Numerical Geodynamics Modelling

(there is no free lunch)

C. Thieulot (c.thieulot@uu.nl)

March 2014

Motivation

2.2. 2D model setup and numerical method

We consider a 2D model domain of 2400 km by 400 km, with an initially horizontally layered lithosphere and underlying mantle (see Fig. 1A). The oceanic crust is subdivided into a 4 km thick upper and an 8 km thick lower crust (see Table S2 for employed material parameters). The thickness of the underlying lithosphere is defined by the 1200 °C isotherm. The initial temperature field of the model is computed numerically by solving the heat diffusion equation in 1D for a half space cooling model, taking into account radioactive heating. To create a thermal heterogeneity at time zero and horizontal coordinate 0 km, the model is divided in two subdomains (left and right) with the right subdomain having a 5 Ma younger thermal age ϒ. The resulting temperature jump is smoothed with an arctan-like interpolant from −200 to 200 km.

The model domain is discretized using quadrilateral elements with quadratic shape functions for velocity and temperature and discontinuous linear shape functions for pressure (Q_2P_{-1}, Cuvelier et al., 1986). Between −500 and 500 km width and depths less than 250 km, node spacing is 2 km in both x- and z-direction. Outside this region, node spacing increases by 2% per element until a maximum spacing of 20 km is reached. To solve Eqs. (1)–(8) on this grid, we use the finite element code MILAMIN_VEP (e.g. Crameri and Kaus, 2010; Kaus, 2010). It employs the finite element method and uses an efficient matrix-assembly method (Dabrowski et al., 2008). This code has been benchmarked vs. analytical solutions as well as vs. other numerical codes (e.g. Kaus, 2010). Advection of properties (composition, temperature, stress etc.) is done by deforming the Lagrangian mesh. Remeshing is applied every 30 timesteps and 2.7 million (initially randomly distributed) markers are used to transfer properties from the old to the new mesh. During remeshing, nodal properties are interpolated to the markers using the element shape functions and then interpolated back to the new mesh. To avoid numerical instabilities, we employ a lower and an upper viscosity cutoff of 10^{18} Pa s and 10^{26} Pa s respectively, as well as the free surface stabilization algorithm (Kaus et al., 2010).

The energy equation is solved with isothermal top and bottom boundaries (273 and 1600 K respectively) and flux-free side boundaries. The mechanical boundary conditions are free surface

Thielmann et al, EPSL 359, 2012

3 DISCRETIZATION AND SOLVERS

The Rhea code is custom written in C. It uses the Message Passing Interface to implement distributed parallelism. For the discretization of the temperature, velocity and the pressure in (1)–(3), we use (tri-)linear finite elements on locally refined hexahedral meshes. These meshes are adapted to resolve features of the velocity, pressure or viscosity fields. Practical challenges, as well as the technical details required for parallel adaptive simulations, are discussed in Section 4. In this section, we focus on the discretization and on the solvers used in Rhea. Because of the large size of the matrices that result from the discretization, linear system cannot be solved using direct factorization-based solvers but have to be solved using iterative solution algorithms.

3.1 Variational formulation of Stokes equations

The finite element discretization is based on the weak form of the system of partial differential equations derived from (1) and (2) by multiplication with admissible test functions $\mathbf{v}$ and q (omitting the differentials d$\boldsymbol{x}$, etc. for brevity),

$$\int_\Omega \left[\nabla\cdot\left(p\mathbf{I}-\mu(\nabla\mathbf{u}+\nabla\mathbf{u}^\top)\right)-\mathbf{f}\right]\cdot\mathbf{v}=0 \quad \text{for all } \mathbf{v}, \qquad (4a)$$

$$\int_\Omega (\nabla\cdot\mathbf{u})\,q=0 \quad \text{for all q}, \qquad (4b)$$

and integration by parts which yields

$$A(\mathbf{u},\mathbf{v})+B(\mathbf{v},p)+E(p,\mathbf{u},\mathbf{v})=F(\mathbf{v}) \quad \text{for all } \mathbf{v}, \qquad (5a)$$

Burstedde et al, GJI 192, 2013

What does Numerical geodynamics modelling mean ?

- Modelling: the process of solving physical problems by appropriate simplification of reality.
- A computer simulation is a simulation, run on a single computer, or a network of computers, to reproduce behavior of a system. (Wikipedia)

Why numerical simulation ?

- because experiments are sometimes impossible
  (life cycle of galaxies, weather forecast, terror attacks)

Why numerical simulation ?

- because experiments are sometimes impossible
  (life cycle of galaxies, weather forecast, terror attacks)
- because experiments are sometimes not welcome
  (avalanches, nuclear tests, medicine)

Why numerical simulation ?

- because experiments are sometimes impossible
  (life cycle of galaxies, weather forecast, terror attacks)
- because experiments are sometimes not welcome
  (avalanches, nuclear tests, medicine)
- because experiments are sometimes very costly and-time consuming
  (protein folding, material sciences)

Why numerical simulation ?

- because experiments are sometimes impossible
  (life cycle of galaxies, weather forecast, terror attacks)
- because experiments are sometimes not welcome
  (avalanches, nuclear tests, medicine)
- because experiments are sometimes very costly and-time consuming
  (protein folding, material sciences)
- because experiments are sometimes more expensive
  (aerodynamics, crash test)

Why numerical simulation ?

- because experiments are sometimes impossible
  (life cycle of galaxies, weather forecast, terror attacks)
- because experiments are sometimes not welcome
  (avalanches, nuclear tests, medicine)
- because experiments are sometimes very costly and-time consuming
  (protein folding, material sciences)
- because experiments are sometimes more expensive
  (aerodynamics, crash test)
- because it's fun.

What can we do ? what is it useful for ?

- Mantle convection

  Trompert & Hansen, Phys. Fluids 10, 1998, Tackley, PEPI 171, 2008, Tosi et al, PEPI 217, 2013

What can we do ? what is it useful for ?

- Mantle convection

  Trompert & Hansen, Phys. Fluids 10, 1998, Tackley, PEPI 171, 2008, Tosi et al, PEPI 217, 2013

- Subduction

  Upton, Tectonics 22, 2003, Billen, Annu. Rev. Earth Planet. Sci. 2008 + 1 million other papers

What can we do ? what is it useful for ?

- Mantle convection

  Trompert & Hansen, Phys. Fluids 10, 1998, Tackley, PEPI 171, 2008, Tosi et al, PEPI 217, 2013

- Subduction

  Upton, Tectonics 22, 2003, Billen, Annu. Rev. Earth Planet. Sci. 2008 + 1 million other papers

- Orogenesis

  Beaumont et al, JGR 105, 2000, Gerbault et al, PEPI 177, 2009, Capitanio, Nature Comm. 480, 2011

What can we do ? what is it useful for ?

- Mantle convection

  Trompert & Hansen, Phys. Fluids 10, 1998, Tackley, PEPI 171, 2008, Tosi et al, PEPI 217, 2013

- Subduction

  Upton, Tectonics 22, 2003, Billen, Annu. Rev. Earth Planet. Sci. 2008 + 1 million other papers

- Orogenesis

  Beaumont et al, JGR 105, 2000, Gerbault et al, PEPI 177, 2009, Capitanio, Nature Comm. 480, 2011

- Salt tectonics

  Poliakov et al, Tectonophys. 226, 1993, Albertz and Beaumont, Tectonics 29, 2010, Gradmann & Beaumont, Tectonics 31, 2012

What can we do ? what is it useful for ?

- Mantle convection

  Trompert & Hansen, Phys. Fluids 10, 1998, Tackley, PEPI 171, 2008, Tosi et al, PEPI 217, 2013

- Subduction

  Upton, Tectonics 22, 2003, Billen, Annu. Rev. Earth Planet. Sci. 2008 + 1 million other papers

- Orogenesis

  Beaumont et al, JGR 105, 2000, Gerbault et al, PEPI 177, 2009, Capitanio, Nature Comm. 480, 2011

- Salt tectonics

  Poliakov et al, Tectonophys. 226, 1993, Albertz and Beaumont, Tectonics 29, 2010, Gradmann & Beaumont, Tectonics 31, 2012

- Delamination/instabilities

  Schott, Tectonophysics 296, 1998, van Wijk, Geology 38, 2010

What can we do ? what is it useful for ?

- Mantle convection

  Trompert & Hansen, Phys. Fluids 10, 1998, Tackley, PEPI 171, 2008, Tosi et al, PEPI 217, 2013

- Subduction

  Upton, Tectonics 22, 2003, Billen, Annu. Rev. Earth Planet. Sci. 2008 + 1 million other papers

- Orogenesis

  Beaumont et al, JGR 105, 2000, Gerbault et al, PEPI 177, 2009, Capitanio, Nature Comm. 480, 2011

- Salt tectonics

  Poliakov et al, Tectonophys. 226, 1993, Albertz and Beaumont, Tectonics 29, 2010, Gradmann & Beaumont, Tectonics 31, 2012

- Delamination/instabilities

  Schott, Tectonophysics 296, 1998, van Wijk, Geology 38, 2010

- Extensional systems

  Huismans et al, JGR 110, 2005, Allken et al, Basin Research 25, 2013,

What can we do ? what is it useful for ?

- Mantle convection

  Trompert & Hansen, Phys. Fluids 10, 1998, Tackley, PEPI 171, 2008, Tosi et al, PEPI 217, 2013

- Subduction

  Upton, Tectonics 22, 2003, Billen, Annu. Rev. Earth Planet. Sci. 2008 + 1 million other papers

- Orogenesis

  Beaumont et al, JGR 105, 2000, Gerbault et al, PEPI 177, 2009, Capitanio, Nature Comm. 480, 2011

- Salt tectonics

  Poliakov et al, Tectonophys. 226, 1993, Albertz and Beaumont, Tectonics 29, 2010, Gradmann & Beaumont, Tectonics 31, 2012

- Delamination/instabilities

  Schott, Tectonophysics 296, 1998, van Wijk, Geology 38, 2010

- Extensional systems

  Huismans et al, JGR 110, 2005, Allken et al, Basin Research 25, 2013,

- Magma transport

  Yamato et al, Tectonophysics 526, 2012

What can we do ? what is it useful for ?

- Mantle convection

  Trompert & Hansen, Phys. Fluids 10, 1998, Tackley, PEPI 171, 2008, Tosi et al, PEPI 217, 2013
- Subduction

  Upton, Tectonics 22, 2003, Billen, Annu. Rev. Earth Planet. Sci. 2008 + 1 million other papers
- Orogenesis

  Beaumont et al, JGR 105, 2000, Gerbault et al, PEPI 177, 2009, Capitanio, Nature Comm. 480, 2011
- Salt tectonics

  Poliakov et al, Tectonophys. 226, 1993, Albertz and Beaumont, Tectonics 29, 2010, Gradmann & Beaumont, Tectonics 31, 2012
- Delamination/instabilities

  Schott, Tectonophysics 296, 1998, van Wijk, Geology 38, 2010
- Extensional systems

  Huismans et al, JGR 110, 2005, Allken et al, Basin Research 25, 2013,
- Magma transport

  Yamato et al, Tectonophysics 526, 2012
- Whole planet evolution

  de Vries et al, EPSL 292, 2010,

What can we do ? what is it useful for ?

- Mantle convection

  Trompert & Hansen, Phys. Fluids 10, 1998, Tackley, PEPI 171, 2008, Tosi et al, PEPI 217, 2013
- Subduction

  Upton, Tectonics 22, 2003, Billen, Annu. Rev. Earth Planet. Sci. 2008 + 1 million other papers
- Orogenesis

  Beaumont et al, JGR 105, 2000, Gerbault et al, PEPI 177, 2009, Capitanio, Nature Comm. 480, 2011
- Salt tectonics

  Poliakov et al, Tectonophys. 226, 1993, Albertz and Beaumont, Tectonics 29, 2010, Gradmann & Beaumont, Tectonics 31, 2012
- Delamination/instabilities

  Schott, Tectonophysics 296, 1998, van Wijk, Geology 38, 2010
- Extensional systems

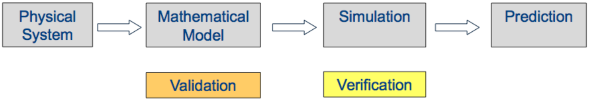
  Huismans et al, JGR 110, 2005, Allken et al, Basin Research 25, 2013,
- Magma transport

  Yamato et al, Tectonophysics 526, 2012
- Whole planet evolution

  de Vries et al, EPSL 292, 2010,
- plume dynamics

  van Hunen & Zhong, GRL 30, 2003, Ueda et al, PEPI 171, 2008, Tosi and Yuen, EPSL 312, 2011 Tan et al, G3 12, 2011

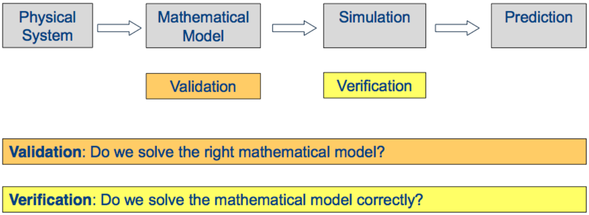
The Main Elements of Simulation



Validation: Do we solve the right mathematical model?

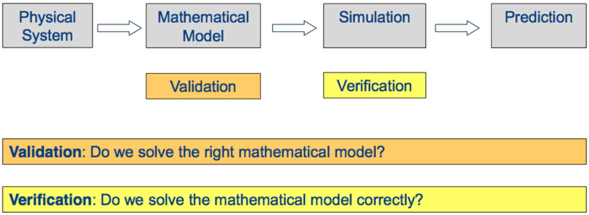
Verification: Do we solve the mathematical model correctly?

The Main Elements of Simulation



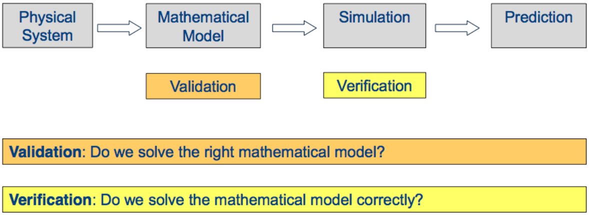
1. construction of a mathematical model for corresponding physical problems with appropriate assumptions. (ODE's, PDE's)

The Main Elements of Simulation



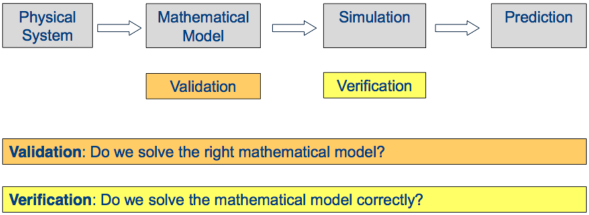
1. construction of a mathematical model for corresponding physical problems with appropriate assumptions. (ODE's, PDE's)
2. development of an appropriate numerical model or approximation to the mathematical model. The numerical model usually needs to be carefully calibrated and validated against pre-existing data and analytical results (Error analysis)

The Main Elements of Simulation



1. construction of a mathematical model for corresponding physical problems with appropriate assumptions. (ODE's, PDE's)
2. development of an appropriate numerical model or approximation to the mathematical model. The numerical model usually needs to be carefully calibrated and validated against pre-existing data and analytical results (Error analysis)
3. theoretical modeling is actual implementation of the numerical model to obtain solutions.

The Main Elements of Simulation



1. construction of a mathematical model for corresponding physical problems with appropriate assumptions. (ODE's, PDE's)
2. development of an appropriate numerical model or approximation to the mathematical model. The numerical model usually needs to be carefully calibrated and validated against pre-existing data and analytical results (Error analysis)
3. theoretical modeling is actual implementation of the numerical model to obtain solutions.
4. interpretation of the numerical results in graphics, charts, tables, or other convenient forms, to support engineering design and operation.

Overview of methods

There are many methods actually used in the community:

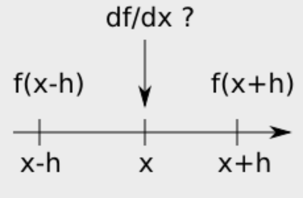
- Finite Differences Method (FDM)
- Finite Element Method (FEM)
- Finite Volume Method (FVM)
- Spectral methods
- Streamline methods

The Finite Differences Method (1)

The derivative of a function f at a point x is defined by the limit

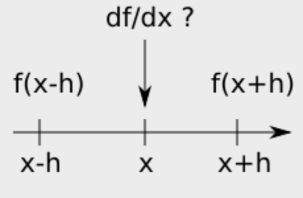
$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h} \simeq \frac{f(x+dx) - f(x)}{dx}$$

The Finite Differences Method (2)

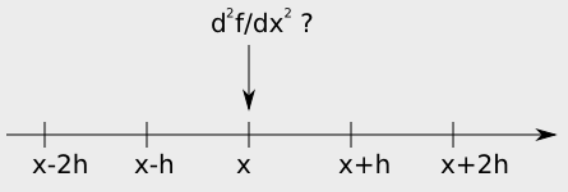


$$\frac{\partial f}{\partial x} = \frac{\Delta f}{\Delta x} = \frac{f(x+h) - f(x-h)}{2h}$$

The Finite Differences Method (2)



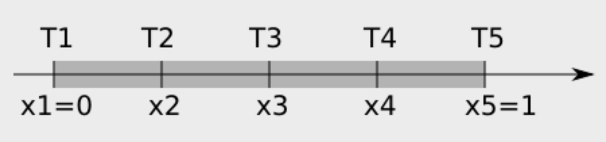
$$\frac{\partial f}{\partial x} = \frac{\Delta f}{\Delta x} = \frac{f(x+h) - f(x-h)}{2h}$$



$$\frac{\partial^2 f}{\partial x^2} = \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial x}\right) = \frac{\left(\frac{\partial f}{\partial x}\right)_{(x+h)} - \left(\frac{\partial f}{\partial x}\right)_{(x-h)}}{2h}$$

The Finite Differences Method (3)

- I wish to solve the PDE $\frac{dT}{dx} = 1$ on the segment $[0 : L]$.
- Obviously, the solution is of the type $T(x) = C$ where C is a constant
- I therefore need one boundary condition, say $T(x = 0) = T_A$



The following relationships then hold:

$$T(x = x_1) = T_A$$
$$\frac{T_2 - T_1}{x_2 - x_1} = 1$$
$$\frac{T_3 - T_2}{x_3 - x_2} = 1$$
$$\frac{T_4 - T_3}{x_4 - x_3} = 1$$
$$\frac{T_5 - T_4}{x_5 - x_4} = 1$$

The Finite Differences Method (4)

- Let us take $x_2 - x_1 = x_3 - x_2 = x_4 - x_3 = x_5 - x_4 = dx = L/(n-1)$
- the previous equations can be rewritten

$$\begin{aligned} T_1 &= T_A \\ T_2 - T_1 &= dx \\ T_3 - T_2 &= dx \\ T_4 - T_3 &= dx \\ T_5 - T_4 &= dx \end{aligned}$$

or,

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} T_1 \\ T_1 \\ T_3 \\ T_4 \\ T_5 \end{pmatrix} = \begin{pmatrix} T_A \\ dx \\ dx \\ dx \\ dx \end{pmatrix}$$

The Finite Differences Method (4)

- Let us take $x_2 - x_1 = x_3 - x_2 = x_4 - x_3 = x_5 - x_4 = dx = L/(n-1)$
- the previous equations can be rewritten

$$\begin{aligned} T_1 &= T_A \\ T_2 - T_1 &= dx \\ T_3 - T_2 &= dx \\ T_4 - T_3 &= dx \\ T_5 - T_4 &= dx \end{aligned}$$

or,

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} T_1 \\ T_1 \\ T_3 \\ T_4 \\ T_5 \end{pmatrix} = \begin{pmatrix} T_A \\ dx \\ dx \\ dx \\ dx \end{pmatrix}$$

- I need to solve a linear system of the type: $\mathbf{A} \cdot \mathbf{X} = \mathbf{B}$

The Finite Differences Method (4)

- Let us take $x_2 - x_1 = x_3 - x_2 = x_4 - x_3 = x_5 - x_4 = dx = L/(n-1)$
- the previous equations can be rewritten

$$\begin{aligned} T_1 &= T_A \\ T_2 - T_1 &= dx \\ T_3 - T_2 &= dx \\ T_4 - T_3 &= dx \\ T_5 - T_4 &= dx \end{aligned}$$

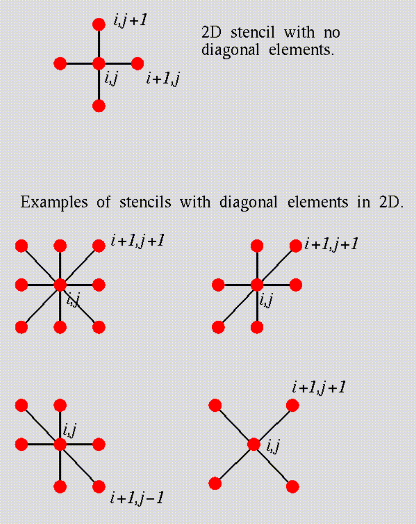
or,

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} T_1 \\ T_1 \\ T_3 \\ T_4 \\ T_5 \end{pmatrix} = \begin{pmatrix} T_A \\ dx \\ dx \\ dx \\ dx \end{pmatrix}$$

- I need to solve a linear system of the type: $\mathbf{A} \cdot \mathbf{X} = \mathbf{B}$
- more points $\rightarrow$ better precision $\rightarrow$ bigger matrix !

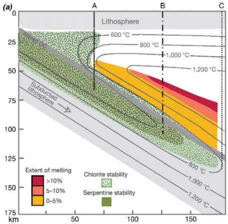
The Finite Differences Method (5)

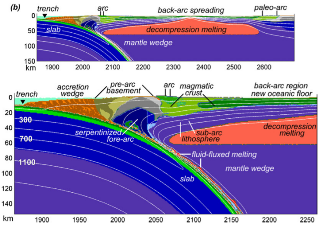
In two-dimensions ? ΔT ? $\nabla \cdot \mathbf{v}$?

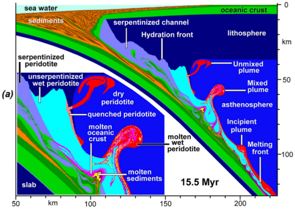


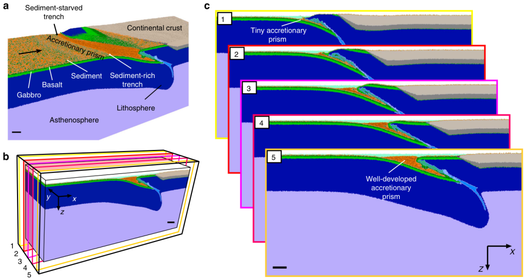
- The red-dot patterns are called stencils.

The Finite Difference Method (6)



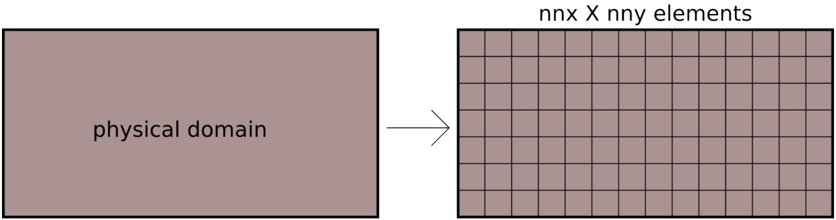


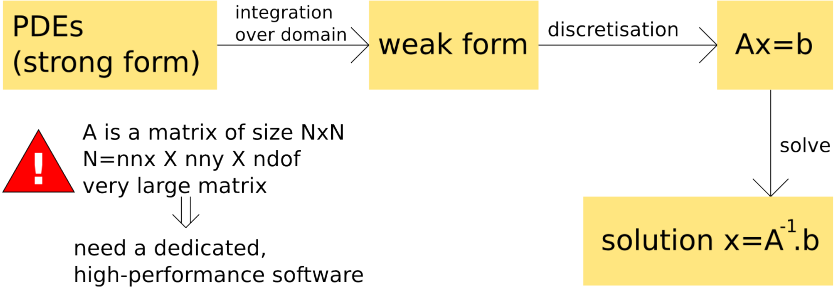




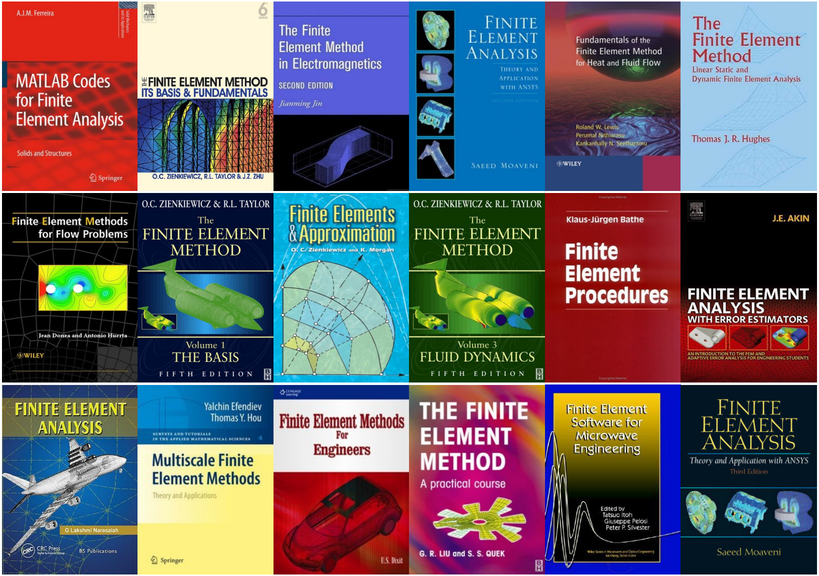
Gerya & Yuen, PEPI 140, 2003; PEPI 163, 2007, Gerya, J. of Geodyn. 52, 2011, Malatesta, Nature Comm. 2013

The Finite Element Method (1)

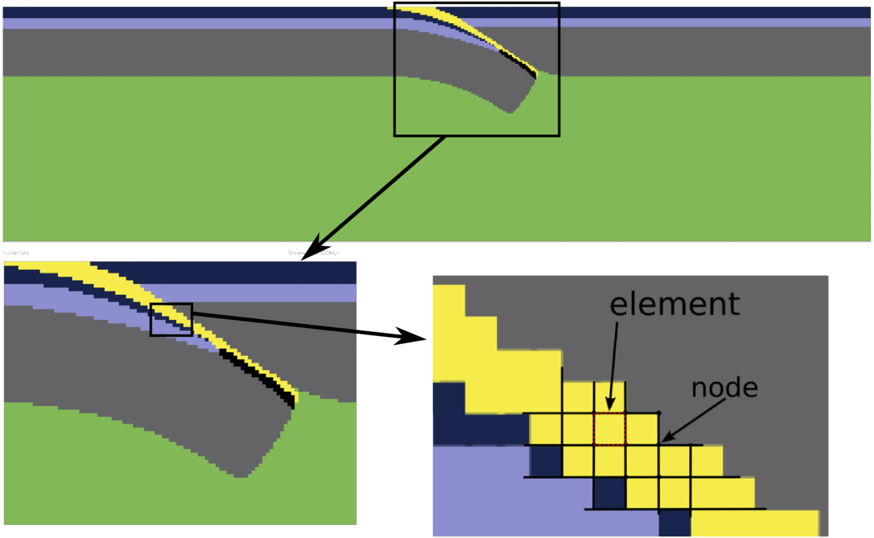




The Finite Element Method (2) - Resources

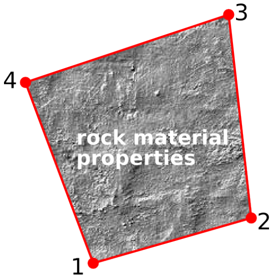


The Finite Element Method (3) - Basic principles



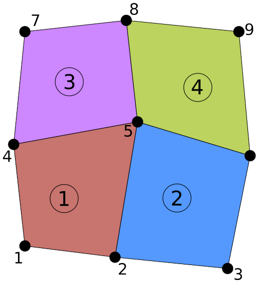
The Finite Element Method (4) - Basic principles

Each element :



$$\begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{pmatrix} \cdot \begin{pmatrix} T_1 \\ T_2 \\ T_3 \\ T_4 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{pmatrix}$$

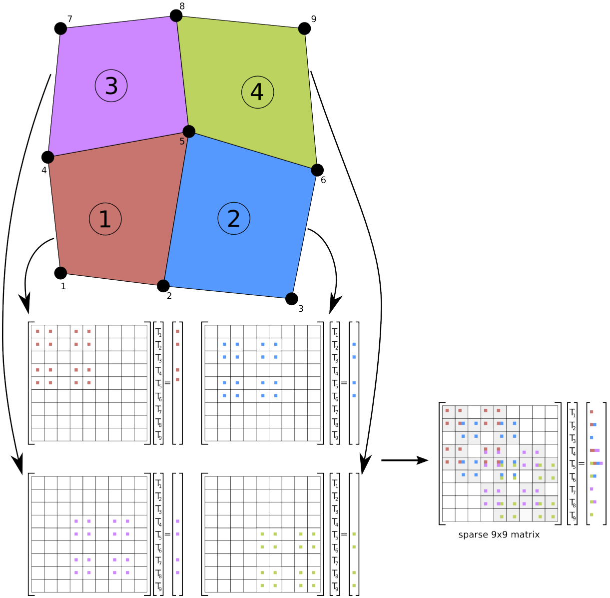
The Finite Element Method (6) - Basic principles



4 elements, 9 nodes

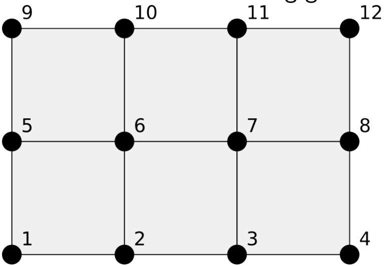
$$
\begin{pmatrix}
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot
\end{pmatrix}
\cdot
\begin{pmatrix}
T_1 \\ T_2 \\ T_3 \\ T_4 \\ T_5 \\ T_6 \\ T_7 \\ T_8 \\ T_9
\end{pmatrix}
=
\begin{pmatrix}
\cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot
\end{pmatrix}
$$

The Finite Element Method (7) - Basic principles



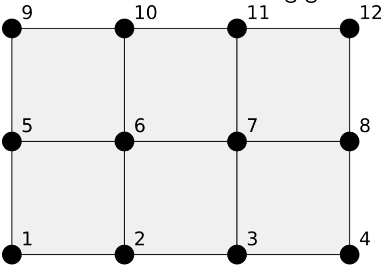
The Finite Element Method (8) - Basic principles

- Let us consider the following grid:



The Finite Element Method (8) - Basic principles

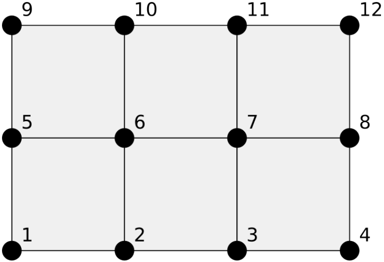
- Let us consider the following grid:



- There are 4x3 nodes and 3x2 elements.

The Finite Element Method (8) - Basic principles

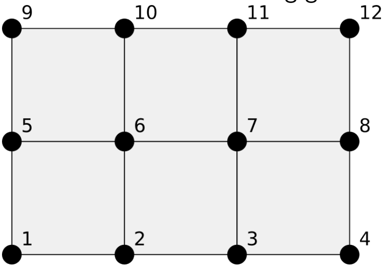
- Let us consider the following grid:



- There are 4x3 nodes and 3x2 elements.
- Heat transport equation: 1 degree of freedom (=unknown) at each node.
  $\rightarrow$ matrix size N=4x3x1=12

The Finite Element Method (8) - Basic principles

- Let us consider the following grid:

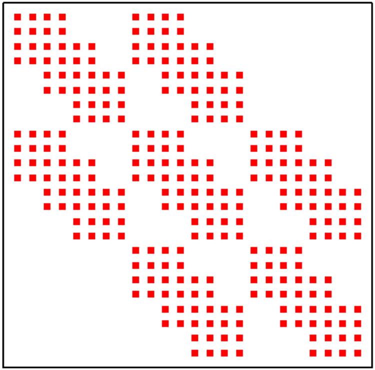


- There are 4x3 nodes and 3x2 elements.
- Heat transport equation: 1 degree of freedom (=unknown) at each node.
  $\rightarrow$ matrix size N=4x3x1=12
- Stokes equation: 2+1 (u, v, p) dofs per node.
  $\rightarrow$ matrix size N=4x3x1=36

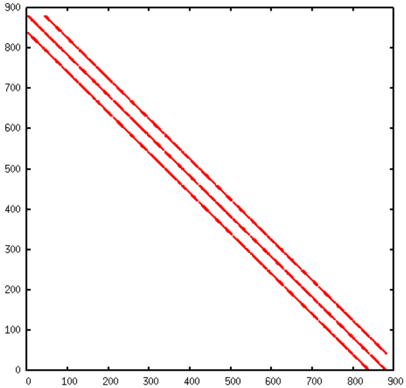
Stokes matrix always larger than temperature matrix !

The Finite Element Method (8) - Basic principles

Nodes only coupled with their nearest neighbours $\rightarrow$ sparse matrix.

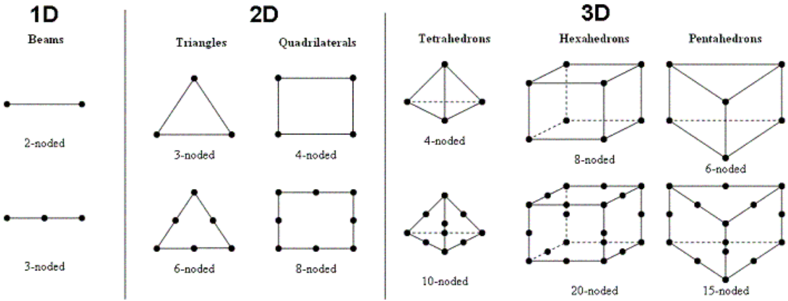


small grid

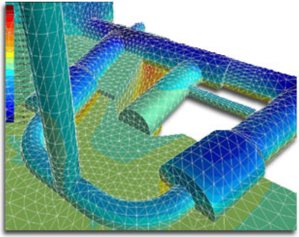
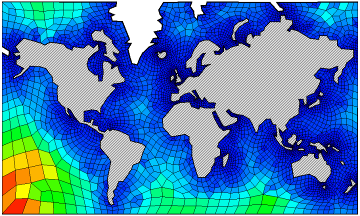
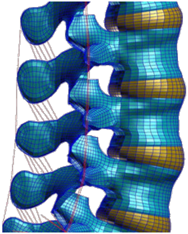


large grid

The Finite Element Method (9) - Elements



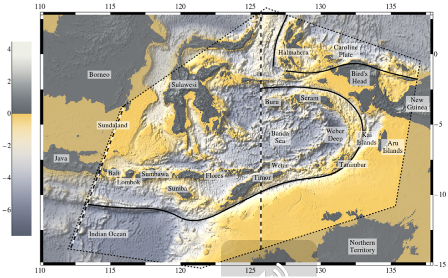
The Finite Element Method (10) - Meshing

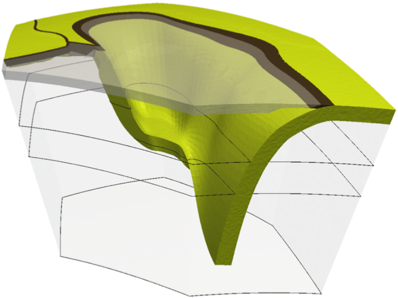




Meshing is can be complex and time consuming, especially in 3D

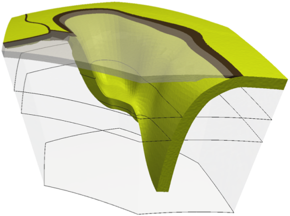
The Finite Element Method (11) - Meshing

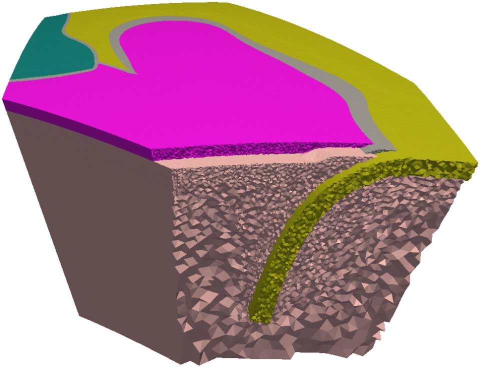
Master student Casper Pranger. "Numerical modelling of the Banda Arcs instantaneous subduction dynamics."



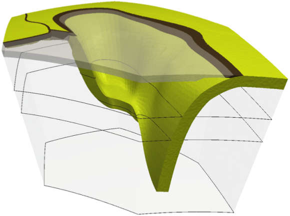


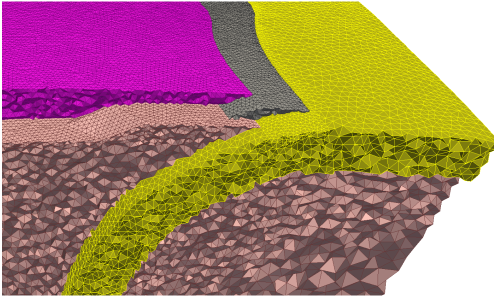
The Finite Element Method (12) - Meshing



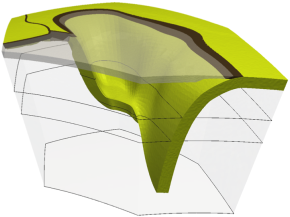


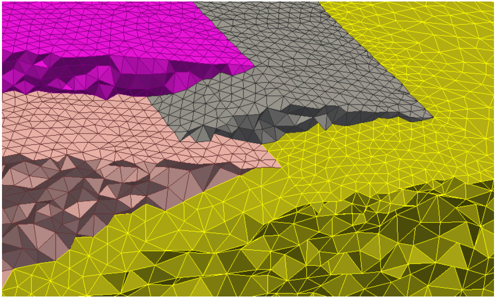
The Finite Element Method (12) - Meshing





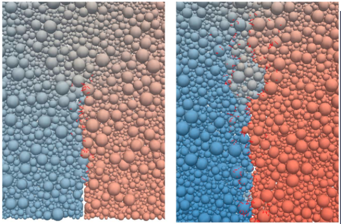
The Finite Element Method (12) - Meshing

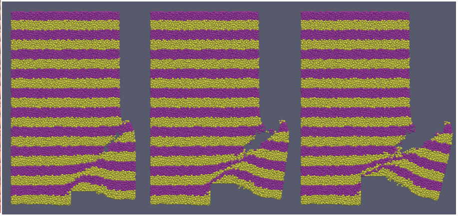




Other methods ?

Discrete Element Method (DEM)





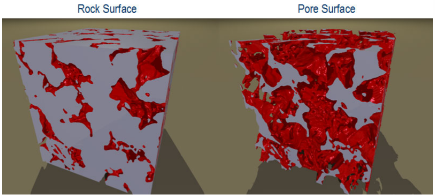
Extension fracture propagation

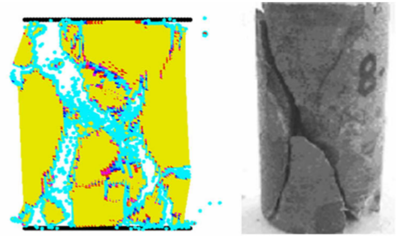
India-Asia collision

Virgo et al, JGR 118, 2013,

Other methods ?

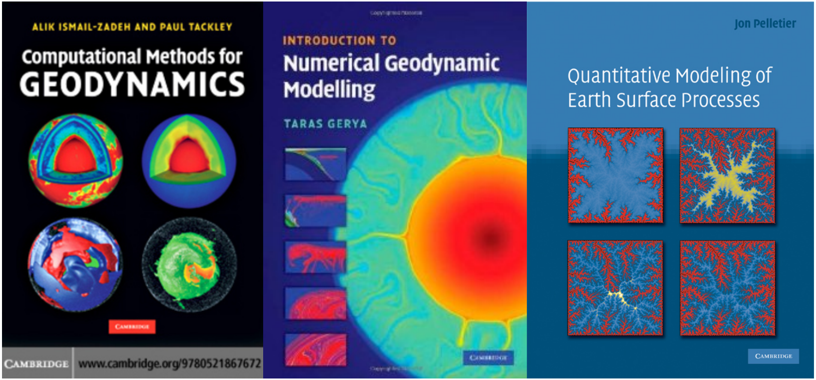
Smoothed Particle Hydrodynamics (SPH)





http://geonumerics.mit.edu/Technologies.aspx, Das & Cleary, Theoretical and Applied Fracture Mechanics 53, 2010

Resources


ALIK ISMAIL-ZADEH AND PAUL TACKLEY
Computational Methods for
GEODYNAMICS
CAMBRIDGE
www.cambridge.org/9780521867672
INTRODUCTION TO
Numerical Geodynamic
Modelling
TARAS GERYA
Jon Pelletier
Quantitative Modeling of
Earth Surface Processes
CAMBRIDGE

Parallelism (1) - Motivation

A simple example: we want ro run a simulation of the whole Earth mantle with a constant resolution of $5km$.

$$V_{mantle} = \frac{4}{3}\pi(R_{out}^3 - R_{in}^3) \simeq 10^{12} km^3$$

$$V_{cell} = 125 km^3$$

Number of cells needed:

$$N_{cell} = \frac{V_{mantle}}{V_{cell}} = 8 \times 10^9$$

Parallelism (1) - Motivation

A simple example: we want ro run a simulation of the whole Earth mantle with a constant resolution of $5km$.

$$V_{mantle} = \frac{4}{3}\pi(R_{out}^3 - R_{in}^3) \simeq 10^{12} km^3$$

$$V_{cell} = 125 km^3$$

Number of cells needed:

$$N_{cell} = \frac{V_{mantle}}{V_{cell}} = 8 \times 10^9$$

Matrix size is approx. 3-4 times the number of cells:

$$N \simeq 25 \times 10^9$$

Using between 9 and 125 markers per cell,

$$N_{markers} \geq 10^{10}$$

Parallelism (1) - Motivation

A simple example: we want ro run a simulation of the whole Earth mantle with a constant resolution of $5km$.

$$V_{mantle} = \frac{4}{3}\pi(R_{out}^3 - R_{in}^3) \simeq 10^{12} km^3$$

$$V_{cell} = 125 km^3$$

Number of cells needed:

$$N_{cell} = \frac{V_{mantle}}{V_{cell}} = 8 \times 10^9$$

Matrix size is approx. 3-4 times the number of cells:

$$N \simeq 25 \times 10^9$$

Using between 9 and 125 markers per cell,

$$N_{markers} \geq 10^{10}$$

$\Rightarrow$ Very large memory footprint & extremely long computational times.

Parallelism (1) - Motivation

A simple example: we want ro run a simulation of the whole Earth mantle with a constant resolution of $5km$.

$$V_{mantle} = \frac{4}{3}\pi(R_{out}^3 - R_{in}^3) \simeq 10^{12} km^3$$

$$V_{cell} = 125 km^3$$

Number of cells needed:

$$N_{cell} = \frac{V_{mantle}}{V_{cell}} = 8 \times 10^9$$

Matrix size is approx. 3-4 times the number of cells:

$$N \simeq 25 \times 10^9$$

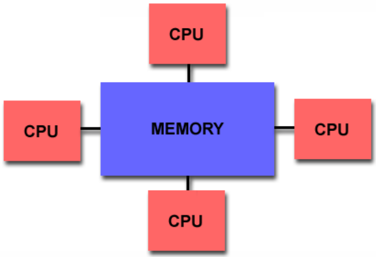
Using between 9 and 125 markers per cell,

$$N_{markers} \geq 10^{10}$$

$\Rightarrow$ Very large memory footprint & extremely long computational times.
$\Rightarrow$ Only way to overcome this: using supercomputers with many processors and large memory capacities.

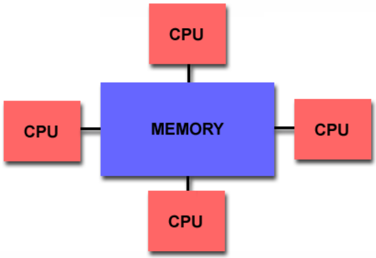
Parallelism (2)

- Shared memory

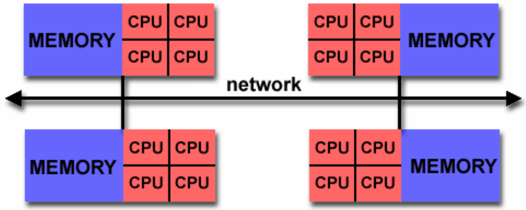


Parallelism (2)

- Shared memory

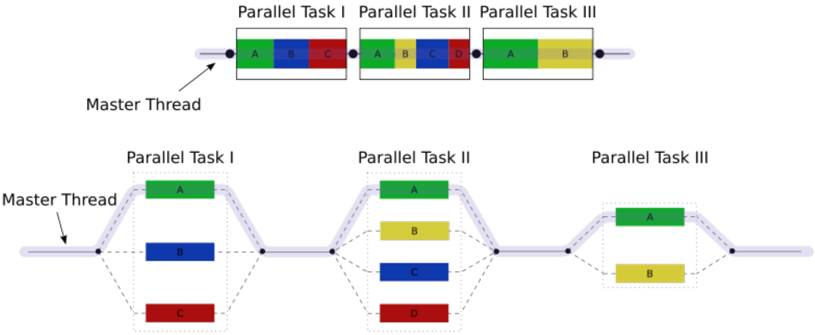


- Distributed memory



Parallelism - Programming paradigms

- OpenMP (1997, Open Multi-Processing) is an API that supports multi-platform shared memory multiprocessing programming in C, C++, and Fortran, on most processor architectures and operating systems, including Solaris, AIX, HP-UX, GNU/Linux, Mac OS X, and Windows platforms.
- It consists of a set of compiler directives, library routines, and environment variables that influence run-time behavior.



Parallelism - Programming paradigms

- MPI (1994, Message Passing Interface) is a standardized and portable message-passing system designed by a group of researchers from academia and industry to function on a wide variety of parallel computers.
- The standard defines the syntax and semantics of a core of library routines useful to a wide range of users writing portable message-passing programs in Fortran or the C programming language.
- There are several well-tested and efficient implementations of MPI, including some that are free or in the public domain.

Parallelism - coding

You can write a code, and then parallelise it.

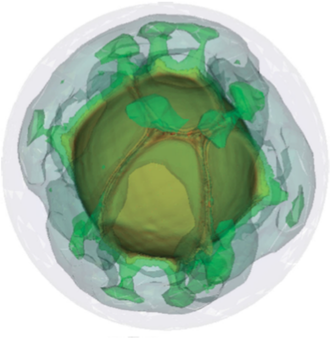
Parallelism - coding

You can write a code, and then parallelise it.

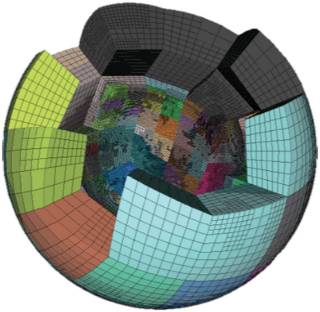
But you shouldn't.

Parallelism - Domain decomposition

An example of domain decomposition for a 3D convection problem in a spherical shell.



Isocontours of the temperature field.



Partitioning of the domain onto 512 proc.

The mesh has 1,424,176 cells. The solution has approximately 54 million unknowns (39 million vel., 1.7 million press., and 13 million temp.)

Kronbichler et al, GJI 191, 2012

Parallelism - Amdahl's law

The speedup of a program using multiple processors in parallel computing is limited by the time needed for the sequential fraction of the program.

Parallelism - Amdahl's law

The speedup of a program using multiple processors in parallel computing is limited by the time needed for the sequential fraction of the program.

Suppose 70% of a program can be sped up if parallelized and run on multiple CPUs instead of one. If α is the fraction of a calculation that is sequential, and $1 - \alpha$ is the fraction that can be parallelized, the maximum speedup that can be achieved by using P processors is given according to Amdahl's Law:

$$\frac{1}{\alpha + \frac{1-\alpha}{P}}$$

Parallelism - Amdahl's law

The speedup of a program using multiple processors in parallel computing is limited by the time needed for the sequential fraction of the program.

Suppose 70% of a program can be sped up if parallelized and run on multiple CPUs instead of one. If α is the fraction of a calculation that is sequential, and $1-\alpha$ is the fraction that can be parallelized, the maximum speedup that can be achieved by using P processors is given according to Amdahl's Law:

$$\frac{1}{\alpha + \frac{1-\alpha}{P}}$$

Using 4 processors: speedup=2.105
Using 8 processors: speedup=2.581
Using 1000 processors: speedup$\simeq$ 3.33

Parallelism - Scaling

- I am running a big task on many processors.

Parallelism - Scaling

- I am running a big task on many processors.
- It goes faster than on one processor !

Parallelism - Scaling

- I am running a big task on many processors.
- It goes faster than on one processor !

- How can I characterise parallel performance ?
- How well does the performance scale with the used ressources ?
- Does it make sense to use more ressources ?

Parallelism - Scaling

- I am running a big task on many processors.
- It goes faster than on one processor !

- How can I characterise parallel performance ?
- How well does the performance scale with the used ressources ?
- Does it make sense to use more ressources ?

⇒ Let's talk about scaling and scalability.

Parallelism - Scaling

In high performance computing there are two common notions of scalability:

Parallelism - Scaling

In high performance computing there are two common notions of scalability:

- The first is strong scaling, which is defined as how the solution time varies with the number of processors for a fixed total problem size.

Parallelism - Scaling

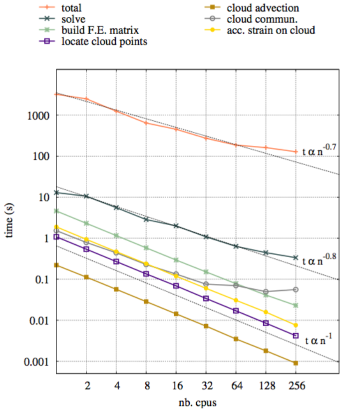
In high performance computing there are two common notions of scalability:

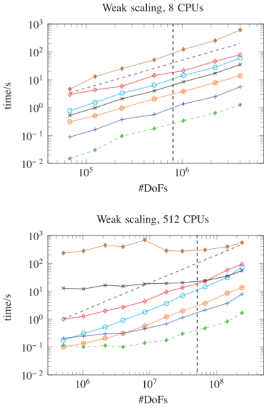
- The first is strong scaling, which is defined as how the solution time varies with the number of processors for a fixed total problem size.
- The second is weak scaling, which is defined as how the solution time varies with the number of processors for a fixed problem size per processor.

Parallelism - Scaling

In high performance computing there are two common notions of scalability:

- The first is strong scaling, which is defined as how the solution time varies with the number of processors for a fixed total problem size.
- The second is weak scaling, which is defined as how the solution time varies with the number of processors for a fixed problem size per processor.





Thieulot, PEPI 188, 2011, Kronbichler et al, GJI 191, 2012

Parallelism - Tools of the trade (1)

- Tablet
- Laptop
- Desktop
- Super Desktop/Server
- Beowulf
- Supercomputer

Parallelism - Tools of the trade (2)

(Super) Desktop computer

- 2.7 Ghz 12-core
- 64Gb RAM memory
- 1Tb flash drive
- ideal for development & running

Parallelism - Tools of the trade (3)

A Beowulf cluster is a computer cluster of what are normally identical, commodity-grade computers networked into a small local area network with libraries and programs installed which allow processing to be shared among them.

The result is a high-performance parallel computing cluster from inexpensive personal computer hardware.

Parallelism - Tools of the trade (3)

Supercomputers. (www.top500.org)

$\sim 300,000$ cores, $710 Gb$ RAM,
peak performance > 20 petaflops, i.e. 20,000 trillion calculations per second.

Parallelism - Tools of the trade (4)

Rank	Site	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	National Super Computer Center in Guangzhou China	**Tianhe-2 (MilkyWay-2)** - TH-IVB-FEP Cluster, Intel Xeon E5-2692 12C 2.200GHz, TH Express-2, Intel Xeon Phi 31S1P NUDT	3120000	33862.7	54902.4	17808
2	DOE/SC/Oak Ridge National Laboratory United States	**Titan** - Cray XK7 , Opteron 6274 16C 2.200GHz, Cray Gemini interconnect, NVIDIA K20x Cray Inc.	560640	17590.0	27112.5	8209
3	DOE/NNSA/LLNL United States	**Sequoia** - BlueGene/Q, Power BQC 16C 1.60 GHz, Custom IBM	1572864	17173.2	20132.7	7890
4	RIKEN Advanced Institute for Computational Science (AICS) Japan	K computer, SPARC64 VIIIfx 2.0GHz, Tofu interconnect Fujitsu	705024	10510.0	11280.4	12660
5	DOE/SC/Argonne National Laboratory United States	**Mira** - BlueGene/Q, Power BQC 16C 1.60GHz, Custom IBM	786432	8586.6	10066.3	3945
6	Swiss National Supercomputing Centre (CSCS) Switzerland	**Piz Daint** - Cray XC30, Xeon E5-2670 8C 2.600GHz, Aries interconnect , NVIDIA K20x Cray Inc.	115984	6271.0	7788.9	2325
7	Texas Advanced Computing Center/Univ. of Texas United States	**Stampede** - PowerEdge C8220, Xeon E5-2680 8C 2.700GHz, Infiniband FDR, Intel Xeon Phi SE10P Dell	462462	5168.1	8520.1	4510
8	Forschungszentrum Juelich (FZJ) Germany	**JUQUEEN** - BlueGene/Q, Power BQC 16C 1.600GHz, Custom Interconnect IBM	458752	5008.9	5872.0	2301

Adaptive Mesh Refinement (1)

Solid earth dynamics are governed by processes that occur over a wide range of time and length scales.

Adaptive Mesh Refinement (1)

Solid earth dynamics are governed by processes that occur over a wide range of time and length scales.
Examples:

- *Plate tectonics*: large-scale motion of plates over Myrs and length 1000's of kilometres and seismic processes that occur at timescales of minutes and less over lengths scales generally under 100km.

Adaptive Mesh Refinement (1)

Solid earth dynamics are governed by processes that occur over a wide range of time and length scales.
Examples:

- *Plate tectonics*: large-scale motion of plates over Myrs and length 1000's of kilometres and seismic processes that occur at timescales of minutes and less over lengths scales generally under 100km.
- *Upwellings associated with mantle convection*: wide range of length scales with large super plumes 1000s of kilometres across with small plumes detaching from their periphery that have thermal and mechanical boundary layers 100s of meters in thickness

Adaptive Mesh Refinement (1)

Solid earth dynamics are governed by processes that occur over a wide range of time and length scales.
Examples:

- *Plate tectonics*: large-scale motion of plates over Myrs and length 1000's of kilometres and seismic processes that occur at timescales of minutes and less over lengths scales generally under 100km.
- *Upwellings associated with mantle convection*: wide range of length scales with large super plumes 1000s of kilometres across with small plumes detaching from their periphery that have thermal and mechanical boundary layers 100s of meters in thickness
- *Thermochemical transport processes* in the mantle where chemical boundaries can be sharp over submeter length scales.

Adaptive Mesh Refinement (1)

Solid earth dynamics are governed by processes that occur over a wide range of time and length scales.
Examples:

- *Plate tectonics*: large-scale motion of plates over Myrs and length 1000's of kilometres and seismic processes that occur at timescales of minutes and less over lengths scales generally under 100km.
- *Upwellings associated with mantle convection*: wide range of length scales with large super plumes 1000s of kilometres across with small plumes detaching from their periphery that have thermal and mechanical boundary layers 100s of meters in thickness
- *Thermochemical transport processes* in the mantle where chemical boundaries can be sharp over submeter length scales.

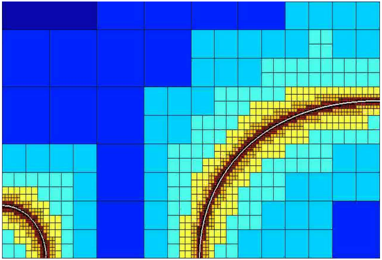
$\Rightarrow$ How can we capture these phenomena with current computing capacities ?

Adaptive Mesh Refinement (2)

- A uniform discretization of the mantle at for instance 1km resolution would result in meshes with nearly 10^{12} elements, which is far beyond the capacity of the largest available supercomputers.

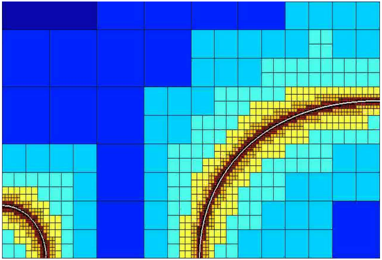
Adaptive Mesh Refinement (2)

- A uniform discretization of the mantle at for instance 1km resolution would result in meshes with nearly 10^{12} elements, which is far beyond the capacity of the largest available supercomputers.
- An alternative is to employ adaptive mesh refinement (AMR) and coarsening methods that can reduce the number of unknowns drastically by placing resolution only where needed.



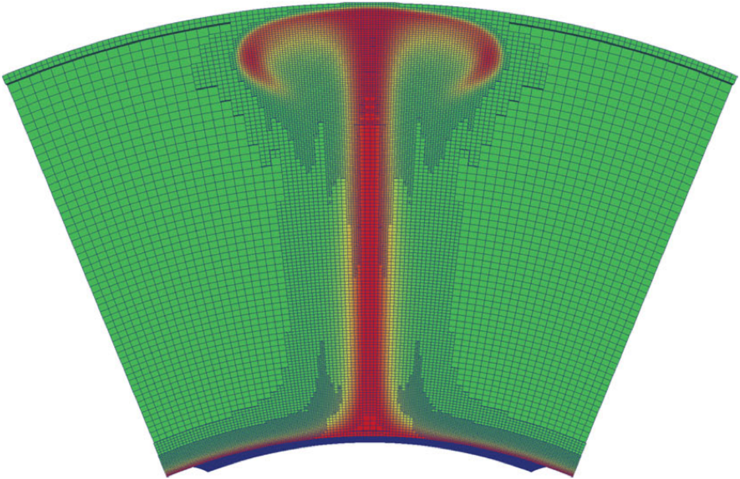
Adaptive Mesh Refinement (2)

- A uniform discretization of the mantle at for instance 1km resolution would result in meshes with nearly 10^{12} elements, which is far beyond the capacity of the largest available supercomputers.
- An alternative is to employ adaptive mesh refinement (AMR) and coarsening methods that can reduce the number of unknowns drastically by placing resolution only where needed.



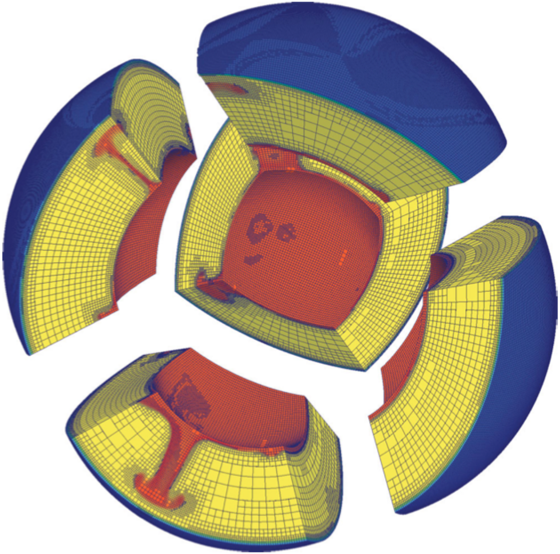
- Unfortunately, the added complexity of AMR methods can also impose significant overhead, in particular on highly parallel computing systems, because of the need for frequent readaptation and repartitioning of the mesh over the course of the simulation.

Adaptive Mesh Refinement (3)



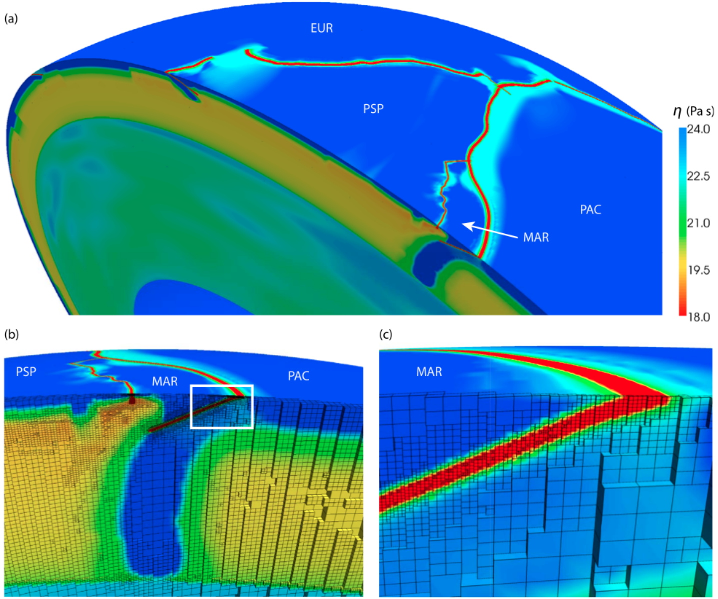
Burstedde et al, GJI 192, 2013

Adaptive Mesh Refinement (3)



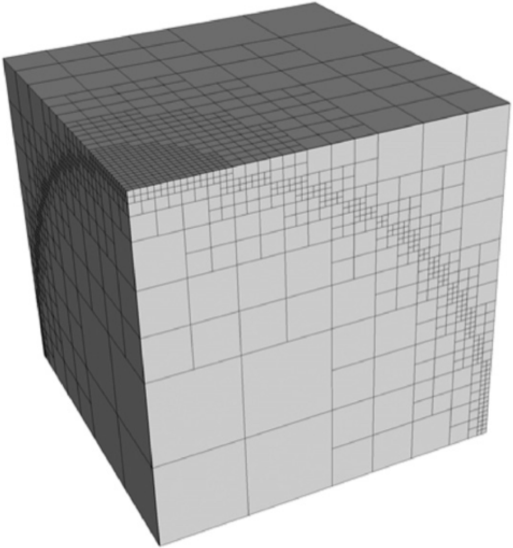
Burstedde et al, GJI 192, 2013

Adaptive Mesh Refinement (3)



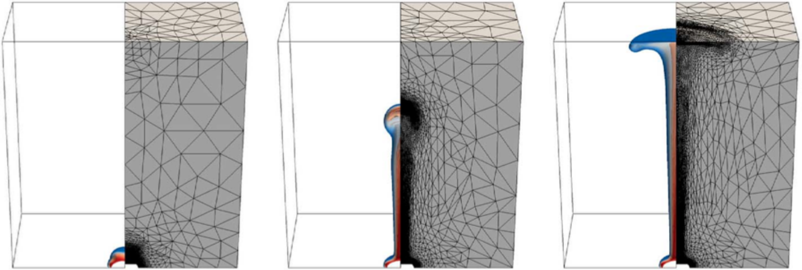
Alisic et al, JGR 117, 2012

Adaptive Mesh Refinement (3)



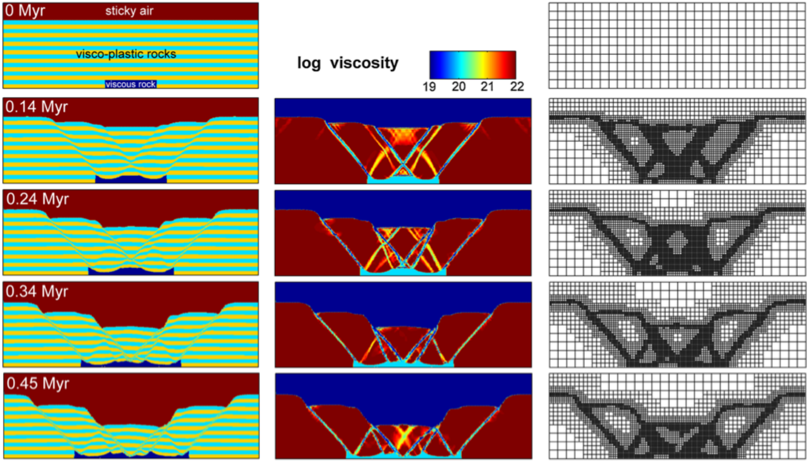
Braun et al, PEPI 171, 2008, Thieulot et al, JGR 113, 2008

Adaptive Mesh Refinement (3)



Davies et al, G3 12, 2011, May et al, J. of Geodyn. 70, 2013

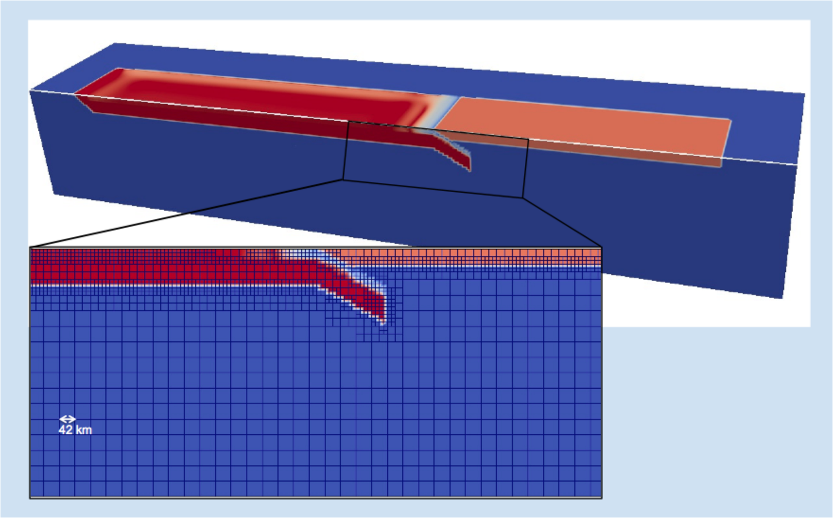
Adaptive Mesh Refinement (3)



AMR+Finite Differences !

Gerya, G3 14, 2013

Adaptive Mesh Refinement (3)



Glerum et al, 2014, In Prep.