Presented at the COMSOL Conference 2010 India

COMSOL Multiphysics in Earth Science Education and Research

R N Singh
INSA Senior Scientist
National geophysical research Institute
Hyderabad
rnsingh@ngri.res.in, 30Oct10

Talk outline

- Introduction
- Main problem of geology
- Numerical modeling as main tool
- Earth science equations and COMSOL Multiphysics
- Effect of erosion/ fluid infiltration on thermal structure of lithosphere
- Concluding remarks

Earth’s processes

- Earth’s materials are in many phases : solid, liquid, gas
- Processes like heat conduction/convection; electromagnetic induction/MHD; elastic , viscous; coupled processes, take place
- Modeling all these physical processes collectively is needed for exploring natural resources, protection against natural hazards and environmental degradation

Basic problem of Earth Science

- Earth's interior is cooling and this leads to all geological phenomena observed at the surface
- Earth's cooling is determined mainly by how heat is lost by bulky mantle, less by crust or core cooling.
- Mantle cools by mode of transport of heat, by solid state convection , no inertia, rotation and highly viscous.
- This process generates deformation of surface region and melts to add to curst and also heat for metamorphism.
- So earth science education and research should have a focus on mantle convection problem both global and local such as underlying and around Indian region for understanding Indian geology.

Mathematical Modeling in earth science

- Conversion of hypothetical ideas of geological processes to mathematical equations, like algebraic and ordinary differential and partial differential equations.
- Optimizing parameters by assimilating geological data with solution of these equations
- Equations used earth sciences is summarized in sequel.

Conservation laws for geodynamics

Conservation of mass:

$$\frac{D\rho}{Dt} + \rho\nabla \bullet \vec{v} = 0$$

$$\frac{D}{Dt} \equiv \frac{\partial}{\partial t} + \vec{v} \bullet \nabla$$

Conservation of momentum:

$$\rho\frac{D\vec{v}}{Dt} = \nabla \bullet \overline{\overline{T}}^{T} + \rho\vec{b}$$

(superscript T refers to transpose of $\overline{T}$)

Conservation of angular momentum:

$$\overline{T} = \overline{T}^{T}$$

Conservation of energy:

$$\rho\frac{DE}{Dt} = \overline{\overline{T}} \bullet \nabla\vec{v} - \nabla \bullet \vec{q} + \rho h$$

Entropy inequality

Here $\rho, \vec{v}, \overline{T}, \vec{b}, E, \vec{q}, h$ and T are density, velocity, stress tensor, force per unit mass, internal energy per unit mass, heat flux vector, internal energy source and temperature

Constitutive relationships fro geodynamics

Hooke's law:

$$\overline{\overline{T}} = \lambda\left(tr\overline{\overline{E}}\right)\overline{\overline{I}} + 2\mu\overline{\overline{E}} \qquad (6)$$

λ and μ are Lame' constants and $\overline{I}$ identity tensor and strain $\overline{E}$ is related to displacement $\vec{u}$ as

$$\overline{\overline{E}} = \frac{1}{2}\left(\nabla\vec{u} + \nabla\vec{u}^{T}\right) \qquad (7)$$

Stokes' law:

$$\overline{T} = \left[-p + \overline{\lambda}\left(tr\overline{\nabla}\right)\right]\overline{I} + 2\overline{\mu}\overline{D} \qquad (8)$$

p – pressure, $\overline{\lambda}$-elastic moduli, $\overline{\mu}$ - coefficient of viscosity, and $\overline{\overline{D}}$ - rate of deformation tensor, related to velocity as

$$\overline{D} = \frac{1}{2}\left(\nabla\vec{v} + \nabla\vec{v}^{T}\right) \qquad (9)$$

Constitutive relationships fro geodynamics

Fourier law:

$$\vec{q} = -k \nabla T$$

(k – thermal conductivity)

Fick's law:

$$\vec{F} = -D \nabla C$$

(C-concentration, D – diffusion coefficient)

Equation of state:

$$\rho = \rho_0 \left[1 - \beta (T - T_0) - \beta_C (C - C_0)\right]$$

where β and β_c are thermal expansion and chemical buoyancy coefficients.

Conservation laws for electromagnetism

4 For electromagnetic phenomena the relevant conservation laws are of those of conservation electric charge and magnetic flux. These Maxwell equations are written in mathematical form as

$$\nabla X\vec{E} = -\frac{\partial}{\partial t}\vec{B} \qquad (13)$$

$$\nabla X\vec{H} = \vec{J} + \frac{\partial\vec{D}}{\partial t} \qquad (14)$$

$$\nabla \bullet \vec{B} = 0 \qquad (15)$$

$$\nabla \bullet \vec{D} = \rho \qquad (16)$$

where $\vec{E}, B, \vec{D}, \vec{H}$, $\vec{J}$ and ρ are electric field, magnetic field, electrical displacement vector, magnetic displacement vector, electric current and electric charge respectively.

Constitutive relationship for electromagnetism

The constitutive relationships for electromagnetic phenomena are:

$$\vec{J} = \sigma\left(\vec{E} + \vec{v} X \vec{B}\right) \quad (17)$$

$$\vec{B} = \mu \vec{H} \quad (18)$$

$$\vec{D} = \varepsilon \vec{E} \quad (19)$$

(σ - electrical conductivity, μ - magnetic permeability, ε – dielectric constant)

Governing equation for geopotential fields

For gravity:

$$\nabla^2 \phi = -4\pi\rho G \quad \textit{with in the body}$$

$$= 0 \quad \textit{outside the body}$$

(ϕ : gravitational scalar potential, G- gravitational constant)

For magnetics:

$$\nabla^2 A = 4\pi \nabla \bullet \vec{M} \quad \textit{inside the body}$$

$$= 0 \quad \textit{outside the body}$$

(A – Magnetic scalar potential, $\vec{M}$ - magnetic dipole moment for unit volume)

Governing equation for elastic earth

For static elastic case:

$$\nabla^4 \vec{u} = 0 \tag{22}$$

$$D\frac{d^4 w}{dx^4} + N\frac{d^2 w}{dx^2} + (\rho_m - \rho_w)gw = q_a \tag{23}$$

(D – Flexural rigidity, N- in plain force, $\rho_m\,(\rho_w)$ - Mantle (water) density, q_a – surface load)

For elastic waves:

$$\rho\frac{\partial^2 u}{\partial t^2} = \mu\nabla^2\vec{u} + (\lambda + \mu)\nabla\nabla \bullet \vec{u} + \rho\vec{b}$$

Governing equation for thermal geophysics

For heat conduction and advection:

$$\rho c_p\left(\frac{\partial T}{\partial t}+\vec{v}\bullet\nabla T\right)=k\nabla^2 T+\rho h$$

(c_p - heat capacity and ρh – heat sources)

For thermal convection:

$$\nabla\bullet\vec{v}=0 \tag{27}$$

$$\rho_0\frac{Dv}{Dt}=-\nabla p+\mu\nabla\bullet\left[(\nabla v)+(\nabla v)^T\right]+\rho_0\vec{b}+\rho_0 g\beta[T-T_0] \tag{28}$$

$$\rho_0 C_v\frac{D}{Dt}T=-k\nabla^2 T+\rho h+\Phi \tag{29}$$

(Φ - viscous dissipation, g – acceleration due to gravity and β -coefficient of thermal expansion)

Equation for geochemical reaction and diffusion

For chemical diffusion:

$$\left(\frac{DC}{Dt}\right) = -D\nabla^2 C + R$$

(C – concentration variable; D – diffusion coefficient, R – chemical reaction rate)

Geochemcial fields in reactive media in are coupled with flow and deformation fields in the porous earth model .

Governing equation for kinematic dynamo

For electrical conduction in moving media:

$$\frac{\partial \vec{B}}{\partial t} = \eta \nabla^2 \vec{B} + \nabla X \left(\vec{v} X \vec{B} \right)$$

where $\eta = (\mu\rho)^{-1}$.

Big three equations

$$0 = \nabla^2 f \ : \text{Potential equation}$$

$$\frac{\partial f}{\partial t} = \nabla^2 f \ : \text{Parabolic equation}$$

$$\frac{\partial^2 f}{\partial^2 t} = \nabla^2 f \ : \text{Wave equation}$$

Solutions of these equations numerically obtained for realistic boundary shapes find large application in earth science data interpretation and forecasting.

Some challenging problems

- Finding past motions in the mantle constrained by observations of past plate motions and present tomography images of the earth. (Navier-Stokes equation constrained optimization)
- Find the core motions from observation of past geomagnetic field (MHD constrained optimization)
- Earthquake processes (equations for elastic waves and deformation, friction on fault, gravity/geoid constrained optimization)
- All using Multiphysics and optimization modules

PDE constrained optimization

- Given physicochemcial process in the earth

  - A set of PDEs, coupled
- Given observations of mechanical and electromagnetic fields
- Minimizing the norm of differences between data and computed data to get the parameters, initial/boundary conditions
- Such problems pervade all areas of earth science

Numerical modeling/ COMSOL Multiphysics

- Geological complexity *in full is* not amenable to analytical tools.
- Differential equations are reduced to algebraic equations in numerical modeling
- These sets of algebraic equations are solved by using computers
- Results are visualized in computer
- COMSOL multiphysics has been used for this purpose.

Effect of erosion/deposition on the thermal structure of a half space

PDE in coefficient form

$$\rho c\left(\frac{\partial T}{\partial t}+(-v)\frac{\partial T}{\partial z}\right)=K\frac{\partial^2 T}{\partial z^2}+A_0\exp(-(z+vt)/d)$$

(T, t, z, v) – (Temperature, time, vertical coordiante, uplift rate)

$(\rho$, c, K) - (density, heat capacity, thermal conductivity)

d - a constant

For deposition sign of v is positive

Erosion.pdf

Effect of CO2 infiltration from depth on the thermal structure of a half space

Defining equation in coefficient form

$$\rho c\left(\frac{\partial T}{\partial t} - v\frac{\partial T}{\partial z}\right) = K\frac{\partial^2 T}{\partial z^2} + A_0 \exp(-z/d)$$

$(T, t, z, v) -$ (Temperature, time, vertical coordinate, fluid velocity)

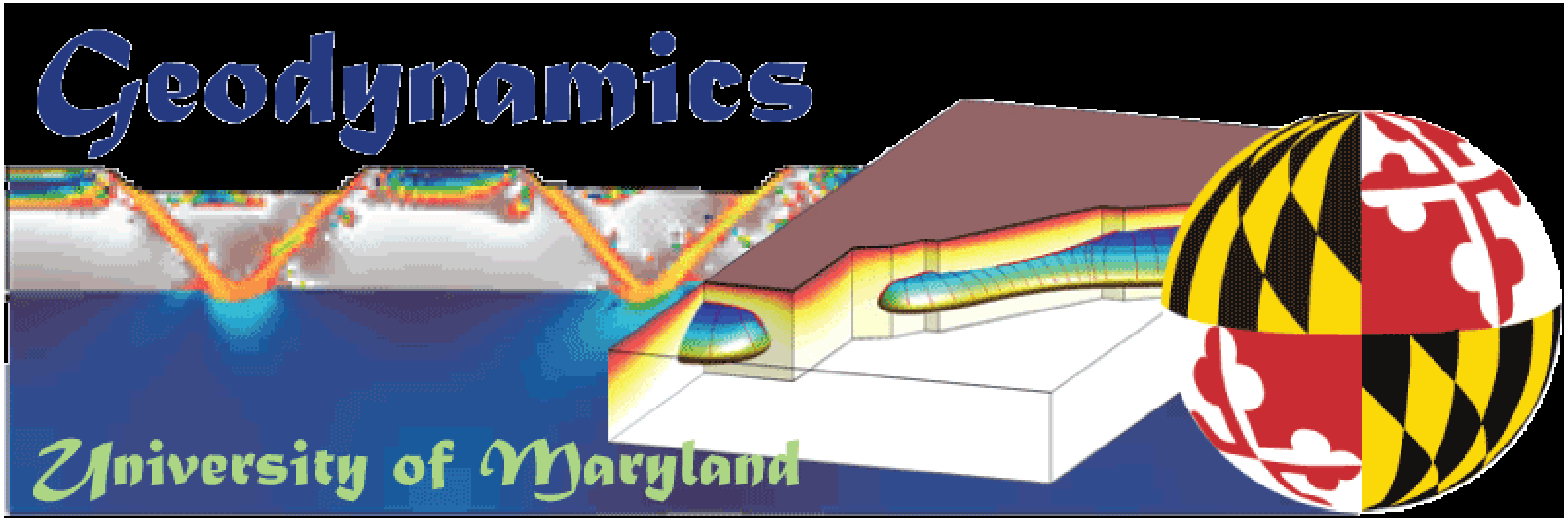
(ρ, c, K) - (density, heat capacity, thermal conductivity)

d - a constant

Advection.pdf

Earth science education

- Collecting observation in ever increasing details and hoping pattern to understand data will emerge: empiricism
- Construction of models of patterns
- Need both instruments and mathematics
- Modeling method for teaching earth science, like Hestenes approach to physics
- COMSOL multiphysics can be used as an excellent tool for such teaching



COMSOL Multiphysics has been used in constructing models of typical geodynamical processes.

http://www.geology.umd.edu/~montesi/Geodynamics/ComsolModels.shtml

An interesting application of COMSOL Multiphysics

Linking Physical and Numerical Modelling in Hydrogeology using Sand Tank Experiments and COMSOL Multiphysics

Kamini Singha[1] and Steven P. Loheide II[2]

[1] Department of Geosciences, Penn State University, Pennsylvania, USA

[2] Department of Civil and Environmental Engineering, University of Wisconsin-Madison, Wisconsin, USA

International J. Sci. Education, 1-25, 2010.

Concluding remarks

- Earth is being observed by many platforms and now observations constitute big data sets.
- All data need to be fitted with a earth model, so multiphysics and data assimilation are needed.
- COMSOL multiphysics has found applications in several areas and this activity is expanding