Using Green’s Functions to Calibrate an Ocean General Circulation Model

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Green’s functions provide a simple yet effective method to test and to calibrate General-Circulation-Model (GCM) parameterizations, to study and to quantify model and data errors, to correct model biases and trends, and to blend estimates from different solutions and data products. The method is applied to an ocean GCM resulting in substantial improvements of the solution relative to observations when compared to prior estimates: overall model bias and drift are reduced and there is a 10% to 30% increase in explained variance. Within the context of this optimization, the following new estimates for commonly used ocean GCM parameters are obtained. Background vertical diffusivity is $(15.1 \pm 0.1) \times 10^{-6} \text{ m}^2/\text{s}$. Background vertical viscosity is $(18 \pm 3) \times 10^{-6} \text{ m}^2/\text{s}$. The critical bulk Richardson number, which sets boundary layer depth, is $Ri_c = 0.354 \pm 0.004$. The threshold gradient Richardson number for shear instability vertical mixing is $Ri_0 = 0.699 \pm 0.008$. The estimated isopycnal diffusivity coefficient ranges from $550 \text{ m}^2/\text{s}$ to $1350 \text{ m}^2/\text{s}$, with the largest values occurring at depth in regions of increased mesoscale eddy activity. Surprisingly, the estimated isopycnal diffusivity exhibits a 5% to 35% decrease near the surface. Improved estimates of initial and boundary conditions are also obtained. The above estimates are the backbone of a quasi-operational, global-ocean circulation analysis system.
1. Introduction

General Circulation Models (GCMs) resolve only a minute fraction of the climate-system degrees of freedom (e.g., Holloway 1999). Sub-grid scale processes, which are not resolved by these models, must therefore be represented using statistical or empirical parameterizations. The discussion herein concerns a method, based on the computation of model Green’s functions, for calibrating these parameterizations. For illustration purposes, the method is applied to an ocean GCM within the context of a global-ocean data-assimilation project.

Example sub-grid scale parameterizations in ocean GCMs are those used to represent the role of eddies, internal waves, small-scale turbulence, etc. For the specific application example discussed here, these processes have been represented using the isopycnal mixing schemes of Redi (1982) and of Gent and McWilliams (1990) and the vertical mixing scheme of Large et al. (1994). These schemes contain empirical “diffusion” coefficients, critical Richardson numbers, etc., whose careful calibration is key to obtaining a realistic representation of the physical processes that have been parameterized.

The conventional approach for calibrating empirical parameterizations is to adjust one parameter at a time using GCM sensitivity studies and comparisons with data. But this approach is suboptimal because empirical parameters depend on each other and on model configuration, initial conditions, surface boundary conditions, etc. Therefore, an optimal set of parameters can only be obtained through the simultaneous adjustment of all of these conditions, a daunting task.

A recent study by Stammer et al. (2003) demonstrates that, using the adjoint method, it is possible to simultaneously adjust the initial and surface boundary conditions of an ocean GCM in order to fit a wide variety of data products. The above study is being extended to include the estimation of the model’s mixing coefficients (D. Stammer, personal communication, 2003). Powerful though it is, however, the adjoint
method has some drawbacks: it is computationally expensive, its implementation is technically demanding, it does not easily accommodate error analysis, and it is not easily applied to chaotic systems.

The Green’s function approach discussed here provides a different set of trade-offs between optimality, computational cost, error description, and ease of implementation. Key advantages relative to the adjoint method are 1) simplicity of implementation, 2) the possibility to obtain complete \textit{a posteriori} error statistics for the parameters being estimated, and 3) improved robustness in the presence of non-linearities. The major drawback of the Green’s function approach is that computational cost increases linearly with the number of control parameters. By comparison, the cost of the adjoint method, while substantial, is largely independent from the number of control parameters. More will be said later about these various trade-offs.

Green’s functions were first used to solve partial differential equations describing electrical, magnetic, mechanical, and thermal phenomena (Challis and Sheard 2003). Green’s functions have also been used to linearize and to solve a wide variety of geophysical inverse problems (e.g., Fan et al. 1999; Gloor et al. 2001; Gray and Haine 2001; Wunsch 1996, and references therein). Application examples that are closely related to the present discussion are those of Stammer and Wunsch (1996) and of Menemenlis and Wunsch (1997), in which model Green’s functions were used to estimate the large-scale, Pacific Ocean circulation. What sets apart the present discussion from the work of Stammer and Wunsch (1996) and of Menemenlis and Wunsch (1997) is the choice of control parameters. Specifically, model Green’s functions are here used to blend existing estimates of initial and surface boundary conditions and to estimate diffusion coefficients, critical Richardson numbers, and relaxation time scales.

The Green’s function approach is described in Sect. 2 using, where possible, the notation of Ide et al. (1997). The power of this approach is best illustrated by example. For this purpose Sects. 3 and 4 discuss the application of the Green’s function approach
to improving the estimates of a quasi-operational, global-ocean circulation analysis system. Summary and concluding remarks follow in Sect. 6.

2. Green’s function approach

At the most basic level, the Green’s function approach described here is a recipe for linearizing a GCM, followed by the application of Gauss’s method of least squares to estimate uncertain GCM parameters. The following discussion assumes that the reader is already familiar with the method of least squares and its application to geophysical data analysis. If not, a brief but excellent introduction is that of Menke (1989).

Algebraically, a GCM can be represented by a set of rules for time-stepping a state vector:

\[ x(t_{i+1}) = M_i (x(t_i), \eta) . \]  

(1)

For the ocean-GCM example herein, state vector \( x(t_i) \) includes temperature, salinity, velocity, and sea-surface height on a predefined grid at discrete time \( t_i \). Function \( M_i \) represents the known GCM time-stepping rules, including initial conditions, boundary conditions, empirical mixing coefficients, etc. Vector \( \eta \) contains a set of uncertain parameters that can be used as “controls” for bringing the GCM simulation closer to observations. For example, vector \( \eta \) can include terms that represent errors in the initial and boundary conditions and in the empirical mixing coefficients. The state estimation problem aims to determine parameters \( \eta \) and their uncertainties given

\[ y^o = H \begin{bmatrix} x(t_0) \\ \vdots \\ x(t_N) \end{bmatrix} + \varepsilon , \]  

(2)

where vector \( y^o \) represents all available observations during the estimation period, \( t_0 \leq t_i \leq t_N \), \( H \) is the measurement function, and residual \( \varepsilon \) represents model and data errors of all kinds.
For the Green’s function approach, Eqs. (1) and (2) are combined, resulting in

\[ y^o = G(\eta) + \varepsilon, \]

where vector \( G(\eta) \) represents the simulated observations. That is, vector \( G(\eta) \) is obtained by integrating the GCM, Eq. (1), from \( t_0 \) to \( t_N \) and then applying measurement function \( H \). Let \( \eta^b \) represent the best prior guess for \( \eta \) and remove all known biases from the observations so that

\[ \langle \eta \rangle = \eta^b \quad \text{and} \quad \langle \varepsilon \rangle = 0, \]

where the angle brackets denote expectation and where \( \mathbf{0} \) is the null vector. The control parameters in vector \( \eta \) can be estimated by minimizing a quadratic cost function

\[ J = (\eta - \eta^b)^T Q^{-1}(\eta - \eta^b) + \varepsilon^T R^{-1} \varepsilon, \]

where superscript \( T \) is the transpose operator and where \( Q \) and \( R \) are weight matrices, usually chosen to coincide with \textit{a priori} error covariance matrices

\[ Q = \langle (\eta - \eta^b)(\eta - \eta^b)^T \rangle \quad \text{and} \quad R = \langle \varepsilon \varepsilon^T \rangle, \]

respectively. Equations (3)–(6) are those of a least-squares minimization problem. Complications arise because the dimensions of \( \eta \) and of \( \varepsilon \) can be huge, because covariance matrices \( Q \) and \( R \) are usually not known, and because function \( G \) is nonlinear. Most practical estimation methods assume that (3) can be usefully linearized about a particular GCM trajectory. If the linearization assumption holds, (3) simplifies to

\[ y^d = y^o - G(\eta^b) = G(\eta - \eta^b) + \varepsilon, \]

where vector \( y^d \) is the model-data difference and \( G \) is a matrix whose columns are the Green’s functions of \( G \). Specifically, the \( j \)-th column of matrix \( G \) is

\[ g_{(j)} = \frac{G(\eta^b + e_j) - G(\eta^b)}{|e_j|}, \]
where $e_j$ is a suitably-scaled perturbation vector that is everywhere zero except for element $j$ and where $|e_j|$ is the amplitude of perturbation $e_j$. That is, each column of $G$ can be computed using a GCM sensitivity experiment. Matrix $G$ is called the data kernel because it relates the data $y^d$ with model parameters $\eta$. The minimization of (5) given (7) is a discrete linear inverse problem with solution

$$\eta^a = \eta^b + PG^T R^{-1} y^d$$

and uncertainty covariance matrix

$$P = \langle (\eta - \eta^a)(\eta - \eta^a)^T \rangle = (Q^{-1} + G^T R^{-1} G)^{-1}.$$  \hspace{1cm} (10)

Discrete linear inverse theory is the subject of a vast literature and many useful tools exist for deriving and for analyzing the solutions (e.g., Menke 1989; Wunsch 1996, and references therein).

The validity of the GCM linearization can be tested \textit{a posteriori} by comparing the residual of Eqs. (3) and (7) for $\eta = \eta^a$. If the linearity assumption holds, then it is expected that $G(\eta^a) - G(\eta^b) \approx G(\eta^a - \eta^b)$. Therefore a reasonable requirement is that

$$\text{abs} \left( G(\eta^a) - G(\eta^b) - G(\eta^a - \eta^b) \right) \ll \text{diag}(R^{1/2}),$$

where operator $\text{abs}(\cdot)$ returns a vector that contains the absolute values of the input-vector elements and operator $\text{diag}(\cdot)$ returns a vector that contains the diagonal elements of the input matrix. If condition (11) is not satisfied, it may be possible to further reduce cost function (5) by using an iterative approach. Specifically, the GCM is re-linearized about $\eta^a$ instead of $\eta^b$, matrix $G$ is recomputed, and a new solution is sought.

3. Ocean state estimation example

The Green’s function approach has been applied to the calibration of a general circulation model, which is used for quasi-operational analysis of the time-evolving
ocean circulation. This analysis is a product of the consortium for Estimating the Circulation and Climate of the Ocean (ECCO), it is maintained at the Jet Propulsion Laboratory (JPL), it is updated approximately once per week, it is freely available (http://ecco.jpl.nasa.gov), and it is being used for a variety of science applications (e.g., Dickey et al. 2002; Fukumori et al. 2004; Gross et al. 2003; Lee and Fukumori 2003; McKinley et al. 2003). The discussion that follows is not meant to be the definitive description of the ECCO/JPL ocean circulation analysis; it is only meant to provide a concrete example for the application of the Green’s function approach.


The ECCO/JPL near-real-time analysis is based on a quasi-global configuration of the Massachusetts Institute of Technology General Circulation Model (MIT GCM) (Marshall et al. 1997). The model grid spans 80°S to 79°N and there are 360 × 224 horizontal grid cells. Zonal grid spacing is 1° of longitude. Meridional grid spacing is 0.3° of latitude within ±10° of the Equator and increases to 1° latitude outside the tropics, as shown on the left panel of Fig. 1. There are 46 vertical levels with thicknesses ranging from 10 to 400 m down to a maximum depth of 5815 m, as shown on the right panel of Fig. 1. Figure 2 shows the model bathymetry. Ocean regions north of 73°N and south of 73°S are not represented in order to permit a 1-hour integration time step. The model employs the K-Profile Parameterization (KPP) vertical mixing scheme of Large et al. (1994) and the isopycnal mixing schemes of Redi (1982) and of Gent and McWilliams (1990) with surface tapering as per Large et al. (1997). Lateral boundary conditions are closed. No-slip bottom, free-slip lateral, and free surface boundary conditions are employed.

The baseline integration spans 1991 to 2000 and is forced at the surface with 12-hourly wind stress and with daily heat and freshwater fluxes from the NCEP meteorological reanalysis (Kistler et al. 2001) with following modifications:

2. The 1945–1993 time-mean COADS heat and freshwater fluxes have further been adjusted so that the spatial integral is zero over the model domain.

3. Model Sea-Surface Temperature (SST) is relaxed to NCEP SST using the formulation of Barnier et al. (1995).


5. Any model temperature that becomes less than $-1.8^\circ C$ is reset to $-1.8^\circ C$.

6. Sea-Surface Salinity (SSS) is relaxed to monthly mean SSS from the World Ocean Database 1998 (WOD98) (Conkright et al. 1999) with a relaxation constant of 60 days.

Isopycnal mixing coefficient is 500 m$^2$/s. Vertical diffusivity is $5 \times 10^{-6}$ m$^2$/s. Horizontal and vertical viscosity are $10^{13}$ m$^4$/s and $10^{-4}$ m$^2$/s, respectively. The model is initialized from rest and from the WOD98 temperature and salinity climatology and integrated for ten years using the 1980–1997 mean NCEP seasonal cycle. It is then integrated from January 1980 to December 1990 using real-time fluxes to obtain January 1991 initial conditions for the baseline integration. These particular choices need not be further justified here, since they are superseded later in this manuscript using the Green’s function approach. Suffice to say that they were the result of dozens of trial-and-error experiments, over the course of several years, by a handful of experienced physical oceanographers.
b. Data used to constrain the baseline integration.

The data that are used to constrain the baseline integration are observations of sea-surface height variability and a collection of vertical temperature profiles. Sea-surface height data are from the NASA/GSFC Pathfinder TOPEX/Poseidon Altimetry Version 9.1 (http://podaac.jpl.nasa.gov). Specifically, colinear sea surface height data are used, which are georeferenced to a specific ground track and are given at 1 s intervals, approximately every 6 km along each track. The data are corrected for all known geophysical, media, and instruments effects, including tides and atmospheric loading. The Pathfinder data are further bin-averaged along each track, consistent with the model resolution.

Vertical temperature profile data from Expendable Bathythermograph (XBT) and from the Tropical Atmosphere Ocean (TAO) array are processed, quality-checked, and made available by D. Behringer (personal communication, 2002). These data are complemented with temperature profiles from the World Ocean Circulation Experiment (WOCE), from the Hawaii Ocean Time Series (HOTS), from the Bermuda Atlantic Time Series (BATS), and from Profiling ALACE (PALACE) floats. Figures 3 and 4 show, respectively, the horizontal and vertical data distributions. For this study, the temperature data are bin-averaged inside each model grid box and for 10-day intervals spanning January 1, 1992 to December 31, 2000.

c. Kalman filter, smoother, and adjoint method

The baseline integration described in Sect. 3a was initially constrained with the data of Sect. 3b using the partitioned Kalman filter and the smoother of Fukumori (2002). As currently implemented, this filter and smoother are used to estimate adiabatic corrections due to errors in the time-varying surface wind stress. But they have not yet been extended to handle model biases nor to correct errors in surface heat and freshwater fluxes and in diabatic processes. In particular, if the stratification of the
baseline integration is in error, the adiabatic corrections needed to match observations of sea-surface height can result in interior temperature and salinity variations that are unrealistic.

A powerful methodology for removing model biases and for correcting errors in surface heat and freshwater fluxes and in diabatic processes is provided by the adjoint model (e.g., Stammer et al. 2003). But at the time that this work was carried out, the available computer resources were insufficient for a complete 1991–2000 adjoint-model optimization using the model configuration just described. Based on the experience of Stammer et al. (2003), a complete adjoint-method optimization may have required the equivalent of some 500 forward-model integrations over the 1991–2000 estimation period. That is, approximately 100 forward and adjoint-model integrations, with each adjoint-model integration requiring approximately four times as much time to complete as a forward-model integration. Also the computer memory and disk storage requirements for an adjoint-model optimization are larger, typically by a factor of 10, or more, than those of the forward integration. This is because of the need to store intermediary model variables in order to reduce recomputations (Heimbach et al. 2002).

It should also be pointed out that the particular GCM configuration, which is used to carry out the work described herein, does not have a well-defined tangent linear for periods longer than about ten days. This is because of sensitivity issues related with the vertical and isopycnal mixing parameterizations. Therefore it is not possible to directly apply the adjoint-model method: some modifications or simplifications of the GCM code are required. By comparison, as is demonstrated below, the Green’s function approach is more robust because it relies on an approximate, not exact, linearization of the GCM.

Finally, the development of a partitioned Kalman filter and smoother or of an adjoint-method optimization require substantial manpower and expertise. By comparison, the computation of model Green’s functions is straightforward. A model Green’s function is derived by perturbing a model parameter relative to the baseline
integration and then integrating the model forward from 1991 to 2000. That is, the computation of a model Green’s function is equivalent to the computation of a model sensitivity experiment.

All the above reasons motivated the development of the Green’s function approach, which is described next, as a way to remove model biases and to correct errors in surface heat and freshwater fluxes and in diabatic processes for the ECCO/JPL ocean circulation analysis.

4. A first Green’s function optimization

A first test of the Green’s function approach is carried out using six sensitivity experiments. For experiments 1–3 the baseline 1991–2000 integration of Sect. 3a is repeated with perturbed vertical diffusivity, vertical viscosity, and isopycnal diffusivity coefficients, as indicated in Table 1. For experiment 4, the time-mean wind stress of the baseline integration is replaced by a time-mean wind stress derived from QuikSCAT (QSCAT) scatterometer data (W. Tang, personal communication, 2002). For experiment 5, a temperature perturbation is generated by Optimal Interpolation (OI) of the observed model data difference and added to the 1991 initial conditions. For experiments 6, the model is reinitialized in 1991 from the January WOD98 temperature and salinity climatology. In terms of the notation of Sect. 2, $G(\eta^b)$ in (8) corresponds to the baseline 1991–2000 integration sampled at the locations and times of the temperature data; $G(\eta^b + e_j)$ in (8) represents the six sensitivity experiments of Table 1, also sampled at the locations and times of the temperature data. The data kernel matrix, $G$ in (7), (9), and (10), is a tall skinny matrix, with six columns and a number of rows equal to the number of data.
a. Cost function

An important step for optimization studies is the definition of cost function $J$ in (5) and, in particular, the specification of prior error covariance matrices $Q$ and $R$ in (6) (e.g., Menemenlis and Chechelnitsky 2000). For the Green’s function approach, the number of observations is generally much larger than the number of parameters being estimated, which simplifies this task. First, the small number of control parameters limits the solution’s degrees of freedom, therefore the choice of $Q$ and of $R$, if they are reasonable, is not expected to change the solution much. Second, the data kernel matrix $G$ is small enough to be defined explicitly, therefore many interesting properties of the solution, for example, the model resolution matrix, can be derived and evaluated. Third, the solution of (9) and (10), once the kernel matrix $G$ has been derived, is very inexpensive, therefore it is possible to use Monte-Carlo methods in order to test particular choices of $Q$ and of $R$, as is done next.

For the first Green’s function optimization we test three different cost functions. In all three cases the form of the cost functions is

$$J = \sum_i \left( \frac{y_i^o - x_i}{\sigma_i} \right)^2,$$

where $y_i^o$ represents temperature data, $x_i$ is the model estimate, $\sigma_i^2$ is the data error variance, and subscript $i$ represents a specific location and time. Cost function (12) implies that the data-error covariance matrix $R$ is diagonal and that there is no a priori information about the parameters to be optimized, that is, $Q^{-1} = 0$. The assumption of diagonal $R$ is justified because the temperature data, which are already bin-averaged inside each model grid box and for 10-day intervals, are further decimated so that each optimization is carried out using $10^4$ randomly-selected observations out of a total of $5 \times 10^6$ bin-averaged temperature observations. The agnostic assumption that $Q^{-1} = 0$ has little impact on the solution because the minimization problem is highly over-determined.
The three cost functions that are tested are labeled Cases 1–3. For Case 1, the \textit{a priori} error variance, $\sigma_i^2$ in (12), is assumed horizontally homogeneous and equal to the data variance at each depth, as shown on Fig. 5. This assumption is a conservative upper bound for data and model representation errors. For Case 2 the \textit{a priori} error variance is assumed horizontally homogeneous but equal to the variance of the model-data difference at each depth, also shown on Fig. 5. Finally for Case 3 the mean \textit{a priori} error variance at each depth is also proportional to the variance of the model-data difference, as is that of Case 2, but it is scaled horizontally by the sea-level anomaly variance observed by the TOPEX/POSEIDON altimeter and shown on Fig. 6.

For Case 3 the \textit{a priori} error variance is further scaled using the following Monte Carlo approach: it is required that the \textit{a posteriori} uncertainty variance of the estimates be approximately equal to the variance of 200 independent estimates, each obtained from an optimization that uses a different random subset of the data.

Columns 5–7 on Table 1 list the optimized parameters and the uncertainties for the three different \textit{a priori} assumptions described above. Uncertainty here refers to twice the square root of the diagonal elements of matrix $P$ in (10), the 95% confidence level if the errors are normally distributed. Admittedly, all three \textit{a priori} error variance estimates are rather \textit{ad hoc}. What matters for the present discussion is that the three cases are radically different. The first case downweighs near-surface data, the second case downweighs seasonal thermocline data, and the third case downweighs high-latitude data. Yet all three cases give similar estimates; the error bars overlap at the 95% confidence level. In particular, the optimized estimates of vertical viscosity and diffusivity and also of initial temperature and salinity conditions are radically different from those that are used in the baseline integration.

Because of coarse resolution, artificial northern boundary conditions, and lack of an interactive sea-ice model, the present model configuration is not expected to be very realistic at high latitudes. Therefore, for the remainder of this article, we use
the spatially varying definition for the \textit{a priori} error variance, that of Case 3, which downweighs the high latitudes.

\textit{b. Linear approximation}

The fundamental assumption that underlies the Green’s function approach is that the estimation problem can be linearized relative to the baseline integration. That is, the optimal solution can be obtained as a linear combination of the baseline and sensitivity experiments. The extent to which this assumption is valid can be evaluated by comparing the optimal linear combination of the baseline and sensitivity experiments with a new model integration, which is carried out using the optimized parameters.

Assuming linearity, the expected cost function reduction relative to the baseline integration is 30\% for the Case-3 parameters, those of column 7 in Table 1. The actual cost function reduction, when the Case-3 parameters are used to carry out a new model integration, is 33\%. This is 3\% better than what would be expected for a perfectly linear problem. While in general we don’t expect such substantial cost function reduction, this preliminary optimization demonstrates that exact linearity is not required for the Green’s function approach to work and that the optimization of a small number of carefully chosen parameters can have a large positive impact on the solution.

On average, for the first Green’s function optimization, the errors due to non-linearity are approximately 25\% of the assumed \textit{a priori} errors in the data and in the model, that is, the right-hand-side of (11) is approximately four times larger than the left-hand-side. Therefore the linear approximation is satisfied and no further iterations are needed in order to optimize the six parameters listed in Table 1.

\textit{c. Linear dependence}

Once the linear approximation has been validated, the kernel matrix $\mathbf{G}$, which is explicitly computed in the Green’s function approach, can be used to ask many
interesting and important “what-if” questions. This capability is a key advantage of the Green’s function approach. Below we use $G$ to determine the hypothetical consequences of estimating the parameters of Table 1 one at a time, to determine the relative contribution of each parameter to cost function reduction, and to infer the robustness of the estimates that have been obtained.

Table 2 lists hypothetical estimates from one-at-a-time optimizations and compares the results to those of Case 3. The table shows that the one-at-a-time estimates differ substantially from those of Case 3. This is because the parameters are linearly dependent on each other. Therefore they cannot be estimated independently. Note that the largest impact on cost function reduction comes first from the vertical diffusivity parameter and second from the initial conditions. This will be explained in Sects. 5f and 5g as resulting primarily from reduction of drift in the upper pycnocline and from compensation of model bias accumulated in that same region during the model spin-up.

To gage the relative contribution of each parameter to cost function reduction, additional hypothetical optimizations are carried out using only five out of the six possible parameters. The results of these optimizations are summarized in Table 3. The table shows that by optimizing only five of the six parameters the cost function reduction ranges from 19.8% to 29.7% as compared to 29.8% for Case 3, in which all six parameters are optimized. In order of decreasing importance for cost function reduction, the parameters are: 1. vertical diffusivity, 2. initial conditions, 3. time-mean wind stress, 4. isopycnal diffusivity, and 5. vertical viscosity.

The hypothetical optimizations summarized in Tables 2 and 3 can also be used to gage the likely impact of increasing the number control parameters, i.e., the number of degrees of freedom of the optimization. For example, one may infer that the estimate of vertical diffusivity is relatively robust since its range is limited from $15.0 \times 10^{-6}$ m$^2$/s to $17.4 \times 10^{-6}$ m$^2$/s. By comparison the estimate of vertical diffusivity is not very robust
since it ranges from $6.0 \times 10^{-6} \text{ m}^2/\text{s}$ to $348 \times 10^{-6} \text{ m}^2/\text{s}$.

5. A Second Green’s function optimization

The encouraging results from the six-parameter optimization discussed above motivated the computation of twenty additional model sensitivity experiments. These additional experiments are summarized in Table 4. Note that these twenty new sensitivity experiments were computed relative to the Case-3 solution of the first Green’s function optimization and that they include a repeat of all six sensitivity experiments listed on Table 1. The end result of this second optimization is a further 10% cost function reduction, as indicated on Table 5. The resulting estimates of vertical mixing coefficients, surface heat and freshwater fluxes, isopycnal diffusivity, surface wind stress, and initial conditions are discussed below, followed by an analysis of improvements in bias, drift, and explained variance relative to earlier solutions and to data.

a. Vertical mixing

Sensitivity experiments 1–4 on Table 4 pertain to the representation of vertical mixing in the model. Notice that the background vertical diffusivity, which had been deemed a relatively robust estimate in the earlier discussion, remains unchanged with a value of $(15.1 \pm 0.1) \times 10^{-6} \text{ m}^2/\text{s}$. This value is consistent with inferences from microstructure and from tracer studies (e.g., Kelley and Scy 1999, and references therein).

The estimate of background vertical viscosity is $(18 \pm 3) \times 10^{-6} \text{ m}^2/\text{s}$, which is approximately six times smaller than the canonical value of $10^{-4} \text{ m}^2/\text{s}$ that is often used for ocean modeling (e.g., Large et al. 2000). A possible explanation for this difference is that the optimal background vertical viscosity is strongly dependent on the values of other model variables, in particular on the values of vertical and isopycnal diffusivity.

Two additional parameters of the Large et al. (1994) KPP scheme, $Ri_c$ and $Ri_0$,
have been estimated. $Ri_c$ is the critical bulk Richardson number, which sets the depth of the oceanic boundary layer. The estimate of $0.354 \pm 0.004$ is 18\% larger than the value suggested by Large et al. (1994). This compensates, in part, for shallow boundary layers depths in the baseline integration relative to the data. $Ri_0$ is a threshold gradient Richardson number for shear instability vertical mixing, which is especially important for equatorial dynamics. The estimated value of $0.699 \pm 0.008$ is the same as that suggested by Large et al. (1994).

**b. Surface heat and freshwater fluxes**

Experiments 5 and 6 are used to adjust the surface salinity and temperature relaxation terms. The estimates shown on Table 4 indicate that the baseline values of the relaxation coefficients are too weak for salinity and too strong for temperature. Figure 7 compares the mean and standard deviation of the resulting estimates of surface heat and freshwater fluxes with those from the NCEP reanalysis. The corrections to the time-mean surface fluxes are substantial, up to 100 W/m$^2$ for heat and 2 m/yr for freshwater, which are values comparable to the time-mean fields themselves.

It is interesting to compare the estimated time-mean surface flux corrections, panels b and f in Fig. 7, to the estimates obtained independently by Stammer et al. (2004, Fig. 3) using the adjoint method. Except for the Equatorial Pacific, the similarities of the two estimates both in pattern and in magnitude are striking. The principal differences between the two estimates occur near the Equator where the meridional grid spacing of the present study is higher than that of Stammer et al. (2004), i.e., 35 km instead of 110 km. A detailed comparison of the two solutions is in preparation.
c. *Isopycnal diffusivity*

Isopycnal diffusivity is estimated as the linear combination of four sensitivity experiments. The objective is to obtain a crude estimate of the time-independent horizontal and vertical variations of this parameter. The first sensitivity experiment is a constant perturbation, similar to experiment 3 in the first Green’s function optimization. The second experiment is a vertically homogeneous but spatially varying perturbation. Following the suggestion of Holloway (1986) the spatial variation of this perturbation is proportional to $|gh/f|$, where $g$ is the acceleration of gravity, $h$ is the standard deviation of observed sea-surface height variations after removing tidal effects and the seasonal cycle, and $f = 2\Omega \sin \phi$ is the Coriolis parameter, where $\Omega$ is the Earth’s rotation rate and $\phi$ is latitude; in the tropics, 23°S to 23°N, $f$ is set equal to $5.7 \times 10^{-5}$ s$^{-1}$ for this computation. The third and fourth sensitivity experiments are also spatially varying as per Holloway (1986) but with exponentially decaying amplitude in the vertical, $\exp(-z/500)$ and $\exp(-z/1000)$, respectively, where $z$ is the depth in m.

Figures 8 and 9 display, respectively, a horizontal map of estimated isopycnal diffusivity at 1000 m depth and vertical profiles of minimum and maximum diffusivity. The estimates range from 550 m$^2$/s to 1350 m$^2$/s and straddle the value of 800 m$^2$/s suggested by Large et al. (1997) but are considerably lower than the 1500 m$^2$/s to 4000 m$^2$/s range that had been inferred by Holloway (1986) using satellite altimeter data. In the vertical, the estimates exhibit a 5% to 35% decrease near the surface. This is contrary to the *a priori* expectation that the estimated isopycnal diffusivity coefficient would be larger near the surface where the eddy kinetic energy is higher. The estimated decrease in near-surface isopycnal diffusivity is in addition to the Large et al. (1997) surface tapering scheme, which has also been applied in this study.
d. Surface wind stress

Surface wind stress is estimated as a linear combination of four sensitivity experiments. The first two experiments perturb the time-mean wind stress while preserving the variability of the NCEP reanalysis. The next two experiments perturb the time variable wind stress. Note that in the baseline integration, the time-mean NCEP wind stress has already been replaced with a time-mean wind stress derived from the COADS climatology, as discussed in Sect. 3a.

Specifically, the first sensitivity experiment, labeled QSCAT, replaces the time-mean wind stress of the baseline integration with a time-mean wind stress derived from QuikSCAT scatterometer data (W. Tang, personal communication, 2002). The second sensitivity experiment, labeled ERS-mean, replaces the time-mean wind stress with that from the ERS-1 and ERS-2 time-mean wind field obtained from CERSAT at IFREMER, Plouzané, France. The third sensitivity experiment, labeled ERS, includes both the time-mean and the time-variability of the CERSAT wind product. Finally, the fourth sensitivity experiment, labeled KFS, replaces the time-variable winds with those estimated by the approximate Kalman filter and smoother described in Sect. 3c.

The optimal surface wind stress estimate is

\[ \tau(r,t) = \overline{\tau}(r) + \tau'(r,t), \]  

where

\[ \overline{\tau}(r) = 0.55 \text{ COADS} + 0.56 \text{ ERS-mean} - 0.11 \text{ QSCAT} \]  

is the time-mean wind stress,

\[ \tau'(r,t) = 1.02 \text{ KFS} + 0.41 \text{ ERS} - 0.43 \text{ NCEP} \]  

is the time-variable wind stress, and \( r \) and \( t \) are space and time coordinates, respectively. The wind stress estimates are compared to the NCEP reanalysis in Fig. 10. The wind stress estimates can also be compared to those obtained independently by Stammer.
et al. (2004, Fig. 9) using the adjoint method. In the large scale, both estimates show an increase in the trade winds over the tropical Pacific and a weakening of the mid-latitude winds, especially above the Southern Ocean. In terms of meridional wind stress changes, both estimates indicate a smaller poleward component at latitudes higher than 30°N. The principal differences between the two estimates is that the adjoint-model solution contains many small-scale wind-stress corrections, especially in western boundary current regions and above the Antarctic Circumpolar Current, which are not present in the Green’s function solution.

The estimated time variability of the surface wind stress is very similar to that estimated by the Kalman filter and smoother, KFS in (15). This is an indication of the consistency and quality of that estimate. But there nevertheless are some small corrections to the KFS wind stress variability, which improve the explained sea-level variance of the Green’s function solution relative to the Kalman filter and smoother solution, as will be shown in Sect. 3h.

e. Initial conditions

Initial conditions are estimated as a linear combination of six experiments. The objective is to remove model bias while minimizing model drift relative to the data. The first two experiments are a repeat of the optimal interpolation and WOD98 initial condition experiments discussed in Section 4, but using the diffusivity, viscosity, and time-mean wind stress estimated by the first Green’s function optimization, Case 3 on Table 1. A third experiment is initialized from a temperature and salinity climatology derived from WOCE data.

The most substantial drift during spin-up, when the model is initialized from a climatology, occurs at high latitudes. In an attempt to minimize this drift, while preserving realistic initial conditions in the tropics, a fourth sensitivity experiment is initialized from a blend of WOD98 and of the 20-year spin-up integration described in
Sect. 3a. Between 20°S and 20°N temperature and salinity is set to WOD98 January values. Poleward of 30°S and of 30°N spin-up initial conditions are used. There is a gradual, sinusoidal transition between the two initial condition estimates in the latitude bands of 20°N–30°N and of 20°S–30°S.

The fifth sensitivity experiment is initialized from the final conditions of the fourth sensitivity experiment and the sixth sensitivity experiment is initialized from the final conditions of the fifth sensitivity experiment. This procedure provides some additional degrees of freedom from which the Green’s function minimization can choose suitable initial conditions.

The estimated initial temperature and salinity conditions are shown in Fig. 11 and are compared to the WOD98 January climatology. Except in some isolated regions, for example, the northern edge of the Antarctic Circumpolar Current, the estimated January 1991 temperature is generally warmer than WOD98 in the upper ocean. This warming relative to WOD98 is most pronounced in the Central Equatorial Pacific, almost 2°C warmer than WOD98, and also in the Gulf Stream and Kuroshio regions.

The estimates of initial salinity also show some large differences, up to 0.2 PSU, relative to the January WOD98 climatology. Particularly striking is the plume of increased salinity at 600 m depth in the Atlantic, flowing out of Gibraltar Strait.

f. Bias

Overall, the Green’s function optimization substantially improves the time-mean, the trend, and the variability of the solution relative to earlier estimate and to data (see Figs. 12–15). The following methodology is used to analyze the temperature data, which are sparse and irregularly sampled in space and in time. The model estimates are first sampled at the exact locations and times of the temperature data. The temperature data and the model estimates are then binned and analyzed in 20°-zonal by 10°-meridional grid cells. Global averages are weighted by area and are obtained by
averaging the results of all grid cells that contains more than 100 temperature samples.

Panel a in Fig. 12 shows that the Green’s function optimization has reduced the bias of the previous solutions relative to data throughout the entire water column. Notice that although the Kalman filter and smoother solution does not change the time-mean winds, it nevertheless impacts the time-mean temperature profile.

The bias reduction of the Green’s function solution is most significant at the base of the Equatorial thermocline as can be seen by comparing panels c and e in Fig. 13. To a large extent this is the result of vertical diffusivity being too weak in the baseline and in the Kalman filter and smoother integrations, hence resulting in a thermocline that is too sharp and too shallow relative to data.

Although the bias of the Green’s function solution relative to data is decreased on a global average when compared to earlier solutions, there are some regions where the bias remains significant. One of these regions is the Indian Ocean, which is too warm by about 1°C in the Green’s function solution at 200 m depth. These residual discrepancies contain information about remaining model parameterization and boundary condition errors. Therefore these discrepancies can guide future model-parameterization improvements and/or the selection of additional model sensitivity experiments.

g. Drift

Given the large changes in 1991 initial conditions relative to those obtained from model spin-up, an important question is whether the bias reduction has taken place at the expense of increased drift in the optimized solution. Panel b of Fig. 12 shows that overall, the Green’s function optimization has also reduced the drift of the solution relative to data. The largest drift reduction compared to the prior Kalman filter and smoother solution is once again at the base of the equatorial thermocline as can be seen by comparing panels c and e in Fig. 14. There are however localized regions where model drift relative to data is larger than that of the baseline and of the Kalman filter
and smoother integrations, for example, in the northern North Atlantic below 1000 m depth. Again these discrepancies can guide future improvements of the solution, for example, in the representation of high-latitude processes and in the formation of deep water masses.

h. Explained variance

Owing to the improved estimate of the time-mean state and to the combination of solutions, the Green’s function optimization also improves model variability of temperature and of sea-surface height relative to data compared to both the baseline and to the prior Kalman filter and smoother integrations. Panel c in Fig. 12 shows that overall the Green’s function solution results in a 10% to 30% increase in explained temperature variance compared to the earlier solutions. Explained variance is here defined as one minus the variance of the analysis-data difference divided by the variance of the baseline-data difference:

$$\text{explained variance} = 1 - \frac{\text{var}(G(\eta^a) - y^o)}{\text{var}(G(\eta^b) - y^o)}.$$  \hspace{1cm} (16)

The spatial pattern of the explained variance relative to the baseline integration is shown in Fig. 15 first for sea-level and second for temperature at the 156-m depth. The Kalman filter and smoother solution, panel a in Fig. 15, already explains a large fraction, up to 50%, of the baseline-data difference for sea-level variability. But overall it degrades the temperature variability, as shown in panel c of Fig. 15. Even though the Kalman filter and smoother solution has more realistic heaving of the water column than the baseline integration, the resulting temperature variability is degraded compared to observations because the time-mean vertical temperature gradient is inaccurate. By comparison, the Green’s function solution improves both the temperature and the sea-level variability, panels b and d in Fig. 15, even though altimetric data have not been used as constraints.
6. Summary and concluding remarks

The work discussed hereinabove demonstrates that Green’s functions provide a simple yet effective method to test and to calibrate GCM parameterizations, to study and to quantify model and data errors, to correct model biases and trends, and to blend estimates from different solutions and data products.

The Green’s function method was applied to an ocean GCM resulting in substantial improvements of the solution relative to observations as compared to prior estimates: overall model bias and drift are reduced and there is a 10% to 30% increase in explained variance. Within the context of this optimization, the following new estimates for commonly used ocean GCM parameters have been obtained. Background vertical diffusivity is \((15.1 \pm 0.1) \times 10^{-6} \text{ m}^2/\text{s}\). Background vertical viscosity is \((18 \pm 3) \times 10^{-6} \text{ m}^2/\text{s}\). The critical bulk Richardson number, which sets boundary layer depth, is \(Ri_c = 0.354 \pm 0.004\). The threshold gradient Richardson number for shear instability vertical mixing is \(Ri_0 = 0.699 \pm 0.008\). The estimated isopycnal diffusivity coefficient ranges from 550 \(\text{m}^2/\text{s}\) to 1350 \(\text{m}^2/\text{s}\), with the largest values occurring at depth in regions of increased mesoscale eddy activity. Surprisingly, the estimated isopycnal diffusivity exhibits a 5% to 35% decrease near the surface. Improved estimates of initial and boundary conditions were also obtained. The above estimates are the backbone of a quasi-operational, global-ocean circulation analysis system whose products are freely available and are being used for a variety of science applications (http://ecco.jpl.nasa.gov).

There remain many aspects of the above solution that can be improved, for example, the warm bias in the Indian Ocean at the 200-m depth, the drift of the solution below 1000 m in the northern North Atlantic, and in general the poor representation of high latitude processes and of deep water mass formation rates. The Green’s function approach provides a powerful mechanism for identifying and for reducing these residual model-data discrepancies in a physically consistent manner.
Compared to other methods, the key advantages of the Green’s function approach are simplicity of implementation, robustness in the presence of non-linearities, and the explicit computation of the data kernel matrix. While the application of an adjoint model or of an approximate Kalman filter and smoother require substantial additional model-development and coding efforts, all that is required for applying the Green’s function approach is the computation of GCM sensitivity experiments. Furthermore, while the adjoint method requires that the exact tangent linear of the GCM be well-behaved, Green’s functions provide an approximate linearization, which can be used to reduce the cost function even when the adjoint model is ill-behaved, as is the case in the above ocean GCM example. Finally, the explicit computation of the data kernel matrix makes available a vast array of tools from discrete linear inverse theory for deriving and for analyzing the solutions.

The key drawback of the Green’s function approach is that computational cost increases linearly with the number of control parameters. Therefore the method is only applicable to situations where a small number of control parameters need to be estimated. Nevertheless the present work demonstrates that a small number of carefully chosen control parameters can result in substantial improvement of the solution. For example, only six control parameters were used in the first test optimization and yet the cost function was reduced by 33%. While in general we don’t expect such substantial cost function reduction to be possible for all problems, it is clear that the Green’s function approach is an extremely powerful tool in the repertoire of ocean state estimation.

What distinguishes the present work from previous applications of Green’s functions to ocean state estimation is the choice of control parameters. Previous applications used model Green’s functions to obtain a coarse-scale representation of ocean GCM dynamics, for example, the GCM response to large-scale, geostrophically-adjusted density or sea-surface height perturbations. The breakthrough here is that rather than
using Green’s functions to approximate GCM dynamics, Green’s functions are instead used to calibrate a small number of key GCM parameters and to blend estimates from existing solutions and data products. This new approach has the advantage of permitting a relatively large impact on the solution from a small number of control variables. Additionally, the representation of GCM dynamics is implicit and exact rather than explicit and approximate.

Work is underway to apply the Green’s function approach to a global, eddy-permitting GCM configuration that includes the Arctic Ocean and an interactive sea-ice model. The Green’s function approach is also being applied to the calibration of an atmospheric GCM and of a coupled ocean-atmosphere climate GCM.

Acknowledgments. This is a contribution of the Consortium for Estimating the Circulation and Climate of the Ocean (ECCO) funded by the National Oceanographic Partnership Program. We are indebted to C. Wunsch for teaching us about inverse methods and for suggesting application of Green’s functions to the ocean circulation inverse problem.


Woodruff, S. D., H. F. Diaz, J. D. Elms, and S. J. Worley, 1998: COADS release 2 data and

Table Captions

**Table 1.** List of sensitivity experiments for the first Green’s function optimization. Column 3 lists the baseline parameters. Column 4 lists the perturbed parameters for each of six sensitivity experiments. Columns 5–7 list the optimized parameters and uncertainty for three different cost functions.

**Table 2.** Optimized parameters for Case 3, Table 1, are compared to parameters estimated one at a time. The last row displays the cost function reduction in percent assuming that the problem is linear. Because the parameters are linearly dependent, the one-at-a-time estimates differ substantially from those of Case 3.

**Table 3.** Optimized parameters for Case 3, from Table 1, are compared to estimates for optimizations where one of the six parameters is not used. The last row displays the cost function reduction in percent assuming that the problem is linear.

**Table 4.** List of sensitivity experiments and optimized parameters for the second Green’s function optimization.

**Table 5.** Cost function reduction relative to baseline integration.
### Tables

<table>
<thead>
<tr>
<th>Exp.</th>
<th>Parameter</th>
<th>Baseline</th>
<th>Perturb.</th>
<th>Case 1</th>
<th>Case 2</th>
<th>Case 3</th>
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<td>QSCAT</td>
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<td>OI</td>
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<td>WOD98</td>
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<td>.67 ± .06</td>
<td>.71 ± .08</td>
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**Table 1.** List of sensitivity experiments for the first Green’s function optimization. Column 3 lists the baseline parameters. Column 4 lists the perturbed parameters for each of six sensitivity experiments. Columns 5–7 list the optimized parameters and uncertainty for three different cost functions.
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Case 3</th>
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<th>Case 7</th>
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<td>—</td>
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<td>—</td>
<td>.60</td>
<td>—</td>
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<td>—</td>
<td>—</td>
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<td>Cost function reduction (%)</td>
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<td>0.14</td>
<td>5.42</td>
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Table 2. Optimized parameters for Case 3, Table 1, are compared to parameters estimated one at a time. The last row displays the cost function reduction in percent assuming that the problem is linear. Because the parameters are linearly dependent, the one-at-a-time estimates differ substantially from those of Case 3.
<table>
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<th>Parameter</th>
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<th>Case 12</th>
<th>Case 13</th>
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<td>—</td>
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<td>Initial temp. &amp; salt</td>
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Table 3. Optimized parameters for Case 3, from Table 1, are compared to estimates for optimizations where one of the six parameters is not used. The last row displays the cost function reduction in percent assuming that the problem is linear.
<table>
<thead>
<tr>
<th>Exp.</th>
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<td>17.7 ± 3.0</td>
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<td>3</td>
<td>(Ri_c), boundary layer depth</td>
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<td>4</td>
<td>(Ri_0), shear instability</td>
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<td>.699 ± .008</td>
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<td>Salinity relaxation (days)</td>
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<td>linear comb.</td>
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<td>11–14</td>
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<td>15–20</td>
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<td>linear comb.</td>
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**Table 4.** List of sensitivity experiments and optimized parameters for the second Green’s function optimization.
<table>
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<tr>
<th>Integration</th>
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<th>Reduction (%)</th>
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<td>Baseline</td>
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<td>Optimization 2</td>
<td>3191</td>
<td>43.1</td>
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**Table 5.** Cost function reduction relative to baseline integration.
**Figure Captions**

**Fig. 1.** The ocean GCM has 360-zonal by 224-meridional by 46-vertical grid cells. Zonal grid spacing is $1^\circ$. The left panel shows meridional grid spacing as a function of latitude. The right panel shows level thickness as a function of depth.

**Fig. 2.** Model bathymetry. The ocean domain spans 73°S to 73°N and excludes the Arctic Ocean.

**Fig. 3.** Horizontal distribution of temperature profiles. Black dots indicate locations of XBT and TAO profiles. Blue dots indicate locations of WOCE profiles. Red dots indicate locations of PALACE profiles. And green and magenta dots indicate locations of HOTS and BATS profiles, respectively.

**Fig. 4.** Vertical distribution of temperature profiles.

**Fig. 5.** Assumed vertical profiles of *a priori* error variance. Case 1 is the mean data variance at each depth. Case 2 is the mean variance of the model-data difference at each depth. Case 3 is proportional to the variance of the model-data difference but has further been scaled as described in the text. The Case-3 *a priori* error variance is that used for both the first and second Green’s function optimizations.

**Fig. 6.** Variance of sea-level anomaly observed by the TOPEX/POSEIDON altimeter during the 1993-2000 period. This map provides horizontal scaling for the Case-3 *a priori* error variance, which is used for weighting the data errors in the cost function.
Fig. 7. Comparison of estimated surface heat and freshwater fluxes with the NCEP reanalysis for the 1993-2000 period: a) estimate of mean heat flux entering the ocean; b) difference of this estimate from NCEP; c) standard deviation of the estimated surface heat flux; d) standard deviation of the difference with NCEP; e) estimate of mean evaporation minus precipitation minus runoff; f) difference of this estimate relative to evaporation minus precipitation from NCEP; g) standard deviation of the estimated evaporation minus precipitation minus runoff; h) standard deviation of the difference with NCEP. Units are W/m² for heat and m/yr for freshwater.

Fig. 8. Estimated isopycnal diffusivity at the 1000-m depth.

Fig. 9. Vertical profile of estimated isopycnal diffusivity.

Fig. 10. Comparison of estimated surface wind stress with the NCEP reanalysis for the 1993-2000 period: a) estimate of mean zonal wind stress; b) difference of this estimate from NCEP; c) standard deviation of the estimated zonal wind stress; d) standard deviation of the difference with NCEP; e) estimate of mean meridional wind stress; f) difference of this estimate from NCEP; g) standard deviation of the estimated meridional wind stress; h) standard deviation of the difference with NCEP. Units are N/m². Positive values are eastward and northward, for zonal and meridional components, respectively.

Fig. 11. Comparison of estimated 1991 initial conditions of potential temperature and of salinity, with the WOD98 January climatology: a) estimate of initial temperature at 156 m; b) estimate of initial temperature at 626 m; c) temperature difference with WOD98 at 156 m; d) temperature difference with WOD98 at 626 m; e) estimate of initial salinity at 156 m; f) estimate of initial salinity at 626 m; g) salinity difference with WOD98 at 156 m; h) salinity difference with WOD98 at 626 m. Units are °C for temperature and PSU for salinity.
Fig. 12. Comparison of the Green’s function solution (GF) to the baseline integration (Base) and to the Kalman filter and smoother solution (KFS): a) global root-mean-square (rms) bias relative to data; b) global rms drift relative to data; and c) percent explained variance of the baseline-data difference. Note that the vertical axis and also the horizontal axis for the bias and drift panels are logarithmic.

Fig. 13. Comparison of 1993-2000 time-mean temperature of the Green’s function and of the Kalman filter and smoother solutions relative to data: a) estimated temperature profile at the Equator down to 500 m depth; b) horizontal map of estimated temperature at the 156-m depth; c) temperature bias relative to data of the Kalman filter and smoother solution at the Equator; d) temperature bias relative to data of the Kalman filter and smoother solution at the 156-m depth; e) temperature bias relative to data of the Green’s function solution at the Equator; and f) temperature bias relative to data of the Green’s function solution at the 156-m depth. Units are °C.

Fig. 14. Comparison of 1993-2000 temperature trend of the Green’s function and of the Kalman filter and smoother solutions relative to data: a) estimated temperature drift at the Equator down to 500 m depth; b) horizontal map of estimated temperature drift at the 156-m depth; c) temperature drift relative to data of the Kalman filter and smoother solution at the Equator; d) temperature drift relative to data of the Kalman filter and smoother solution at the 156-m depth; e) temperature drift relative to data of the Green’s function solution at the Equator; and f) temperature drift relative to data of the Green’s function solution at the 156-m depth. Units are °C/yr.

Fig. 15. Percent explained variance of the baseline-data residual for a) sea-surface height variability of the Kalman filter and smoother solution, b) sea-surface height variability of the Green’s function solution, c) temperature variability at 156 m of the Kalman filter and smoother solution, and d) temperature variability at 156 m of the Green’s function solution.
Fig. 1. The ocean GCM has 360-zonal by 224-meridional by 46-vertical grid cells. Zonal grid spacing is 1°. The left panel shows meridional grid spacing as a function of latitude. The right panel shows level thickness as a function of depth.
Fig. 2. Model bathymetry. The ocean domain spans 73°S to 73°N and excludes the Arctic Ocean.
Fig. 3. Horizontal distribution of temperature profiles. Black dots indicate locations of XBT and TAO profiles. Blue dots indicate locations of WOCE profiles. Red dots indicate locations of PALACE profiles. And green and magenta dots indicate locations of HOTS and BATS profiles, respectively.
Fig. 4. Vertical distribution of temperature profiles.
Fig. 5. Assumed vertical profiles of \textit{a priori} error variance. Case 1 is the mean data variance at each depth. Case 2 is the mean variance of the model-data difference at each depth. Case 3 is proportional to the variance of the model-data difference but has further been scaled as described in the text. The Case-3 \textit{a priori} error variance is that used for both the first and second Green’s function optimizations.
Fig. 6. Variance of sea-level anomaly observed by the TOPEX/POSEIDON altimeter during the 1993-2000 period. This map provides horizontal scaling for the Case-3 *a priori* error variance, which is used for weighting the data errors in the cost function.
Fig. 7. Comparison of estimated surface heat and freshwater fluxes with the NCEP reanalysis for the 1993-2000 period: a) estimate of mean heat flux entering the ocean; b) difference of this estimate from NCEP; c) standard deviation of the estimated surface heat flux; d) standard deviation of the difference with NCEP; e) estimate of mean evaporation minus precipitation minus runoff; f) difference of this estimate relative to evaporation minus precipitation from NCEP; g) standard deviation of the estimated evaporation minus precipitation minus runoff; h) standard deviation of the difference with NCEP. Units are W/m$^2$ for heat and m/yr for freshwater.
Fig. 8. Estimated isopycnal diffusivity at the 1000-m depth.
Fig. 9. Vertical profile of estimated isopycnal diffusivity.
Fig. 10. Comparison of estimated surface wind stress with the NCEP reanalysis for the 1993-2000 period: a) estimate of mean zonal wind stress; b) difference of this estimate from NCEP; c) standard deviation of the estimated zonal wind stress; d) standard deviation of the difference with NCEP; e) estimate of mean meridional wind stress; f) difference of this estimate from NCEP; g) standard deviation of the estimated meridional wind stress; h) standard deviation of the difference with NCEP. Units are N/m². Positive values are eastward and northward, for zonal and meridional components, respectively.
Fig. 11. Comparison of estimated 1991 initial conditions of potential temperature and of salinity, with the WOD98 January climatology: a) estimate of initial temperature at 156 m; b) estimate of initial temperature at 626 m; c) temperature difference with WOD98 at 156 m; d) temperature difference with WOD98 at 626 m; e) estimate of initial salinity at 156 m; f) estimate of initial salinity at 626 m; g) salinity difference with WOD98 at 156 m; h) salinity difference with WOD98 at 626 m. Units are °C for temperature and PSU for salinity.
Fig. 12. Comparison of the Green’s function solution (GF) to the baseline integration (Base) and to the Kalman filter and smoother solution (KFS): a) global root-mean-square (rms) bias relative to data; b) global rms drift relative to data; and c) percent explained variance of the baseline-data difference. Note that the vertical axis and also the horizontal axis for the bias and drift panels are logarithmic.
Fig. 13. Comparison of 1993-2000 time-mean temperature of the Green’s function and of the Kalman filter and smoother solutions relative to data: a) estimated temperature profile at the Equator down to 500 m depth; b) horizontal map of estimated temperature at the 156-m depth; c) temperature bias relative to data of the Kalman filter and smoother solution at the Equator; d) temperature bias relative to data of the Kalman filter and smoother solution at the 156-m depth; e) temperature bias relative to data of the Green’s function solution at the Equator; and f) temperature bias relative to data of the Green’s function solution at the 156-m depth. Units are °C.
Fig. 14. Comparison of 1993-2000 temperature trend of the Green’s function and of the Kalman filter and smoother solutions relative to data: a) estimated temperature drift at the Equator down to 500 m depth; b) horizontal map of estimated temperature drift at the 156-m depth; c) temperature drift relative to data of the Kalman filter and smoother solution at the Equator; d) temperature drift relative to data of the Kalman filter and smoother solution at the 156-m depth; e) temperature drift relative to data of the Green’s function solution at the Equator; and f) temperature drift relative to data of the Green’s function solution at the 156-m depth. Units are °C/yr.
Fig. 15. Percent explained variance of the baseline-data residual for a) sea-surface height variability of the Kalman filter and smoother solution, b) sea-surface height variability of the Green’s function solution, c) temperature variability at 156 m of the Kalman filter and smoother solution, and d) temperature variability at 156 m of the Green’s function solution.