Numerical Geodynamics Modelling

(there is no free lunch)

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

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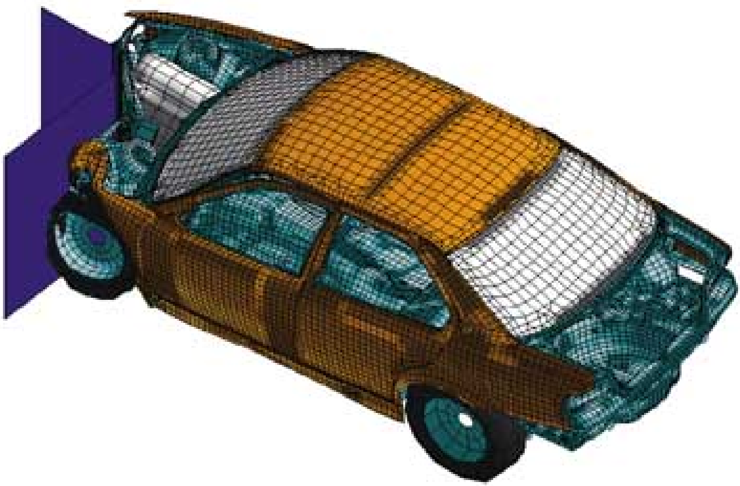
Kinematical description (1)

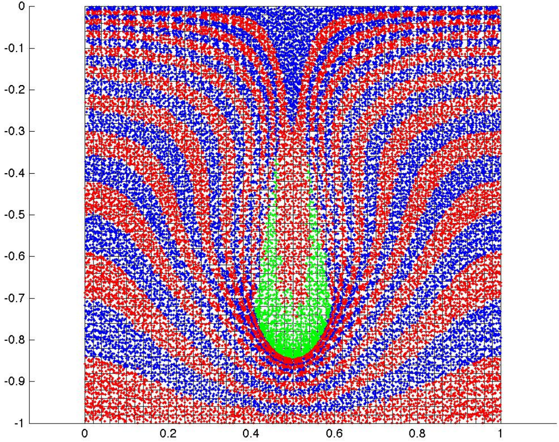
Lagrangian $\rightarrow$ the mesh deforms



$\rightarrow$ Finite Element method

Kinematical description (2)

Eulerian $\rightarrow$ the mesh does not deform

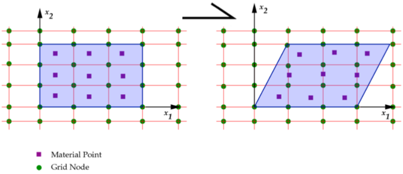


$\rightarrow$ Finite Difference Method, Finite Element Method

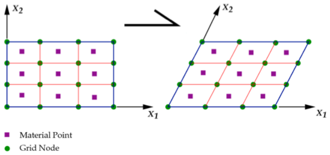
Gerya & Yuen, PEPI, 2007, Braun et al, PEPI, 2008, Jadamec & Billen, JGR, 2012

Kinematical description (2)

In Eulerian methods the mesh is fixed



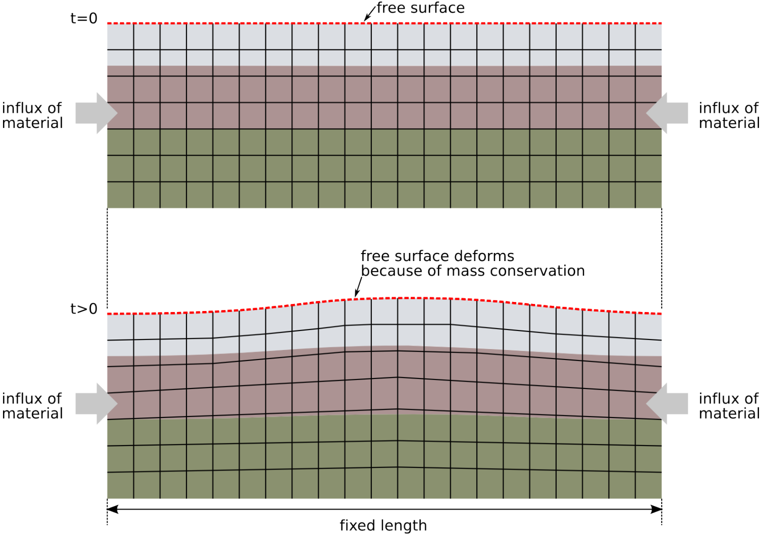
In Lagrangian methods the mesh deforms



	+	−
Lagrangian	Follows surfaces	Needs remeshing
Eulerian	No remeshing	Extra effort to follow surfaces

Kinematical description (3)

Arbitrary Lagrangian-Eulerian → the mesh somewhat deforms



→ Finite Element method

Fullsack, GJI 1995, Thieulot, PEPI 2011

Kinematical description (3)

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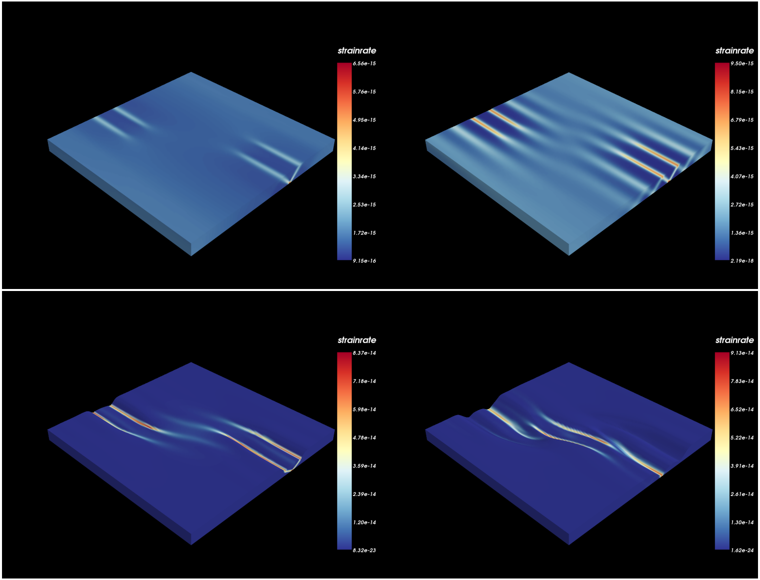

Allken et al, JGR 2011, G^3 2012

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There are three essential features needed to properly model free surfaces:

- A scheme is needed to describe the shape and location of a surface,
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- Lagrangian formulation (or ALE): no special requirement
- Eulerian formulation: the mesh cannot conform to the Earth's surface $\rightarrow$ we need to model the air too.

Free surface (2) - Sticky air

- This method requires the addition of a fluid layer in the model domain.
- pb: air viscosity $< 10^{-5} Pa.s$ vs mantle viscosity $\sim 10^{21} Pa.s$
- air is replaced by a proxy, i.e. a fluid with low density and a sufficiently small viscosity.
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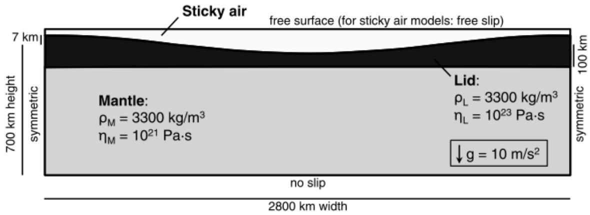

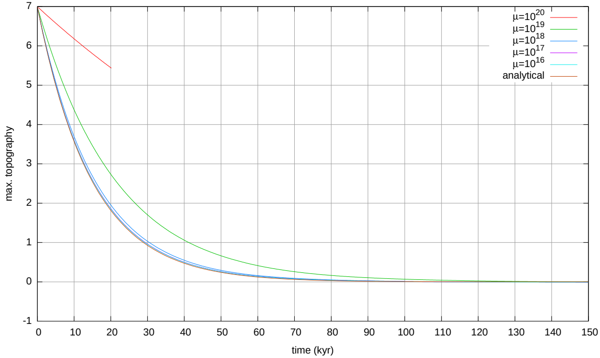

Crameri et al, GJI 189, 2012

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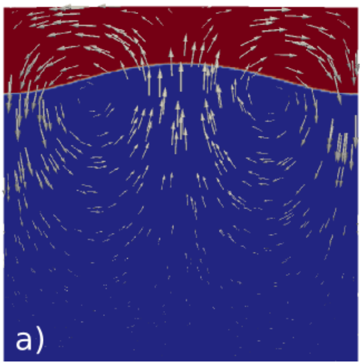
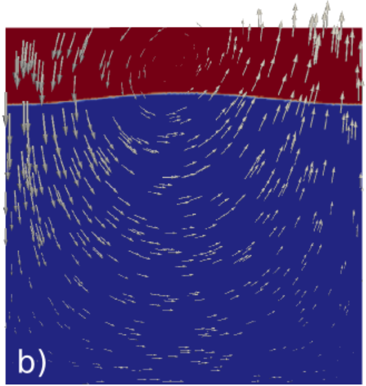


dt small



dt large

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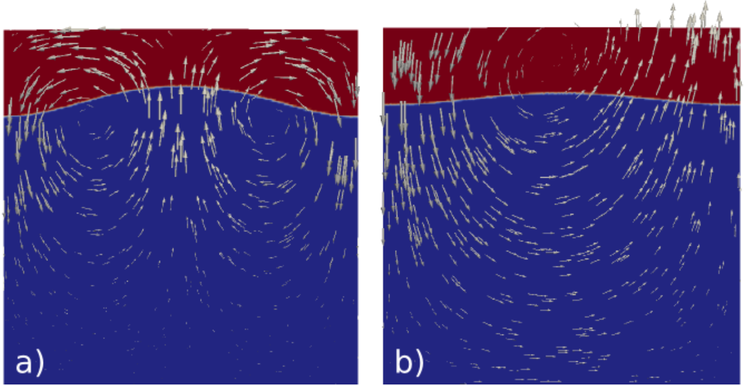
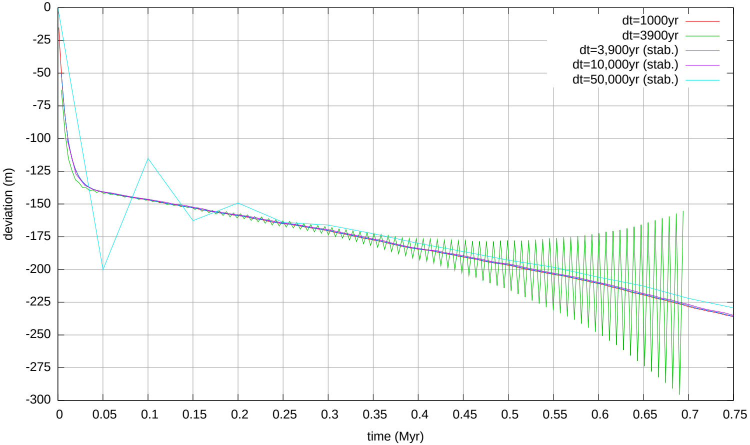


dt small — *dt* large

$\Rightarrow$ Need for stabilisation !

Free surface (5) - stabilisation



Kaus et al, PEPI 181, 2010, Duretz, Gcubed, 2011, Quinquis et al, Tectonophysics 497, 2011

2D vs 3D

Earth is 3D. Why are 99% of all modelling papers 2D ?

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	2D	3D	ratio
grid	100x100	100x100x100	
# nodes	10^4	10^6	
# dofs	3×10^4	4×10^6	> 100
memory solver	$< 10 Mb$	$\sim 100 Gb$	$> 10^5$
solve time	$\sim 1s$	$1h$	> 1000
# tracers	$5^2 \times 10^4$	$5^3 \times 10^6$	500

$\Rightarrow$ 100-fold increase in memory and computational time
$\hookrightarrow$ optimised code, dedicated methods, parallelism, ...

2D vs 3D

Jadamec & Billen, 2012: *The mesh contains 960 x 648 x 160 elements in the longitudinal, latitudinal, and radial directions, respectively. Models were run using 360 processors on Lonestar, a Linux cluster, for approximately 48 hours per job in models with the composite viscosity and for less time in models with the Newtonian only viscosity.*

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Li et al, EPSL 2013: *The Cartesian spatial domain is resolved by 501x341x165 grid points with the resolution of 2x2km in the x-y plane and 4 km in the along-strike z-direction. The lithological structure of the model is represented by a dense grid of about 330 million randomly distributed markers used for advecting various material properties and temperatures.*

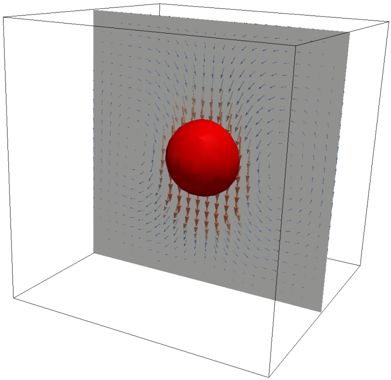
Boundary conditions (1)

- Free slip (flow tangential to boundary) Jadamed & billen, JGR, 2012, Leng & Gurnis, 2011
- No-slip (no flow along the boundary)
- kinematical (precribed velocity) Gurnis et al, Gcubed, 2004
- stress (prescribed stress)
- Open boundaries are implemented by constraining zero tangential velocity on the boundary and by imposing a lithostatic pressure condition for the normal stress on the boundary Chertova et al, 2012.

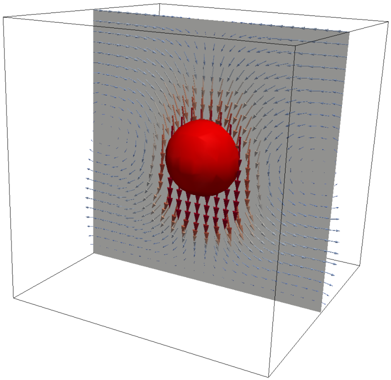
Your model is only as good as the boundary conditions you apply.

Boundary conditions (2) - Open Boundary conditions

$$-\nabla p + \nabla(2\mu\dot{\epsilon}) = \rho g \qquad p = p_{lith} + \delta p$$



free slip side walls



open b.c. side walls

Boundary conditions (3) - Open Boundary conditions

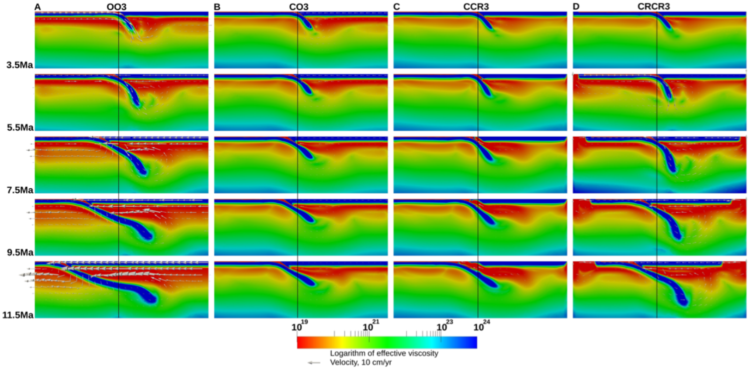
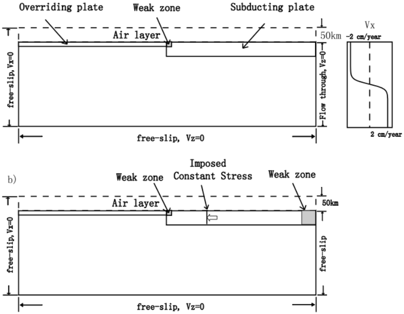


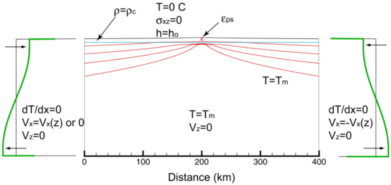
Fig. 4. Evolution of the subduction process for model OO3 with open boundaries, model CO_3 closed left and open right boundary, model CCR3 with closed right and left boundaries with spreading centre on the right boundary and model CRCR3 with closed boundaries. Arrows show the direction and magnitude of flow field. Identical scaling of the velocity vectors applies to all cases.

Chertova et al, Solid Earth 3, 2012

Boundary conditions (4) - In/Outflow



Leng & Gurnis, 2011



Gurnis et al, 2004

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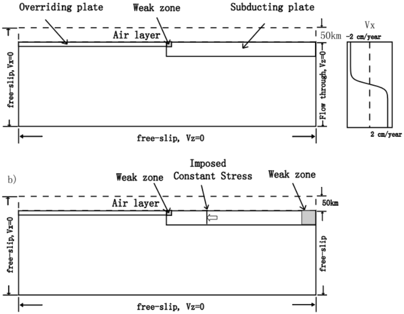

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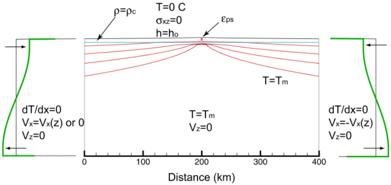

Gurnis et al, 2004

Eulerian computational domain + incompressible flow:
$\Rightarrow$ inflow must balance outflow !

The art of benchmarking (1)

- ASPECT $>$ 500,000 lines
- ELEFANT $>$ 100,000 lines
- Complex codes are made of multiple algorithms interacting with each other:
  Solving Stokes Eq + Solving Temp. Eq. + Advecting material + Phase change + brittle-ductile transition +Surface processes + ...

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This process is called *benchmarking*

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Since (1) is not always possible, (2) is widely used:

"A comparison of numerical surface topography calculations: an evaluation of the sticky air method", Crameri et al, GJI 189, 2012

"A community benchmark for 2-D Cartesian compressible convection in the Earths mantle", King et al, GJI 180, 2010

"A comparison of methods for the modeling of thermochemical convection", van Keken, JGR 102, 1997

"The numerical sandbox: comparison of model results for a shortening and an extension experiment", Buiter et al, 2006

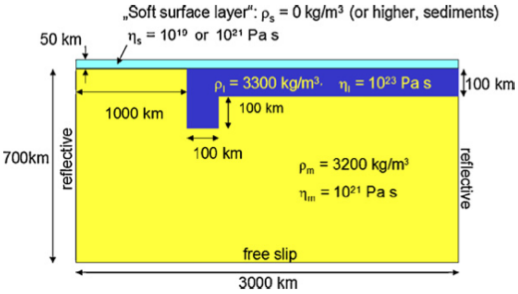
"3D convection at infinite Prandtl number in Cartseian geometry - a benchmark comparison", Busse et al, 1993

"A two- and three-dimensional numerical comparison study of slab detachment", C. thieulot et al, 2014 ?

"A benchmark comparison of spontaneous subduction modelsTowards a free surface", H. Schmeling et al, PEPI 2008

The art of benchmarking (2) - Example

Schmeling et al, PEPI, 2008



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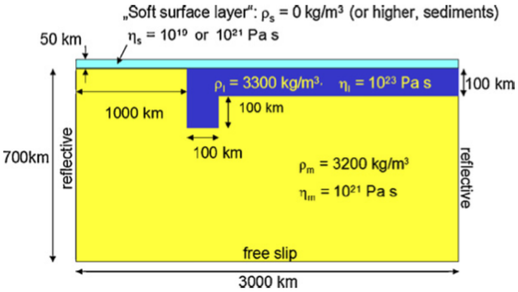

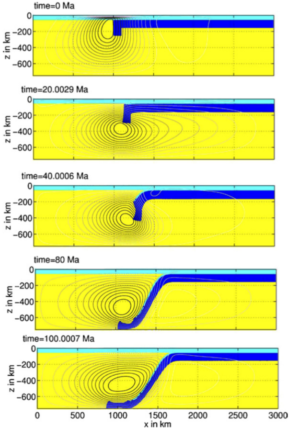

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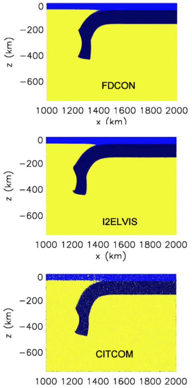

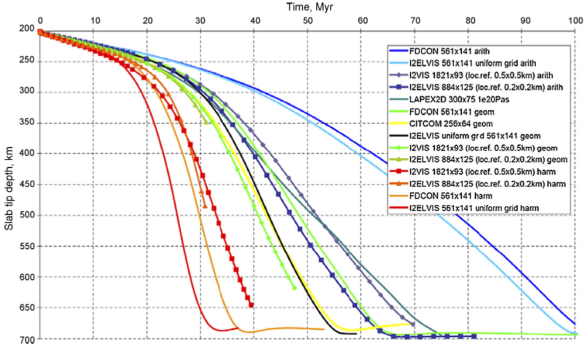

Material tracking (1)

- The Earth consists of an upper crust, a middle crust, a lower crust, a lithospheric mantle, an asthenospheric mantle, sediments, melts, ...
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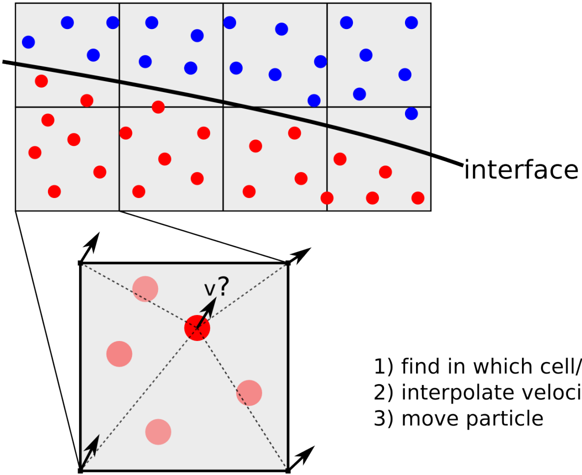
- The Earth consists of an upper crust, a middle crust, a lower crust, a lithospheric mantle, an asthenospheric mantle, sediments, melts, ...
  $\Rightarrow$ realistic setups require multiple materials.
- This is not unique to Geodynamics, but very common in CFD too.
- Multiple methods have been designed over the past decades
  - marker-and-cell (MAC) , Particle-in-Cell (PIC)
    McKee et al, Computers & Fluids, 2008, Gerya book
  - Compositional fields
    ASPECT manual, ConMan code
  - Level set functions
    hillebrand, subm. 2014
  - Particle Level set
    Braun et al, PEPI 2008, Samuel & Evonuk, C3, 2010
  - Marker-Chain
    van Keken et al, JGR 1997
  - all kinds of hybrid methods

None is perfect, none is trivial, none is the best.

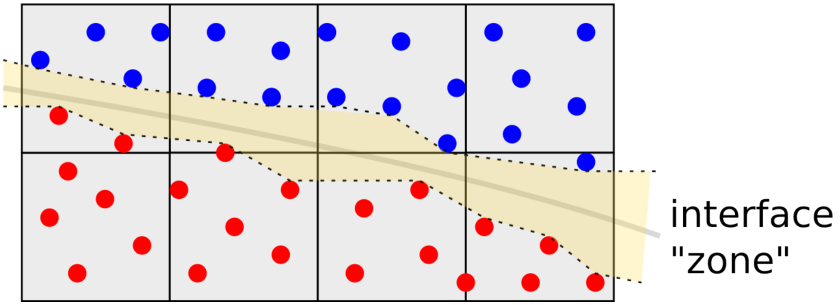
Material tracking (2) - particle/marker advection

Purely Eulerian grid, particles/markers are used to track crustal and lithospheric material.



1) find in which cell/elt the particle is
2) interpolate velocity on particle
3) move particle

Material tracking (3) - particle/marker advection



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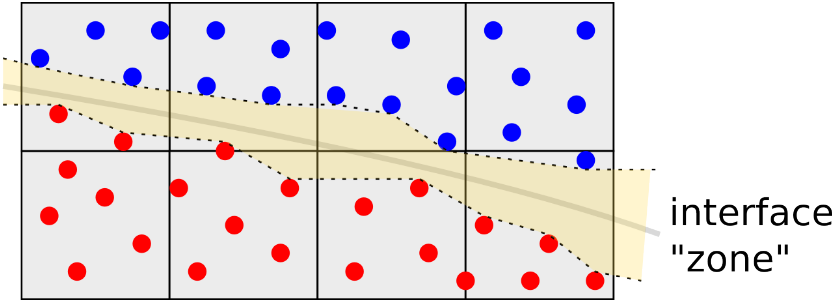

If average spacing between particles is $\sim 500m$, free surface is known with $\pm 250m$ precision.

Material tracking (4) - particle/marker advection

Task 1: "Find in which cell/element the particle is"

Assuming a 3D simulation with 100x100x100 grid and 10 particles per cell, doing 1000 timesteps.
$\rightarrow 10^6$ cells , 10^7 particles

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Do not use the force Luke ...

Material tracking (5) - particle/marker advection

Task 2: "interpolate velocity on particle"

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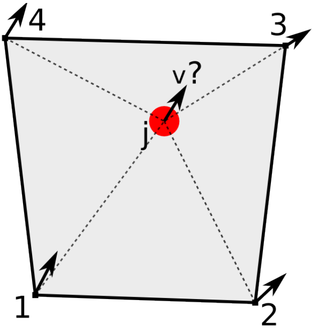
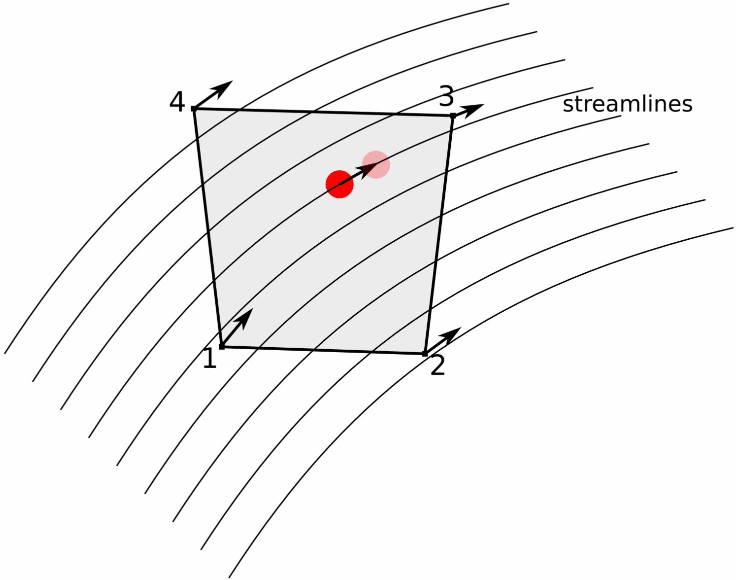


u(xj,yj)=fct(u1,u2,u3,u4, x1,x2,x3,x4,y1,y2,y3,y4)

v(xj,yj)=fct(v1,v2,v3,v4, x1,x2,x3,x4,y1,y2,y3,y4)

Material tracking (6) - particle/marker advection

Task 3: "move particle with velocity v"



Material tracking (7) - particle/marker advection

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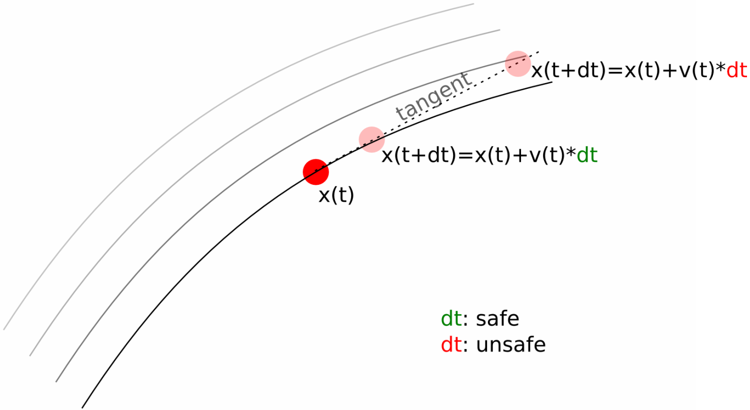

$\Rightarrow$ small *dt* is better, but increases computational time.

Material tracking (8) - particle/marker advection

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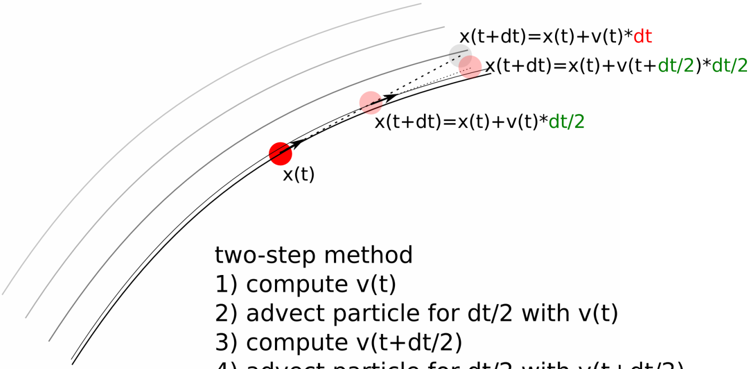

two-step method
1) compute v(t)
2) advect particle for dt/2 with v(t)
3) compute v(t+dt/2)
4) advect particle for dt/2 with v(t+dt/2)

Solvers (1)

- Most methods yield a very large linear system of equations. $N \simeq 10^6 - 10^8$
- Corresponding matrices are *very* sparse (nonzero terms $< 0.001\%$ of matrix terms)
- A solver is a piece of code which solves the system as efficiently as possible (and possibly in parallel)

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There are two main types of solvers

- Direct
- Iterative

Solvers (2) - Direct Methods

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- They can reuse the factorized matrix and apply it to the solutions of multiple right-hand sides.

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- They are harder to parallelize efficiently on a large number of processors

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- Therefore, when solving a problem with an iterative method, you can observe the error estimate in the solution decrease with the number of iterations.
- For well-conditioned problems, this convergence should be quite monotonic. If you are working on problems that are not as well-conditioned, then the convergence will be slower.

Solvers (2) - an example of iterative method

The Gauss-Seidel method is an iterative technique for solving a square system of n linear equations with unknown x:

$$A\mathbf{x} = \mathbf{b}.$$

It is defined by the iteration

$$L_*\mathbf{x}^{(k+1)} = \mathbf{b} - U\mathbf{x}^{(k)},$$

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In more detail, write out A, x and b in their components:

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix}, \qquad \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}, \qquad \mathbf{b} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}.$$

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The system of linear equations may be rewritten as:

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The Gauss-Seidel method now solves the left hand side of this expression for x, using previous value for x on the right hand side. Analytically, this may be written as:

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The procedure is generally continued until the changes made by an iteration are below some tolerance, such as a sufficiently small residual.

Code structure

- One or multiple folders containing fortran/C/C++/matlab files
- Makefile/configure file
- Cookbooks
- Post-processing tools

Languages


Perl
JavaScript
PHP
Markup
DOSBatch
Tcl-Tk
LabVIEW
Logic-based
Logo
Visual
Haskell
Occam
Scala
Functional
Simula
Miranda
C++
SQL
.NET
XML
Simkin
Moto
CLU
Pascal
VisualBasic
Euphoria
RPG
Cocoa
Pliant
Python
ObjectiveCaml
Database
BETA
MATLAB
Cobol
Maple
Prototype-based
DataStructured
Erlang
Declarative
Ruby
UML
GLSL
ICI
Turing
ABC
Eiffel
Delphi
Scripting
Multiparadigm
Squeak
Ada
Yorick
Assembly
Mumps
Verilog
CurlyBracket
Groovy
PowerBuilder
S-Lang
Object-Oriented
LaTeX
Clean
Oberon
Scheme
Java
Clojure
ADL
Fortran
IDL
Bistro
Caml
FP
BASIC
HyperCard
Procedural
PostScript
Prolog
Reflective
HTML
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Should you write your own code ?

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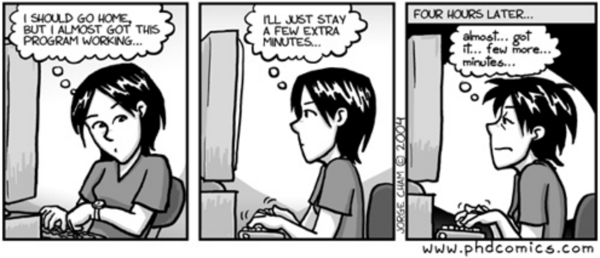
- Spending more time debugging (not fun) than coding (fun)



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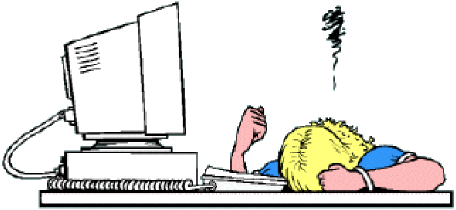
- Legacy code: you inherit a code written 20 years ago by your supervisor, in a deprecated language, and consequently modified by 5 generations of phd students ...



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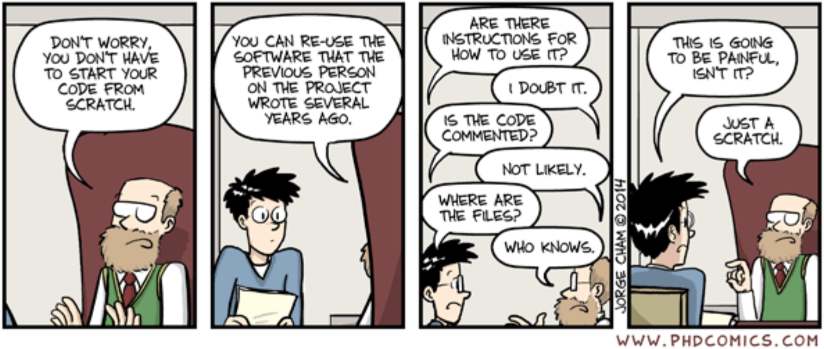

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Let's read the papers and learn some more.

Journals

- GJI: Geophysical Journal International
- JGR: Journal of Geophysical Research
- G3: Geochemistry, Geophysics, Geosystems