

Application of the MITgcm Modeling Framework for Global Ocean State Estimation in ECCO

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Outline

- The ocean state estimation framework
 - The optimization / optimal control problem
 - The MIT general circulation model (MITgcm) and its adjoint
 - Observations, uncertainties, control variables
 - Examples of some residual misfits
- Some example results
 - Decadal variations in North Atlantic heat and volume transport
 - Decadal variations in global sea-level patterns
- Future directions
 - Coupled ocean/sea-ice estimation
 - A truly global grid including the Arctic
 - Moving toward higher resolution
- OpenAD: a new tool for automatic differentiation
 - MITgcm sensitivity application
- Outlook
 - Long-term goals
 - Problems and challenges





Ocean State Estimation





Least-squares optimization / optimal control problem

Given:

- a set of (possibly different types of) observations
- a numerical model & set of initial/boundary conditions, parameters
- Question: (estimation / optimal control problem) Find "optimal" model trajectory consistent with available observations

Approach: seek minimum of least square cost function

$$\min_{\vec{u}} \left\{ \mathcal{J}(\vec{u}) \right\} = \min_{\vec{u}} \left\{ \sum_{i} \left[\mathsf{model}_{i}(\vec{u}) - \mathsf{data}_{i} \right]^{2} \right\}$$

 \longrightarrow seek $\nabla_u \mathcal{J}(\vec{u})$ to infer update $\Delta \vec{u}$ from variation of controls \vec{u}

$$\vec{u}^{n+1} = \vec{u}^n + \Delta \vec{u}$$

- Results: see ECCO (Stammer et al., 2002/03)
 - optimal/consistent ocean state estimate
 - adjusted initial/boundary value estimates









Some algebra

		vv.i.t	. control variab		_ шс
${\mathcal J}$:	$ec{u}$	⊨→	$\vec{v} = \mathcal{M}(\vec{u})$	⊢→	$\mathcal{J}(\mathcal{M}(ec{u}))$
TLM :	\deltaec{u}	↦	$\delta \vec{v} = M \cdot \delta \vec{u}$	⊨	$\delta \mathcal{J} = ec abla_u \mathcal{J} \cdot \delta ec u$
ADM :	$\delta^* \vec{u} = \vec{\nabla}_u \mathcal{J}^T$	\leftarrow	$\delta^*ec v$	$\leftarrow\!$	$\delta \mathcal{J}$

Need $\vec{\nabla}_{u} \mathcal{T}_{u_0}$ of $\mathcal{T}(\vec{u}_0) \in \mathbb{R}^1$ w.r.t. control variable $\vec{u} \in \mathbb{R}^m$

- $\vec{v} = \mathcal{M}(\vec{u})$ nonlinear model
- M, M^T tangent linear (TLM) / adjoint (ADM)
- $\delta \vec{u}$, $\delta^* \vec{u}$ perturbation / dual (or sensitivity)

$$\vec{\nabla}_u \mathcal{J}^T |_{\vec{u}} = M^T |_{\vec{v}} \cdot \vec{\nabla_v} \mathcal{J} |_{\vec{v}}$$

 $TLM: m(\sim n_x n_y n_z)$ integrations @ $1 \cdot$ (#forward) ADM: 1 integration @ $\gamma \cdot$ (#forward)





Automatic Differentiation (AD)

Model code

Adjoint code

 $\vec{v} = \mathcal{M}_{\Lambda} \left(\mathcal{M}_{\Lambda-1} \left(\dots \left(\mathcal{M}_{0} \left(\vec{u} \right) \right) \right) \right) \quad \delta^{*} \vec{u} = M_{0}^{T} \cdot M_{1}^{T} \cdot \dots \cdot M_{\Lambda}^{T} \cdot \delta^{*} \vec{v}$

Automatic differentiation:

each line of code is elementary operator \mathcal{M}_{λ}

- \rightarrow rules for differentiating elementary operations
- \longrightarrow yield elementary Jacobians M_{λ}
- \longrightarrow composition of M_{λ} 's according to chain rule

yield full tangent linear / adjoint model

TAMC / TAF source-to-source tool (Giering & Kaminski, 1998)

• model \mathcal{M} • independent \vec{u} • dependent \mathcal{J} $\left\{\begin{array}{l} \mathsf{TAMC}/\mathsf{TAF} \\ \mathsf{ADM} \ M^{T}, \text{ or} \\ \mathsf{gradient} \ \delta^{*}\vec{u} = \vec{\nabla}_{u}\mathcal{J} \end{array}\right.$





TAF: Transformation of Algorithms in Fortran http://www.fastopt.de

- Commercial successor of TAMC
- Source-to-source tool for F77/F90/F95 code
- Produces readable derivative code
- Recompute all by default + Efficient Recomputation Algorithm (ERA)
- Flow directives enable
 - insertion of taping or checkpointing directives to disk or memory
 - ignore passive routines
 - active I/O handling
 - self-adjointness
 - application of implicit function theorem for iterative loops
 - handle hand-written derivative code
 - adjoint checkpointing ("Divided Adjoint" DIVA)

Has been applied to various large-scale geophysical (Earth system) and high-performance CFD codes

Giering & Kaminski: Recipes of adjoint code construction. ACM Trans. Math. Software (TOMS), 1998.





Storing vs. recomputation: the critical feature of checkpointing for time-stepping algorithms (I)

Example of a simple time-stepping box model

- DO t = 1, nTimeSteps
 - · calculate density

$$\rho = -\alpha T + \beta S$$

• calculate thermohaline transport

$$U = U(\rho(T, S))$$

• calculate tracer advection

$$\frac{d}{dt}Tr = f(Tr, U)$$

calculate timestepping and update tracer fields $Tr = \{T, S\}$





END DO



Storing vs. recomputation: the critical feature of checkpointing for time-stepping algorithms (II)

$$\frac{dT_3}{dt} = U(T_3 - T_2), \text{ for } U \ge 0$$

diffT3 = u * (T3 - T2)

derivative $\delta \texttt{diffT3}$:

$$\delta \texttt{diffT3} \,=\, \frac{\partial \texttt{diffT3}}{\partial \texttt{U}} \delta \texttt{U} \,+\, \frac{\partial \texttt{diffT3}}{\partial \texttt{T}_2} \delta \texttt{T}_2 \,+\, \frac{\partial \texttt{diffT3}}{\partial \texttt{T}_3} \delta \texttt{T}_3$$

in matrix form:

$$\begin{pmatrix} \delta \text{diffT3} \\ \delta \text{T}_3 \\ \delta \text{T}_2 \\ \delta \text{U} \end{pmatrix}^{\lambda} = \begin{pmatrix} 0 & -\text{U} & \text{U} & \text{T3} - \text{T1} \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} \delta \text{diffT3} \\ \delta \text{T}_3 \\ \delta \text{T}_2 \\ \delta \text{U} \end{pmatrix}^{\lambda-1}$$





Storing vs. recomputation: the critical feature of checkpointing for time-stepping algorithms (III)

Transposed relationship yields:

$$\begin{pmatrix} \delta^* \text{diffT3} \\ \delta^* \text{T}_3 \\ \delta^* \text{T}_2 \\ \delta^* \text{U} \end{pmatrix}^{\lambda-1} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ -\text{U} & 1 & 0 & 0 \\ \text{U} & 0 & 1 & 0 \\ \text{T3} - \text{T1} & 0 & 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} \delta^* \text{diffT3} \\ \delta^* \text{T}_3 \\ \delta^* \text{T}_2 \\ \delta^* \text{U} \end{pmatrix}^{\lambda}$$

and thus adjoint code:

adT3	=	adT3		-	۱	u*;	add	lif	ET3
adT2	=	adT2		+	1	u*	add	lif	ET3
adU	=	adu	+	(ТЗ-Т2	2)*	add	lif:	ET3
addiffT3	=	0							

Note: state T2, T3, U are required to evaluate derivative at each time step, in reverse order!





Storing vs. recomputation: the critical feature of checkpointing for time-stepping algorithms (IV)

- Adjoint = transpose of TLM
- \rightarrow evaluated in reverse order
- → model state at every time step required in reverse
- \rightarrow all state stored or recomputed

Solution: Checkpointing

(e.g. Griewank, 1992, Restrepo et al., 1998) balances storing vs. recomputation







Adjoint parallel and I/O primitives

- domain decomposition (tiles) & overlaps (halos)
- split into extensive on-processor and global phase



Global communication/arithmetic op.'s supported by MITgcm's intermediate layer (WRAPPER) which need hand-written adjoint forms

	operation/primitive	forward		reverse
•	communication (MPI,):	send	\longleftrightarrow	receive
•	arithmetic (global sum,):	gather	\longleftrightarrow	scatter
•	active parallel I/O:	read	\longleftrightarrow	write





New controls, parameter activity, and *incremental* improvement of an AD-generated adjoint model

Total depth in partial cell formulation

$$H(i,j) = \sum_{k} \frac{h_c(i,j,k)}{\Delta r_f(k)}$$

- $\Delta_r(k)$: full cell thickness of layer k
- $h_c(i, j, k)$: fractional cell thickness

$$h_c(i, j, k) \begin{cases} = 1 & \text{for } k < k_{low} \\ = \frac{h_{low}(i, j)}{6} \in (0, 1] & \text{for } k = k_{low} \\ = 0 & \text{for } k > k_{low} \end{cases}$$

► Variation of *H*

$$\delta H(i,j) = \sum_{k} \frac{\delta h_c(i,j,k)}{\Delta r_f(k)} \Delta r_f(k) = \frac{\delta h_{low}(i,j)}{\Delta r_f(k_{low})}$$

> Zonal volume transport U through cell face A_x

$$U = uA_x = u\Delta x \,\Delta r_f \, \boldsymbol{h_w}$$

 \blacktriangleright δU is quadratic for active A_x : product rule

$$\delta U = \delta u A_x + u \delta A_x = \Delta x \Delta r_f \left(\delta u \mathbf{h}_w + u \delta \mathbf{h}_w \right)$$



The MIT general circulation model (MITgcm)

Parallel implementation of a general-purpose grid-point algorithm for a Boussinesq or non-Boussinesq fluid, hydrostatic or non-hydrostatic, in curvilinear coordinates.



- z-level or pressure vertical coordinates (ocean atmosphere isomorphism)
- nonlinear free surface and z^{*} vertical coordinates
- finite-volume formulation with partial cells
- various parameterization schemes (GM/Redi, KPP, Leith, Smagorinsky)
- thermodynamic/dynamic sea-ice model (Hibler-type)
- ocean biogeochemical model
- cubed-sphere global grid topology





The ECCO-GODAE setup

- 1 degree horiz. Resolution, covering 80N to 80S
- 23 vertical levels
- GM/Redi eddy parameterization, KPP vertical mixing scheme
- covers 1992 to 2004 (nov through 2006)
- forcing: 6-hourly NCEP air-sea fluxes



run_xp/grid,ields.Depth.data.000000000.1x1.lev1 min/avg/max=35 / 3.36e+03 / 5.7e+03



Control variables

- 3-dim. initial conditions
 - temperature, salinity
- 2-dim. time-varying surface forcings:
 - Version 2:
 - heat flux, freshwater flux,
 - zonal/meridional windstress
 - Version 3:
 - surface air temperature, specific humidity, precipitation,
 - downwelling shortwave radiation,
 - zonal/meridional wind speed
- 3-dim. internal model parameters (experimental)
 - mixing coefficients (Stammer, 2005)
 - eddy stress parameterization (Ferreira et al., 2005)
 - bottom topography (Losch and Heimbach, 2007)





A large-scale optimal control problem

ECCO-GODAE state estimation: problem size (version 2)

Dimensionality:

• grid @ $1^{\circ} \times 1^{\circ}$ resolution: $n_x \cdot n_y \cdot n_z = 360 \cdot 160 \cdot 23$	1,324,800
 model state: 17 3D + 2 2D fields 	$\sim 2 \cdot 10^7$
 timesteps: 15 years @ 1-hour time step 	131,400
 control vector initial temperature (T), salinity (S) 	$\sim 1.5 \cdot 10^8$
 time-dependent surface forcing (every 2 days) cost function: observational elements: 	$\sim 2.5 \cdot 10^8$
Computational size (per iteration):	
 – 96 processors @ 2GB per proc. (SGI Altix) 	

- I/O: 20 GB input, 35GB output
- time: 28 hours per iteration @ 96 processors
- What we would ideally want:
 - $1/16^{\circ} \times 1/16^{\circ}$ resol., 1000 years, full model error covariance ...





Misfits: summary of cost function reduction iteration 193 vs. 177 (G. Forget)







Misfits: Mean Dynamic Topography (MDT) from satellite gravity

RMS difference: GRACE-based MDT by CLS (Rio, 1995) vs. various OSE products *Vossepoel, JGR (2007)*





Misfits: Sea Level Anomaly (SLA) from satellite altimetry





tpccst.30dayav_timemean: mn:0,mx:8.3e+00,av:3.6e-01,sd:2.7e-01





Misfits: in-situ XBT costs for v2.193





Southern Elephant Seals as Oceanographic Samples (SEaOS)

CTD-type observations from seals in SO

Sea Mammal Research Unit, University St. Andrews, UK, British Antarctic Survey (M. Meredith)







2006/11/8 11:44:13 ps: SEAOS_iter3.05_T_wfedav_cost_vertsummean_1dep__10.psc, data: /sea/raid0/diana/seaos/T_wfedav_cost_vertsummean

Application: Decadal variations in Atlantic poleward heat and mass transports (I)

Vol 438|1 December 2005|doi:10.1038/nature04385

nature

TERS

Slowing of the Atlantic meridional overturning circulation at 25° N

Harry L. Bryden¹, Hannah R. Longworth¹ & Stuart A. Cunningham¹

Table 1 | Meridional transport in depth classes across 25° N

	1957	1981	1992	1998	2004
Shallower than 1,000 m depth					
Gulf Stream and Ekman	+35.6	+35.6	+35.6	+37.6	+37.6
Mid-ocean geostrophic	-12.7	-16.9	-16.2	-21.5	-22.8
Total shallower than 1,000 m	+22.9	+18.7	+19.4	+16.1	+14.8
1,000-3,000 m	-10.5	-9.0	-10.2	-12.2	-10.4
3,000-5,000 m	-14.8	-11.8	-10.4	-6.1	-6.9
Deeper than 5,000 m	+2.4	+2.1	+1.2	+2.2	+2.5

Values of meridional transport are given in Sverdrups. Positive transports are northward.









Application: Decadal variations in Atlantic poleward heat and mass transports (II)

- Historical hydrographic section A5 at 26°N the North Atlantic
 - Bryden et al 2005 (Nature): "Slowing of the Atlantic overturning circulation"
 - UK RAPID program to measure elements of MOC via moorings
- The ECCO-GODAE data-constrained estimate for 1993-2004





Application: Decadal variations in Atlantic poleward heat and mass transports (III)

Transports & Trends:



- ECCO-GODAE estimate yields no significant trend in heat transport, and only marginally significant trend in volume transport;
- serious sampling/aliasing issues expected in the Bryden et al. estimate;
- results remain fragile in view of remaining uncertainties





ECCO-GODAE solution version 2, iteration 216 (v2.216)

• Science goal:

investigate patterns of decadal sea-level variability and its partition into steric and mass-change contributions

• What is needed:

- accurate heat and freshwater forcing
- accurate treatment of surface boundary condition
- numerical accuracy, ensuring tracer conservation
- closed property budgets
- uncertainty estimates in altimetric data
- → Accuracy required to match 2-3 mm/y (sub-)global mean sea-level rise as inferred from altimetry





Application: decadal sea-level patterns (II)

• Need to remove air-sea flux imbalances

	mean	intercept	$_{\rm slope}$
	[cm/year]	$[\mathrm{mm/sec}]$	$[\mathrm{mm/sec}^2]$
NCEP/NCAR-I ocean $E-P$	15.1	4.90E-9	9.29E-12
NCEP/NCAR-I ocean $E - P - R$	6.2	1.92E-9	9.29E-12
ECCO-GODAE ocean $E - P - R$	3.9	1.35E-9	-14.99E-12
NCEP/NCAR-I global $E - P$	6.1	$\sim 1.90 ext{E-9}$	5.14E-12
NCEP/DOE-II global $E-P$	-73.9	\sim -19.00 E-9	-740.00E-12







Application: decadal sea-level patterns (III)

- Approach to remove air-sea flux imbalances:
 - Impose additional constraint in cost function for overall balance in
 - Evaporation Precipitation Runoff
 - Net heat flux penalized at "observed" 1 W/m²
 - Adjusted (ECCO) fluxes are balanced as result of adjoint-based optimization within residual errors
 - Misfit in time-varying SSH anomalies are successfully reduced to levels of v2.199 (status quo ante)
 - Balance is achieved over full 1993 to 2004 period (alternative per-year balancing is conceivable).





Application: decadal sea-level patterns (IV)

- Vertical partition in density trends due to
 - trends in temperature T
 - trends in salinity S
 - trends in T, S





Wunsch et al., 2007: Decadal trends in sea level patterns. (submitted to J. Clim.)





ECCO-GODAE v3.27 (experimental) atmos. boundary layer & sea-ice model

Sea-ice concentration: daily model vs. NSIDC

(National Snow and Ice Data Center)

Iteration 0

Iteration 27





ECCO-GODAE v3.27 (experimental)

Atmospheric state adjustment (controls)

surface air temperature



precipitation



-1.5 -1 -0.5 0 0.5 1 1.5

specific humidity



zonal wind speed



4 -3 -2 -1 0 1 2 3 4



Version 4: SPGrid - a truly global grid (related to cubed-sphere grid)

L(at) L(on) P(olar) C(ap) specifics: (Hill et al., MWR 2007, submitted)

- Topologically equivalent to cubed-sphere
- Nominally 1° (i.e. zonal spacing)
- Lat/Lon between 81°S and 65°N
- Telescopic from 0.25° to 0.8° between 25°N/S
- Isotropic to 81°S
- 90 x 90 polar cap North of ~65°N











Version 4: matching the adjoint to the cubed-sphere topology





Toward high-resolution state estimation (I)

ECCO2: High-Resolution Global-Ocean and Sea-Ice Data Synthesis @ NASA/Ames

MIT

Marshall, Campin, Heimbach, Hill, Mazloff, Wunsch

JPL

Fu, Kwok, Lee, Menemenlis, Zlotnicki **GSFC** Rienecker, Suarez **ARC** Henze, Taft **HARVARD** Tziperman, Zanna **GFDL** Adcroft **ARGONNE** Hovland, Utke





Toward high-resolution state estimation (II)

Eddy permitting state estimation in the Southern Ocean

M. Mazloff (Ph.D. thesis)

- 78⁰ South to 24.7⁰ South
- 1/6⁰ Horizontal resolution;
- 42 depth levels (partial cells)
- similar setup to ECCO-GODAE
- atmospheric boundary layer scheme
- adjoint generated via AD tool TAF
- sea-ice model
- KPP, GM/Redi parameterizations
- currently optimizing year 2005
- 600 processor adjoint on SDSC's DataStar (IBM SP4) supercomputer





Toward high-resolution state estimation (III)

Eddy permitting state estimation in the Southern Ocean (cont'd)





OpenAD: a new open-source automatic differentiation tool http://www.mcs.anl.gov/OpenAD

@ ANL: J. Utke, B. Norris, M. Strout, P. Hovland
@ Rice: N. Tallent, G. Mellor-Crummy, M. Fagan
@ MIT: P. Heimbach, C. Hill, D. Ozyurt, C. Wunsch
@ RWTH: U. Naumann





Tool design emphases:

- modularity
- flexibility
- use of open-source components
- new algorithmic approaches
 - XML-based languageindependent transformation
 - basic block preaccumulation
 - other optimal elimination methods
 - control flow & call graph reversal
 - taping & hierarchical checkpointing





OpenAD: a new open-source automatic differentiation tool http://www.mcs.anl.gov/OpenAD



Utke et al., 2007: submitted to ACM Transactions on Math. Software (TOMS).

Open64:

(code parsing)

- lexical/syntactic/semantic analysis
- canonicalizer
- intermediate representation

OpenAnalysis:

(static code analysis)

- build call / control flow graphs
- code analysis, activity, side-effects

whirl2xaif / xaif2whirl:

(representing the numerical core)

 representation in languageindependent XAIF format

xaifBooster:

(transforming the numerical core)

apply differentiation algorithms



Atlantic meridional heat transport: 5 year sensitivities at 4° resolution (OpenAD)



First *MITgcm* application using *OpenAD*, and with implemented checkpointing at the time-stepping level.

Extend adjoint integration of heat flux sensitivities backward in time (here at coarser resolution).

Confirms role of propagating waves (Rossby waves, Kelvin waves) over these time scales in fast signal propagation over long distances.



Atlantic meridional heat transport: 10 year sensitivities at 4° resolution (OpenAD)











Outlook (I)

- Observations and uncertainties
 - new types (e.g. acoustic tomography, time-varying GRACE)
 - determining scales, errors, and covariances
 - sparsity of observations
 - satellites: maintaining long-term climate-relevant missions
 (similar to weather satellites, but look at 20- to 50-year horizon)
- Model and adjoint
 - high-resolution adjoint and exponential sensitivity growth (linked to Lyapunov exponent, predictability horizon, ...)
 - representation error due to model vs. obs. scales mismatch
 - model error, and model error covariances
 - long-term state estimation (100 to 1000 year time scales)
 - coupled atmosphere-ocean problem (fast vs. slow timescales)
 - scientific interpretations of remaining misfits (inconsistencies)





Outlook (II)

- Optimization
 - is a gradient-descent method the best method?
 - are there other/better methods out there for large-scale optimization that we should know?
- Sustaining the effort
 - transfer from science to operational community
 - sustained (and increasing) compute power required
 - Who takes on the challenge of maintaining climate-relevant observational record (in particular satellite)?

state estimation remains essential:

Ability to synthesize, in an optimal manner, all available observations and best known physics/dynamics (a model) to derive a full state of the ocean that is consistent with known physics and observations, and yields closed budgets to enable analysis of the nature and causes of variability and change.





An early vision, ca. 1982:

Acoustic Tomography and Other Answers



Forecasting?

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."
C. Garrett and C. Wunsch, Eds., <u>SIO Reference Series 84-5</u>, March 1984

