COMSOL Multiphysics in Earth Science Education and Research

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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 crust 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:
\[
\frac{D\rho}{Dt} + \rho \nabla \cdot \vec{v} = 0
\]

Conservation of momentum:
\[
\rho \frac{D\vec{v}}{Dt} = \nabla \cdot \vec{T}^T + \rho \vec{b}
\]

(superscript T refers to transpose of \( \vec{T} \))

Conservation of angular momentum:
\[
\vec{T} = \vec{T}^T
\]

Conservation of energy:
\[
\rho \frac{DE}{Dt} = \vec{T} \cdot \nabla \vec{v} - \nabla \cdot \vec{q} + \rho h
\]

Entropy inequality

Here \( \rho, v, \vec{T}, \vec{b}, E, \vec{q}, h \) 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 for geodynamics

Hooke’s law:

$$\bar{T} = \lambda \left( \text{tr} \bar{E} \right) \bar{I} + 2\mu \bar{E}$$  \hspace{1cm} (6)

$\lambda$ and $\mu$ are Lame’ constants and $\bar{I}$ identity tensor and strain $\bar{E}$ is related to displacement $\bar{u}$ as

$$\bar{E} = \frac{1}{2} \left( \nabla \bar{u} + \nabla \bar{u}^T \right)$$  \hspace{1cm} (7)

Stokes’ law:

$$\bar{T} = \left[ -p + \lambda \left( \text{tr} \nabla \right) \right] \bar{I} + 2\mu \bar{D}$$  \hspace{1cm} (8)

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

$$\bar{D} = \frac{1}{2} \left( \nabla \bar{v} + \nabla \bar{v}^T \right)$$  \hspace{1cm} (9)
Constitutive relationships for 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 \( \beta \) and \( \beta_c \) 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

\[ \nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \]  \hspace{1cm} (13)

\[ \nabla \times \vec{H} = \vec{J} + \frac{\partial \vec{D}}{\partial t} \]  \hspace{1cm} (14)

\[ \nabla \cdot \vec{B} = 0 \]  \hspace{1cm} (15)

\[ \nabla \cdot \vec{D} = \rho \]  \hspace{1cm} (16)

where \( \vec{E}, \vec{B}, \vec{D}, \vec{H}, \vec{J} \) and \( \rho \) 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:

\[ J = \sigma (E + v \times B) \]  \hspace{1cm} (17)

\[ \dot{B} = \mu \dot{H} \]  \hspace{1cm} (18)

\[ \dot{D} = \varepsilon \dot{E} \]  \hspace{1cm} (19)

(\( \sigma \) - electrical conductivity, \( \mu \) - magnetic permeability, \( \varepsilon \) - dielectric constant)
Governing equation for geopotential fields

For gravity:
\[ \nabla^2 \phi = -4\pi \rho G \quad \text{within the body} \]
\[ = 0 \quad \text{outside the body} \]
(\( \phi \): gravitational scalar potential, \( G \): gravitational constant)

For magnetics:
\[ \nabla^2 A = 4\pi \nabla \cdot \vec{M} \quad \text{inside the body} \]
\[ = 0 \quad \text{outside the body} \]
(\( A \): Magnetic scalar potential, \( \vec{M} \): magnetic dipole moment for unit volume)
For static elastic case:

\[ \nabla^4 \ddot{u} = 0 \]  
(22)

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

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

For elastic waves:

\[ \rho \frac{\partial^2 u}{\partial t^2} = \mu \nabla^2 \ddot{u} + (\lambda + \mu) \nabla \nabla \cdot \ddot{u} + \rho \dddot{b} \]
Governing equation for thermal geophysics

For heat conduction and advection:

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

( \( c_p \) - heat capacity and \( \rho h \) - heat sources)

For thermal convection:

\[
\nabla \cdot \vec{v} = 0
\]

\[
\rho_0 \frac{D\vec{v}}{Dt} = -\nabla p + \mu \nabla \cdot \left[ (\nabla \vec{v}) + (\nabla \vec{v})^T \right] + \rho_0 \bar{b} \cdot \rho_0 g \beta [T - T_0]
\]  \hspace{1cm} (27)

\[
\rho_0 C_v \frac{D}{Dt} T = -k \nabla^2 T + \rho h + \Phi
\]  \hspace{1cm} (29)

( \( \Phi \) - viscous dissipation, \( g \) - acceleration due to gravity and \( \beta \) - 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:

\[
\frac{\partial \mathbf{B}}{\partial t} = \eta \nabla^2 \mathbf{B} + \nabla \times \left( \nu \mathbf{X} \mathbf{B} \right)
\]

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 physicochemical 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

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

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

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

d - a constant

For deposition, sign of \(v\) is positive
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)

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

d - a constant
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.

An interesting application of COMSOL Multiphysics

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

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Concluding remarks

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