An Overview of Numerical Methods for Earth Simulations

Part 1: Earth Simulation Issues

Part 2: Overview of Methods for Large Deformation

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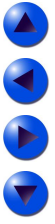
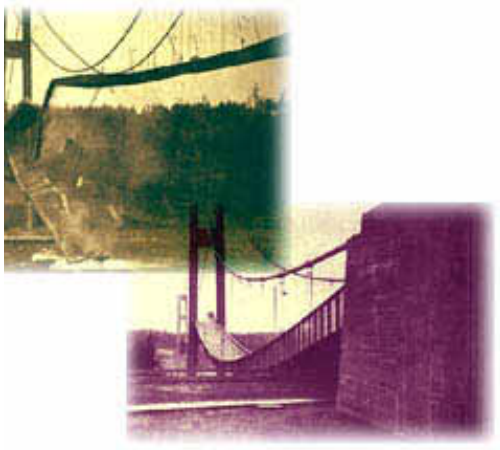


Why do we model things ?

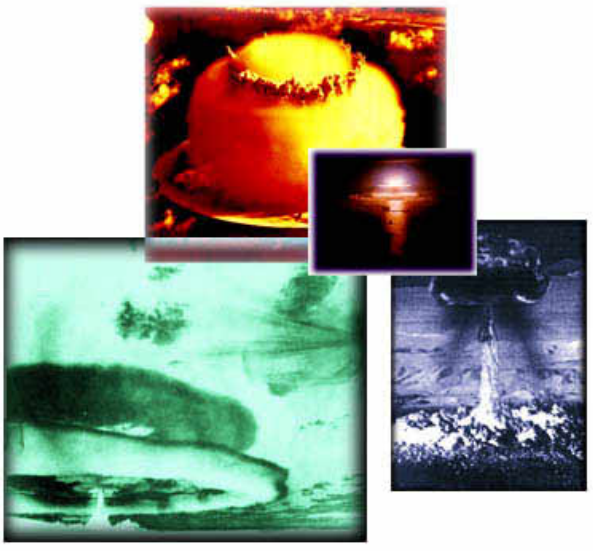


(1) Stability of structures — test *before* you build something expensive

Why do we model things ?

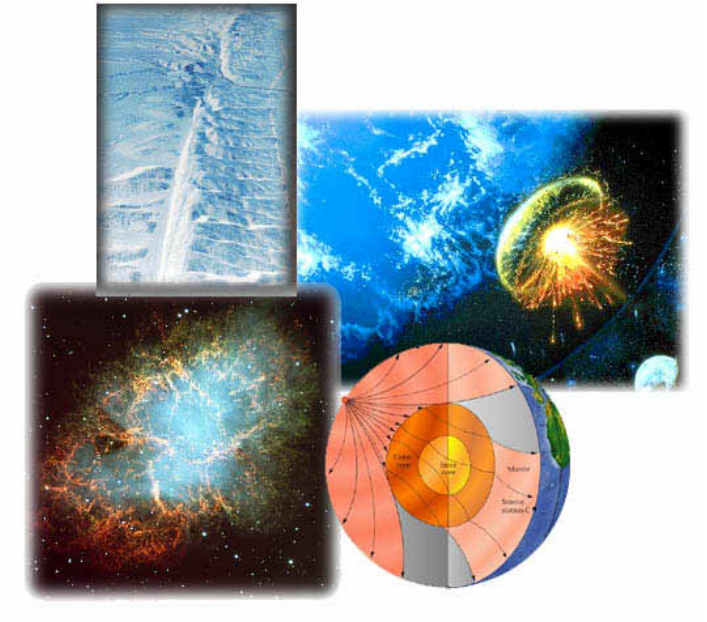
(2) Safety — a lot more safety testing per dollar

Why do we model things ?



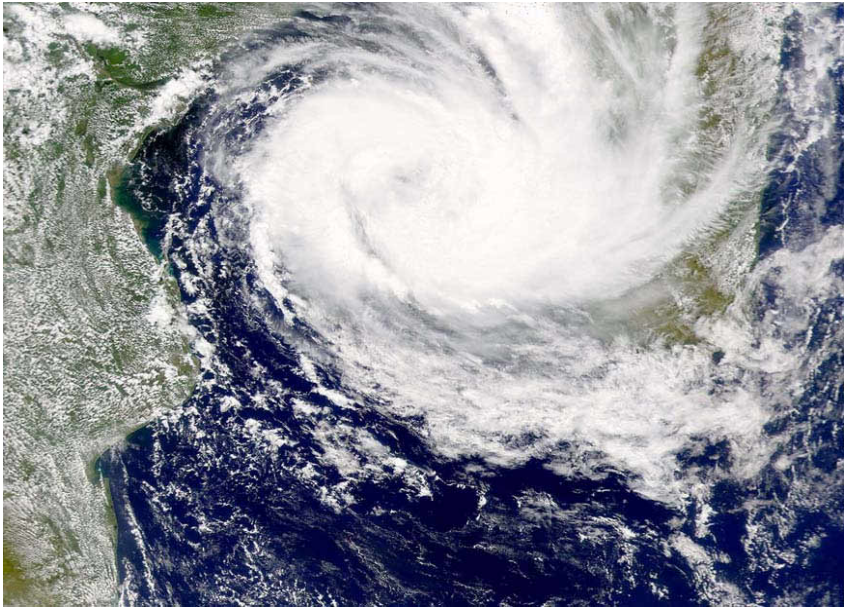
(3) Some things are too risky and/or unethical
. . . extermination of humanity

Why do we model things ?



(4) Impossible experiments: astrophysics, plate tectonics

Why do we model things ?



(5) Or forecasting the evolution of complex systems.

Inside the Earth

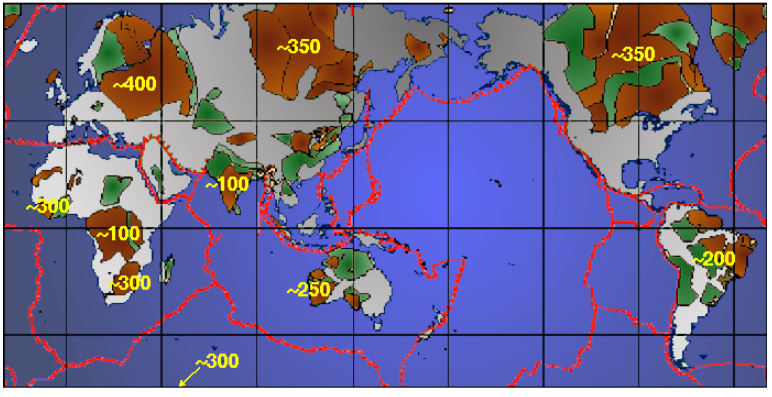
A cursory glance at the earth: we barely scrape the surface and still there's an enormous amount going on

Inside the Earth

We can also see a wealth of information at the surface both on the land

Cratons, Root Depths & Plate Boundaries

(after Stoddard & Abbott, 1996)



Archean crust overlying tectosphere

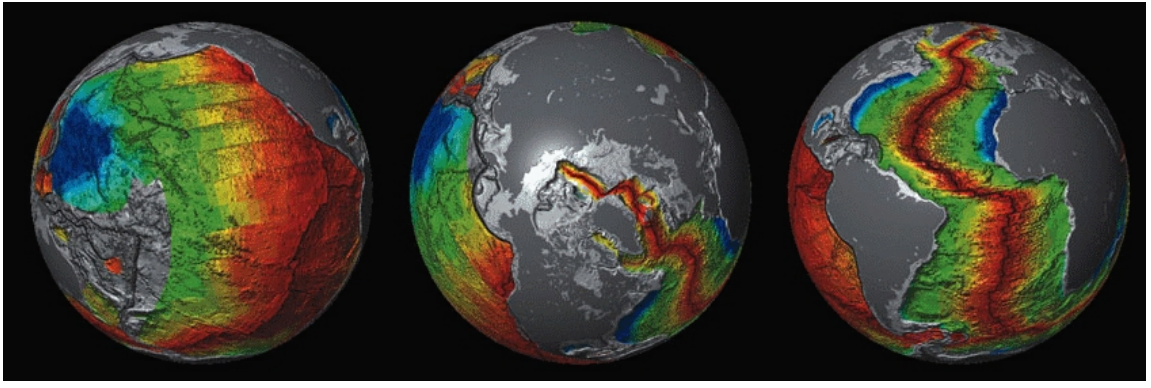
Early Proterozoic crust (>1.6 Ga) overlying tectosphere

Younger crust not underlain by tectosphere

100 Approximate seismic root thicknesses (Polet & Anderson, 1995)

Inside the Earth

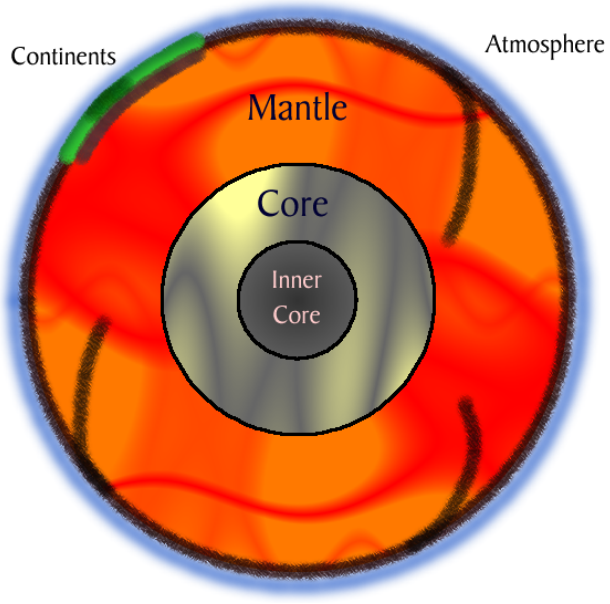
And in the ocean basins — using the right set of spectacles . . .



Here the age of the oceanic lithosphere as it rumbles along from mid-ocean ridge to trench.

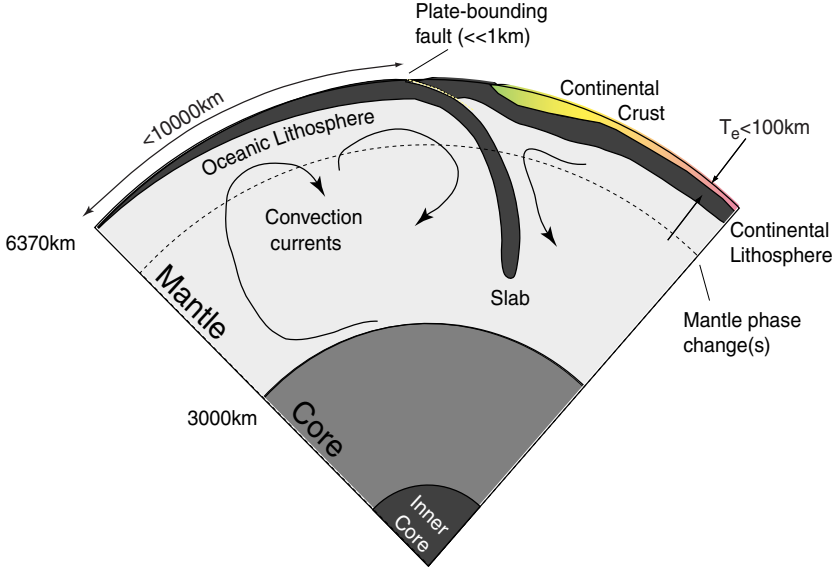
Inside the Earth

Seismology allows us to probe the internal structure instantaneouly



Inside the Earth

But to understand the time evolution we need to use models of the processes which unwind too slowly for us to wait and see.



Mathematical Earth Models

The starting point for mantle convection modeling is usually Navier-Stokes equation for fluid flow

$$\frac{1}{\mathrm{Pr}}\frac{D\boldsymbol{u}}{Dt} - \nabla \cdot \boldsymbol{\sigma}' = \mathrm{Ra}T\mathbf{z}$$

where Pr is the Prandtl number, and Ra is the Rayleigh number.

$$\frac{D}{Dt} \equiv \frac{\partial}{\partial t} + (\mathbf{u} \cdot \nabla)$$

But this term is usually small since the Prandtl number (η/κ) is absolutely enormous in the Earth.

This means there is no time dependent term left in the momentum equation. We therefore have to use implicit methods for the solution.

Mathematical Earth Models

Assume incompressibility

$$\nabla \cdot \boldsymbol{u} = 0$$

In a purely viscous formulation there is no way to represent (physical) fluid compressibility directly since this is an elastic property.

And an equation for thermal evolution

$$\frac{DT}{Dt} - \kappa \nabla^2 T = Q$$

Note the reappearance of a time-dependent term ! The coupled thermal/mechanical problem does evolve in time.

Obviously this is highly simplified — but it is a starting point, and it is the traditional place to start for the large-scale problem.

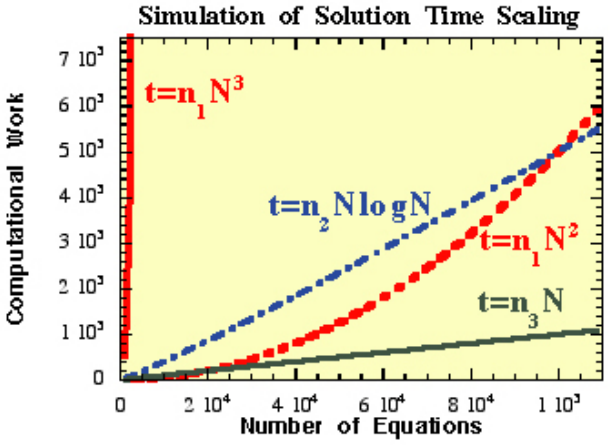
Multigrid methods

- In geodynamics, the fact that inertia is negligible leaves the equation of motion independent of time and it can only be solved implicitly.
- The traditional implicit solver in FEM: build the matrix equation and solve it directly exploiting banded nature of matrix for efficiency. Unfortunately it is N^3 or, at best, N^2 process.
- For 3D etc, this is unacceptable. Iterative methods can do much better: preconditioned conjugate gradient ($N \log N$) or multigrid (N)

Multigrid methods

Time as function of number of unknowns for several

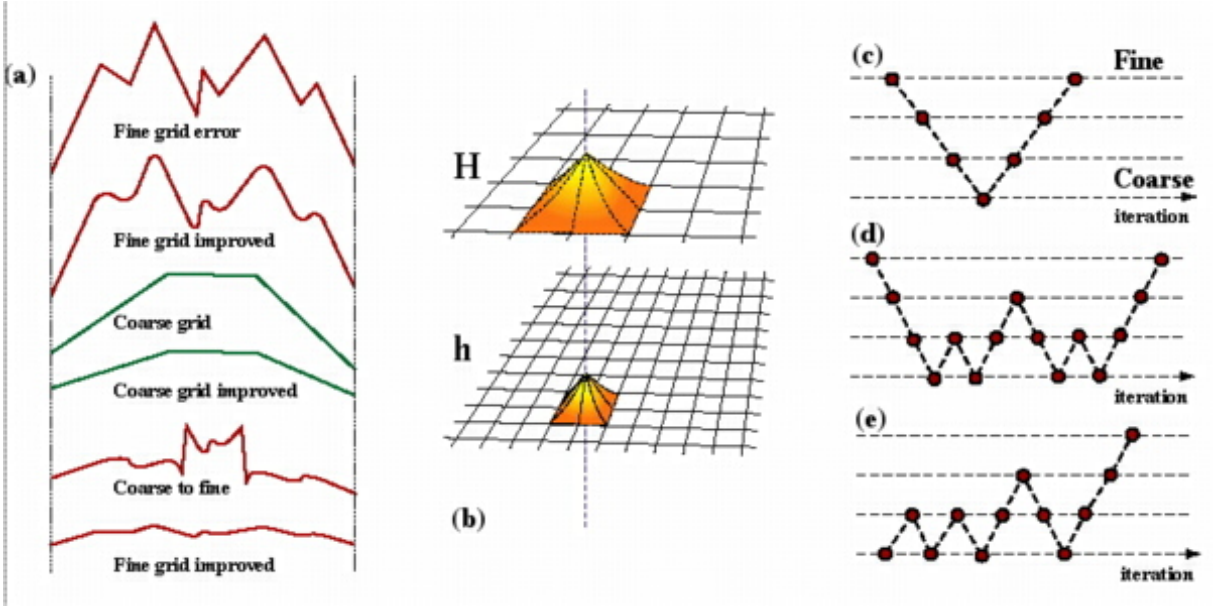
Choice of solution method for large problems



methods

Multigrid methods

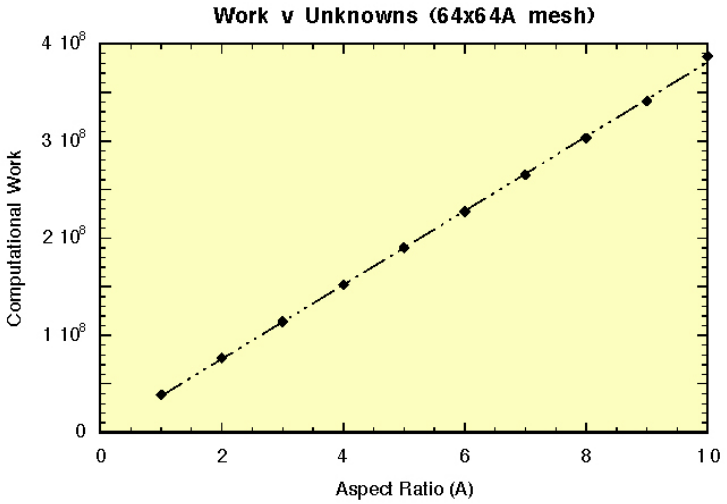
Multigrid methods work by interleaving iterative solutions on a nested set of grids (geometrically or conceptually (AMG))



Iterative scheme should be of a “smoothing” variety.

Multigrid methods

It really does work. Here is the timing for an ever growing set of convection simulations.



Off the shelf codes ?

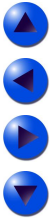
Most off-the-shelf codes were originally intended to solve problems in engineering

- Testing of a man-made structure (e.g. against failure)
- Optimization of product design
- Analysis of structural response (e.g. bridge oscillations)
- Flow of “simple fluids” through complex geometries (e.g. aircraft design)

. . . and that sort of thing

Geoscience requirements

Geological modeling is associated with a different set of requirements:



Geoscience requirements

Geological modeling is associated with a different set of requirements:

- Very large deformation of solid materials including
  - accurate tracking of material (compositional) interfaces
  - accurate tracking of history variables (e.g. $\tau_{\text{yield}}(\varepsilon)$)
  - high Deborah number viscoelasticity ($\overset{\triangledown}{\tau}$ term)
  - evolution of oriented microstructure ( )

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- Strongly evolving rheology
- Complex geometry emerges from simple structures through non-linearity of rheology
- Uncertainty of material properties
  - a different style of modeling (forward models not definitive)
  - ensembles of models to classify regimes / inversion strategies (e.g. Wijns et al, JSG, 2001)

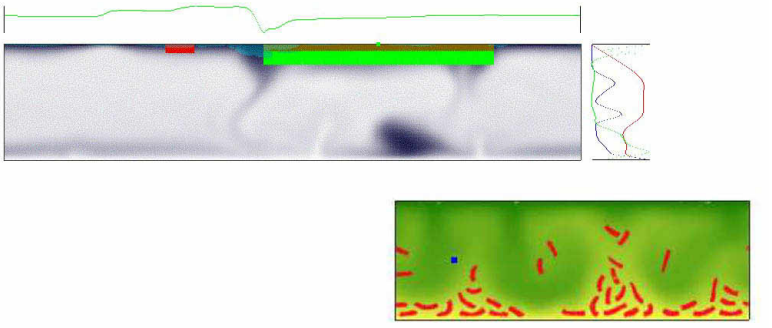
Geology ≠ engineering

(1) Large deformation ?

Geology ≠ engineering

(2) Not a spectacular success ... and no longer of interest

Geology ≠ engineering



(3) Compare that with what we need to do on scales from the whole planet to a few grains of sediment

Geology ≠ engineering

(4) Where we are presented with materials whose properties we don't know well at the time of deformation, or even which of the materials were actually *there* at the time.

Geology ≠ engineering

(5) Where materials have a number of nested “characteristic” scales.

Geology ≠ engineering

(6) And where macro/microstructures may interact during deformation to produce far-from-linear evolution. (Computer shown for scale)

Geology ≠ engineering

(7) And where the system may localize with or without some material evolution during shear band formation.

Where to begin

Problems need to be

- Written in a mathematical form, i.e. the *model*
- Rendered finite so it can fit onto a computer

The finite version of the problem then needs to be solved

- Efficiently
- Accurately

The choice of model and solution method should suit the physics of the problem to satisfy efficiency and accuracy !

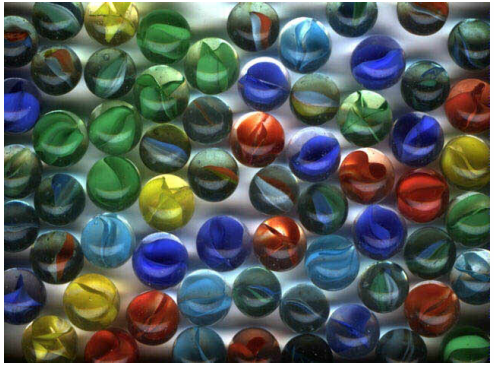
Finite Problems

Some problems are already finite — there is an obvious mapping between the computational points and real objects

(1) A discrete structure — naturally finite

Finite Problems

Some problems are already finite — there is an obvious mapping between the computational points and real objects



(2) Granular structures — naturally finite
OK as long as we can compute all the grains

Finite Problems

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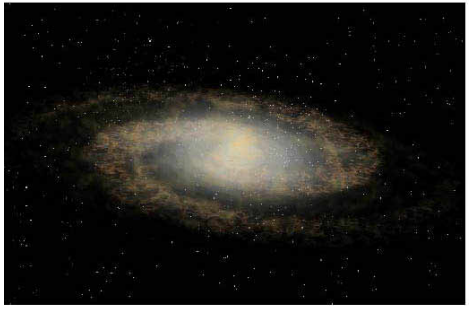

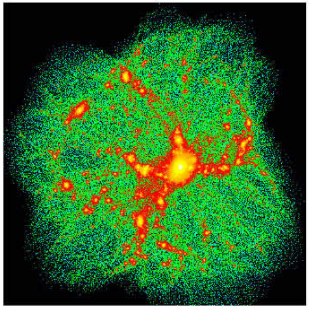

(3) Really big grains — a finite number of stars in the galaxy, galaxies in the universe

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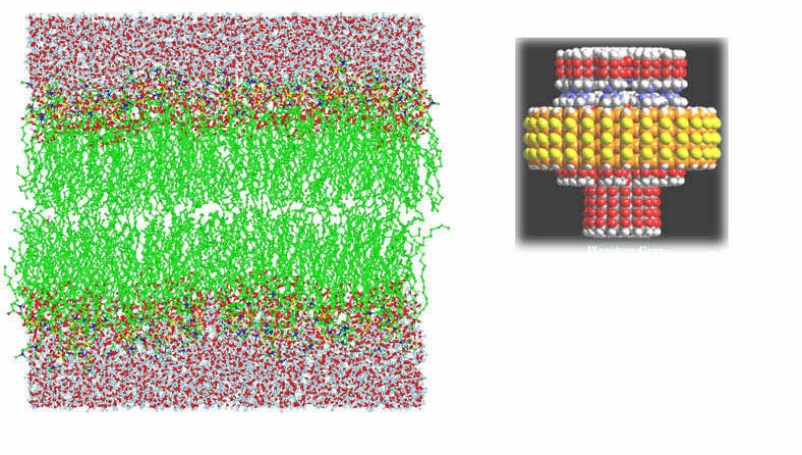

(4) Atom by atom — OK for very small things

Not-finite Problems

In other cases the computational points don't have direct counterparts in the physical system. Continuum *models* of physical phenomena are built assuming an infinitely divisible medium. The *model* must be made finite by

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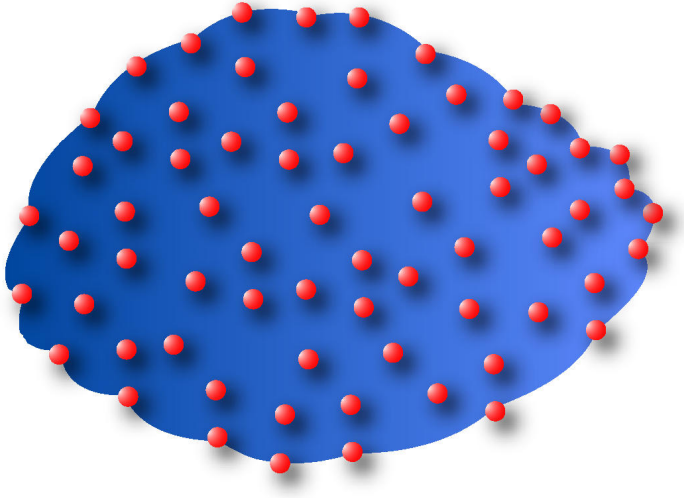
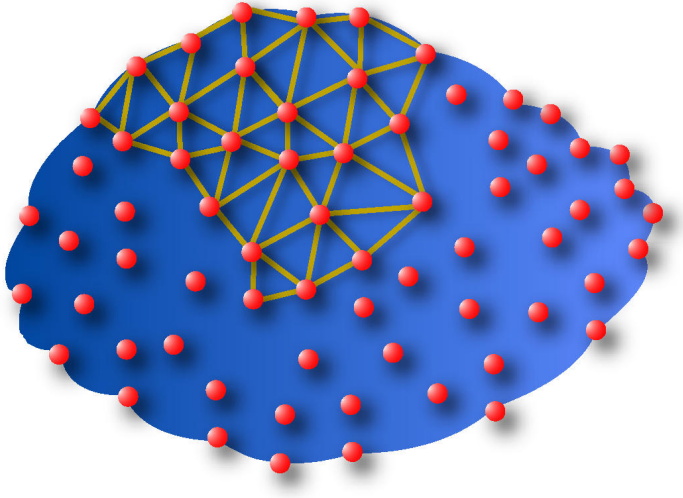
- Solving at a finite number of points (spatial)



Not-finite Problems

In other cases the computational points don't have direct counterparts in the physical system. Continuum *models* of physical phenomena are built assuming an infinitely divisible medium. The *model* must be made finite by

- Solving at a finite number of edges/volumes (spatial)



Not-finite Problems

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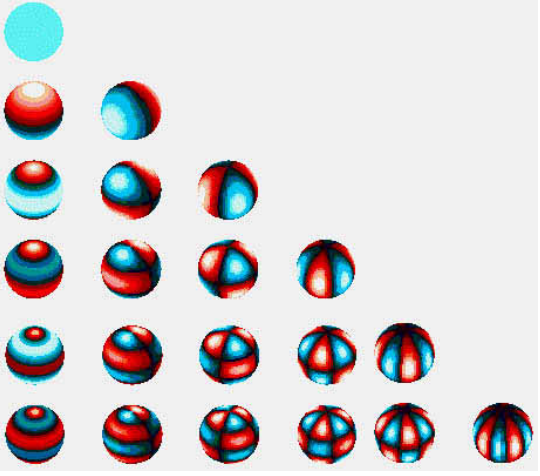
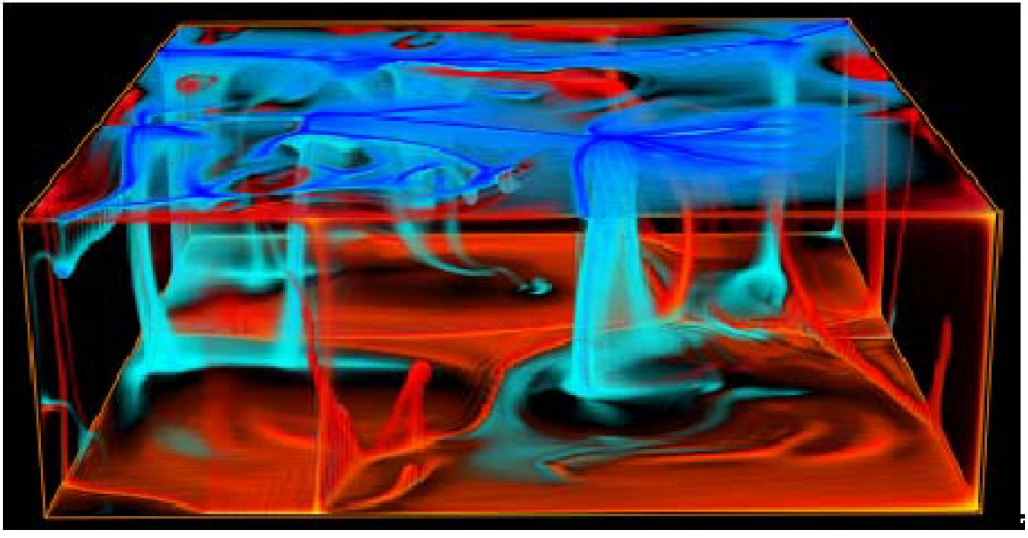
- Solving with a truncated set of mathematical functions (spectral)



Eulerian Formulation

Sufficiently diffusive quanities can be modeled with a fixed mesh of computational points *(Dubuffet et al, 2001, GRL)*



Quickly and efficiently with high resolution.
But must deal with $u.\nabla T$ term at high Peclet number.

Large Deformation & Meshes

If we want to track history, we need to track material points.
As material points move, the mesh they define distorts.

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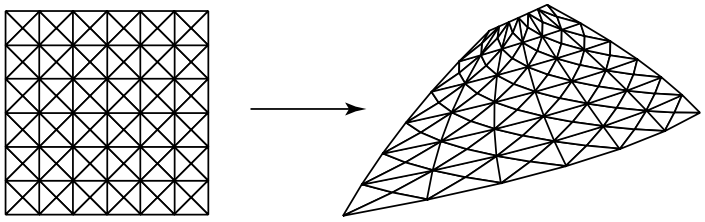

Even modest deformation can make a mesh unusable

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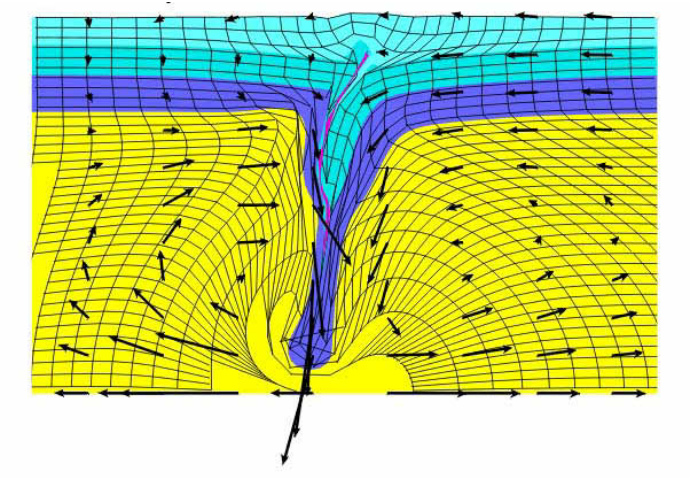

(Beaumont & coworkers)

We actually want an immodest amount of deformation

Large Deformation & Meshes

If we want to track history, we need to track material points.
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We need to remesh . . .

Large Deformation & Meshes

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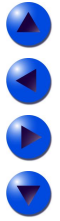
We need to remesh . . .

or devise a solution strategy which does not rely on a (distorting) mesh

Discretization Examples

There are a great many different strategies for solving large deformation problems.



Discretization Examples

There are a great many different strategies for solving large deformation problems.

- Discrete Element Methods
  - E.g. Sakaguchi et al., Burbidge & Braun, the Quakes group ...
  - Meshless method
  - Fracture, separation, granular materials — lots of particles needed

Discretization Examples

There are a great many different strategies for solving large deformation problems.

- Smooth Particle Hydrodynamics Methods
  - E.g. Barton et al. ...
  - Meshless continuum method — essential boundary conditions can be troublesome.
- FLAC
  - Conceptually a hybrid between DEM and classical continuum methods

Discretization Examples

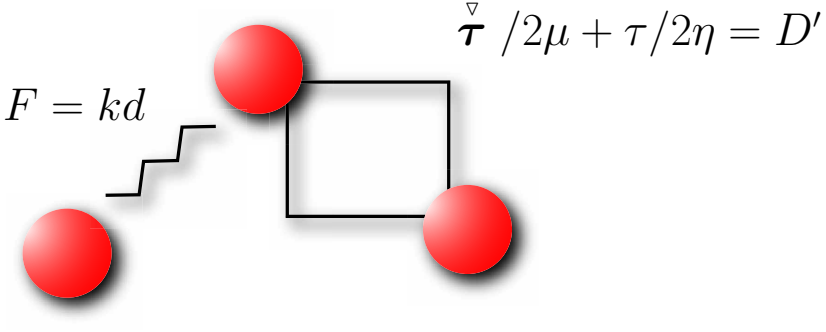
There are a great many different strategies for solving large deformation problems.

- Finite Element Derived Methods
  - Dynamic Remeshing
  - ALE
  - Natural Element Method
  - Element Free Galerkin & Reproducing Kernel Methods (cf SPH)
  - Lagrangian Integration Point FEM
  - Point Interpolation Method

Mathematically (computationally) these all share common, modular core — which is slow.
And meshless strategies may suffer boundary condition issues.

Generalization

It's just about some computational points interacting - the trick is to choose the right way for the points to interact which matches the physics

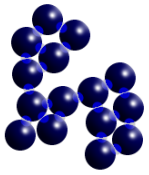


To produce a matrix problem something like:

$$K_{ij}u_j = \sum F_i$$

which can be solved by some textbook method

Strategies in sync with Physics



Short range

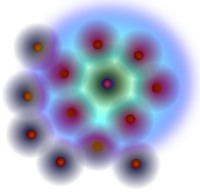
Interaction through local contacts - directional, dynamic interactions.

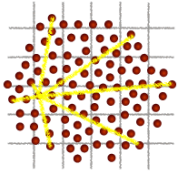
E.g. granular materials in gas-like flow, waves propagating through solids.

Medium range

Interaction with more than immediate neighbours

Where long-range forces exist - gravity, viscosity in momentum dominated flow





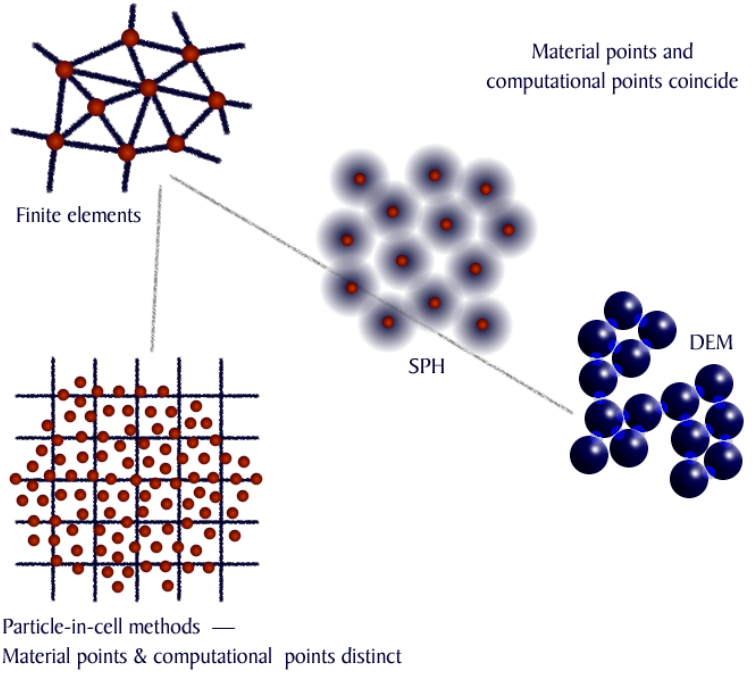
Long range

Strong Interaction with all other points

Where long-range forces dominate - slow, creeping flow

Consider how the forces behave, whether the system is naturally finite

Strategies in sync with Physics



What information the computational points carry, whether they are material points, are there fast computational "short-cuts" for some methods to help accelerate the calculation (e.g. multigrid on structured grid).

FEM

The strength of FEM is to build standardized matrix problems from any differential equation

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(1) Strong form

$$\tau_{ij,j} - p_{,i} - f_i = 0$$

$$u_{i,i} = 0$$

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$$\tau_{ij,j} - p_{,i} - f_i = 0$$

$$u_{i,i} = 0$$

(2) Equivalent weak form

$$\int_\Omega N_(i,j)\tau_{ij} d\Omega - \int_\Omega N_{i,i} p d\Omega - \int_\Omega N_i f_i d\Omega = 0$$

FEM

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(2) Equivalent weak form

$$\int_\Omega N_(i,j)\tau_{ij}d\Omega - \int_\Omega N_{i,i}pd\Omega - \int_\Omega N_i f_i d\Omega = 0$$

(3) Equivalent matrix form

$$\begin{pmatrix} K & G \\ G^T & 0 \end{pmatrix} \begin{pmatrix} u \\ p \end{pmatrix} = \begin{pmatrix} F \\ 0 \end{pmatrix}$$

FEM

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(3) Equivalent matrix form

$$\begin{pmatrix} K & G \\ G^T & 0 \end{pmatrix} \begin{pmatrix} u \\ p \end{pmatrix} = \begin{pmatrix} F \\ 0 \end{pmatrix}$$

(4) Where the coefficients come from a standard form computed element by element

$$k^e_{ab} = \int_{\Omega^e} B^T_a D B_b d\Omega^e$$

(D is a matrix of material properties, B an incarnation of the consitutive law). The full k_{ab} coefficients come from summing the element contributions — That's basically the interaction rule for two node points, and this is the machinery for generating it for a given continuum expression

FEM

We like FEM because it's ...

- Flexible
  - Wide variety of meshes
  - Interchangeable constitutive relationships
  - Robust to strong gradients in material properties
- Modular
  - Plug in solvers
  - Standard form for most differential equation systems
  - Plug in element types
- Versatile
  - Just look at all those FEM-like strategies !

But the generality comes at a price: it runs slowly.

FEM Pros & Cons

Mesh free (and *mesh-lite*^{TM}) methods are cool, but can be even slower, may have trouble applying boundary conditions, and convergence proofs are not always available.

Achilles heal:
calculating everything on the fly for all elements which means we cannot take advantage of known symmetries (cf. typical strategies in finite differences)

But if we *really* use this recalculation property creatively... the weakness becomes a strength

Lagrangian Integration Point FEM

Consider the element integrals:

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These are expressed as the sum over a finite number of sample points (cf Simpson's rule in 1D)

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$$\int_{\Omega^e} \phi d\Omega^e \leftarrow \sum_p w_p \phi(x_p)$$

So why not write this:

$$k^e_{ab} = \sum_{p=1}^{n_{\text{ep}}} w_p B^T_a(x_p) D_p B_b(x_p)$$

allowing the material properties to vary at the sample point ?

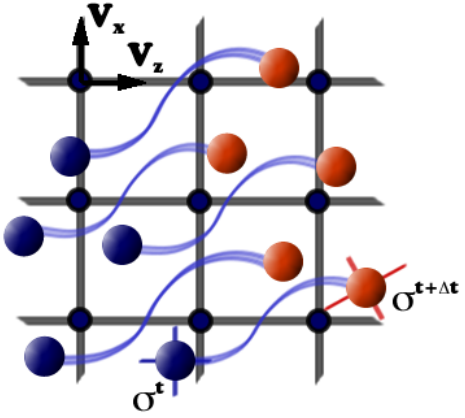
Lagrangian Integration Point FEM

And why not allow the integration points to be material points ?

Lagrangian Integration Point FEM

And why not allow the integration points to be material points ?

$$x_p^{t+\Delta t} = x_p^t + \Delta t \sum_{\text{nodes}} v_n N_n(x_p)$$



Which is ok as long as we remember to recompute integration schemes dynamically

Lagrangian Integration Point FEM

If this is done then we can:

- Track the entire history of the problem at the integration points
- Produce a self consistent averaging process back to the mesh
- Decouple computational point evolution and material point evolution
- Handle boundary conditions correctly
- Use meshes designed for multigrid

At the expense of:

- Speed (again)
- Inherent smoothness
- Complexity (but it's not *that* bad)

LIP — integration schemes

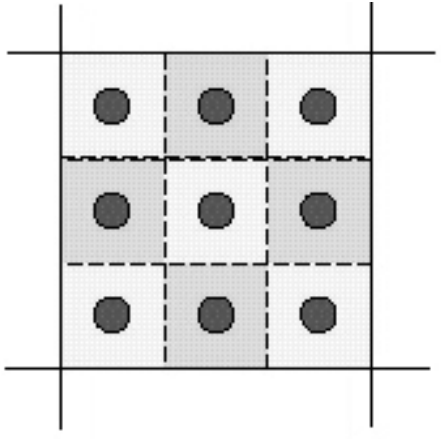
Material points are used as integration points

$$\int_{\Omega^e} \phi d\Omega^e \leftarrow \sum_p w_p \phi(x_p)$$

but this means that it is not possible to work out in advance what the locations, x_p or the weights, w_p for each integration point should be. Locations are given, weights must be calculated.

LIP — integration schemes

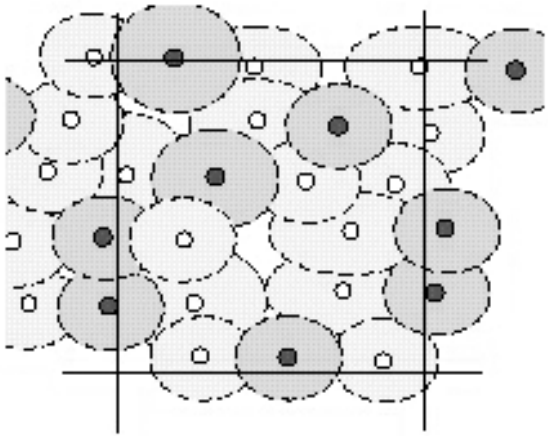
This is not such a problem for regular arrays of material points



Where equal weights may make sense. We can make a correspondance between local volume and particle weight. But the particle distribution is usually not regular ...

LIP — integration schemes

With uneven distributions of particles



the local volume is also distorted and probably crosses element boundaries. In problems where there is a delicate balance between large forces this can be an issue.
However, we know some properties of the integration scheme

LIP — integration schemes

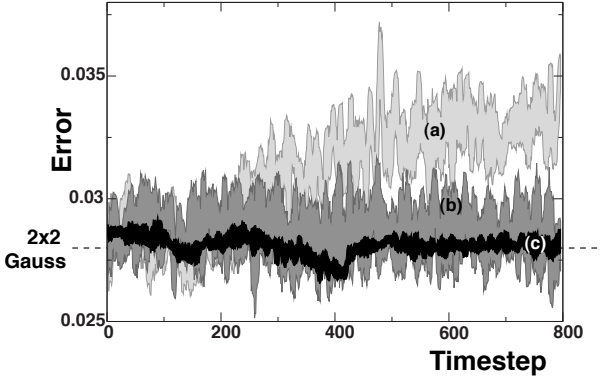
The constraints can be derived from convergence conditions for specific elements:

$$\begin{aligned}
\sum_{p=1}^{\mathrm{n_{ep}}} w_p &= 2 && \text{(constant terms)} \\
\sum_{p=1}^{\mathrm{n_{ep}}} w_p x_p &= 0 && \text{(linear terms)} \\
\sum_{p=1}^{\mathrm{n_{ep}}} w_p x_p^2 &= \frac{2}{3} && \text{(quadratic terms)} \\
\sum_{p=1}^{\mathrm{n_{ep}}} w_p x_p^3 &= 0 && \text{(cubic terms)}
\end{aligned} \qquad (1)$$

which we can apply through an iterative scheme (approximately) for a given distribution of particles assuming an initial guess at the set of w_p.

LIP — integration schemes

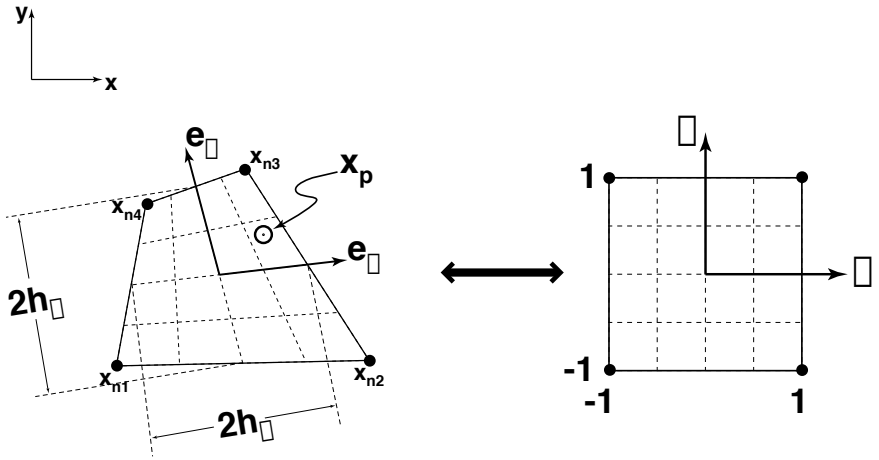
On average such a procedure can be as accurate as a standard Gaussian quadrature scheme



Although with considerably more work required.

LIP — Coordinate Mappings

It is necessary to be able to map both from an arbitary location in the master element domain to the element's global coordinate (as normal) and also from any point in the global (distorted) element back to the master element.



LIP — Coordinate Mappings

Guess an initial value of $\boldsymbol{\xi}_p$ and use this to predict the global coordinates $\boldsymbol{x}_p^0$,

$$\boldsymbol{\xi}_p = (0,0)$$
$$\boldsymbol{x}_p^0 = \left(\sum_{n=1}^{\mathrm{n_{en}}} N_n(\boldsymbol{\xi}_p) x_n, \sum_{n=1}^{\mathrm{n_{en}}} N_n(\boldsymbol{\xi}_p) y_n \right)$$

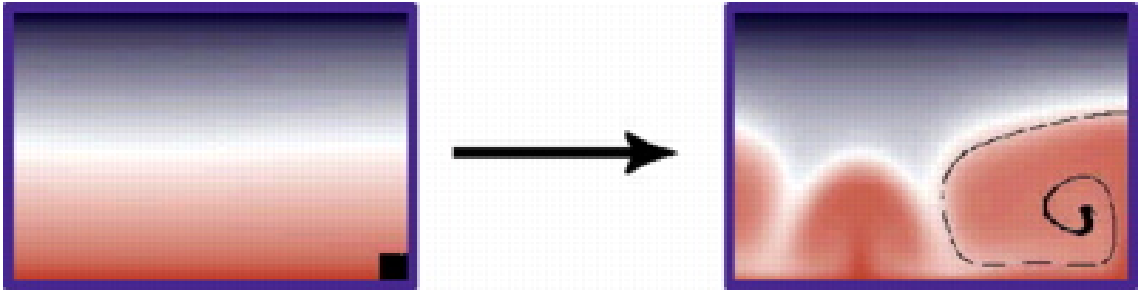
We compute $\boldsymbol{\xi}_p$ through a number of corrector steps:

$$\xi_p \leftarrow \xi_p + \beta \left(e_{\xi x} x_p^i + e_{\xi y} x_p^i \right) / h_\xi$$
$$\eta_p \leftarrow \eta_p + \beta \left(e_{\eta x} x_p^i + e_{\eta y} x_p^i \right) / h_\eta$$
$$\boldsymbol{x}_p^{i+1} = \left(\sum_{n=1}^{\mathrm{n_{en}}} N_n(\boldsymbol{\xi}_p) x_n, \sum_{n=1}^{\mathrm{n_{en}}} N_n(\boldsymbol{\xi}_p) y_n \right)$$

This is a useful coordinate system to test if a point is in an element.

LIP — Particle splitting

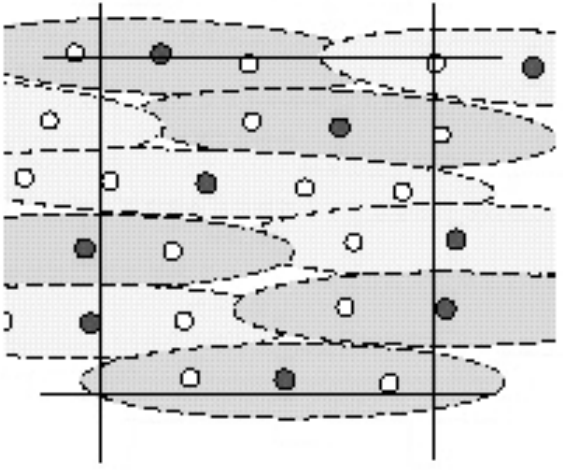
Initially small aspect-ratio local volumes do not stay that way



Which makes it inappropriate to associate a fixed local volume to a given material point.

LIP — Particle splitting

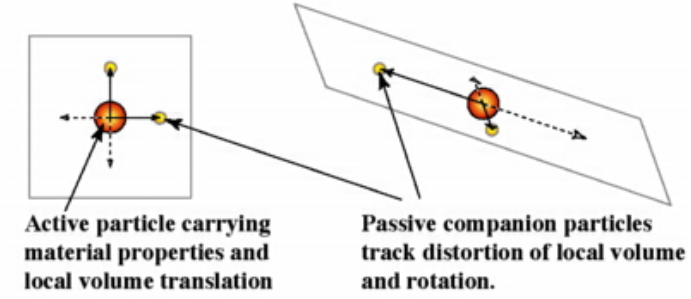
But a judicious splitting of particles can reduce this effect



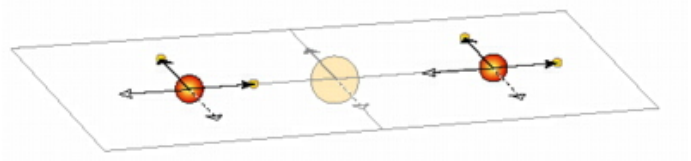
and in some cases is absolutely necessary to avoid the appearance of holes in the distribution of integration points (e.g. near a stagnation point in the fluid).

LIP — Particle splitting

One strategy for the splitting is based on the strain ellipse at the material point



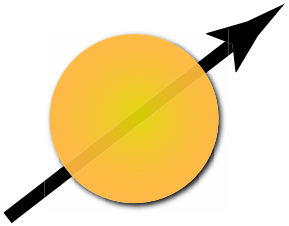
which can be calculated in many ways (such as this) but which always produces a heavy storage burden.



but then it is also necessary to have a merging algorithm.

Formulations using material points

In an orthotropic material (which has a unique direction) we follow a director attached to the material points.



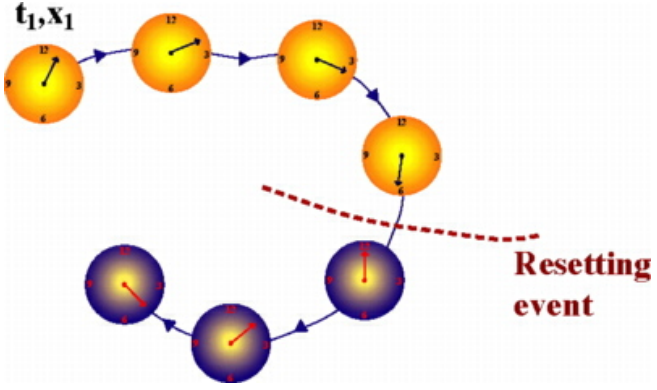
The contribution to the stiffness matrix depends upon the direction of the director at the point and the material orthotropy at that point. The director is updated from the grid velocity gradient.

$$\dot{n}_i = \tilde{\omega}_{ij} n_j$$

$$\tilde{\omega}_{ij} = v_{i,j} - \delta_{ij} \left(v_{k,l} n_k n_l \right)$$

Formulations using material points

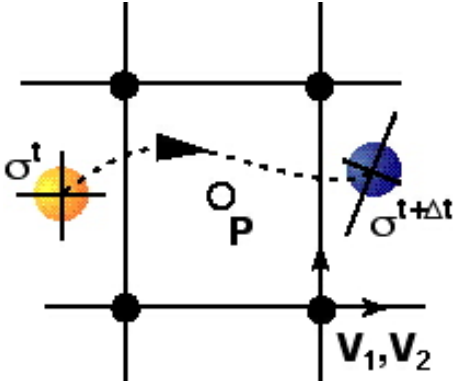
In materials with history we can track any kind of clock(s) on the particles



Many examples ! Including tracking of pressure / temperature / time paths, non-equilibrium phase changes or irreversible transformations, material history (strain dependent damage), the evolution of grain-sizes during deformation.

Formulations using material points

Implementation of viscoelasticity (stress history required in a viscous-based formulation)



$$\frac{\overset{\nabla}{\boldsymbol{\tau}}}{2\mu} + \frac{\boldsymbol{\tau}}{2\eta} = \hat{\boldsymbol{D}}_v + \hat{\boldsymbol{D}}_e = \hat{\boldsymbol{D}}$$

Formulations using material points

$\overset{\triangledown}{\boldsymbol{\tau}}$ is the Jaumann corotational stress rate for an element of the continuum, μ is the shear modulus and η is shear viscosity. $\hat{\boldsymbol{D}}$ is the deviatoric part of $\boldsymbol{D}$.

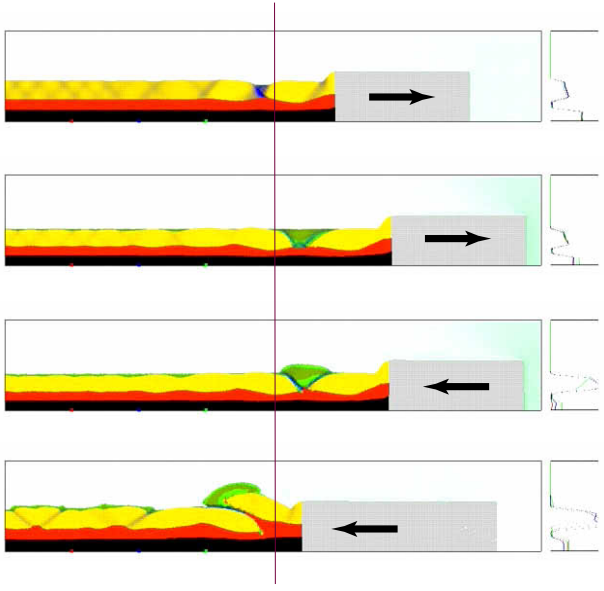
$$\overset{\triangledown}{\boldsymbol{\tau}} = \dot{\boldsymbol{\tau}} + \boldsymbol{\tau}\mathbf{W} - \mathbf{W}\boldsymbol{\tau}$$

where $\mathbf{W}$ is the material spin tensor,

$$W_{ij} = \frac{1}{2}\left(\frac{\partial V_i}{\partial x_j} - \frac{\partial V_j}{\partial x_i}\right)$$

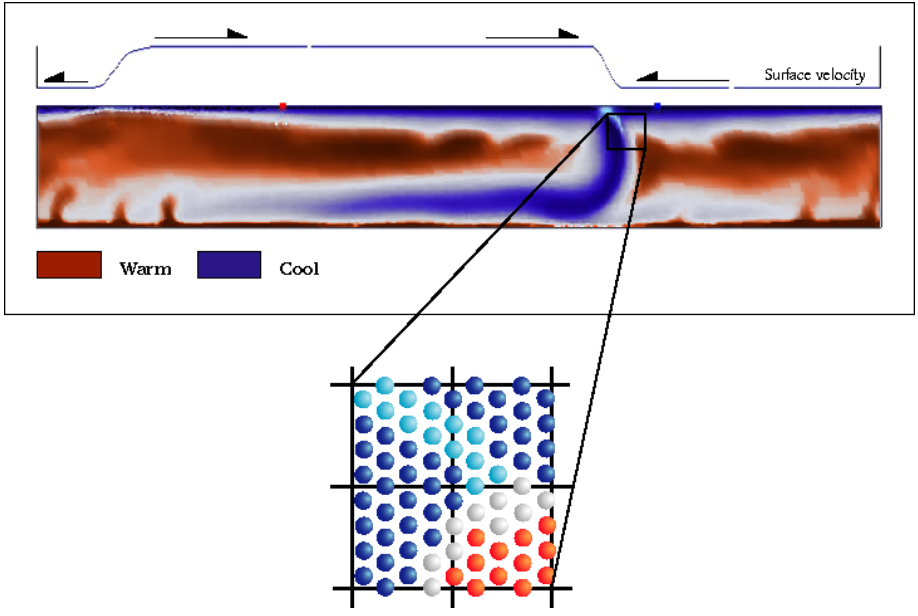
The $\boldsymbol{W}$ terms account for material spin during advection which reorients the elastic stored-stress tensor.

Lagrangian Integration Point FEM



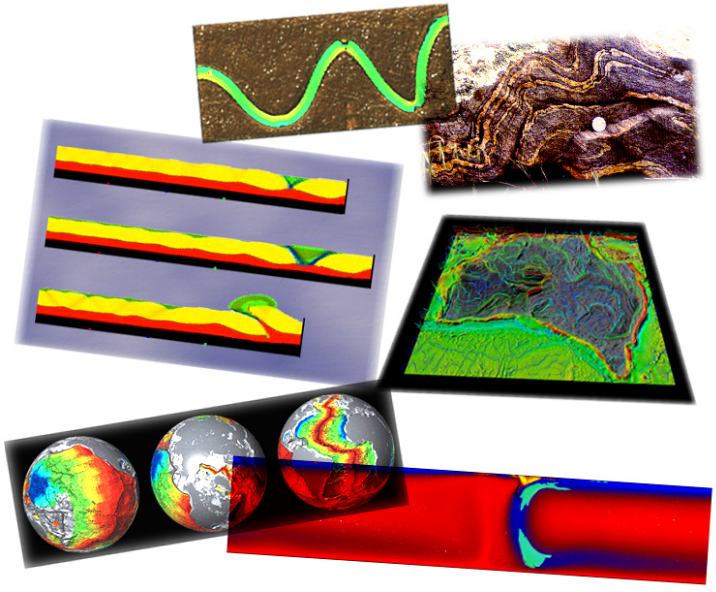
Example: The extension of a layered crust/mantle with sedimentation, followed by compression. Demonstrates the reactivation of basin structures upon inversion.

Lagrangian Integration Point FEM



Example: mantle convection simulation with “brittle” rheology in the lithosphere which allows the development of a mobile surface mode (otherwise it would be in stagnant lid mode)

Lagrangian Integration Point FEM



Various examples of modeling and data where non-linearity dominates the outcome.

Progress (October 2001)

Algorithm in 2D developed and tested for

- Fluids with interfaces
- Viscous materials with history
- Viscoelastic materials / yielding
- Anisotropic viscoelastic materials
- Cosserat materials (partial)

Simple meshes, geometrical multigrid, simple boundary conditions.

Progress (October 2001)

Collaboration with VPAC (ACcESS partner) & Univ. of Sydney

- 3D Prototype *(tested)*
- Arbitrary mesh generation
- Algebraic Multigrid
- Parallel code

Work in progress . . . due mid 2002

Progress (October 2001)

Some relevant publications

- Moresi, L. Mühlhaus, H.-B. and Dufour, F., Particle-in-cell solutions for creeping viscous flows with internal interfaces. In Bifurcation and Localization in soils and Rocks 99. Mhlhaus, Dyskin, A. and Pasternak, E. (ed), Balkema: Rotterdam, In Press 2001
- Moresi, L. Mühlhaus, H.-B. and Dufour, F. Viscoelastic formulation for modelling of plate tectonics. In Bifurcation and Localization in soils and Ro cks 99. Mhlhaus, Dyskin, A. and Pasternak, E. (ed), Balkema: Rotterdam, In Press 2001.
- Dufour, F. Mühlhaus, H-B., Moresi, L., A particle in cell formulation for large deformation in cosserat continua, In Bifurcation and Localization in soils and Rocks 99. Mhlhaus, Dyskin, A. and Pasternak, E. (ed), Balkema: Rotterdam, In Press, 2001
- Louis Moresi, Frédéric Dufour, Hans Mühlhaus, Mantle convection models with viscoelastic/ brittle lithosphere: Numerical methodology and plate tectonic modeling, Pure Applied Geophys., In Press, 2001
- H-B Mühlhaus, L.N Moresi, B. Hobbs, and F Dufour, Large Amplitude Folding in Finely Layered Viscoelastic Rock Structures, Pure Applied Geophys, In Press 2001
- Moresi, Louis, Dufour, Frédéric and Mühlhaus, Hans (2001) A Lagrangian integration point finite element method for large deformation modeling of viscoelastic geomaterials. Journal Computational Physics, Submitted 2001.

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