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Computational Geodynamics: Problems, Methods, Results and Perspectives

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INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

Eight Workshop
“Non-Linear Dynamics and Earthquake Prediction”
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COMPUTATIONAL GEODYNAMICS:

PROBLEMS, METHODS, RESULTS & PERSPECTIVES

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Computational Geodynamics

Problems, Methods, Results and Perspectives

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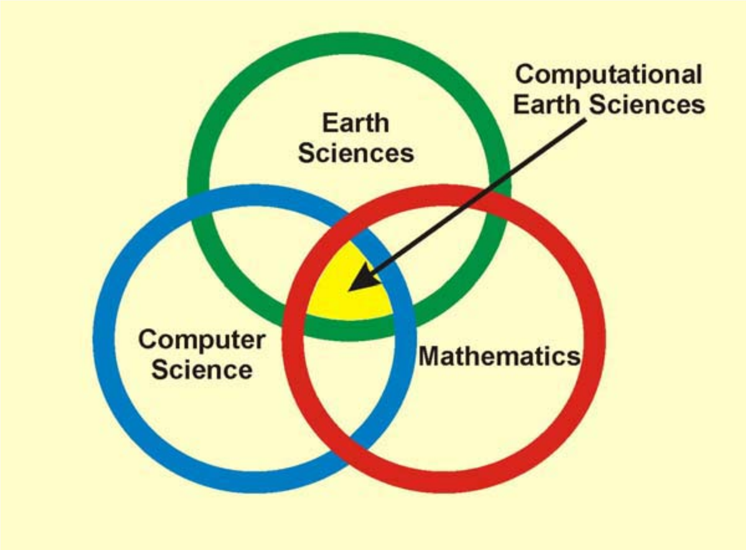
Outline

- ✓ Introduction
- ✓ Computational Geodynamics
  - History
  - Basics of numerical modelling
- ✓ Results
- ✓ Perspectives and Challenges



Computational Earth Sciences are a blending of these three areas to obtain a better understanding of some phenomena through a judicious match between the problem, a computer architecture, and algorithms.

Computational approach to problems of Earth dynamics

is inherently **multi-disciplinary**:
it requires of its practitioners a firm grounding in *applied mathematics* and *computer science* in addition to a command of *one or more disciplines in Earth sciences (geophysics , geology and geomechanics)*.

- **Computer science** provides the tools, ranging from networking and visualization tools to algorithms, that match modern computer architectures.
- **Mathematics** provides means to establish credibility of algorithms, such as error analysis, exact solutions and expansions, uniqueness proofs and theorems.

The characteristics of
Computational Earth Science
problems can be summarized as those:

- having a precise mathematical statement;
- requiring an in-depth knowledge of Earth dynamics;
- being intractable by traditional analytical, analogue or even numerical methods;
- having a significant scope.

HISTORY

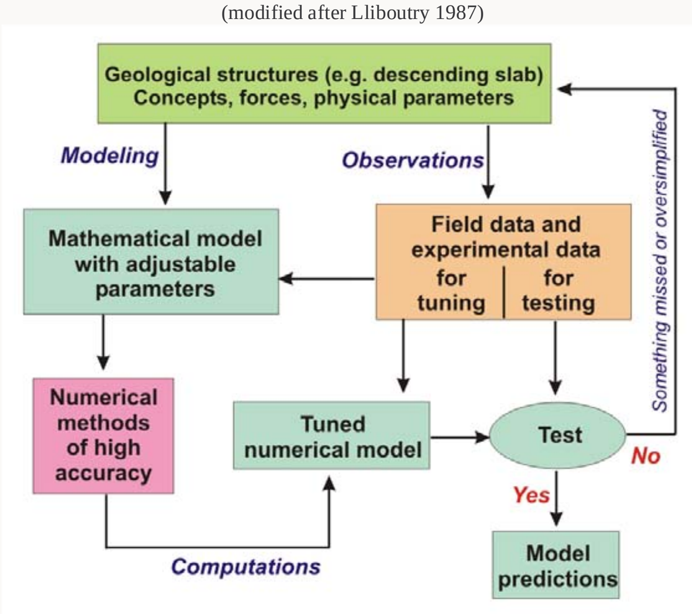
- The field of Fluid Geodynamics was born in the late 1960's with the general acceptance of the plate tectonics paradigm.
- At the beginning, simple analytic models were developed to explain plate tectonics and its associated geological structures. These models were highly successful in accounting for many of the first order behaviors of the Earth.
- The necessity to go beyond these basic models to make them more realistic and better understand the Earth shifted the emphasis to numerical simulations. These numerical models have grown increasingly complex and capable over time with improvements in computational power and numerical algorithms. This has resulted in a development of the new branch of science: **computational geodynamics**.

3-D numerical modelling

"A model which images any detail of the reality is as useful as a map of scale 1:1"
(Joan V. Robinson, economist)

Sketch of Numerical Modeling

(modified after Lliboutry 1987)



Mathematical Statement

- ✓Governing Equations
- ✓Boundary and Initial Conditions

Governing Equations

- ✓Conservation of momentum (Stokes equation)
- ✓State equation
- ✓Incompressibility condition
- ✓Rheological equation (dependence of effective viscosity on temperature, pressure and stress)
- ✓Heat balance equation
- ✓Advection equation for density, viscosity or chemical components .

Governing Equations

The equations for **conservation of momentum**

$$\rho \left(\frac{\partial \vec{u}}{\partial t} + < \vec{u}, \nabla > \vec{u} \right) = - \nabla p + \operatorname{div} (\mu \, e_{ij}) + \vec{F} = 0,$$

where

$$\operatorname{div} (\mu e_{ij}) = \left(\sum_{m=1}^{3} \frac{\partial \, (\mu e_{m1})}{\partial x_m}, \sum_{m=1}^{3} \frac{\partial \, (\mu e_{m2})}{\partial x_m}, \sum_{m=1}^{3} \frac{\partial \, (\mu e_{m3})}{\partial x_m} \right)$$

$$e_{ij} = e_{ij}(\vec{u}) = \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i},$$

the **incompressibility** condition $\operatorname{div} \vec{u} = 0$

the equation for *P*- and *T*-dependent viscosity

$$\mu(t, x, T) = \mu_*(t, x) \exp\left(\frac{E + \rho_* g x_3 V}{RT} - \frac{E_0 + \rho_0 g_0 l_0 V_0}{RT_0}\right).$$

Governing Equations

the **heat balance** equation

$$\frac{\partial}{\partial t}(\rho c T) + < \vec{u}, \nabla(\rho c T) > = \operatorname{div} (k \nabla T) + \mu \Phi + \rho Q,$$

where

$$\Phi = \frac{1}{2} \sum_{i=1}^{3} \sum_{j=1}^{3} (e_{ij})^2,$$

the **state** equation

$$\rho(t, x, T) = \rho_*(t, x)(1 - \alpha(T(t, x) - T_0)),$$

the **advection** equations for thermally unperturbed density and viscosity

$$\frac{\partial \rho_*}{\partial t} + < \nabla \rho_*, \vec{u} > = 0, \quad \frac{\partial \mu_*}{\partial t} + < \nabla \mu_*, \vec{u} > = 0,$$

Dimensionless Equations

In the Boussinesq and infinite Prandtl number approximation

$$\mathrm{La}\cdot\nabla p=\mathrm{div}\,(\;\mu\, e_{ij}\;)-\mathrm{La}\cdot\rho\,\vec{e}_3,\quad \mathrm{div}\;\vec{u}=0,$$

$$\frac{\partial}{\partial t}(\rho_* T)+<\vec{u},\nabla(\rho_* T)>=\Delta T+\mathrm{Di}\cdot\mu\Phi,$$

$$\rho(t,x,T)=\rho_*(t,x)(1-\alpha_0 T_0(T(t,x)-1)),$$

$$\frac{\partial\rho_*}{\partial t}+<\nabla\rho_*,\vec{u}>=0,\quad \frac{\partial\mu_*}{\partial t}+<\nabla\mu_*,\vec{u}>=0,$$

$$\mu(t,x,T)=\mu_*(t,x)\exp\left(\frac{E_0+\rho_* x_3 p_0 V_0}{RTT_0}-\frac{E_0+p_0V_0}{RT_0}\right).$$

$$\mathrm{La}=\frac{\rho_0 g_0 l_0^3}{\mu_0\kappa_0}\qquad \mathrm{Di}=\frac{\mu_0\kappa_0}{c_0\rho_0 T_0 l_0^2}$$

Boundary and Initial Conditions

Model domain $\Omega=(0,l_1)\times(0,l_2)\times(0,l_3)$.

At the **initial time** $t_0=0$:

$$T(0,x)=T_*^0(x),\quad \rho_*(0,x)=\rho_*^0(x),\quad \mu_*(0,x)=\mu_*^0(x),\quad x\in\Omega.$$

At the **boundary faces** $\Gamma(x_i=0)$ and $\Gamma(x_i=l_i)$ $(i=1,2,3)$:

Impermeability conditions with perfect slip:

$$\partial\vec{u}_\tau/\partial\vec{n}=0,\quad <\vec{u},\vec{n}>=0\quad \text{at }\Gamma.$$

$\vec{n}$ the outward unit normal vector at a point on the boundary Γ, $\vec{u}_\tau$ the projection of the velocity vector onto the tangent plane at the same point on Γ.

Impermeability conditions with no-slip conditions:

$$\vec{u}=0\quad \text{at }\Gamma.$$

Boundary and Initial Conditions

For the **temperature** on the vectical model boundaries heat flux = 0 (homogeneous Neumann problem):

$$\Gamma(x_1 = 0, x_1 = l_1): \quad \partial T/\partial x_1 = 0, \quad t \geq 0,$$
$$\Gamma(x_2 = 0, x_2 = l_2): \quad \partial T/\partial x_2 = 0, \quad t \geq 0.$$

On the horizontal model boundaries (nonhomogeneous Dirichlet problem):

$$\Gamma(x_3 = 0): \quad T(t, x_1, x_2, 0) = T_1(t, x_1, x_2), \quad t \geq 0,$$
$$\Gamma(x_3 = l_3): \quad T(t, x_1, x_2, l_3) = T_2(t, x_1, x_2), \quad t \geq 0.$$

Introduction of Vector Potential

The **vector potential** $\vec{\psi} = (\psi_1, \psi_2, \psi_3)$ and
the **vector velocity** $\vec{u} = (u_1, u_2, u_3)$

$$u_1 = \frac{\partial \psi_3}{\partial x_2} - \frac{\partial \psi_2}{\partial x_3}, \; u_2 = \frac{\partial \psi_1}{\partial x_3} - \frac{\partial \psi_3}{\partial x_1}, \; u_3 = \frac{\partial \psi_2}{\partial x_1} - \frac{\partial \psi_1}{\partial x_2}.$$

We apply the **curl** operator (curl$(\nabla p) = 0$ and div (curl$\vec{\psi}$) = 0):

$$\sum_{i=1}^{3}\left[\frac{\partial^2(\mu\, e_{i3})}{\partial x_2 \partial x_i} - \frac{\partial^2(\mu\, e_{i2})}{\partial x_3 \partial x_i}\right] = (\mathrm{La}(1 + \alpha_0 T_0) - \mathrm{Ra}T)\frac{\partial \rho_*}{\partial x_2} - \mathrm{Ra}\rho_* \frac{\partial T}{\partial x_2},$$

$$\sum_{i=1}^{3}\left[\frac{\partial^2(\mu\, e_{i3})}{\partial x_1 \partial x_i} - \frac{\partial^2(\mu\, e_{i1})}{\partial x_3 \partial x_i}\right] = (\mathrm{La}(1 + \alpha_0 T_0) - \mathrm{Ra}T)\frac{\partial \rho_*}{\partial x_1} - \mathrm{Ra}\rho_* \frac{\partial T}{\partial x_1},$$

$$\sum_{i=1}^{3}\left[\frac{\partial^2(\mu\, e_{i2})}{\partial x_1 \partial x_i} - \frac{\partial^2(\mu\, e_{i1})}{\partial x_2 \partial x_i}\right] = 0,$$

$$\mathrm{La} = \frac{\rho_0 g_0 l_0^3}{\mu_0 æ_0}, \quad \mathrm{Ra} = \alpha_0 T_0 \mathrm{La}, \quad \mathrm{Di} = \frac{\mu_0 æ_0}{c_0 \rho_0 T_0 l_0^2}.$$

Two-Component Representation of Vector Velocity Potential

(Ismail-Zadeh et al., 2001)

$$\vec{u} = \mathrm{curl}\vec{\psi}, \quad \vec{\psi} = (\psi_1, \psi_2, \psi_3), \quad \psi_3 = 0,$$

where

$$\psi_1 = \psi_1(t, x_1, x_2, x_3) = \int_0^{x_3} u_2(t, x_1, x_2, \xi)\, d\xi + \frac{\partial \varphi}{\partial x_1},$$

$$\psi_2 = \psi_2(t, x_1, x_2, x_3) = -\int_0^{x_3} u_1(t, x_1, x_2, \xi)\, d\xi + \frac{\partial \varphi}{\partial x_2},$$

$$\psi_3 = \psi_3(t, x_1, x_2, x_3) = 0,$$

$\varphi = \varphi(t, x_1, x_2)$ an arbitrary sufficiently smooth scalar function with a compact support in the rectangular domain $(0, l_1) \times (0, l_2)$.

$$u_1 = -\partial\psi_2/\partial x_3,\; u_2 = \partial\psi_1/\partial x_3,\; u_3 = \partial\psi_2/\partial x_1 - \partial\psi_1/\partial x_2.$$

Numerical Approach

- ✓Approximation of the mathematical problem
- ✓Numerical techniques used

Approximation of the Problem

Consider the uniform rectangular grid covering Ω:

$$\Omega_{ijk} = (x_1^i, x_2^j, x_3^k), \quad 0 \le i \le n_1, 0 \le j \le n_2, 0 \le k \le n_3.$$

The vector potential $\vec{\psi}$ is approximated by a linear combination of tricubic basis functions expressed as products of appropriate cubic splines:

$$\psi_p(t, x_1, x_2, x_3) \approx \sum_{i=0}^{n_1} \sum_{j=0}^{n_2} \sum_{k=0}^{n_3} \psi_{ijk}^{(p)}(t) s_i^{(p1)}(x_1) s_j^{(p2)}(x_2) s_k^{(p3)}(x_3), \quad p = 1, 2.$$

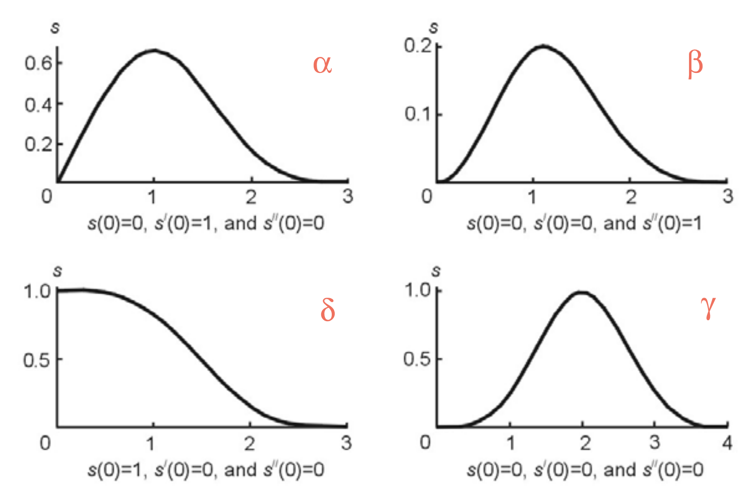
Density and viscosity are approximated by linear combinations of appropriate trilinear basis functions at fine grid

$$\rho_*(t, x_1, x_2, x_3) \approx \sum_{i=0}^{n_1} \sum_{j=0}^{n_2} \sum_{k=0}^{n_3} \rho_{ijk}(t) \tilde{s}_i^{(1)}(x_1) \tilde{s}_j^{(2)}(x_2) \tilde{s}_k^{(3)}(x_3),$$

$$\mu_*(t, x_1, x_2, x_3) \approx \sum_{i=0}^{n_1} \sum_{j=0}^{n_2} \sum_{k=0}^{n_3} \mu_{ijk}(t) \tilde{s}_i^{(1)}(x_1) \tilde{s}_j^{(2)}(x_2) \tilde{s}_k^{(3)}(x_3).$$

Approximation of the Problem

Cubic splines used in the modelling



Numerical Techniques

Numerical Method for Solving the Stokes Equation

Approximations of vector potential, density, and viscosity are substituted into the variational equation. A system of linear algebraic equations with a positive define band matrix for unknown coefficients is obtained. The coefficients are determined on each time step by solving the system of linear algebraic equations iteratively by conjugate gradient or by Gauss–Seidel methods.

Numerical Method for Solving the Advection Equation

- The advection equations has characteristics described by the system of ordinary differential equations

$$dx(t)/dt = \mathbf{u}(t, x(t))$$

- Both density and viscosity retain constant values along the characteristics

$$\rho_*(t, x(t)) = \rho_0(x(0)), \quad \mu_*(t, x(t)) = \mu_0(x(0)).$$

Numerical Techniques

Numerical Method for Solving the Heat Equation

Temperature is approximated by finite-differences:

$$\frac{\partial T(t_n, x_1^i, x_2^j, x_3^k)}{\partial x_1} = \frac{T_{i+1,j,k}^n - T_{i-1,j,k}^n}{2h_1}, \quad h_1 = x_1^i - x_1^{i-1},$$

$$\frac{\partial^2 T(t_n, x_1^i, x_2^j, x_3^k)}{\partial x_1^2} = \frac{T_{i+1,j,k}^n - 2T_{i,j,k}^n + T_{i-1,j,k}^n}{2h_1}$$

Temperature is computed by an implicit alternating-direction method:

$$r^{(k)} = \tau\nabla^2 T^{(k)} + \mathbf{u}\cdot\nabla T^{(k)}, \quad \left[1 - \frac{\tau}{2}\frac{\partial^2}{\partial x_3^2}\right]T^* = r^{(k)},$$

$$\left[1 - \frac{\tau}{2}\frac{\partial^2}{\partial x_2^2}\right]T^{**} = T^*, \quad \left[1 - \frac{\tau}{2}\frac{\partial^2}{\partial x_1^2}\right]T^{***} = T^{**}, \quad T^{(k+1)} = T^{(k)} + T^{***}.$$

Parameter τ is chosen in such a way as to guarantee the stability of the FDM:

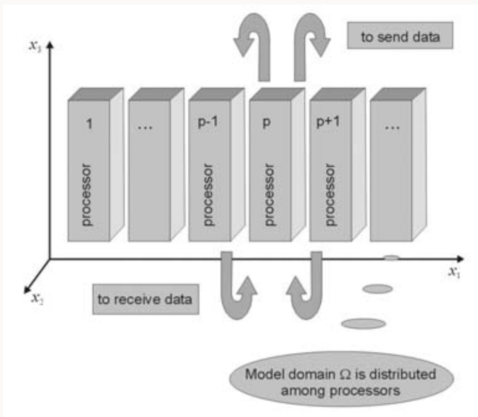
$$\tau = \frac{1}{8}\frac{dx}{u_{\max}}, \quad dx = \left[h_1^2 + h_2^2 + h_3^2\right]^{1/2}, \quad u_{\max} = \max\left\{|u_i(x)| : x \in \overline{\Omega},\ i = 1,2,3\right\}$$

Verification

A few tests were done to check the accuracy of the method

- Benchmark with another numerical codes (Busse et al., 1993)
  in a reasonable agreement (constant viscosity and temperature dependent)
- Conservation of mass at each time step
  relative change of mass about 0.1% per 200 time steps
- Element refinement
- Accuracy of the vector velocity potential
  relative error for the grid 30x30x30 remained within 0.3% for right-hand sides having reasonable numbers of periods
- Comparison with an analytical solution for the Stokes equation combined with the advection equation for density (Trushkov, 2002).

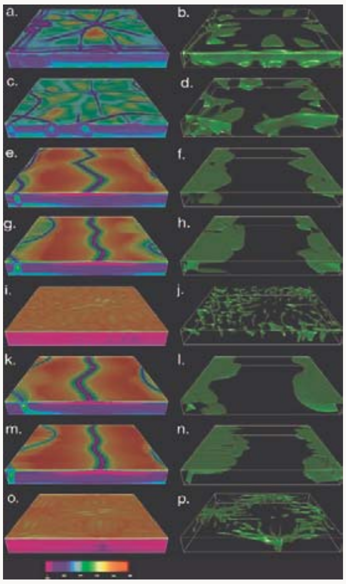
Parallel Computing using MPI

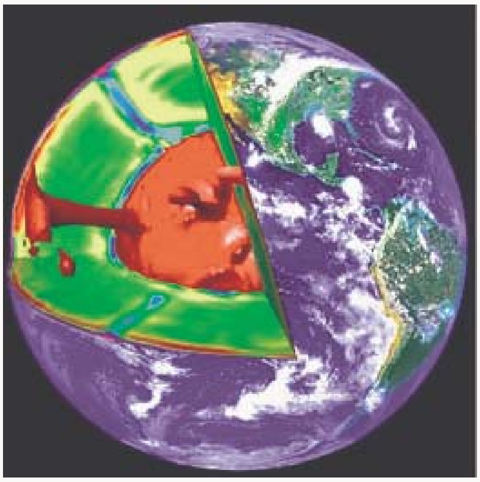


Discrete Stokes equation, characteristic equation, and heat equation are solved at parallel processors.

Numerical modelling and its results

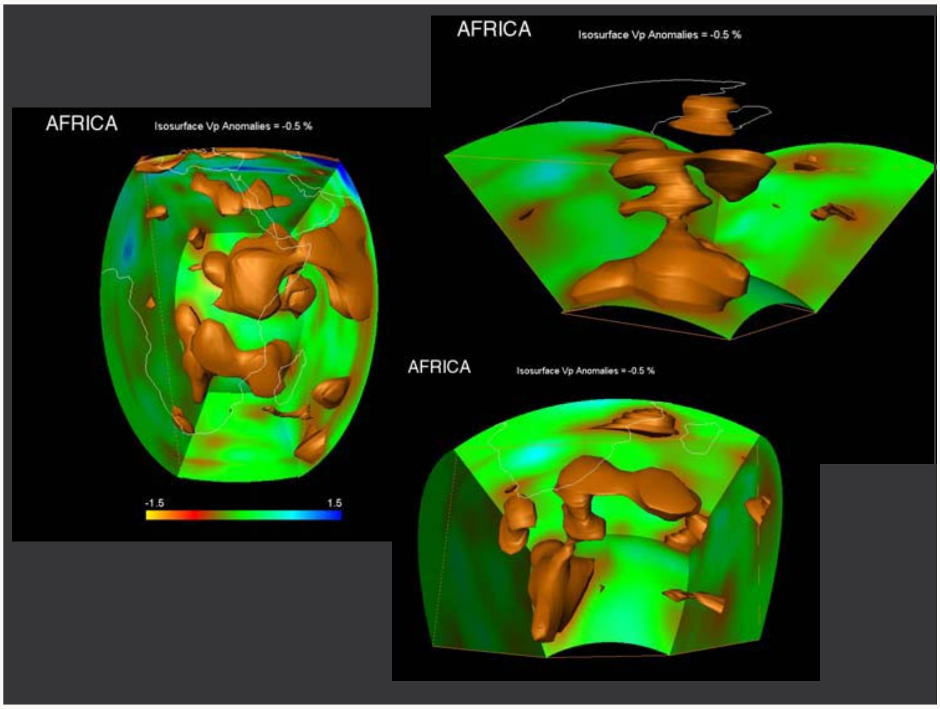
Thermal convection in the mantle



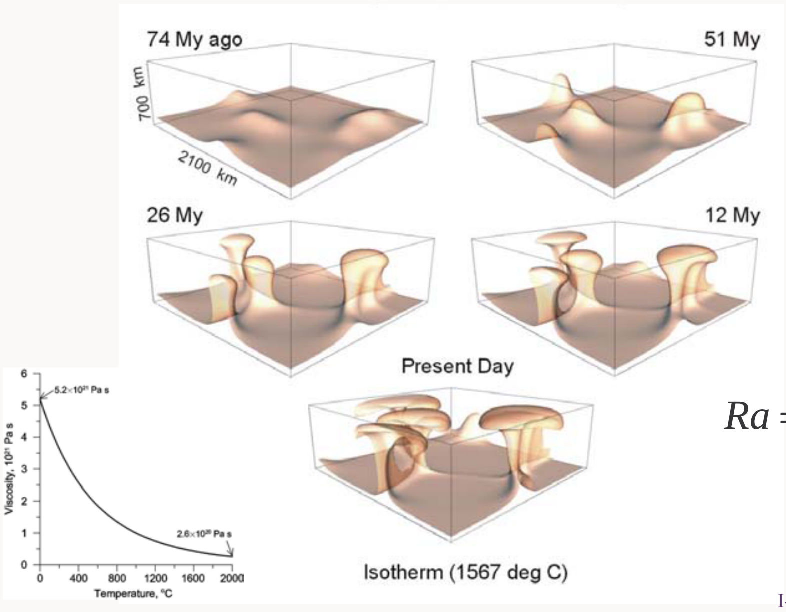


I-Z et al., 2002

Tackley et al., 1999



Mantle plume evolution



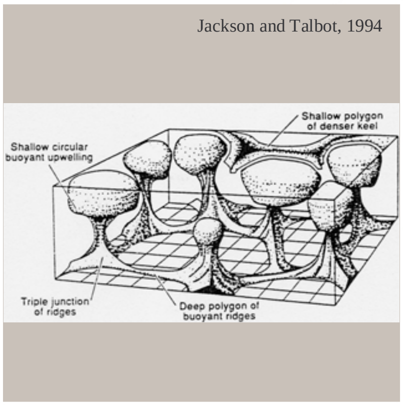
$$Ra = 10^6$$

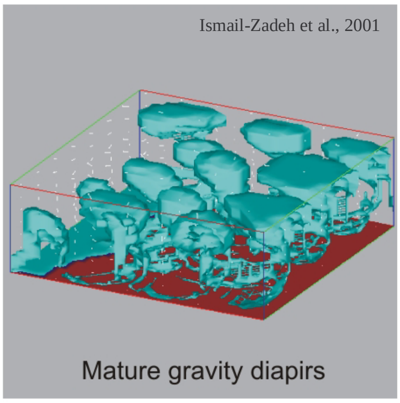
I-Z et al., 2004

Salt Diapirism

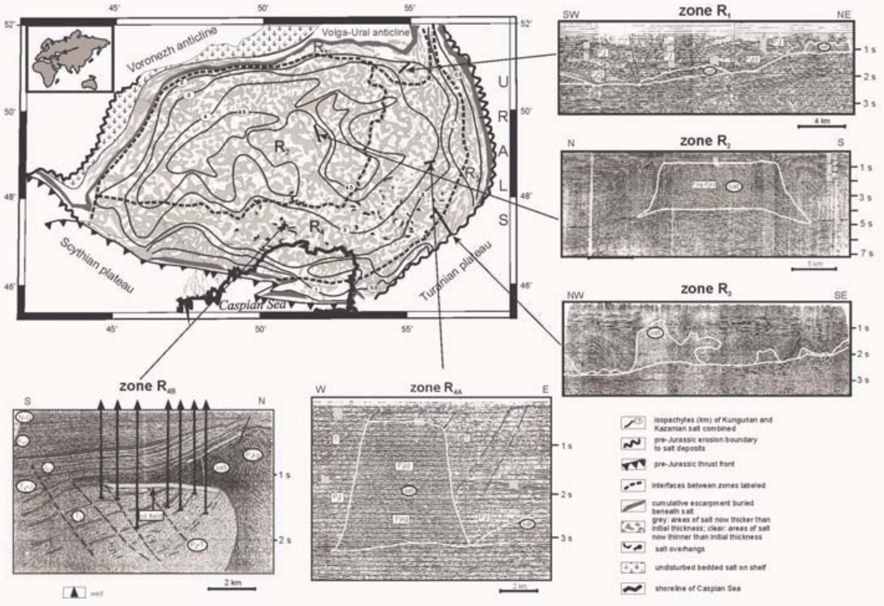
3D Model Examples

Rayleigh-Taylor Problem

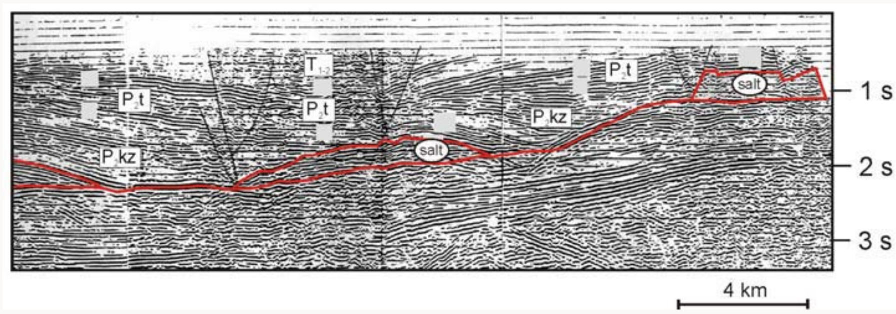




Pricaspian Salt Basin



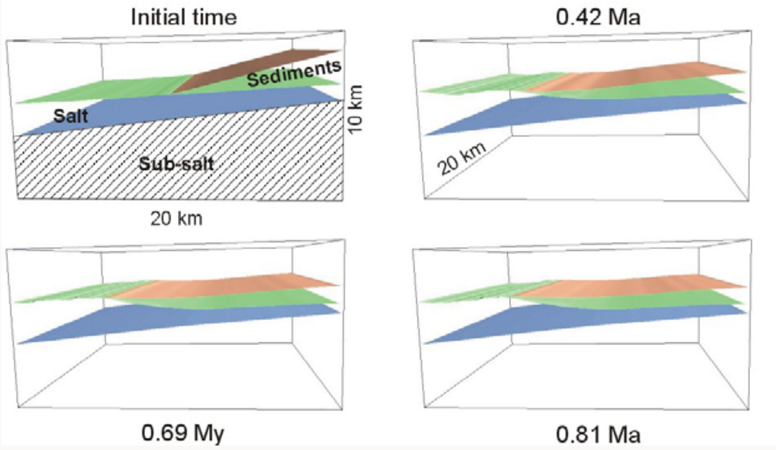
Case study 1 - 2D structures



Viscosities and densities of the sedimentary layers are assumed to be 10^{20} Pa s and 2.65×10^3 kg m^{-3} for the overburden layer, 10^{18} Pa s and 2.24×10^3 kg m^{-3} for salt, and 10^{21} Pa s and 2.7×10^3 kg m^{-3} for the subsalt layer, respectively.

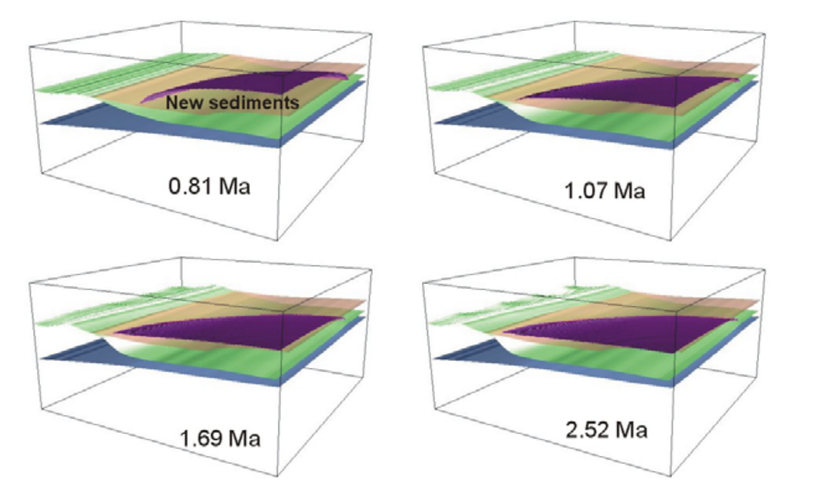
Case study 1 - 2D structures

Evolution (front view) of a salt wall in a sedimentary basin. At time t=0 an inclined salt layer is overlain by sediments at the eastern part of the model region.

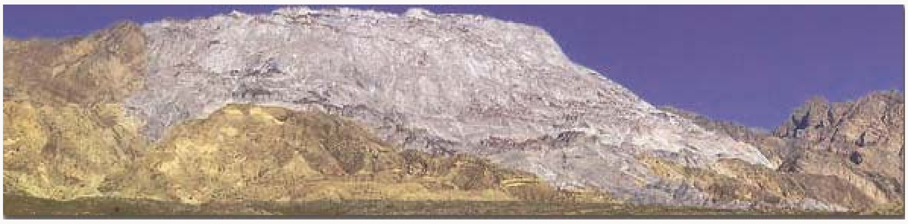


Case study 1 - 2D structures

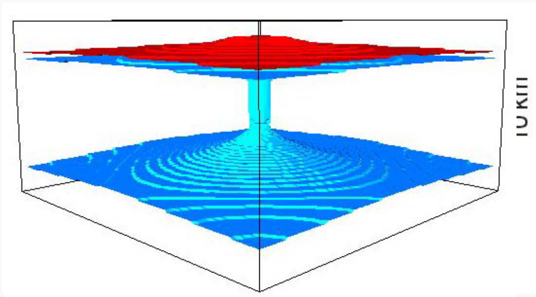
A new portion of sediments is added to the structure at the southeastern corner of the model region

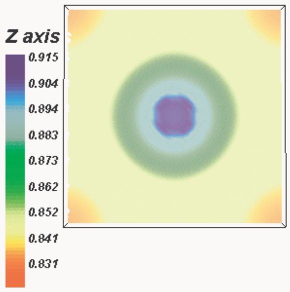


Case study 2 - extrusion

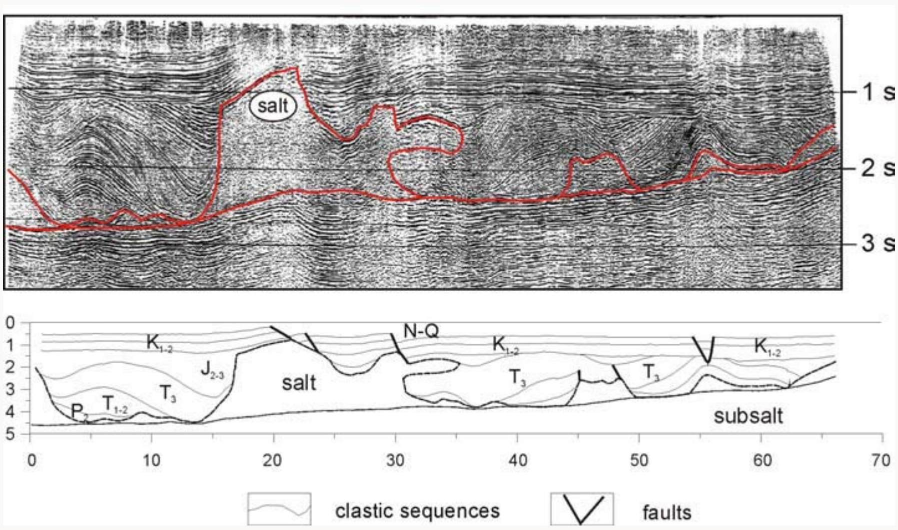


1-km-high summit dome of Kuh-e-Namak, Hormuz salt basin, Zagros Mountains, southwestern Iran

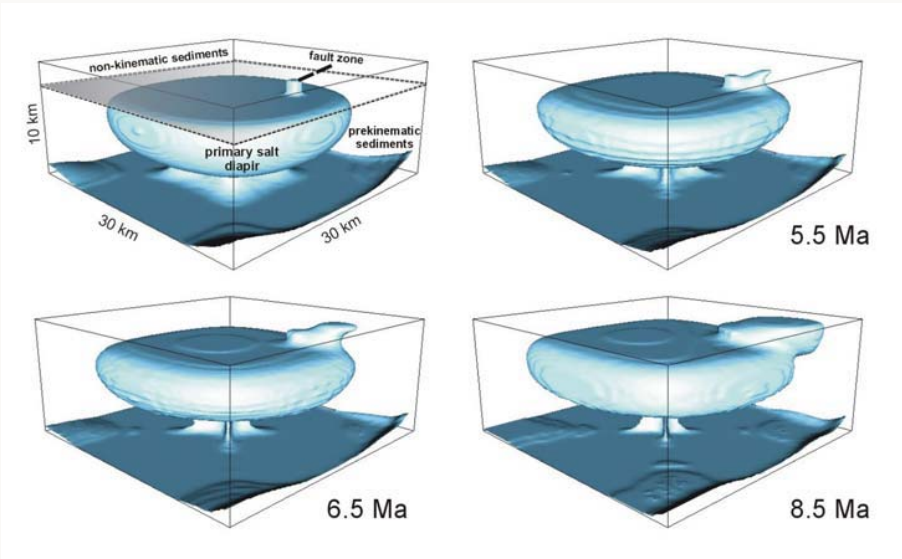




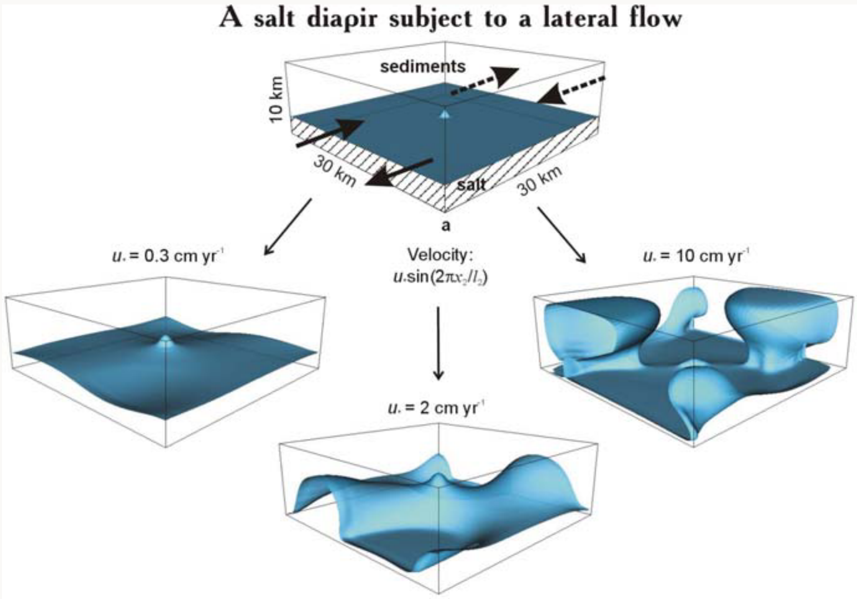
Case study 3 - second diapirism



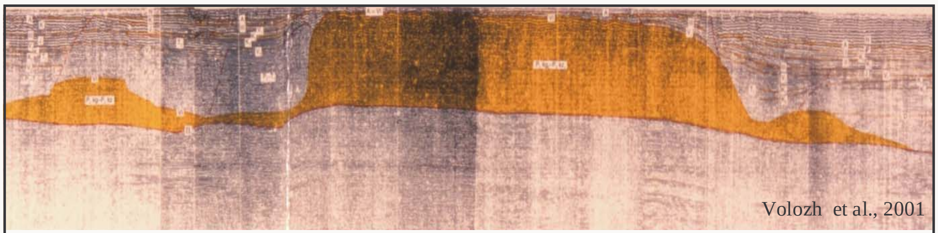
Case study 3 - second diapirism



Case study 4 - lateral flow

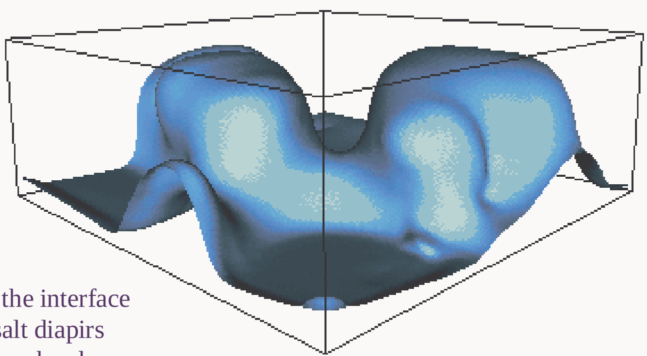


Inverse Modelling of Gravity Overturns



Volozh et al., 2001

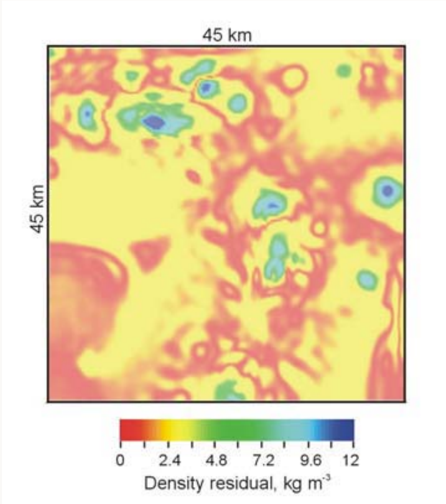
Restoration of Salt Structures



Evolution of the interface between salt diapirs and their overburden

Ismail-Zadeh et al., 2004

Restoration errors - density residual



$$\delta\rho(x_1, x_2) = \left[\int_0^h \left(\rho(x_1, x_2, x_3) - \tilde{\rho}(x_1, x_2, x_3) \right)^2 dx_3 \right]^{1/2}$$

Perspectives and challenges

Perspectives

"A new level of mathematical modeling and numerical solution does not merely involve the analysis of a single medium but must encompass the solution of multi-physics problems involving fluids, solids, their interactions, chemical and electro-magnetic effects; must involve multi-scale phenomena from the molecular to the macroscopic scales; must include uncertainties in the given data and solution results" (*J. Bathe*, 2003)

Challenge 1

Effective numerical schemes for fluid and solid geodynamics

Numerous publications exist on the numerical solutions of fluid flows and solid deformations, but the numerical methods proposed are far from satisfactory. "Ideal" solution schemes would be much more predictive, reliable and effective.

Clearly, major advances are still possible.

Challenge 2

The development of numerical procedures for multi-geophysics problems

Major areas are given by deformations of the crust and lithosphere and fluid flows, including heat transfer and chemical effects (sedimentary basins and mantle convection) and hydro-magnetic effects (core geodynamo), fully coupled to structures (lithospheric plates). Advances have been made for simulations in these fields, but significant further progress can be accomplished.

Challenge 3

The development of numerical procedures for multi-scale problems

Many phenomena in geodynamics involve multiple scales (sedimentary basins, mantle plumes, hierarchical structure of the lithosphere, etc).

The spanning of scales in analyses of the problems provides an exciting challenge.

Challenge 4

The analysis of complete cycles of the Earth system

At present, largely, only parts of the whole system are analysed and optimised. There is a need to extensively develop

"virtual laboratories"

in which complete cycles of the Earth system could be optimised.

Challenge 5

Education

The powerful tools for analysis are only of value if they are used with

sound scientific judgement.

This judgment must be created by a strong, basic and exciting education in the Universities and International Centres and ongoing, life-long education in practice.

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