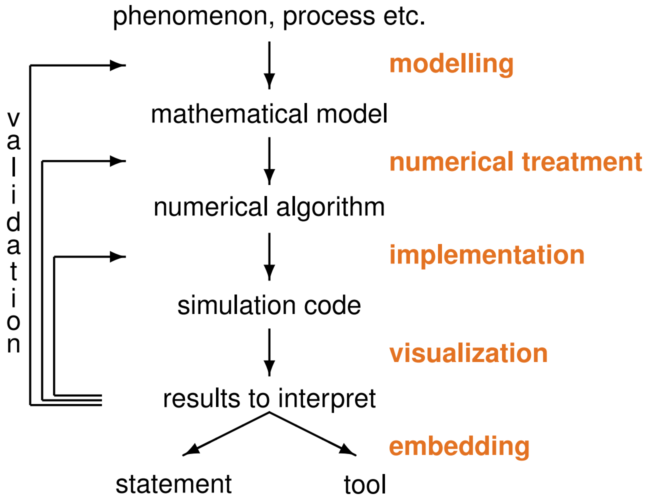
Scientific Computing II

Overview

Michael Bader

Summer 2015

Remember: The Simulation Pipeline



Topic #1: Solving Systems of Linear Equations

Focussing on

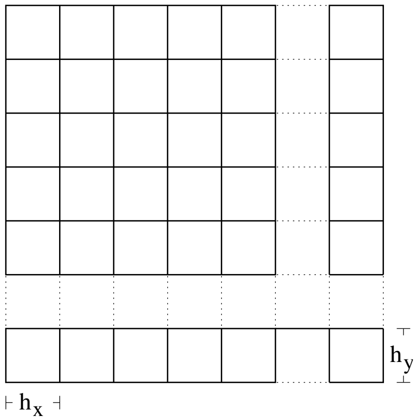
- large systems: 10^6–10^9 unknowns
- sparse systems: typically only $\mathcal{O}(N)$ non-zeros in the system matrix (N unknowns)
- systems resulting from the discretization of PDEs

Topics

- relaxation methods (as smoothers)
- multigrid methods
- Conjugate Gradient methods
- preconditioning

Recall: Finite Volume Model for Heat Equation

- object: a rectangular metal plate
- model as a collection of small connected rectangular cells



- compute the temperature distribution on this plate!

A Finite Volume Model (2)

- model assumption: temperatures in equilibrium in every grid cell
- heat flow across a given edge is proportional to
  - temperature difference $(T_1 - T_0)$ between the adjacent cells
  - length h of the edge
- e.g.: heat flow across the left edge:

$$q_{i,j}^{(\text{left})} = k_x \left(T_{i,j} - T_{i-1,j}\right) h_y$$

  note: heat flow **out of** the cell (and $k_x > 0$)
- heat flow across all edges determines change of heat energy:

$$\begin{aligned} q_{ij} &= k_x \left(T_{ij} - T_{i-1,j}\right) h_y + k_x \left(T_{ij} - T_{i+1,j}\right) h_y \\ &+ k_y \left(T_{ij} - T_{i,j-1}\right) h_x + k_y \left(T_{ij} - T_{i,j+1}\right) h_x \end{aligned}$$

A Steady-State Model

...and a large system of linear equations

- heat sources: consider additional source term $F_{i,j}$ due to
  - external heating
  - radiation
- $F_{i,j} = f_{i,j} h_x h_y$ ($f_{i,j}$ heat flow per area)
- equilibrium with source term requires $q_{i,j} + F_{i,j} = 0$:

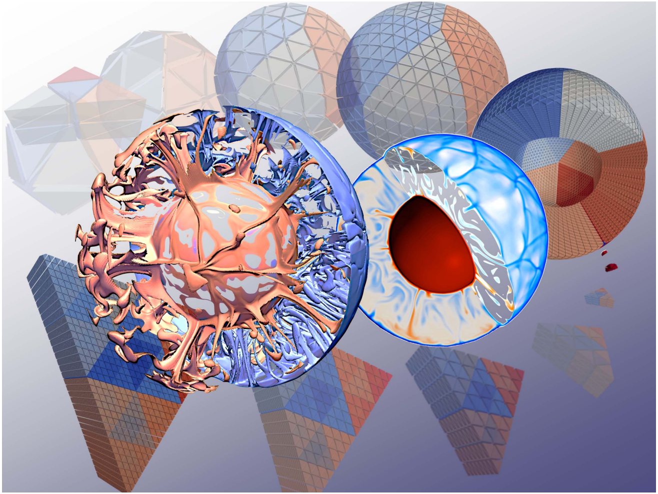
$$\begin{aligned} f_{i,j} h_x h_y &= -k_x h_y \left(2T_{i,j} - T_{i-1,j} - T_{i+1,j} \right) \\ &\quad -k_y h_x \left(2T_{i,j} - T_{i,j-1} - T_{i,j+1} \right) \end{aligned}$$

- leads to large system of linear equations
- $1/h^2$ unknowns, sparse system matrix (only 5 entries per row)

$\rightarrow$ **will be our model problem!**

Multigrid: HHG for Mantle Convection

(Rüde et al., 2013; project: TERRA NEO)



Multigrid: HHG for Mantle Convection (2)

Mantle Convection on PetaScale Supercomputers:

- mantle convection modeled via Stokes equation (“creeping flow”)
- linear Finite Element method on an hierarchically structured tetrahedral mesh
- requires solution of global pressure equation in each time step

Weak Scaling of HHG Multigrid Solver on JuQueen:

- geometric multigrid for Stokes flow via pressure-correction
- pressure residual reduced by 10^{-3} (A) or 10^{-8} (B)

Nodes	Threads	Grid points	Resolution	Time: (A)	(B)
1	30	$2.1 \cdot 10^{07}$	32 km	30 s	89 s
4	240	$1.6 \cdot 10^{08}$	16 km	38 s	114 s
30	1 920	$1.3 \cdot 10^{09}$	8 km	40 s	121 s
240	15 360	$1.1 \cdot 10^{10}$	4 km	44 s	133 s
1 920	122 880	$8.5 \cdot 10^{10}$	2 km	48 s	153 s
15 360	983 040	$6.9 \cdot 10^{11}$	1 km	54 s	170 s

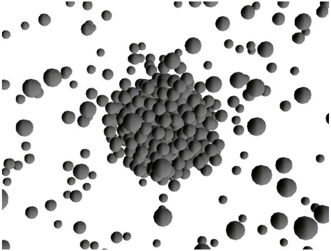
Topic #2: Molecular Dynamics

Discuss large part of the simulation pipeline:

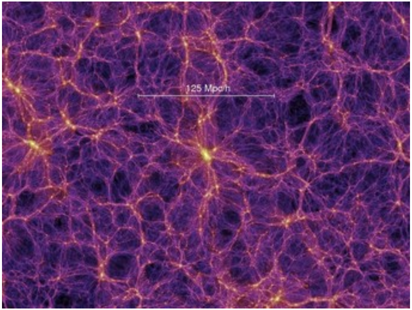
- modelling: potentials, forces, systems of ODE
- numerics: suitable numerical methods for the ODEs
- implementation: short-range vs. longe-range forces
- visualisation? (well, actually not the *entire* pipeline . . .)

Focussing on

- large systems: 10^6–10^9 particles
- short-range vs. long-range forces
- N-body methods, parallelization



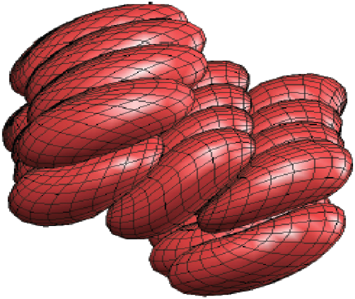
N-Body Methods: Millennium-XXL Project



(Springel, Angulo, et al., 2010)

- *N*-body simulation with $N = 3 \cdot 10^{11}$ "particles"
- compute gravitational forces and effects
  (every "particle" correspond to $\sim 10^9$ suns)
- simulation of the generation of galaxy clusters
  plausibility of the "cold dark matter" model

N-Body Methods: Particulate Flow Simulation



(Rahimian, . . . , Biros, 2010)

- direct simulation of blood flow
- particulate flow simulation (coupled problem)
- Stokes flow for blood plasma
- red blood cells as immersed, deformable particles

Part I

Organisation

Exams, ECTS, Modules

ECTS, Modules

- 5 ECTS (2+2 lectures/tutorials per week)
- CSE: compulsory course
- Biomed. Computing/Computer Science: elective/Master catalogue
- others?

Tutorials:

- tutor: Arash Bakhtiari
- time and day: **to be discussed . . .**

Exam:

- written exam at end of semester
- based on exercises presented in the tutorials