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?

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CO_2 ...

- ... in the atmosphere: 800 Giga (10^9) tons
  pre-industrial: 600 Gigatons
- ... in the oceans: 40'000 Gigatons (atmosphere:ocean 1:50)

O=C=O

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

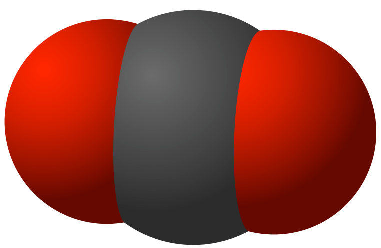


Image: Jacek FH GNU FDL

- 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?

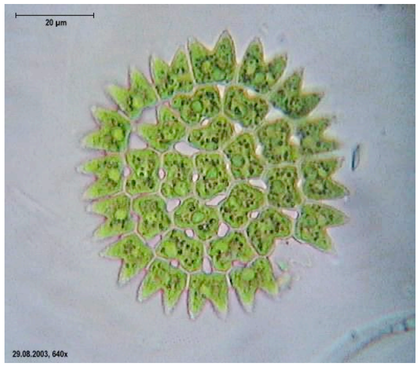
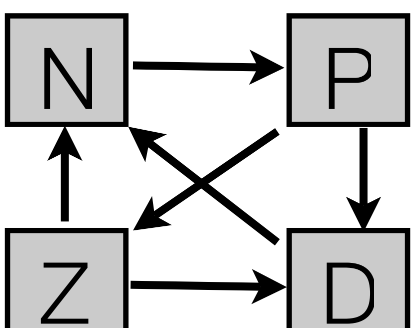


Bild: Dr. Ralf Wagner
GNU FDL

Image: MAR-ECO Øystein Paulsen GNU FDL



- "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

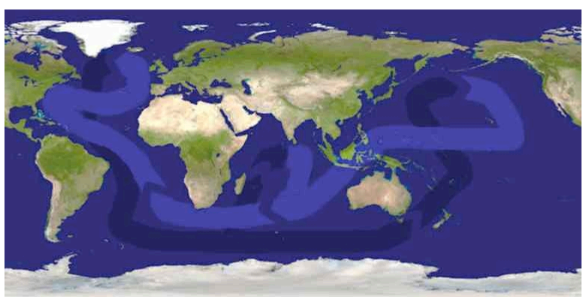
Coupled Ocean Biogeochemistry

First concept:

use
computed
circulation

Ocean
circulation

Biogeo-
chemistry



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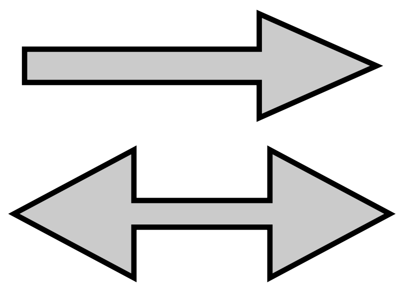
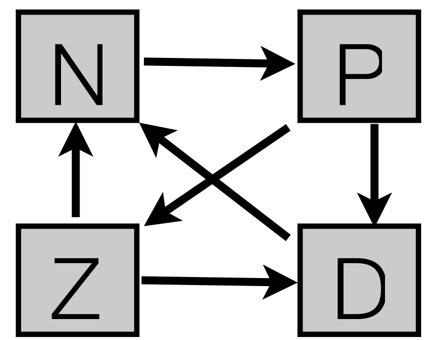


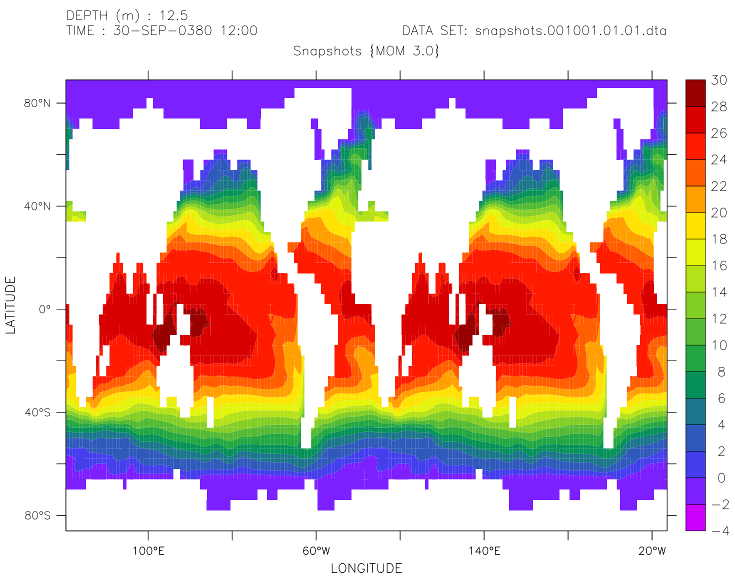


Second concept:

full
interaction

Differences

Ocean circulation



potential temperature (deg C)

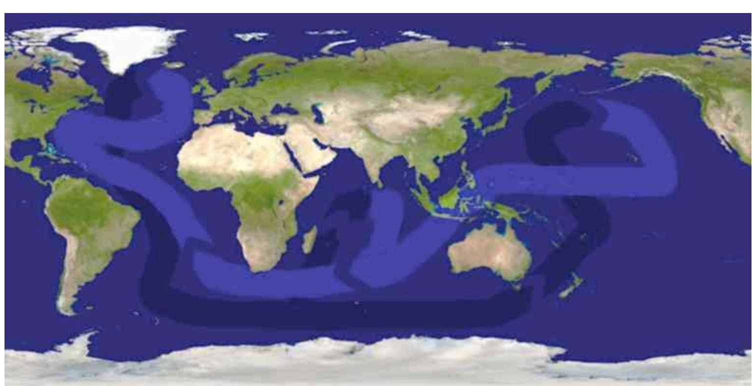


Bild: Nerd GNU FDL

- 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 yeras needed to reach steady seasonal cycle
- Thus: Simplifications, modeling, model parameters

Ocean Circulation

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

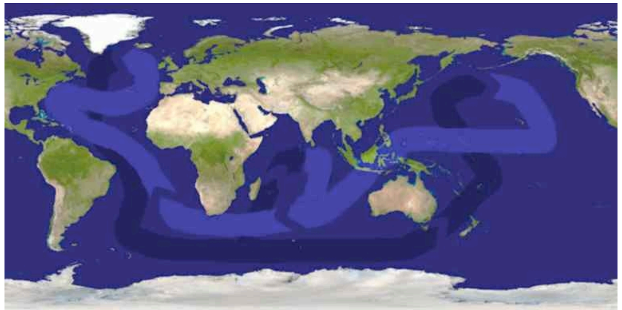


Image: Nerd GNU FDL

$$\begin{aligned} \vec{v}_t - \operatorname{div}(\nu\nabla\vec{v}) + \vec{v}\cdot\nabla\vec{v} + \nabla p &= -2\vec{\Omega}\times\vec{v} - \rho\vec{g} \\ \operatorname{div}\vec{v} &= 0 \\ S_t - \operatorname{div}(\nu\nabla S) + \vec{v}\cdot\nabla S &= 0 \\ T_t - \operatorname{div}(\nu\nabla T) + \vec{v}\cdot\nabla T &= 0 \\ \rho &= \rho(T,S) \end{aligned}$$

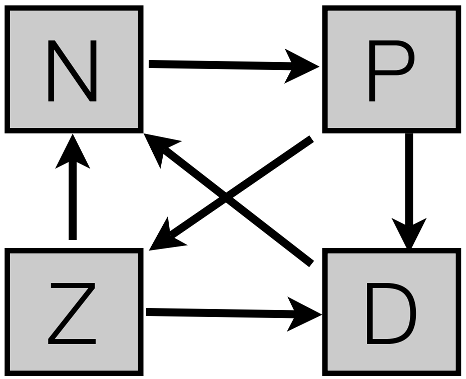
- numerical solution available (MITgcm, MOM, OPA ...)

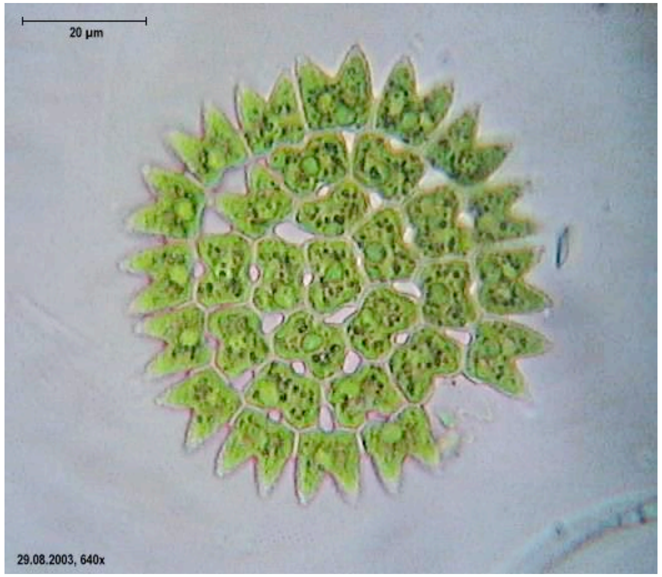
- takes some 1000s years model time to become "steady", i.e. no change from year to year, i.e. periodic

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

Biogeochemistry





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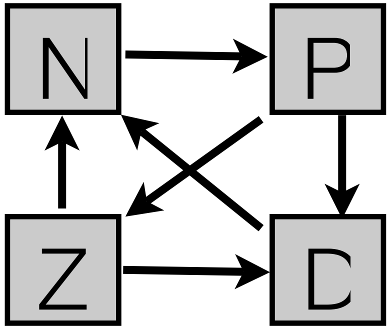
... and Biogeochemistry

- Linear transport/advection-diffusion equations with nonlinear coupling/forcing:

$$\frac{\partial c_i}{\partial t} = \underbrace{\mathrm{div}(\kappa \nabla c_i)}_{\text{diffusion}} - \underbrace{\mathrm{div}(\vec{v} c_i)}_{\text{advection}} + \underbrace{q_i(c_1, \ldots, c_N, T, S, p)}_{\text{tracer coupling}}$$

- 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

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

- 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):

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

- i.e. a fixpoint of Φ

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:

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

- Requires Jacobian $\left(\frac{\partial \Phi}{\partial c} - I\right)$
- where the Jacobian of Φ is mainly given by the matrices A_k and the q'_k
- remember:

$$c^{k+n} = \underbrace{\Phi_{k+n-1} \circ \cdots \circ \Phi_{k+1} \circ \Phi_k}_{=:\Phi}(c^k) \qquad \frac{dc_i}{dt} = A(t)c_i(t) + q(c(t), t)$$

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:
  # Newton * # linear iterations <-> # 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

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- 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:

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

- 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

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

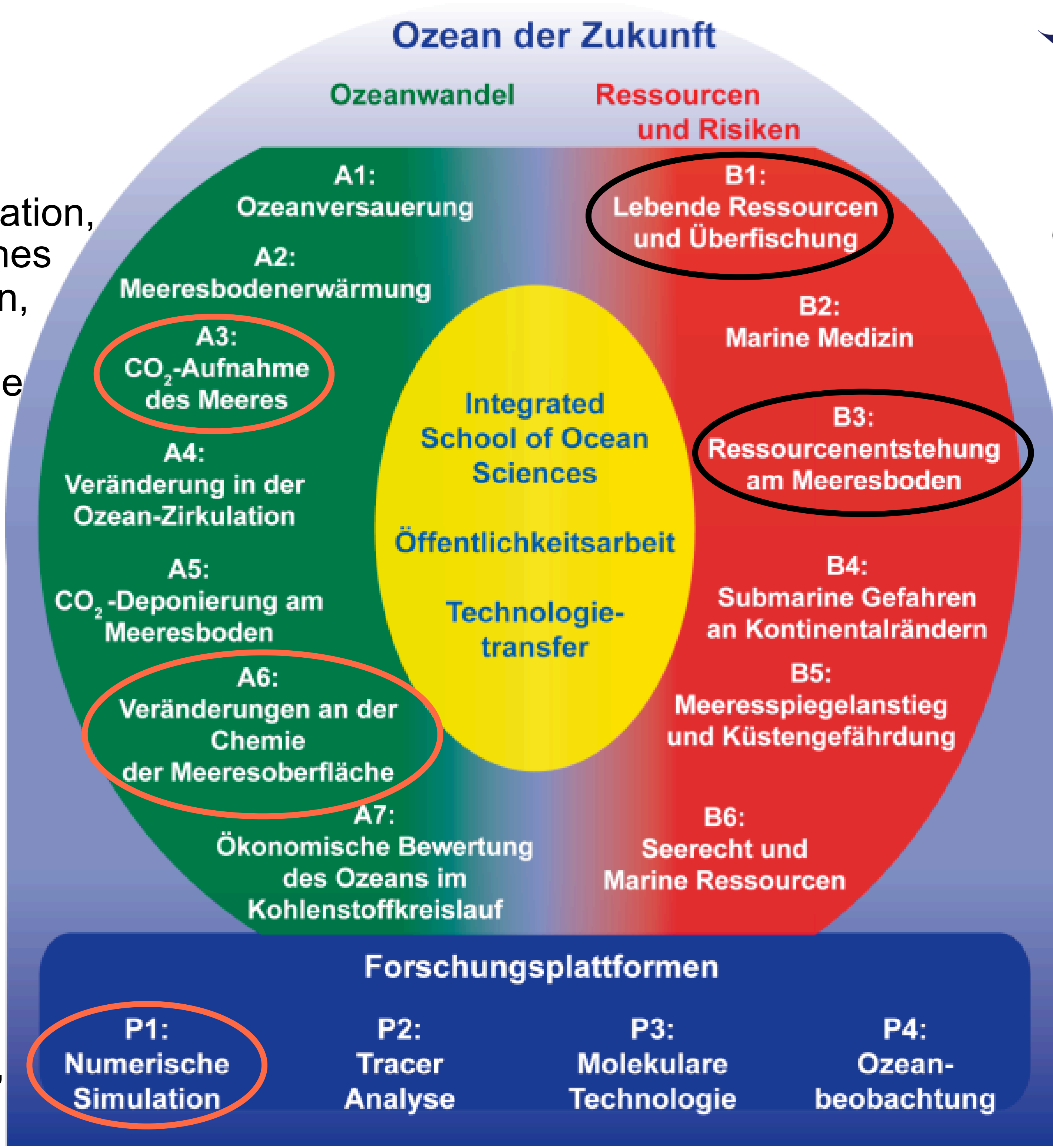
$$
\begin{aligned}
q(c) &= \begin{pmatrix} 0 & 0 & \gamma_2 & \mu_4 & \mu_5 \\ 0 & -\mu_2 & 0 & 0 & 0 \\ 0 & 0 & -\mu_2 & 0 & 0 \\ 0 & (1-\sigma)\mu_2 & 0 & -\mu_4 & 0 \\ 0 & \sigma\mu_2 & 0 & 0 & -\mu_5 \end{pmatrix} c \\
&+ \begin{pmatrix} -J(c_1, c_2)c_1 \\ J(c_1, c_2)c_1 - G(c_2)c_3 \\ \gamma G(c_2)c_3 - \mu c_3^2 \\ (1-\sigma)((1-\gamma_1)G(c_2)c_3 + \mu_3 c_3^2) \\ \sigma((1-\gamma_1)G(c_2)c_3 + \mu_3 c_3^2) \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ 0 \\ -\omega\frac{\partial c_4}{\partial z} \\ 0 \end{pmatrix}
\end{aligned}
$$

$$
G(c_2) = \frac{g\epsilon c_2^2}{g + \epsilon c_2^2}
$$

Summary

- CO_2 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 ...

Parameter-
optimierung,
Datenassimilation,
Algorithmisches
Differenzieren,
Ozean +
Biogeochemie



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Optimierung/
Steuerung bei
ökonomischen
Modellen (ODEs)

Inverse
Modellierung
Stokes +
nicht-
Newtonische
Fluide

Parameter-
identifikation

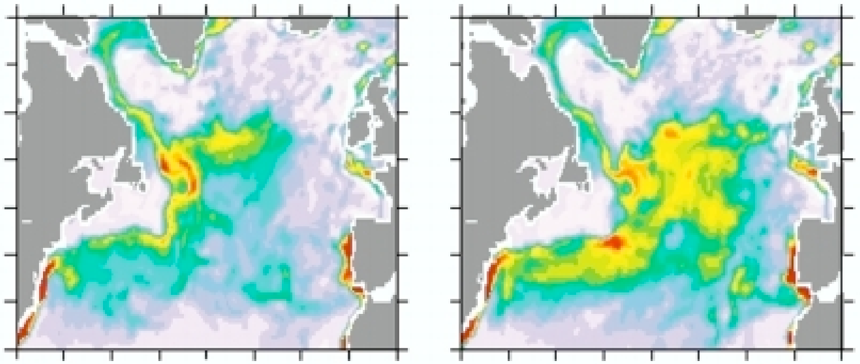
Numerik,
Optimierung,
Kopplung

The Christian Albrechts University Kiel
invites to the

4. Scientific Computing Seminar

with special emphasis on

Parameter Estimation, Optimization and Inverse Modeling in Geosciences



16.-18.06.2008, Kiel

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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.

Thank you!!!