

# Scientific Computing II

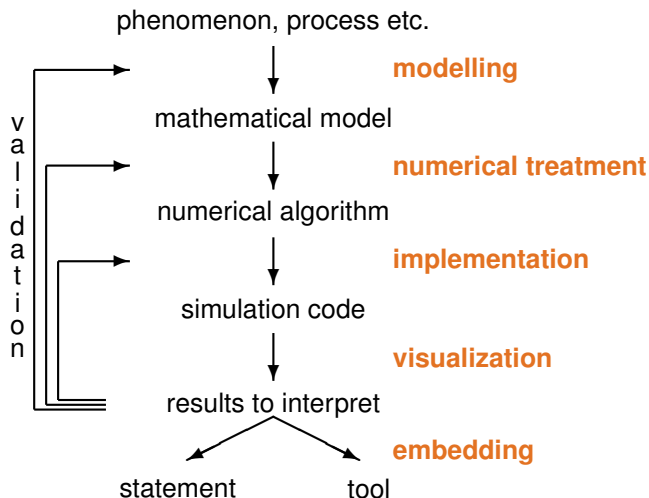
Overview

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# Remember: The Simulation Pipeline



# Topic #1: Solving Systems of Linear Equations

## Focussing on

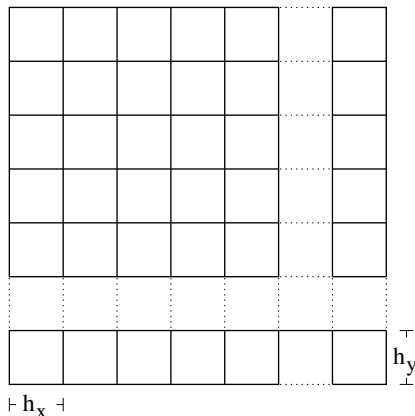
- large systems:  $10^6$ – $10^9$  unknowns
- sparse systems: typically only  $\mathcal{O}(N)$  non-zeros in the system matrix ( $N$  unknowns)
- systems resulting from the discretization of PDEs

## 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:

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

note: heat flow **out of** the cell (and  $k_x > 0$ )

- heat flow across all edges determines change of heat energy:

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

# 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  $q_{i,j} + F_{i,j} = 0$ :

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

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

→ **will be our model problem!**

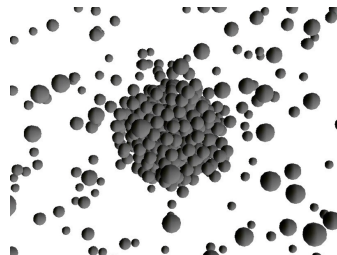
## Topic #2: Molecular Dynamics

### Discuss large part of the simulation pipeline:

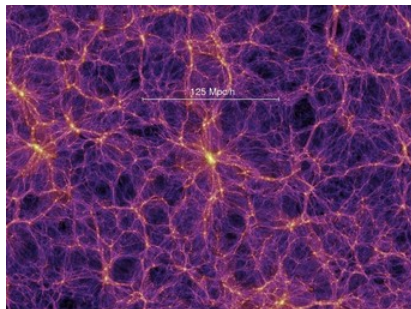
- modelling: potentials, forces, systems of ODE
- numerics: suitable numerical methods for the ODEs
- implementation: short-range vs. long-range forces
- visualisation? (well, actually not the *entire* pipeline ...)

### 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

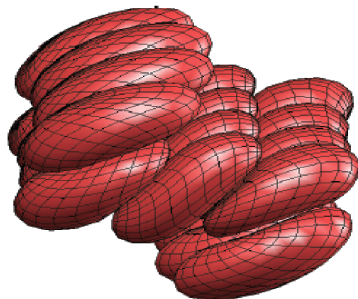


(Springel, Angulo, et al., 2010)

- $N$ -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:

- tutors: Philipp Neumann, Wolfgang Eckhardt
- Monday 10-12, lecture room MI 02.07.023, starting Apr 22

## Exam:

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