CO$_2$ Uptake of the Ocean - Parameter Optimization in Biogeochemical Models

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Outline

• Why study CO2 uptake?

• How is it working?

• What are the models?

• Computing a steady seasonal cycle

• Full Jacobian Approach for optimization

• Brief look inside a biogeochemical model

• What is Future Ocean?
Why study CO\(_2\) uptake?

- ... in the atmosphere: 800 Giga (10\(^9\)) tons
  pre-industrial: 600 Gigatons

- ... in the oceans: 40'000 Gigatons (atmosphere:ocean 1:50)

- ... exchange atmosphere-ocean: 90 Gigatons/year

- today: 6 Gigatons emissions/year,
  2 Gigatons are dissolved in the oceans
  ocean decreases global warming, but: acidification

- questions: future CO\(_2\) uptake?
  how much remains in the ocean?
  feedback effects: changes due to global warming?
  sequestration opportunities, techniques, safety?
  fertilization to increase uptake?
"Who" is taking up CO$_2$?

- "biological pump":
  - photosynthesis of phytoplankton
  - phytoplankton as nutrient of zooplankton
  - dead organic material sinking to the bottom, little mixing of surface and bottom layers

- "carbon pump":
  - sinking of calcium carbonate (inorganic)
  - All that happens in the ocean circulation
Coupled Ocean Biogeochemistry

First concept:
- Use computed circulation

Second concept:
- Full interaction

Bild: Nerd GNU FDL
Differences

Ocean circulation

- Equations are standard
- Some parts are focus of current research (e.g. diffusion)
- Time-dependent, 3-D, nonlinear
- Small scales: resolving turbulence would need about $10^{28}$ points
- Thousands years needed to reach steady seasonal cycle
- Thus: Simplifications, modeling, model parameters
Ocean Circulation

- Ocean model (Navier-Stokes + tracer equations, hydrostatic + Boussinesq approximations)

\[
\begin{align*}
\vec{v}_t - \text{div}(\nu \nabla \vec{v}) + \vec{v} \cdot \nabla \vec{v} + \nabla p &= -2\tilde{\Omega} \times \vec{v} - \rho \vec{g} \\
\text{div} \vec{v} &= 0 \\
S_t - \text{div}(\nu \nabla S) + \vec{v} \cdot \nabla S &= 0 \\
T_t - \text{div}(\nu \nabla T) + \vec{v} \cdot \nabla T &= 0 \\
\rho &= \rho(T, S)
\end{align*}
\]

- numerical solution available (MITgcm, MOM, OPA ...)

- takes some 1000s years model time to become "steady", i.e. no change from year to year, i.e. periodic
Differences

- Transport equations, nonlinear coupling, easier compared to ocean model

- Not clear how many tracers to include

  - NPZD model: nutrients, phytoplankton, zooplankton, detritus

  - more tracers -> more equations -> more parameters -> but more information?

- Modeling is current research topic
... and Biogeochemistry

- Linear transport/advection-diffusion equations with nonlinear coupling/forcing:
  \[
  \frac{\partial c_i}{\partial t} = \text{div}(\kappa \nabla c_i) - \text{div}(\bar{v} c_i) + q_i(c_1, \ldots, c_N, T, S, p)
  \]
  - diffusion
  - advection
  - tracer coupling

- for tracers, e.g. nutrients, phyto-, zooplankton, detritus

- Different numbers of tracers, equations, many parameters

- "more tracers -> better results" is not naturally true

- local (in gridpoints, except for sinking) biochemical processes in source terms \( q \)

- given "steady" circulation: separated tracer computation into a "steady" state, starting from uniform distribution, again 1000s of years model time
The seasonal cycle

- Using pre-computed velocity, temperature, salinity the biogeochemical equations

\[
\frac{\partial c_i}{\partial t} = \text{div}(\kappa \nabla c_i) - \text{div}(\vec{v}c_i) + q_i(c_1, \ldots, c_N, T, S, p)
\]

- can be written as

\[
\frac{dc_i}{dt} = A(t)c_i(t) + q(c(t), t)
\]

- where \(A(t)\) can be pre-computed as Transition Matrix [Khatiwala et. al. '04]

- Time discretization gives for the vectors of tracers: \(c^{k+1} = \Phi_k(c^k)\)

- Looking for a periodic solution (steady seasonal cycle):

\[
c^{k+n} = \Phi_{k+n-1} \circ \cdots \circ \Phi_{k+1} \circ \Phi_k(c^k) =: \Phi
\]

- i.e. a fixpoint of \(\Phi\)
Computing the steady seasonal cycle

• Pseudo time-stepping (this is done by now): Compute until for some $k$ ($n$ fixed):

$$ c^{k+n} = \Phi(c^k) = c^k $$

• vs. Newton's method for the fixpoint equation:

$$ \Phi(c) = c \iff \Phi(c) - c = 0 $$

• Requires Jacobian

$$ \left( \frac{\partial \Phi}{\partial c} - I \right) $$

• where the Jacobian of $\Phi$ is mainly given by the matrices $A_k$ and the $q'_k$

• remember:

$$ c^{k+n} = \Phi_{k+n-1} \circ \cdots \circ \Phi_{k+1} \circ \Phi_k(c^k) =: \Phi $$

$$ \frac{dc_i}{dt} = A(t) c_i(t) + q(c(t), t) $$
Inexact Newton & Preconditioning

- The linear system in the Newton steps can be solved inexactly/iteratively (GMRES etc.) and needs only matrix-vector products with $A_k, q'_k$.

- Two nested iterations, only useful if it needs less matrix-vector multiplications than the pseudo time-stepping:
  
  \[ \# \text{Newton} \times \# \text{linear iterations} \leftrightarrow \# \text{pseudo time-steps} \]

- Preconditioning:
  \[
  \left( \frac{\partial \Phi}{\partial c} - I \right)^{-1} \approx - \sum_{k=0}^{K} \left( \frac{\partial \Phi}{\partial c} \right)^k
  \]

- again reduces to multiplication with $A_k$ and $q'_k$.

- Use bigger timesteps for the biogeochemics for the preconditioner.
Computing a derivative for optimization

- Looking for a steady seasonal cycle/fixpoint, depending on parameters $p$:

  $$\Phi(c(p), p) = c(p)$$

- Taking the derivative w.r.t to the parameter vector:

  $$\frac{\partial \Phi}{\partial c} c'(p) + \frac{\partial \Phi}{\partial p} = c'(p) \iff \left( \frac{\partial \Phi}{\partial c} - I \right) c'(p) = -\frac{\partial \Phi}{\partial p}. $$

- Same system matrix as for the computation of the steady seasonal cycle.

- To be tested against classical adjoint technique or oneshot method for pseudo-timestepping (see Adel Hamdi's talk)
Looking inside a biogeochemical model

- Oschlies, Garcon 1999: \(c=(N,P,Z,D,DOM)\)

\[
q(c) = \begin{pmatrix}
0 & 0 & \gamma_2 & \mu_4 & \mu_5 \\
0 & -\mu_2 & 0 & 0 & 0 \\
0 & 0 & -\mu_2 & 0 & 0 \\
0 & (1-\sigma)\mu_2 & 0 & -\mu_4 & 0 \\
0 & \sigma\mu_2 & 0 & 0 & -\mu_5 \\
\end{pmatrix} c
\]

\[
+ \begin{pmatrix}
-J(c_1, c_2)c_1 \\
J(c_1, c_2)c_1 - G(c_2)c_3 \\
\gamma G(c_2)c_3 - \mu c_3^2 \\
(1-\sigma)((1-\gamma_1)G(c_2)c_3 + \mu_3 c_3^2) \\
\sigma((1-\gamma_1)G(c_2)c_3 + \mu_3 c_3^2) \\
\end{pmatrix}
\]

\[
+ \begin{pmatrix}
0 \\
0 \\
0 \\
0 \\
-\omega \frac{\partial c_4}{\partial z} \\
0 \\
\end{pmatrix}
\]

\[
G(c_2) = \frac{g\epsilon c_2^2}{g + \epsilon c_2^2}
\]
Summary

• CO2 uptake is a crucial point in climate research

• One-way coupling between ocean circulation + biogeochemistry allows to precompute circulation

• Newton to obtain steady seasonal cycle, exploiting structure of Jacobian

• Optimization: up to now: GA, finite differences, aim: Full Jacobian approach + Algorithmic Differentiation of biogeochemical part, one-shot approach

• Analysis of model equations w.r.t. existence, uniqueness

• Work in progress ...
Parameteroptimierung, Datenassimilation, Algorithmisches Differenzieren, Ozean + Biogeochemie

Öffentlichkeitsarbeit

Inverse Modellierung Stokes + nicht-Newtonische Fluide

Optimierung/Steuerung bei ökonomischen Modellen (ODEs)
The Christian Albrechts University Kiel invites to the

4. Scientific Computing Seminar

with special emphasis on

Parameter Estimation, Optimization and Inverse Modeling in Geosciences

Workshop Program

Keynote Speakers
The following experts confirmed do give survey talks of 50 minutes:

- Dr. Peter Bayer (ETH Zürich)
- Prof. Roland Becker (Université de Pau et des Pays de l’Adour)
- Prof. Michael Hinze (Uni Hamburg)
- Prof. Rupert Klein (ZIB Berlin und PKI Potsdam)
- Dr. Samar Khatiwala (New York)
- Dr. Michael Vossbeck (FastOpt, Hamburg)
- Prof. Andrea Walther (TU Dresden)

Contributed talks - Call for Papers

We offer the possibility to deliver 30 minutes talks. Please send an abstract within 11 April 2008 via the registration link.

16.-18.06.2008, Kiel

Thank you!!!