Model Green’s Functions
(a simple but effective way to adjust model parameters)

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In 1828, an English miller from Nottingham published a mathematical essay that generated little response. George Green’s analysis, however, has since found applications in areas ranging from classical electrostatics to modern quantum field theory.
Green’s Functions for linear differential equations

Let $L$ be an arbitrary linear differential operator.

A Green's function, $G(x,y)$, is defined as the impulse response of this linear operator, that is:

$$LG(x,y) = \delta(x - y),$$

where $\delta(x-y)$ is the Dirac delta function applied at location $y$.

By linear superposition, Green’s functions can be used to solve a differential equation with arbitrary forcing term, $Lu(x) = f(x)$.

The solution is the convolution: $u(x) = \int G(x,y) f(y) \, dy$. 
Model Green’s Functions estimation approach

**GCM:** A General Circulation Model can be represented by a set of rules for time stepping a state vector $x(t_i)$ one time step in the future:

$$x(t_{i+1}) = M(x(t_i), \eta)$$

where $M$ represents the known time stepping rules and vector $\eta$ represents perturbations to a set of model parameters. Vector $\eta$ is assumed to be a noise process with zero mean and covariance matrix $Q$. 
Model Green’s Functions estimation approach

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x(t_{i+1}) = M(x(t_i), \eta)
\]

where \( M \) represents the known time stepping rules and vector \( \eta \) represents perturbations to a set of model parameters. Vector \( \eta \) is assumed to be a noise process with zero mean and covariance matrix \( Q \).

**Data:** The state estimation problem aims to estimate parameters \( \eta \) given a set of observations:

\[
y = H(x) + \epsilon
\]

where \( H \) is the measurement function, and residual \( \epsilon \) is a noise process assumed to have zero mean and covariance matrix \( R \). For the Green’s function approach, the data equation is rewritten:

\[
y = G(\eta) + \epsilon
\]

where \( G \) is the convolution of measurement function \( H \) with GCM dynamics \( M \).
Model Green’s Functions estimation approach

**Cost function:** Control parameters $\eta$ can be estimated by minimizing a quadratic cost function:

$$ J = \eta^T Q^{-1} \eta + \varepsilon^T R^{-1} \varepsilon $$

where superscript $T$ is the transpose operator and superscript $-1$ denotes a matrix inversion.
Model Green’s Functions estimation approach

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Linearization: To minimize this cost function, the GCM and data equations are linearized about a baseline simulation $x_b (\eta = 0)$. For “small” perturbations:

$$ G(\eta) \approx G(0) + G\eta $$

where matrix $G$ is an $n \times p$ matrix, $n$ is the dimension of observation vector $y$, and $p$ is the dimension of parameter vector $\eta$. Matrix $G$ can be determined by performing a series of GCM sensitivity experiments. Specifically, each column of matrix $G$ is obtained by perturbing the corresponding element in parameter vector $\eta$ and then carrying out a GCM integration over the estimation period.
Model Green’s Functions estimation approach

Minimization: The minimization of cost function $J$ subject to the linearized model-data constraints has solution:

$$\eta_a = PG^TR^{-1}y_d$$

where $y_d$ is the model-data residual, that is, $y_d \equiv y - G(0)$, and $P$ is the uncertainty covariance matrix:

$$P = (Q^{-1} + G^TR^{-1}G)^{-1}$$
Model Green’s Functions estimation approach

Minimization: The minimization of cost function \(J\) subject to the linearized model-data constraints has solution:

\[
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\]

where \(y_d\) is the model-data residual, that is, \(y_d \equiv y_o - G(0)\), and \(P\) is the uncertainty covariance matrix:

\[
P = ( Q^{-1} + G^TR^{-1}G )^{-1}
\]

Solution: The optimized solution \(x_a\) is:

\[
x_a = x_b + (G^TR^{-1}G)^{-1}R^{-1}y_d
\]

where \(x_b = M(x, \eta = 0)\) is from the baseline simulation and it is assumend that there is no prior information about control parameters, i.e., \(Q^{-1} \approx 0\).

If linearization assumption holds, we will have: \(x_a \approx M(x, \eta_a)\).
Figure 26. All measurements and models of the ocean can be interconnected to provide global estimates of the state of the three-dimensional ocean. Some side benefits accrue — e.g. improved estimates of the earth’s gravity field.

Taken from: **C. Wunsch**, in "A Celebration in Geophysics and Oceanography 1982. In Honor of Walter Munk on his 65th birthday."
Example application:
Large-Scale Circulation of the Pacific Ocean from Satellite Altimetry
(Stammer and Wunsch, 1996)

Figure 10, p. 137.

Figure 23. Estimates of seasonal surface elevation anomalies relative to the 1-year mean and related geostrophic currents. Fields represent (a) spring, (b), summer, (c) fall, and (d) winter, with spring starting at the beginning of March. Positive and negative values are drawn by bold, and thin lines, respectively. Contour increment is 1 cm. The reference vector represent 4 cm/s.
Example application: Linearization of an Oceanic General Circulation Model for Data Assimilation and Climate Studies (Menemenlis and Wunsch, 1997)

Fig. 9. Response of the four-level GFDL model to a 0.05°C perturbation, between 100- and 600-m depth, at the end of month 16. A two-dimensional low-pass spatial filter with cutoff wavelength of 16° has been applied to smooth scales not resolved by the reduced-order linear model. The heavy dot indicates the initial location of the disturbance.
3. Model description

The current study was initiated using the GFDL numerical code and model output from a global eddy-resolving integration by Semtner and Chervin (1992). These results are reported in sections 6 and 7. We have now switched over to the newly developed MIT GCM. This model is used to carry out the perturbation analysis reported in section 4 and will be the focus of our future assimilation efforts. The above models and their configurations are briefly described below.

a. MIT model

In its current configuration, the MIT GCM (Marshall et al. 1997a,b) solves the incompressible Navier–Stokes
Example application:
Basin-Scale Ocean Circulation from Combined Altimetric, Tomographic and Model Data (Menemenlis et al., 1997)
**Example application:**


**Fig. 1.** The ATOC acoustic array is superimposed on a map of the root-mean-square (rms) sea level anomaly from 4 years (January 1993 to December 1996) of TOPEX/POSEIDON altimetric measurements. Red lines indicate the sections used in the present study and are referenced by letter labels. Yellow lines show additional sections along which the acoustic propagation has been observed, but for which the data were not used here. Data assimilation was carried out in the region bounded by the outer white rectangle, and heat content estimates were obtained inside the inner white rectangle. Much, but not all, of the elevation anomalies represent seasonal thermal changes within the ocean, with the acoustic data providing a stable spatial average that is otherwise difficult to obtain. The ATOC region, being on the eastern side of the ocean, shows comparatively weak variability. Nevertheless, it is evident that the different acoustic sections will, during any 10-day period, have potentially very different anomalies.

**Fig. 3.** The range-averaged sea level anomaly along the acoustic sections inferred by several independent methods: (i) thick black lines indicate the ATOC acoustic measurements converted to equivalent sea surface height for comparison with the altimeter data, (ii) thin black lines are from the TOPEX/POSEIDON altimeter data, (iii) dashed lines represent the climatological thermal anomaly converted to sea surface height, (iv) blue lines are the GCM estimates, and (v) the asterisks along section v1 are the XBT data. Uncertainties are indicated for the acoustic estimates: the possible errors are largest along section v1 because the upper ocean variability is unresolved due to a lack of surface-reflecting rays near the receiver.
**Example application:**
Using Green’s Functions to Calibrate an Ocean General Circulation Model (Menemenlis et al., 2005)

**Table 4. List of sensitivity experiments and optimized parameters for the second Green’s function optimization.** For experiment 6, the optimized parameter is indicated as a factor multiplying the $\partial Q/\partial T$ fields of Barnier et al. (1995).

<table>
<thead>
<tr>
<th>Expt</th>
<th>Parameter</th>
<th>Baseline</th>
<th>Optimized</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Vertical diffusivity ($10^{-6}$ m$^2$ s$^{-2}$)</td>
<td>5</td>
<td>$15.1 \pm 12$</td>
</tr>
<tr>
<td>2</td>
<td>Vertical viscosity ($10^{-6}$ m$^2$ s$^{-2}$)</td>
<td>100</td>
<td>$17.7 \pm 3.0$</td>
</tr>
<tr>
<td>3</td>
<td>$R_i$, boundary layer depth</td>
<td>0.300</td>
<td>$0.354 \pm 0.004$</td>
</tr>
<tr>
<td>4</td>
<td>$R_i$, shear instability</td>
<td>0.700</td>
<td>$0.699 \pm 0.008$</td>
</tr>
<tr>
<td>5</td>
<td>Salinity relaxation (days)</td>
<td>60</td>
<td>$44.5 \pm 1.2$</td>
</tr>
<tr>
<td>6</td>
<td>Temperature relaxation ($\partial Q/\partial T$)</td>
<td>1.000</td>
<td>$1.630 \pm 0.008$</td>
</tr>
<tr>
<td>7–10</td>
<td>Isopycnal diffusivity (m$^2$ s$^{-2}$)</td>
<td>500</td>
<td>Linear combination</td>
</tr>
<tr>
<td>11–14</td>
<td>Surface wind stress</td>
<td>NCEP/COADS</td>
<td>Linear combination</td>
</tr>
<tr>
<td>15–20</td>
<td>Initial conditions</td>
<td>SPINUP</td>
<td>Linear combination</td>
</tr>
</tbody>
</table>

- 43% decrease in cost function
- significant reduction in model bias and drift
- 10–30% increase in explained variance
**Example application:**
Using Green’s Functions to Calibrate an Ocean General Circulation Model (Menemenlis et al., 2005)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Case 3</th>
<th>Case 4</th>
<th>Case 5</th>
<th>Case 6</th>
<th>Case 7</th>
<th>Case 8</th>
<th>Case 9</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vertical diffusivity ($10^{-6}$ m$^2$ s$^{-2}$)</td>
<td>15.4</td>
<td>17.4</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>Vertical viscosity ($10^{-6}$ m$^2$ s$^{-2}$)</td>
<td>46</td>
<td>—</td>
<td>348</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>Isopycnal diffusivity (m$^2$ s$^{-2}$)</td>
<td>572</td>
<td>—</td>
<td>—</td>
<td>399</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>Time-mean wind stress</td>
<td>0.43</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>0.72</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>Initial temperature</td>
<td>0.11</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>0.60</td>
<td>—</td>
</tr>
<tr>
<td>Initial temperature and salt</td>
<td>0.71</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>2.5</td>
</tr>
<tr>
<td>Cost function reduction (%)</td>
<td>29.8</td>
<td>19.4</td>
<td>0.58</td>
<td>0.14</td>
<td>5.42</td>
<td>6.46</td>
<td>14.2</td>
</tr>
</tbody>
</table>
**Example application:**
Using Green’s Functions to Calibrate an Ocean General Circulation Model (Menemenlis et al., 2005)

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Figure 12a 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 smoother solution corrects the temporal variability, it nevertheless has a measurable impact on 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 Figs. 13c and 13e. To a large extent this is the result of vertical diffusivity being too weak in the baseline and in the 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...
Example application:
Using Green’s Functions to Calibrate an Ocean General Circulation Model (Menemenlis et al., 2005)

Fig. 14. Potential temperature trend, 1993–2000: (a) Green’s function estimate at the equator down to 500-m depth; (b) Green’s function estimate at the 156-m depth; (c) smoother drift relative to data at the equator; (d) smoother drift relative to data at the 156-m depth; (e) Green’s function drift relative to data at the equator; and (f) Green’s function drift relative to data at the 156-m depth. Units are °C yr⁻¹.
**Example application:**
Using Green’s Functions to Calibrate an Ocean General Circulation Model (Menemenlis et al., 2005)

**Fig. 8.** Estimated isopycnal diffusivity in m² s⁻¹ at the 1000-m depth.

**Fig. 9.** Vertical profile of estimated isopycnal diffusivity.
Example application:
Ocean Carbon-cycle Model Intercomparison Project 3 (OCMIP-3)
(Mikaloff Fletcher et al. 2006, 2007; Gruber et al. 2009)

Figure 2. The 24 regions used for the ocean inversion. The region numbers show the aggregation from the original 30 regions [Mikaloff Fletcher et al., 2003] to the 24 regions used in this study.
Example application:
Ocean Carbon-cycle Model Intercomparison Project 3 (OCMIP-3) (Mikaloff Fletcher et al. 2006, 2007; Gruber et al. 2009)

Figure 1. Air-sea CO₂ fluxes for 10 regions, ordered by latitude and Ocean basin (positive: outgassing; negative: uptake). (a) Comparison of contemporary air-sea fluxes of CO₂. Shown are the ocean inversion estimates (this study), the new pCO₂-based estimates of Takahashi et al. [2008], the mean estimates based on results from the 13 ocean biogeochemistry models that participated in the second phase of the Ocean Carbon-cycle Model Intercomparison Project (OCMIP-2) [Watson and Orr, 2003], and the mean estimates from the TransCom-3 project based on the interannual (level 3) inversions of atmospheric CO₂ [Baker et al., 2006]. The uncertainties for the OCMIP-2 estimates reflect the (unweighted) standard deviation across the 13 models, while the uncertainties for the TransCom estimates were obtained by quadrature of the within and between model errors reported by Baker et al. [2006]. (b) Weighted mean estimates of the natural, anthropogenic, river-induced, and contemporary air-sea fluxes of CO₂ based on our ocean inversion [Mikaloff Fletcher et al., 2006, 2007]. The results are aggregated to 10 regions from the 23 regions solved for in the inversion for reasons of clarity. Error bars denote the cross-model weighted standard deviation of the mean. The anthropogenic and contemporary CO₂ fluxes are for a nominal year of 1995.
Example application: Ocean Carbon-cycle Model Intercomparison Project 3 (OCMIP-3) (Mikaloff Fletcher et al. 2006, 2007; Gruber et al. 2009)

Figure 5. Ocean interior distributions of the tracers reflecting the exchange of CO$_2$ across the air-sea interface, displayed as global-scale section plots organized around the Southern Ocean in the center. (a) Distribution of anthropogenic CO$_2$, $C_{ant}$, estimated using the $\Delta C^*$ method of Gruber et al. [1996]. (b) Distribution of the gas exchange component of natural CO$_2$, $\Delta C_{gas ex}$, following Gruber and Sarmiento [2002]. The inversion interprets these distributions by determining, given ocean circulation and mixing, a set of surface ocean fluxes that most closely matches these observations. Also shown are isolines of potential density anomalies, $\sigma_0$ (density referenced to the ocean surface minus 1000 kg m$^{-3}$), along which most of the oceanic flow occurs. Major ocean circulation features are indicated by schematic arrows. Figure 5 is based on data taken from GLODAP [Key et al., 2004]. NADW: North Atlantic Deep Water, CDW: Circumpolar Deep Water; SAMW: Subantarctic Mode Water; AAIW: Antarctic Intermediate Water.
Example application:
Ocean Carbon-cycle Model Intercomparison Project 3 (OCMIP-3) (Mikaloff Fletcher et al. 2006, 2007; Gruber et al. 2009)

Table 1. Evaluation of Model Skill Based on Comparisons Between CFC-11 Model Simulations and the GLODAP Gridded CFC Data Set

<table>
<thead>
<tr>
<th>Model</th>
<th>Correlation</th>
<th>Normalized Std. Dev.</th>
<th>Model Skill</th>
<th>Inverse Anthropogenic CO₂ Uptake, Pg C yr⁻¹</th>
<th>Forward Anthropogenic CO₂ Uptake, Pg C yr⁻¹</th>
</tr>
</thead>
<tbody>
<tr>
<td>BERN</td>
<td>0.89</td>
<td>1.04</td>
<td>0.81</td>
<td>2.05</td>
<td>N.A.</td>
</tr>
<tr>
<td>ECCO</td>
<td>0.96</td>
<td>0.89</td>
<td>0.91</td>
<td>2.01</td>
<td>N.A.</td>
</tr>
<tr>
<td>MIT</td>
<td>0.91</td>
<td>1.00</td>
<td>0.85</td>
<td>2.22</td>
<td>N.A.</td>
</tr>
<tr>
<td>NCAR</td>
<td>0.95</td>
<td>0.98</td>
<td>0.91</td>
<td>2.18</td>
<td>2.36</td>
</tr>
<tr>
<td>PRINCE-LL</td>
<td>0.90</td>
<td>1.18</td>
<td>0.80</td>
<td>1.85</td>
<td>1.90</td>
</tr>
<tr>
<td>PRINCE-HH</td>
<td>0.93</td>
<td>1.05</td>
<td>0.87</td>
<td>2.33</td>
<td>2.43</td>
</tr>
<tr>
<td>PRINCE-LHS</td>
<td>0.93</td>
<td>1.04</td>
<td>0.86</td>
<td>1.99</td>
<td>2.04</td>
</tr>
<tr>
<td>PRINCE-2</td>
<td>0.93</td>
<td>1.03</td>
<td>0.87</td>
<td>2.17</td>
<td>2.24</td>
</tr>
<tr>
<td>PRINCE-2a</td>
<td>0.91</td>
<td>1.05</td>
<td>0.85</td>
<td>2.25</td>
<td>2.35</td>
</tr>
<tr>
<td>UL</td>
<td>0.87</td>
<td>1.00</td>
<td>0.77</td>
<td>2.81</td>
<td>2.95</td>
</tr>
<tr>
<td>Mean</td>
<td>0.92</td>
<td>1.02</td>
<td>0.85</td>
<td>2.18</td>
<td>2.32</td>
</tr>
</tbody>
</table>

a Also tabulated are forward and inverse estimates of the global total anthropogenic CO₂ uptake (Pg C yr⁻¹, scaled to 1995). Forward results are from OCMIP-2 [Dutay et al., 2002; Watson and Orr, 2003].
b Normalized Std. Dev. is defined as the standard deviation of the modeled field divided by the corresponding standard deviation of the observed field.
c Following Taylor [2001].

Tracer Green’s Functions from old 2-deg ECCO solution was among solutions with highest correlation, lowest standard error, and highest model skill relative to CFC-11 observations!
References

George Green

Atmospheric tracer inversions

Ocean circulation estimates

Ocean carbon inversions

Joint ocean-atmosphere carbon dioxide inversions
Comparison with representer method

The representer method (see Andrew Bennett’s books and publications) was developed for data-sparse inverse modeling problems.

Both the Green’s Functions and representer approaches provide a reduced orthogonal basis sets for inversions. The two methods are mirror images of each other.

The representer method should be used when the number of available observations is small. The optimized solution is projected on the “observable” parameter space.

The Green’s Functions approach should be used when the number of control parameters is small. The optimized solution is projected on the “controllable” parameter space.
Comparison with adjoint method

The Green’s function approach has been called a poor-man’s adjoint.

Advantages relative to the adjoint method are simplicity of implementation, the possibility of offline experimentation with different cost functions, improved robustness in the presence of nonlinearities, and complete a posteriori error statistics for the parameters being estimated.

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.
Summary and concluding remarks

Green’s functions provide a simple yet effective method to test and to calibrate general circulation model 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.

They can be applied to pretty much any general circulation model since all that is required is forward-model sensitivity experiments.

They are a better way to adjust uncertain model parameterizations than ad-hoc or one-at-a time parameter adjustments.

In the absence of adjoint model, or for strongly nonlinear systems, they can be used for preliminary model adjustments.
Model Green’s Functions cheat sheet

Least squares method based on computation of model Green’s functions.

Used for, e.g., atmospheric tracer inversions (Enting and Mansbridge, 1989; Tans et al., 1990; Bousquet et al., 2000), ocean circulation estimates (Stammer and Wunsch, 1996; Menemenlis et al., 1997a, b; ATOC 1998, 2005; Nguyen et al., 2011), ocean carbon inversions (Gloor et al., 2003; Mikaloff Fletcher et al., 2006; 2007; Gruber et al., 2009; Brix et al., 2015), and joint ocean-atmosphere carbon dioxide inversions (Jacobson et al., 2007a; 2007b).

GCM: \[ x(t_{i+1}) = M(x(t_i), \eta) \]
x(t_i) is the ocean model state vector at time \( t_i \)
\( M \) represents the numerical model
\( \eta \) is a set of control parameters.

Data: \[ y = H(x) + \varepsilon = G(\eta) + \varepsilon \]
y is the available observations
\( H \) is the measurement model
\( G \) is a function of \( M \) and \( H \)
\( \varepsilon \) is additive noise

Cost function: \[ J = \varepsilon^T R^{-1} \varepsilon \]
\( J \) is quadratic cost function
\( R \) is estimate of covariance matrix of \( \varepsilon \)

Linearization: \[ G(\eta) \approx G(0) + G\eta \]
\( G \) is a kernel matrix whose columns are computed using a GCM sensitivity experiment for each parameter in vector \( \eta \).
\( G(0) \) is from baseline GCM integration.

Solution: \[ x_a = x_b + (G^T R^{-1} G)^{-1} R^{-1} (y - G(0)) \]
\( x_a \) is optimized solution that minimizes cost function \( J \).
\( x_b \) is the solution of the baseline simulation.