the pure forward calculation in Fig. 9 except,

752 nearly invisibly, near the terminal time. (b) Estimate of the state vector after application of  
753 the smoothing algorithm, and which changes the state as far back as its initial conditions. (c)  
754 Deviation of the terminal state estimate from the core data, along with one standard errors  
755  $\sqrt{P(t_f)} = \sqrt{P(t_f, +)}$  (d)  $C_h^{\text{a priori}}(t)$  (solid), and the estimated  $C_h(t) = q(t) + \tilde{u}(t)$  (dashed).  
756 Horizontal dashed lines are the modern and LGM global means, the latter the AS03 estimate.  
757 The estimated value of  $C_h(t)$  remains below the global mean LGM salinity, as the deep maximum  
758 is controlled by the initial conditions in contrast to the solution of AS03 which reached 37.1 g/kg.  
759 (e) Last 5000 years of  $\tilde{u}(t)$ , and the one standard deviation uncertainty from  $\pm\sqrt{Q(t)}$ . Except  
760 at the very end,  $\tilde{Q}(t, +)$  differs negligibly from  $Q(t)$ . (f) Terminal state from the Kalman filter  
761 just prior to the invocation of the terminal data (identical to the forward solution; solid line.  
762 Dashed line is the core data, dotted line the terminal state. Note that the Lagrange multiplier  
763 solution, the Kalman filter solution, and the smoothed solution are identical at  $t = t_f$ .

764 13. Core 1093 with a constant (“flat”) prior of 34.93 g/kg, the mean of  $C_h^{\text{a priori}}(t)$ . (a) The  
765 solution as run forward in the Kalman filter sweep. (b) The same solution as modified by the  
766 smoothing sweep. (c) Deviation of the terminal state (either from Lagrange multipliers or the  
767 Kalman filter or the smoother) from the core data. (d) Flat, a priori control  $q(t)$  (solid line)  
768 and the final estimated  $C_h(t) = q(t) + \tilde{u}(t)$ . (e) Last 5000 years of  $\tilde{u}(t)$  and the one standard  
769 deviation uncertainty. (f) Comparison of the prediction,  $\tilde{\mathbf{x}}(t_f, -), \tilde{\mathbf{x}}(t_f, +) = \tilde{\mathbf{x}}(t_f)$ , and the  
770 Core 1093 data.

771 14. Same as Fig. 12 except for  $w = -|k|$  m/s. Again  $\tilde{C}_h(t)$  is always below the LGM mean.

772 15. Same as Figs. 12, except for Core 1063 on the Bermuda Rise. The terminal state does  
773 not well-match the core data in terms of depth and this solution probably should be rejected.

774 16. Core 1093 (Southwest Indian Ridge) results using 300m length,  $w = -|k|$  and an initial  
775 time of -200 ky with the sea level curve treated as twice periodic over 100 ky. (a) The misfit to  
776 the core data and (b,c) the final control are shown. Now structure appears as far back as -60  
777 ky, and includes an excursion above the LGM mean at around -38ky although not statistically  
778 significant.

779 17. Same as Fig. 17 except for Core 1063 on the Bermuda Rise.

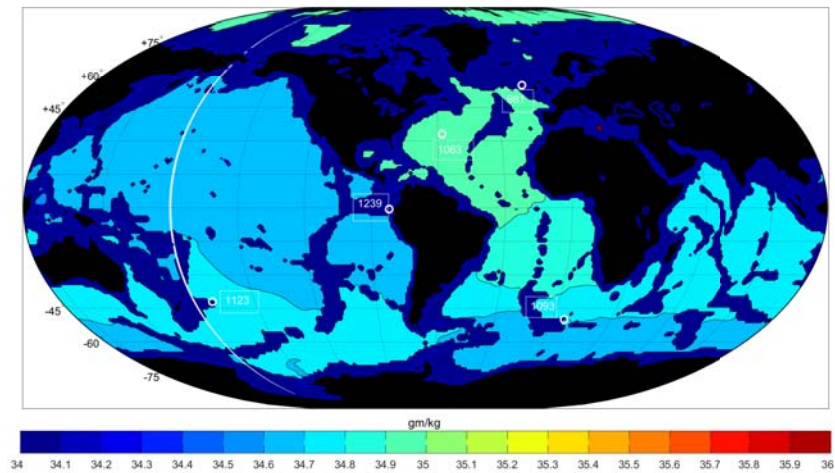


Figure 1: Core positions—white circles—used by Miller et al. (2015), Adkins and Schrag (2003). Shown on a chart of the modern 20-year average salinity at 3600 m from the ECCO 4 state estimate (e.g., Forget et al., 2015). The focus of attention here is on the North Atlantic core near Bermuda and the South Atlantic one southwest of the Cape of Good Hope. A modern average salinity calculated from these 5 positions might be useful but would not be very accurate. See Table 1 for descriptive references of each core, and the greatly varying water depths at each site. In the modern ocean, the North Atlantic at 3600 m is more saline than the Southern Ocean. The modern full volume average salinity is about 34.7 g/kg. The average value at this depth today is about 34.75 g/kg (not area weighted) and about 34.74 g/kg when weighted. A suite of charts for modern salinity and other properties in section and latitude-longitude form is available in the online WOCE Atlas. Variations are complex and defy a simple verbal description. In particular note that strong zonal structures in salinity exist in the abyssal Southern Ocean; it is not zonally homogeneous.



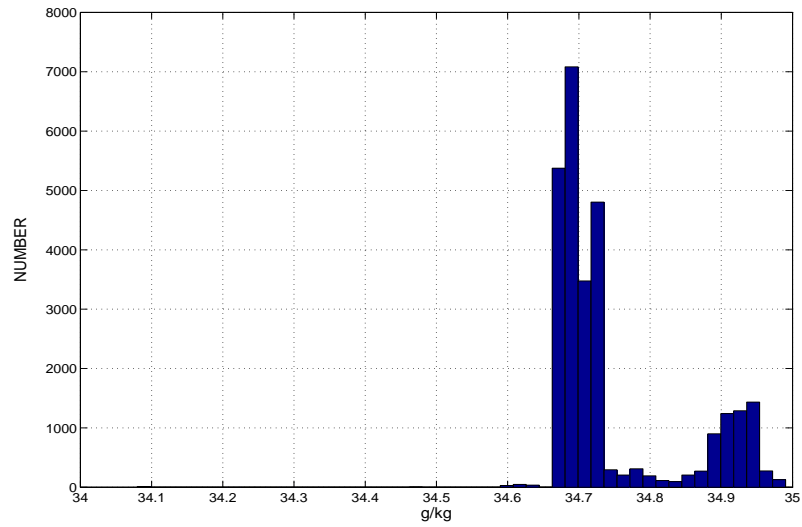


Figure 2: Histogram of the modern ocean salinity at 3600m as a time average over 20 years from the ECCO state estimate (Forget et al., 2015). Perhaps the glacial ocean was more homogeneous? The two modes roughly correspond to North Atlantic Deep Water and Antarctic Bottom Waters. The probability of an accurate global average from any handful of values is low and note that the core tops here lie at considerably different water depths (Table 1).

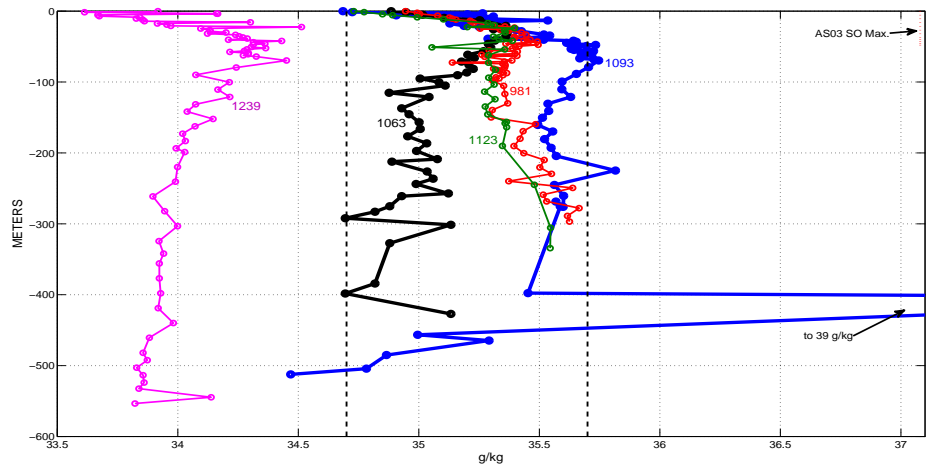


Figure 3: Salinity, g/kg over the full measured depth in each of the five cores. This paper focusses on Cores 1063, 1093 plotted as thicker lines. See Table 1 for a reference and geographical label for each core. Vertical dashed lines are the approximate modern global volume mean salinity, 34.7 g/kg and the approximate LGM value of 35.7 g/kg. and dotted line fragment shows the LGM maximum value of  $C_h(t)$  estimated for this core by Adkins and Schrag (2003).

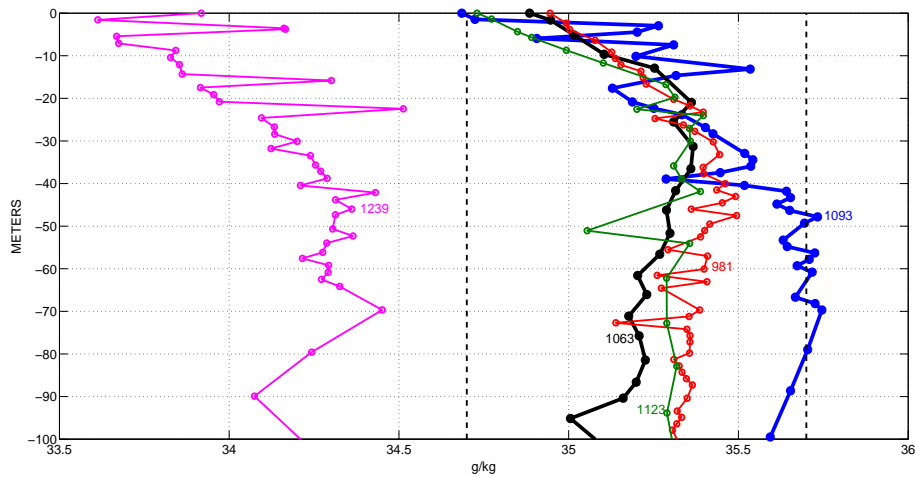


Figure 4: Same as Fig. 3 except expanded to show only the top 100m. The maximum measured value in core 1093 lies near the estimated LGM mean of 35.7 (vertical dashed line), but does not exceed it except slightly in short, possibly noise, events. Thick lines are the data from the two cores analyzed, 1063, 1093. Approximate modern mean salinity of 34.7 g/kg is also shown as a vertical dashed line. The salinity increase with depth in the much fresher Core 1239 is almost as large as that appearing in Core 1093. Near surface, the core is either undersampled, or the data are extremely noisy.

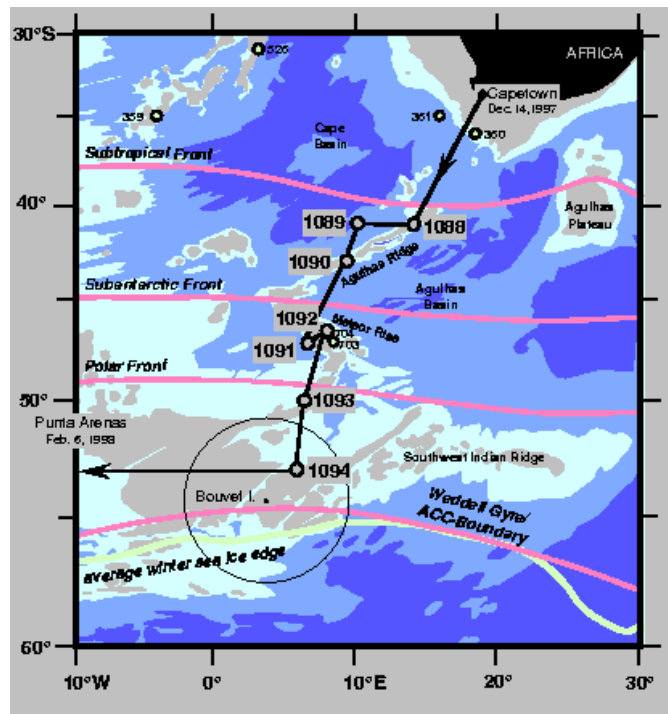


Figure 5: Location of ODP Core 1093 on the Southwest Indian Ridge. See Gersonde et al. (1999).

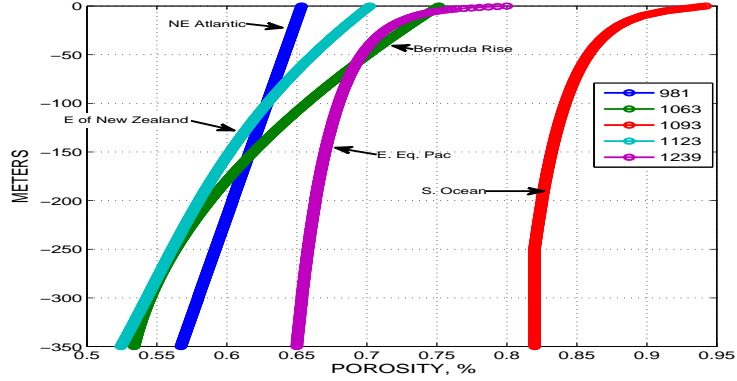


Figure 6: Measured porosity from all five cores. Tortuosity is assumed to follow Eq. (4). In the present calculations the corresponding diffusivity,  $k$ , is taken to be constant with depth. Experiments with linear  $k$  produced only slight changes from the solutions with a constant value.

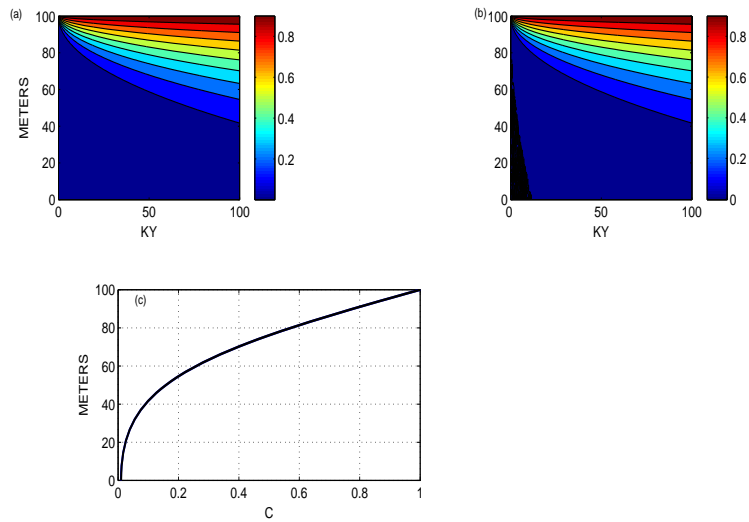


Figure 7: Time-depth profile of a numerical solution using a Dufort-Frankel method (Roache, 1976) (a), and the analytic solution from Carslaw and Jaeger (1986, P. 101) for a zero-initial condition, (b) for  $w = 0, k = 2 \times 10^{-10} \text{m}^2/\text{s}$  in a 100 meter length “core” over a duration of 100,000 years. Panel (c) shows the terminal profile in the two solutions which are visually indistinguishable. Time scale zero is at -100 ky BP.

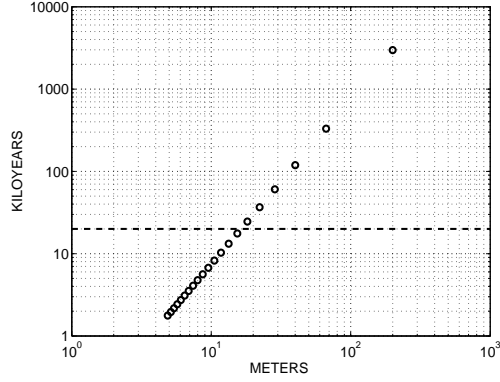


Figure 8: Time for a particular vertical scale to decay to 1% of its initial value (from Eq. 5). Horizontal dashed line is at 20 ky.

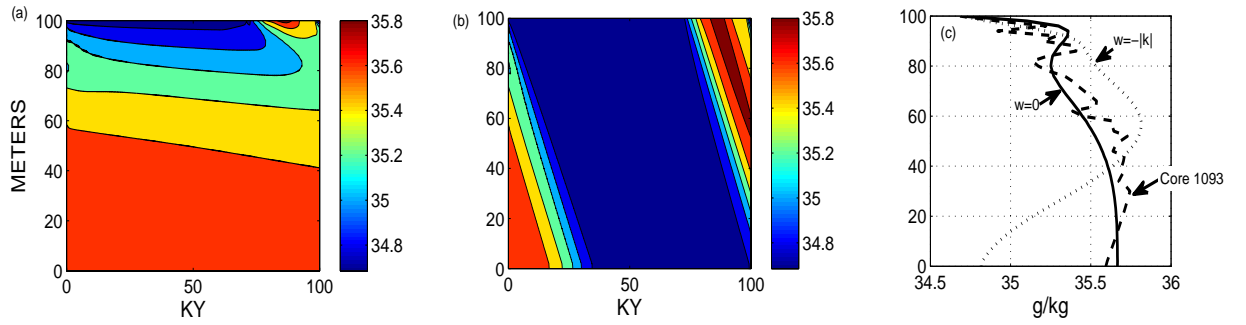


Figure 9: (a) Forward solution, with pure diffusion, using the quasi-periodic condition: starting with the observed Core 1093 at  $t = -100$  ky and forced by  $q(t) = C_h^{\text{a priori}}(t)$ . Much of the terminal structure originates with the initial conditions, although some small scale-structure is lost in the terminal-time profile (solid line) in (c). (b) Shows the forward calculation with the same initial and boundary conditions, except now  $w = -|k|$  m/s. All of the initial condition data is swept out of the system before the end. (c) Observed terminal data (dashed) and the two terminal states for  $w = 0$ , and  $w = -|k|$ .

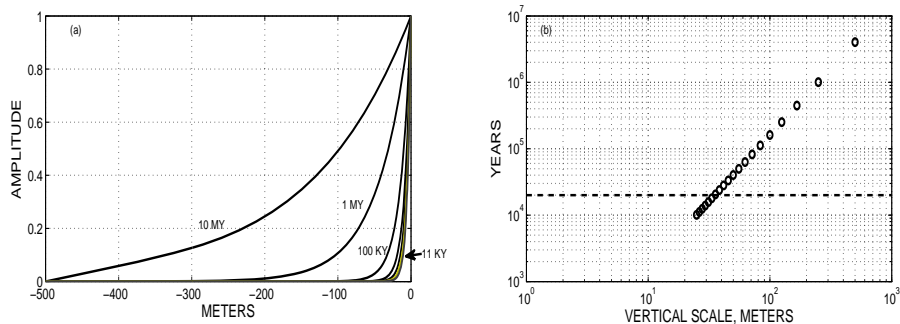


Figure 10: (a) Amplitude (Eq. 6) of the steady-periodic state component of  $c(z)$  for different forcing periods using the same value of  $k$ . Short period (“high” frequency) responses rapidly diminish with depth. A 500 m depth was used because of the dependence on the zero boundary condition at the core bottom. (b) 99% decay times of the transient element of periodic surface forcing against vertical scale. Horizontal dashed line is at 20 ky.

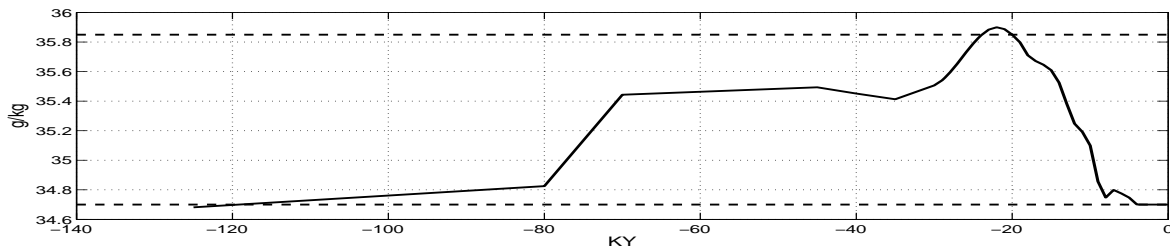


Figure 11: Estimated global mean salinity from the sea level change curve (Miller, 2014, Miller et al., 2015, from a variety of sources). The direction of the time axis has been converted to the physics convention from the geological “age”. This curve becomes the prior boundary condition  $C_h^{\text{a priori}}(t)$ . Dashed lines are the estimated volume average modern (lower) and LGM salinities (upper), the latter the value used by Adkins and Schrag (2003). Here the time scale represents time before the present.

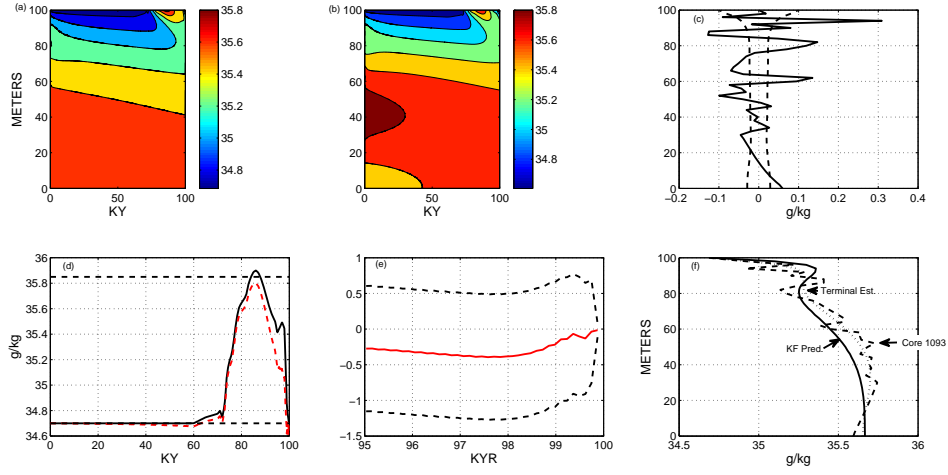


Figure 12: (a) Kalman filter solution, Core 1093, pure diffusion ( $w = 0$ ) and the sea level prior. The filter solution is identical to that shown from the pure forward calculation in Fig. 9 except, nearly invisibly, near the terminal time. (b) Estimate of the state vector after application of the smoothing algorithm, and which changes the state as far back as its initial conditions. (c) Deviation of the terminal state estimate from the core data, along with one standard errors  $\sqrt{P(t_f)} = \sqrt{P(t_f, +)}$  (d)  $C_h^{\text{a priori}}(t)$  (solid), and the estimated  $C_h(t) = q(t) + \tilde{u}(t)$  (dashed). Horizontal dashed lines are the modern and LGM global means, the latter the AS03 estimate. The estimated value of  $C_h(t)$  remains below the global mean LGM salinity, as the deep maximum is controlled by the initial conditions in contrast to the solution of AS03 which reached 37.1 g/kg. (e) Last 5000 years of  $\tilde{u}(t)$ , and the one standard deviation uncertainty from  $\pm\sqrt{Q(t)}$ . Except at the very end,  $\tilde{Q}(t, +)$  differs negligibly from  $Q(t)$ . (f) Terminal state from the Kalman filter just prior to the invocation of the terminal data (identical to the forward solution; solid line. Dashed line is the core data, dotted line the terminal state. Note that the Lagrange multiplier solution, the Kalman filter solution, and the smoothed solution are identical at  $t = t_f$ .

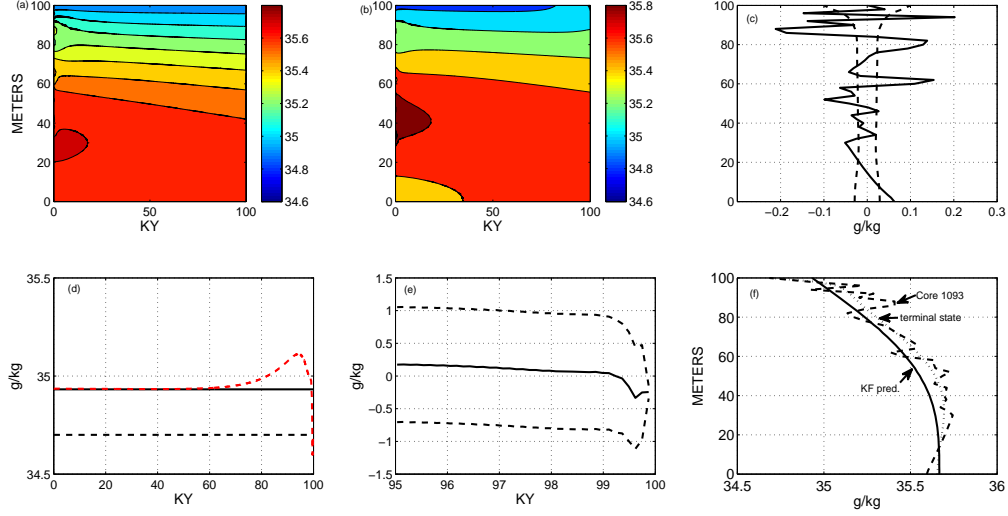


Figure 13: Core 1093 with a constant (“flat”) prior of 34.93 g/kg, the mean of  $C_h^{\text{a priori}}(t)$ . (a) The solution as run forward in the Kalman filter sweep. (b) The same solution as modified by the smoothing sweep. (c) Deviation of the terminal state (either from Lagrange multipliers or the Kalman filter or the smoother) from the core data. (d) Flat, a priori control  $q(t)$  (solid line) and the final estimated  $C_h(t) = q(t) + \tilde{u}(t)$ . (e) Last 5000 years of  $\tilde{u}(t)$  and the one standard deviation uncertainty. (f) Comparison of the prediction,  $\tilde{\mathbf{x}}(t_f, -), \tilde{\mathbf{x}}(t_f, +) = \tilde{\mathbf{x}}(t_f)$ , and the Core 1093 data.

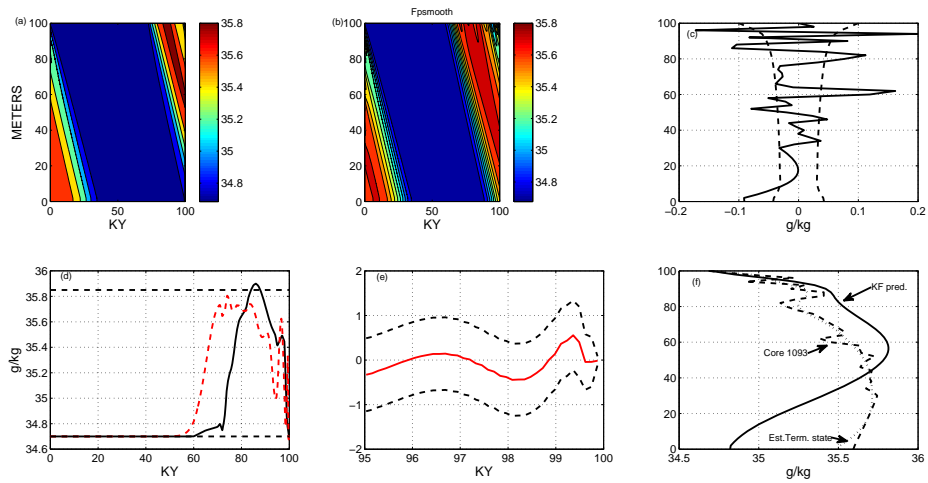


Figure 14: Same as Fig. 12 except for  $w = -|k|$  m/s. Again  $\tilde{C}_h(t)$  is always below the LGM mean.



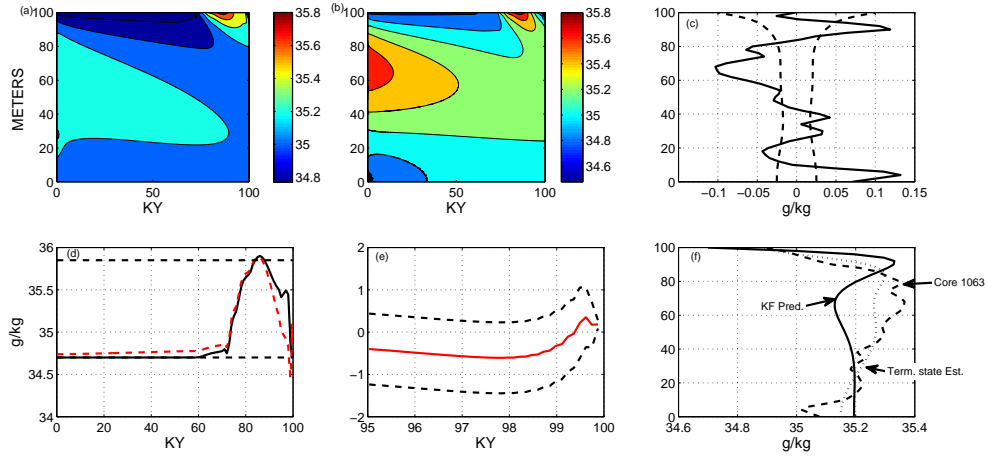


Figure 15: Same as Figs. 12, except for Core 1063 on the Bermuda Rise. The terminal state does not well-match the core data in terms of depth and this solution probably should be rejected.

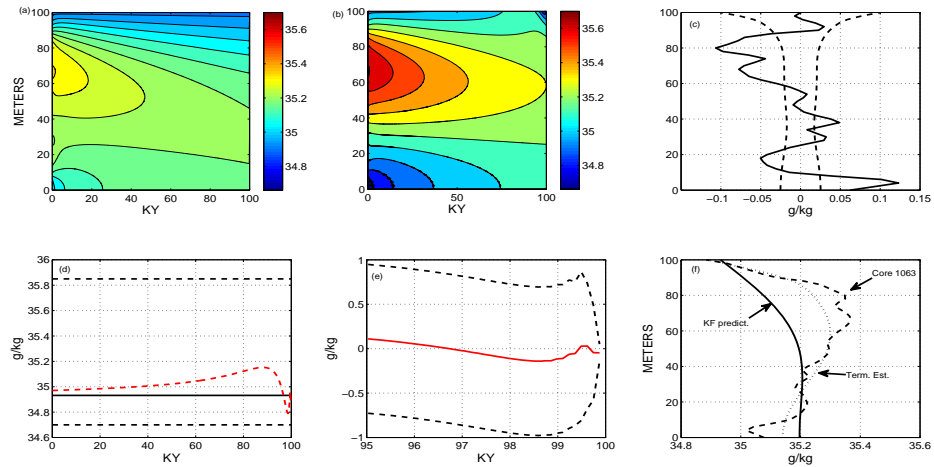


Figure 16: Same as Fig. 15 except for a constant prior  $C_h^{\text{a priori}}(t)$ .

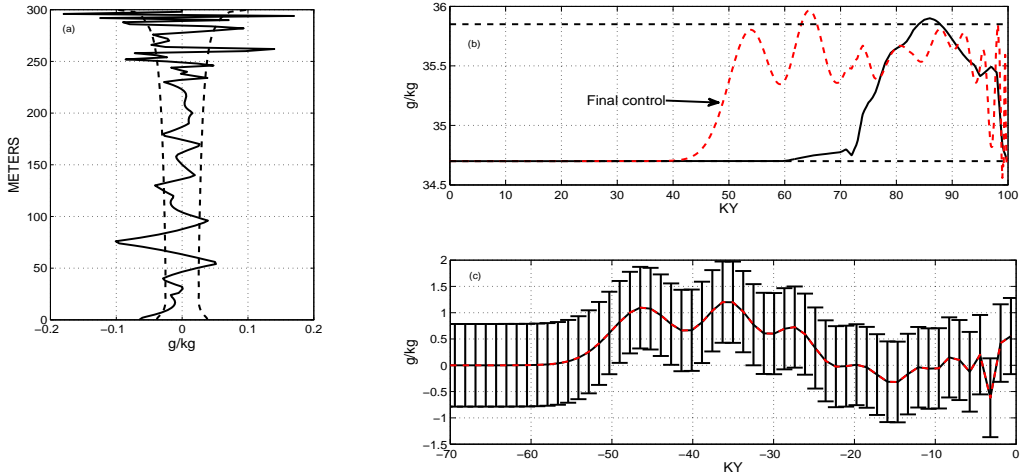


Figure 17: Core 1093 (Southwest Indian Ridge) results using 300m length,  $w = -|k|$  and an initial time of -200 ky with the sea level curve treated as twice periodic over 100 ky. (a) The misfit to the core data and (b,c) the final control are shown. Now structure appears as far back as -60 ky, and includes an excursion above the LGM mean at around -38ky although not statistically significant.

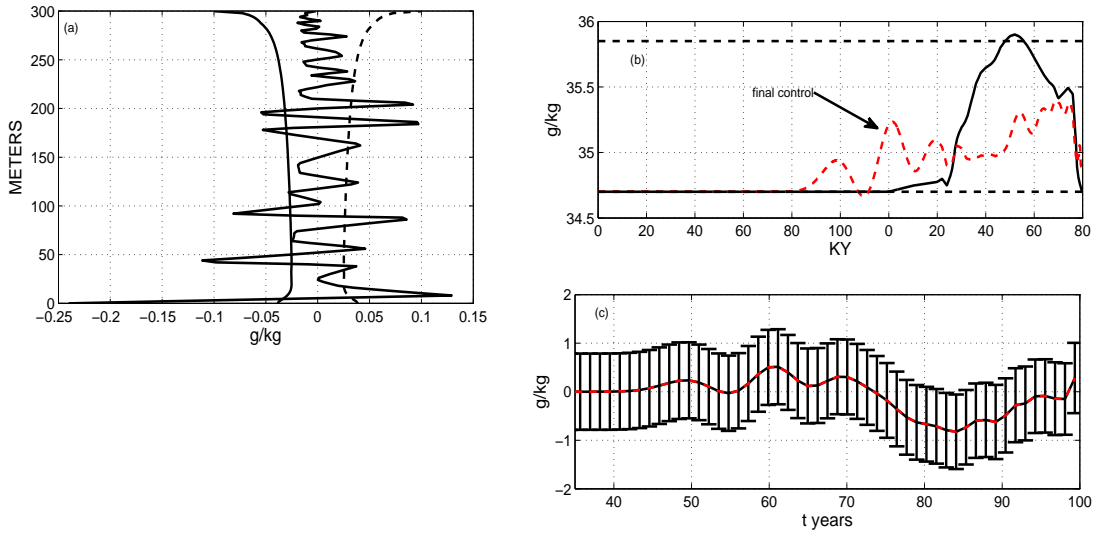


Figure 18: Same as Fig. 17 except for core 1063 on the Bermuda Rise.