The Abdus Salam
International Centre for Theoretical Physics

United Nations
Educational, Scientific and
Cultural Organization

IAEA
International Atomic Energy Agency

1864-12

Ninth Workshop on Non-linear Dynamics and Earthquake Predictions

1 - 13 October 2007

Inverse Problems and Data Assimilation in Non-Linear Sciences

Alik T. Ismail-Zadeh

Geophysical Institute
University of Karlsruhe
Karlsruhe, Germany
&
International Institute of Earthquake Prediction
Theory & Mathematical Geophysics
Moscow, Russia

United Nations Educational Scientific and Cultural Organization
and
International Atomic Energy Agency

THE ABDUS SALAM
INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

Ninth Workshop
"Non-Linear Dynamics and Earthquake Prediction"
1 October to 13 October 2007

INVERSE PROBLEMS AND DATA ASSIMILATION

IN NON-LINEAR EARTH SCIENCES

Alik T. Ismail-Zadeh

Geophysical Institute, University of Karlsruhe,
Hertzsrt. 16, Karlsruhe 76187, Germany.
E-mail: Alik.Ismail-Zadeh@gpi.uka.de

International Institute of Earthquake Prediction Theory and
Mathematical Geophysics, Russian Academy of Sciences,
84/32 Profsoyuznaya ul., Moscow 117997, Russia.

MIRAMARE-TRIESTE
October 2007

Inverse Problems and Data Assimilation

IN NON-LINEAR EARTH SCIENCES

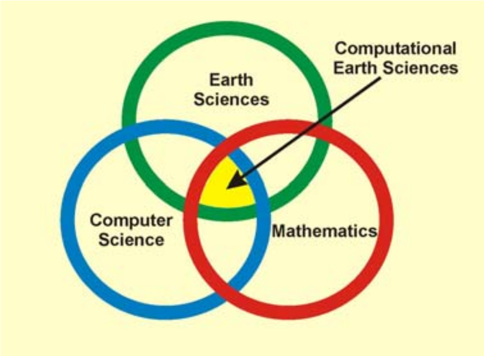
$$\frac{\partial T(t_n, x_1^i, x_2^j, x_3^k)}{\partial x_1} = \frac{T_{i+1,j,k}^n - T_{i-1,j,k}^n}{2h_1}, \quad h_1 = x_1^i - x_1^{i-1},$$

$$\frac{\partial^2 T(t_n, x_1^i, x_2^j, x_3^k)}{\partial x_1^2} = \frac{T_{i+1,j,k}^n - 2T_{i,j,k}^n + T_{i-1,j,k}^n}{2h_1} = \mathrm{K}_1(T^n),$$

Alik Ismail-Zadeh

Karlsruhe University, Germany / Russian Academy of Sciences, Moscow

Great advances in understanding of the complex Earth system and in computational tools, permitting accurate numerical modelling and forecasting, are transforming the geoscience.



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 non-linear dynamics of the Earth

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.

Mathematical Model of Geophysical Problem

Many geophysical problems can be described by mathematical models (MM), i.e., by a set of partial differential equations and boundary and/or initial conditions defined in a specific domain.

A MM links the causal characteristics of a geophysical process with its effects.

The causal characteristics of the process include, for example, parameters of the initial and boundary conditions, coefficients of the differential equations, and geometrical parameters of a model domain.

Direct and Inverse Problems

The aim of the *direct mathematical problem* is to determine the relationship between the *causes* and *effects* of the geophysical process and hence to find a solution to the mathematical problem for a given set of parameters and coefficients.

An *inverse problem* is the opposite of a direct problem. An inverse problem is considered when there is a lack of information on the causal characteristics (but information on the effects of the geophysical process exists).

Inverse Problems

Inverse problems can be subdivided into

(i) time-reverse problems (e.g., to restore the development of a geodynamic process)
(ii) coefficient problems (e.g., to determine the coefficients of the model equations and/or boundary conditions)
(iii) geometrical problems (e.g., to determine the location of heat sources in a model domain or the geometry of the model boundary),
(iv) and some others.

Inverse Problems

Jacques Hadamard
(1865 – 1963)

Andrei Tikhonov
(1906 – 1993)

Jacques-Louis Lions
(1928 – 2001)

Inverse (Time-Reverse) Problems

The mantle is heated from the core and from inside due to decay of radioactive elements. Since mantle convection is described by heat advection and diffusion, one can ask:

Is it possible to tell, from the present temperature estimations of the Earth, something about the Earth's temperature in the geological past?

Even though heat diffusion is irreversible in the physical sense, it is possible to predict accurately the heat transfer backwards in time using data assimilation techniques without contradicting the basic thermodynamic laws.

Inverse (Time-Reverse) Problems

Inverse (time-reverse) problems of geodynamics **(thermal convection in the Earth's mantle) will be the subject of the several lectures during the Workshop.**

The principal result of such inversion is to restore dynamics of the Earth's interior in the geological past.

In other words, the present observations (mantle temperature, velocity, etc.) can be *assimilated* into the past to constrain the initial conditions for the mantle temperature and velocity.

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**

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

where

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

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

the **incompressibility** condition 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

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

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

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

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):

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

Properly and Improperly Posed Problems

Inverse problems are often ill-posed. Jacques Hadamard introduced the idea of ***well- (and ill-) posed*** problems in the theory of partial differential equations (Hadamard 1902).

A mathematical model for a geophysical problem has to be ***well-posed*** in the sense that it has to have the properties of existence, uniqueness, and stability of a solution to the problem. Problems for which at least one of these properties does not hold are called ***ill-posed***.

The requirement of stability is the most important one. If a problem lacks the property of stability then its solution is almost impossible to compute because computations are polluted by unavoidable errors. If the solution of a problem does not depend continuously on the initial data, then, in general, the computed solution may have nothing to do with the true solution.

Improperly Posed Problems

The inverse problem of Earth dynamics (thermal convection in the mantle) is an ill-posed problem, since the backward heat problem, describing both heat advection and conduction through the mantle backwards in time, possesses the properties of ill-posedness.

In particular, the solution to the problem does not depend continuously on the initial data. This means that small changes in the present-day temperature field may result in large changes of predicted mantle temperatures in the past

Example

Consider 1D diffusion problem backward in time.

$$T_t = T_{xx}\,, \qquad 0 \le x \le \pi\,,\quad t \le 0\,,$$
$$T(t,0) = 0 = T(t,\pi)\,, \qquad t \le 0\,,$$
$$T(0,x) = \varphi_n(x)\,, \qquad 0 \le x \le \pi\,.$$

At initial time (or final time with respect to the forward problem) we assume that $\varphi_n(x)$ takes the following two forms:

$$\varphi_n(x) = \frac{1}{4n+1}\sin((4n+1)\cdot x) \quad \text{and} \quad \varphi_0(x) \equiv 0$$

Note that

$$\max_{0\le x\le\pi} \left|\varphi_n(x) - \varphi_0(x)\right| \le \frac{1}{4n+1} \to 0 \quad \text{at} \quad n \to \infty$$

The following two solutions of the problem correspond to the two chosen functions of φ respectively:

$$T_0 \equiv 0 \quad \text{at} \quad \varphi_n(x) = \varphi_0$$

$$T_n = \frac{1}{4n+1}\exp(-(4n+1)^2\cdot t)\cdot\sin((4n+1)\cdot x) \quad \text{at} \quad \varphi_n(x) = \varphi_n$$

At t = -1 and x = $\pi/2$ we obtain

$$T_n(-1,\pi/2) = \frac{1}{4n+1}\exp((4n+1)^2) \to \infty \quad \text{at} \quad n \to \infty$$

Therefore, two closely set initial functions φ_n and φ_0 are associated with two different solutions. Hence, **a small error in initial data can result in large errors in the solution of the backward diffusion problem**.

Numerical Approach

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

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

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

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

Numerical Techniques

Numerical Method for Solving the Stokes Equation

- Finite element method is used to solve the Stokes 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:

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

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

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:

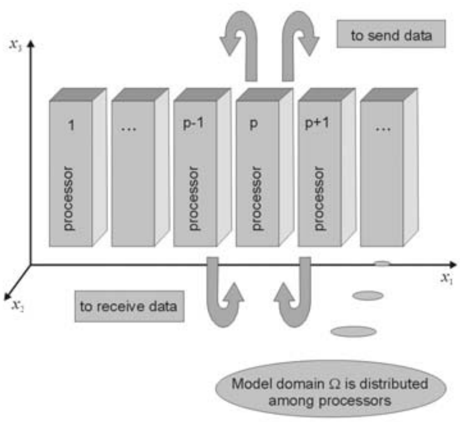
$$\tau = \frac{1}{8}\frac{dx}{u_{\max}}, \quad dx = \left[h_1^2 + h_2^2 + h_3^2\right]^{1/2}, \quad u_{\max} = \max\left\{|u_i(x)| : x \in \overline{\Omega},\ i = 1,2,3\right\}$$

Verification

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

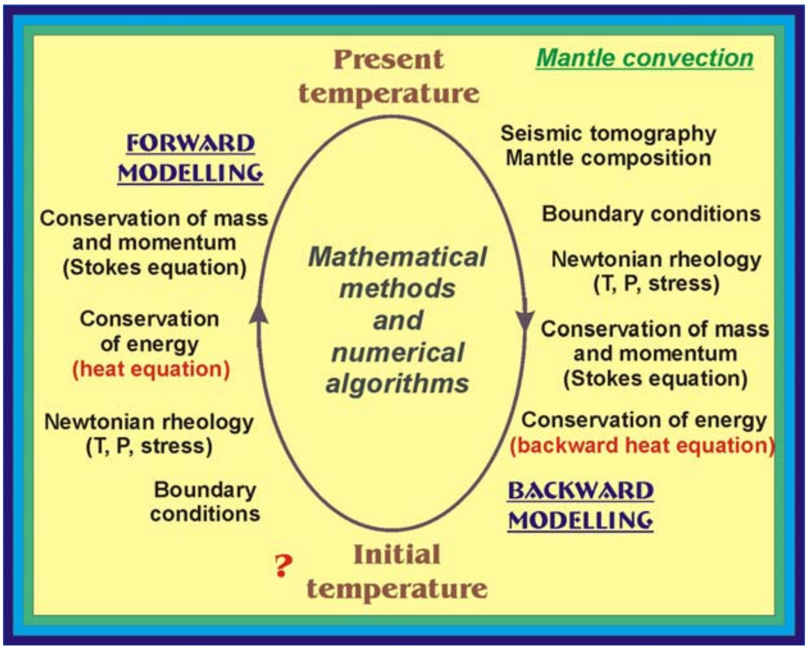
- Benchmark with another numerical codes (Busse et al., 1993)
  in a reasonable agreement (constant viscosity and temperature dependent)
- Conservation of mass at each time step
  relative change of mass about 0.1% per 200 time steps
- Element refinement
- Accuracy of the vector velocity potential
  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



The model problem is solved at parallel processors.

Two Approaches to Numerical Modeling

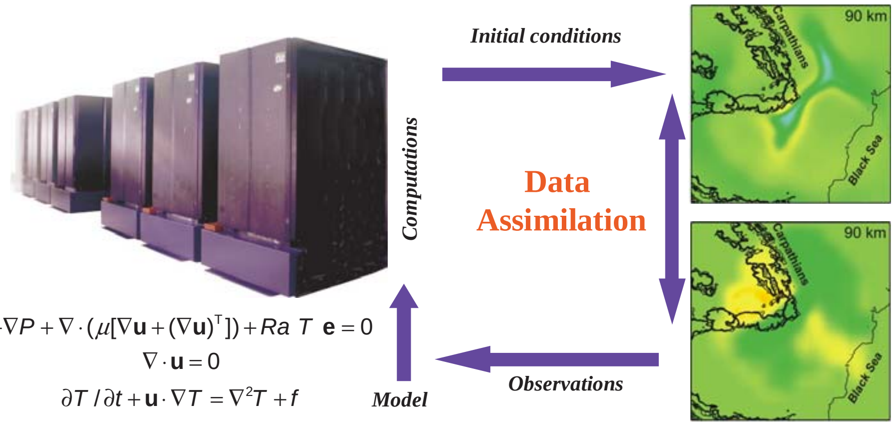


Data Assimilation

Data assimilation **can be defined as the incorporation of present (observations) and past data (initial conditions) in an explicit dynamic model to provide time continuity and coupling among the physical fields (e.g., velocity, temperature).**

The basic principle of data assimilation is to consider the initial condition as a control variable and to optimize the initial condition in order to minimize the discrepancy between the observations and the solution of the model.

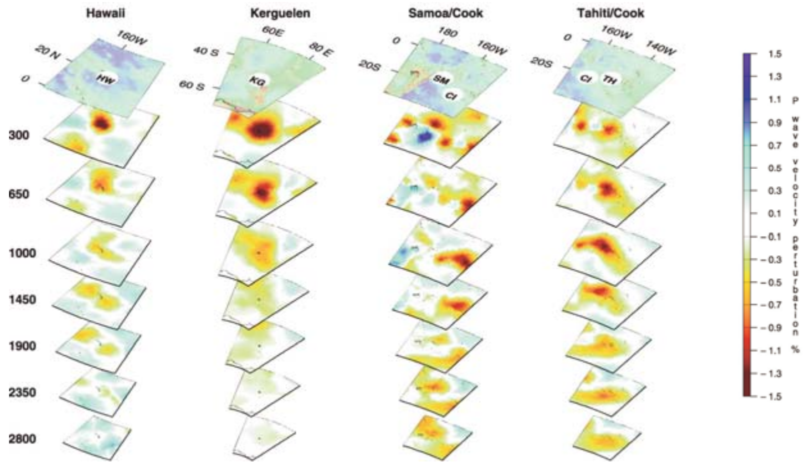
Data Assimilation in Geodynamics



$$-\nabla P + \nabla \cdot (\mu[\nabla \mathbf{u} + (\nabla \mathbf{u})^T]) + Ra\ T\ \mathbf{e} = 0$$
$$\nabla \cdot \mathbf{u} = 0$$
$$\partial T / \partial t + \mathbf{u} \cdot \nabla T = \nabla^2 T + f$$

Why data assimilation?

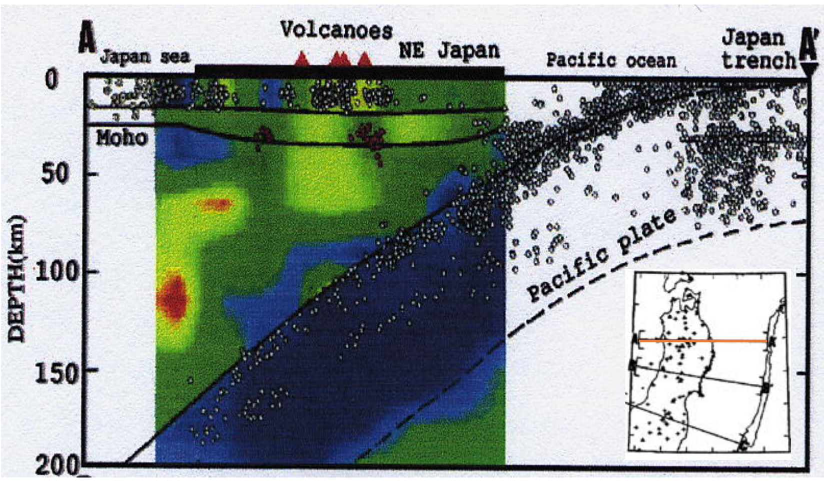
To restore the temperature, composition, and movements in the mantle and to predict the Earth's heat budget evolution



Montelli et al., *Science*, 2004

Why data assimilation?

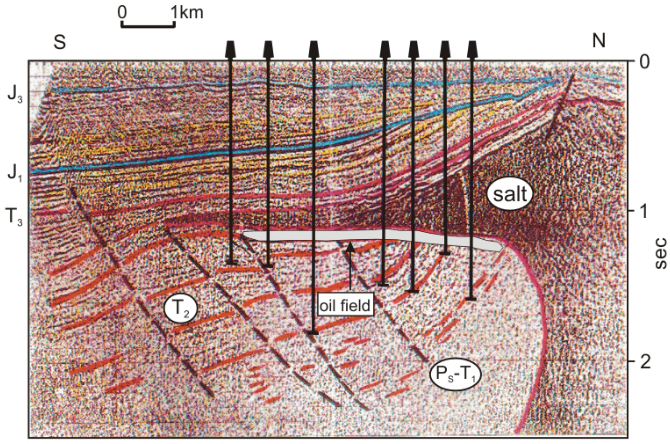
To understand the origin and evolution of the present high and low velocity anomalies in a particular region



Zhao, *PEPI*, 2001

Why data assimilation?

To reconstruct structural and geothermal evolutions of sedimentary basins (particularly, complicated by salt tectonics)

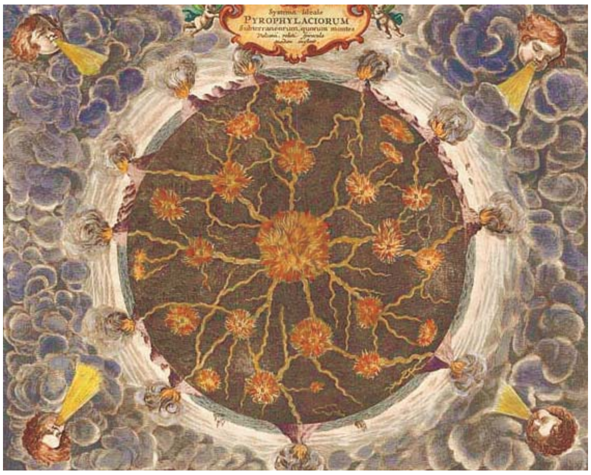


Salt diapirism in the Pricaspian basin, Russia & Kazakhstan

Volozh, Talbot & Ismail-Zadeh, *AAPG Bull.*, 2003

Data Assimilation Methods in Models of the Earth

„Primitive method“ (ca. 1668)



The Jesuit scholar *A.Kircher* was one of the first compilers of semi-scientific knowledge about the physical features of the world.

Data Assimilation Methods in Models of Geodynamics

- **Backward advection method** (**BAD**)

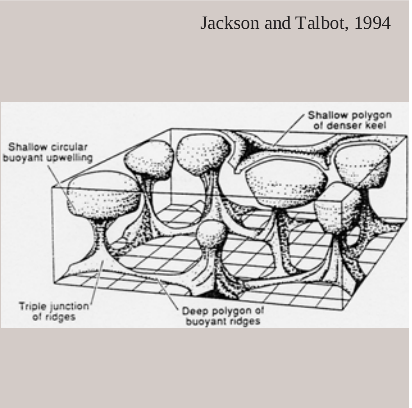
Steinberger and O’Connell, *GJI*, 1998.

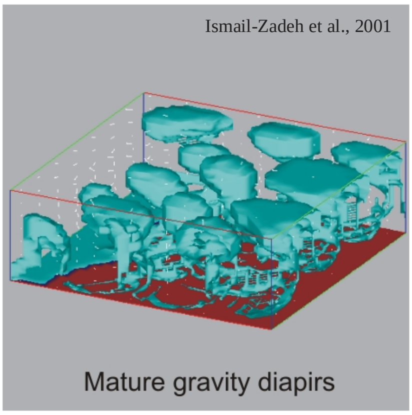
Ismail-Zadeh et al., *Tectonophysics*, 2001, 2004.

Conrad and Gurnis, *G³*, 2003.

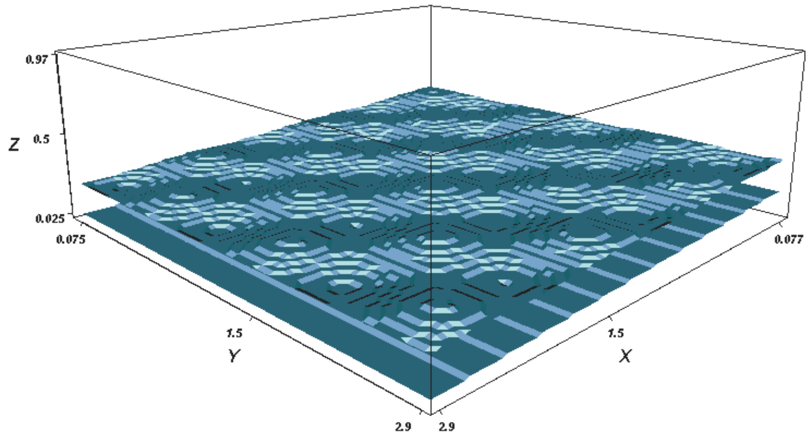
Salt Diapirism

Rayleigh-Taylor Problem



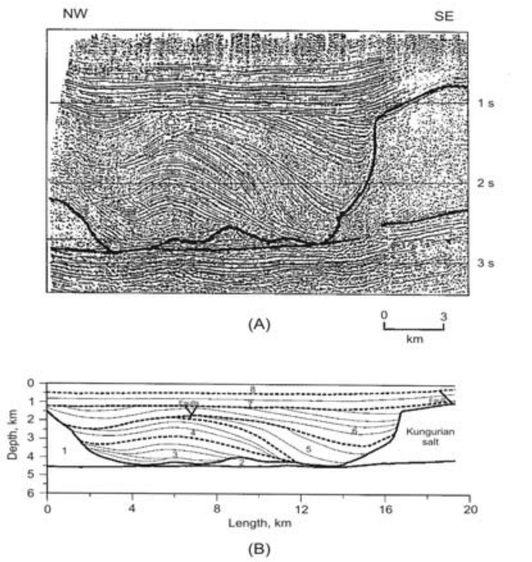


Salt Diapirism



Seismic Profile

Depth-converted Profile

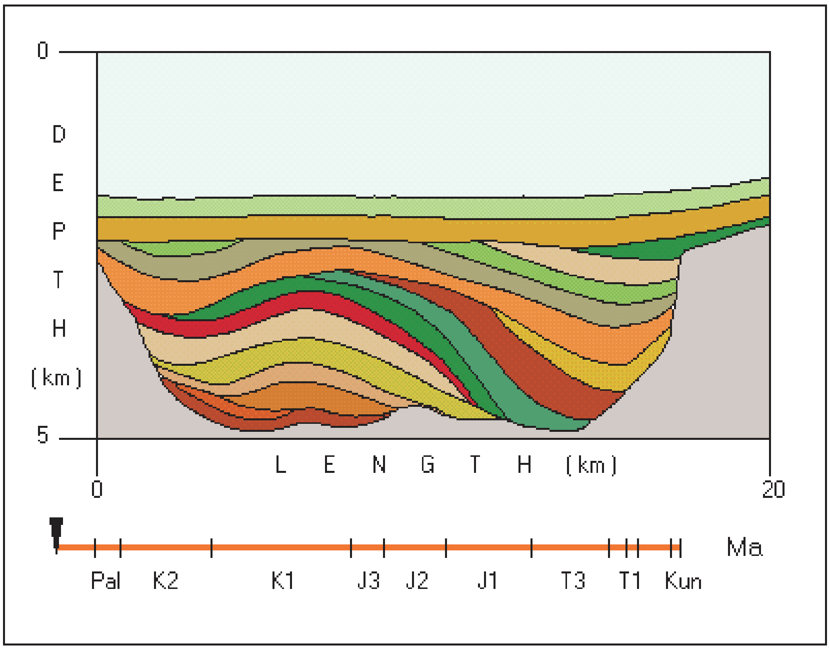


Seismic profile (A) through the south-eastern part of the Pricaspian basin and its depth-conversion (B) with salt related structures as indicated:

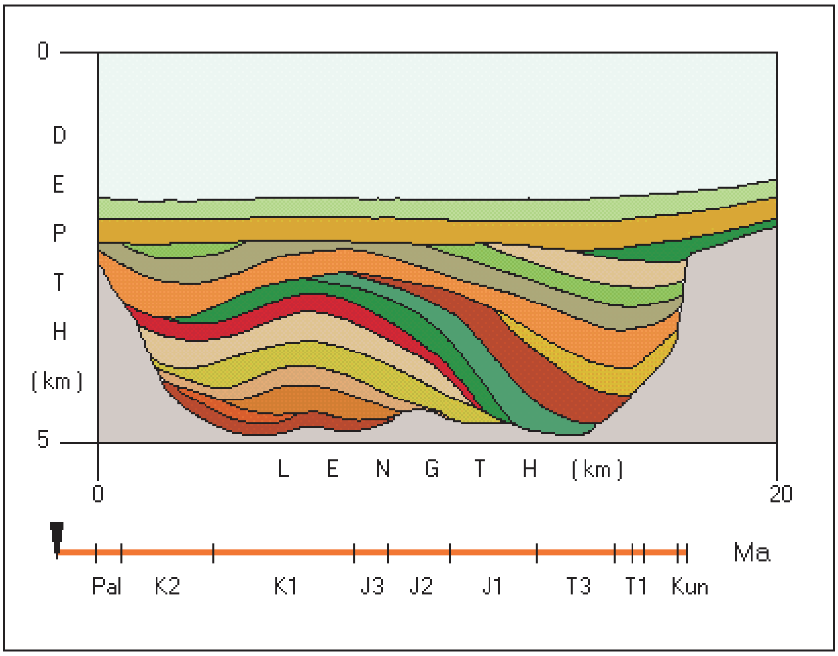
1, salt dome; 2, residual salt high; 3-8, sedimentary layers of salt overburden: 3, Lower Kazanian (258-255 Ma); 4, Upper Kazanian (255-253 Ma); 5, Tatarian (253-245 Ma); 6, Lower Triassic (245-241); 7, Middle Triassic to Lower Cretaceous (241-90 Ma); and 8, Upper Cretaceous to Quaternary (90-0 Ma).

Ismail-Zadeh et al., 2001

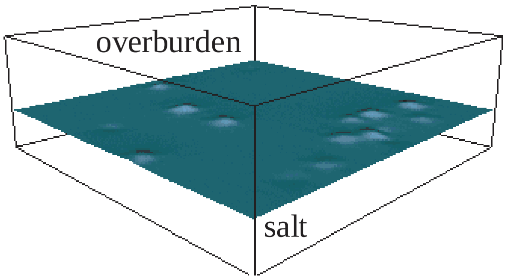
Restoration of the cross-section



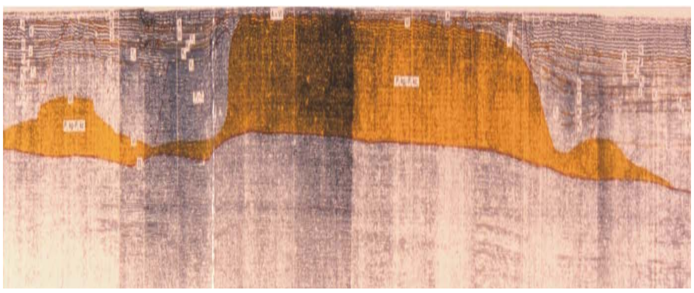
Movie of the Restoration



Forward Modeling of Salt Diapirism

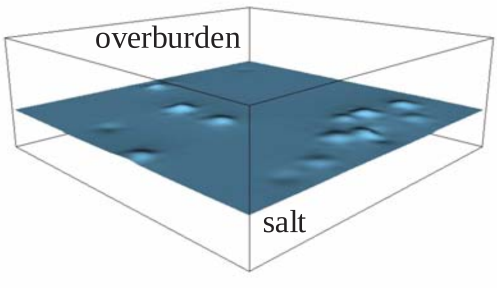


Evolution of the interface between salt and its overburden

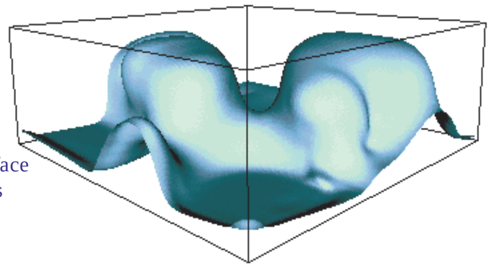


Ismail-Zadeh et al., 2004

Initial state of small perturbations



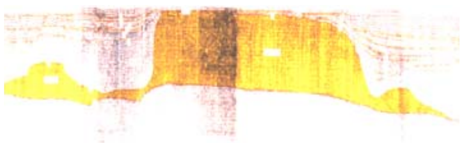
Backward Modeling of Salt Diapirism

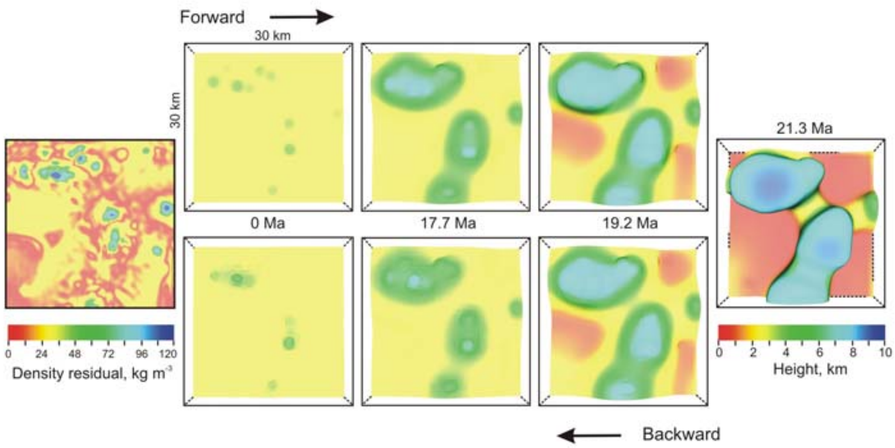


Evolution of the interface between salt and its overburden

Ismail-Zadeh et al., 2001

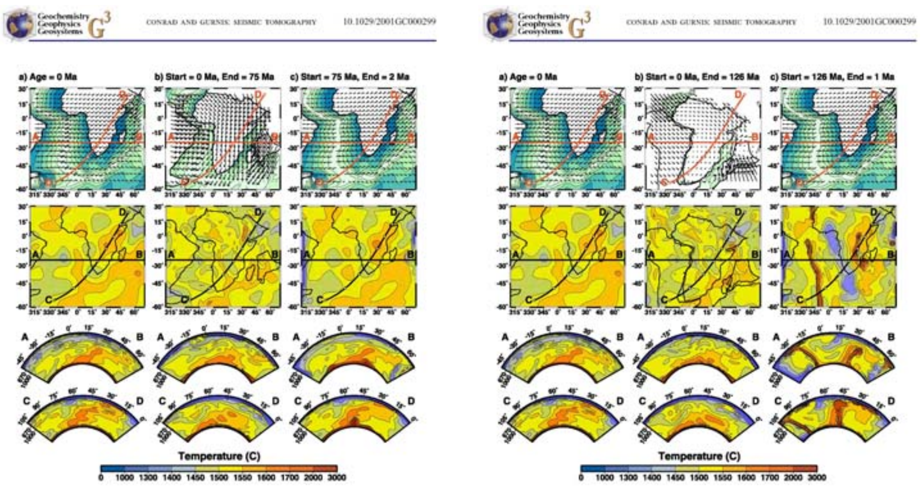
BAD method applied to restore salt structures





• **Backward advection method** (**BAD**)

Conrad and Gurnis, *G*^{3}, 2003.



Data Assimilation Methods in Models of Geodynamics

• Backward advection method (BAD)
  - Ismail-Zadeh et al., *Tectonophysics*, 2001, 2004.
  - Conrad and Gurnis, *G*^{3}, 2003.

• Sequential filtering (SFL)
  - Hager and O'Connell, *JRG*, 1979.
  - Bunge et al., *Phil. Trans. Roy. Soc. A* , 2002.

• Variational method (VAR)
  - Bunge et al., *GJI*, 2003.
  - Ismail-Zadeh et al., *CMMP*, 2003; *PEPI*, 2004; *JGR*, 2006.

• Quasi-reversibility method (QRV)
  - Ismail-Zadeh et al., *GJI*, 2007.