

Advanced Programming in Engineering

Intro (Stefan – s.luding@utwente.nl)

Wouter den Otter, Vanessa Magnanimo, Thomas Weinhart,
Anthony Thornton, Stefan Luding
MSM, CTW, MESA+, UTwente, NL



Contents

- **Why** is this class important for me?
- **What** will I learn in this class?

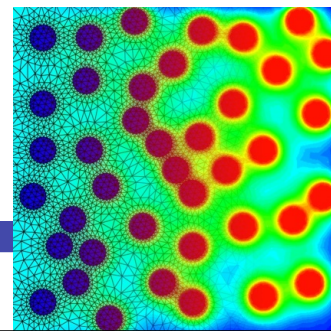
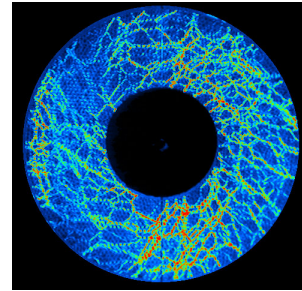


Why is the class important for me?

Computations are everywhere in engineering problems.

Many problems are resolved with the aid of computers and dedicated programs today. It is important to be able to understand & implement numerical algorithms

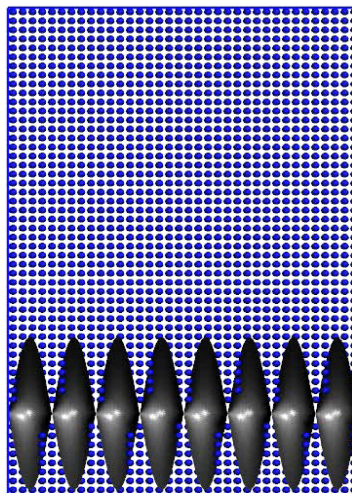
Is it really important for an engineer to be familiar with computers and programming languages?



Open source

Based on:

- HGrid
- MicroMacro



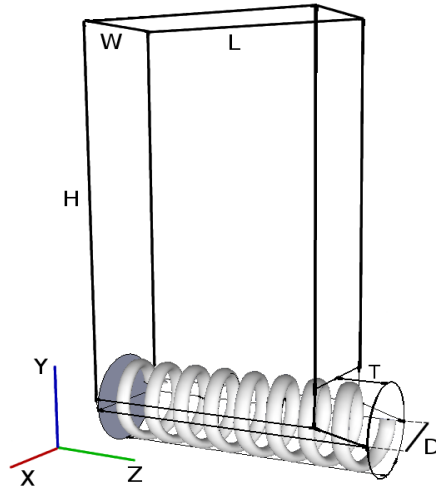
Dosing application example ...

MERCURYDPM

Open source

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- HGrid
- MicroMacro



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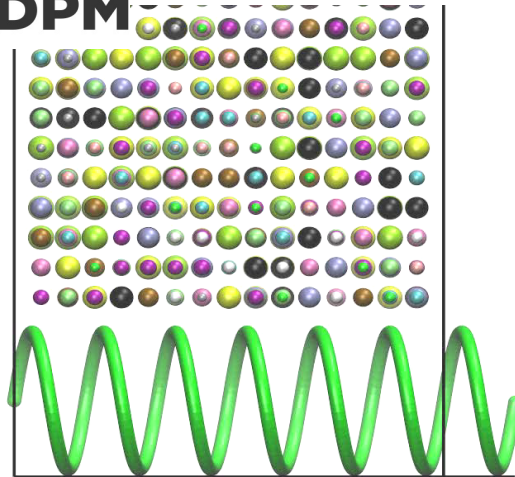
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msm

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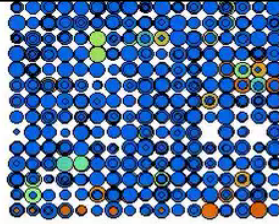


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flowable powder



© Marco Ramaioli, Nestle

msm (screw hidden)

Dosing application example ...

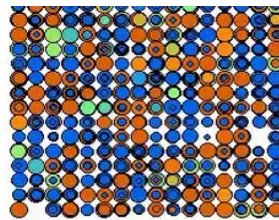
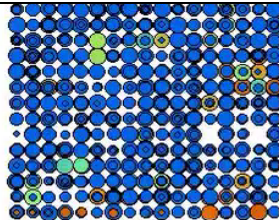


Open source

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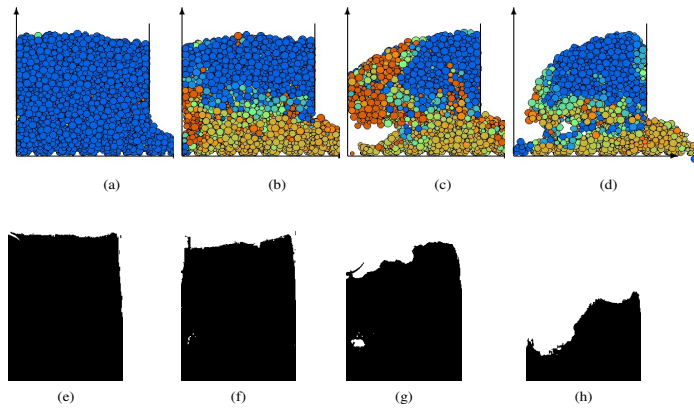
**flowable powder vs.
sticky, chunky powder**



msm (screw hidden) 0.5.1006 MSM 2013

Dosing application example ...

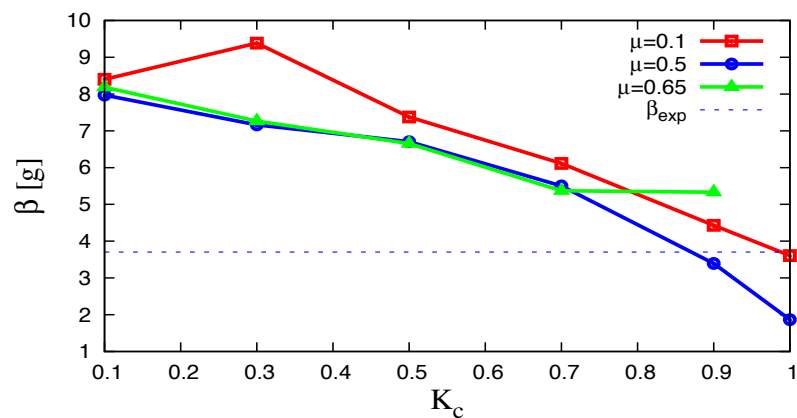
Dosing: DEM vs. experiment



*Based on O. I. Imole, D. Krijgsman, T. Weinhart, V. Magnanimo, E. C. Montes, M. Ramaioli, and S. Luding.

Experiments and Discrete Element Simulation of the Dosing of Cohesive Powders in a Canister Geometry. In preparation, PhD-thesis, O. I. Imole 2014

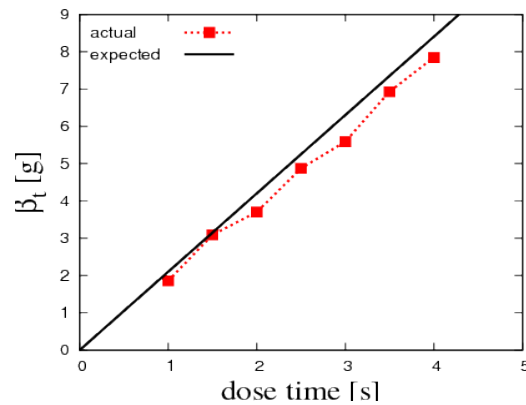
Dosing – parameter calibration



*Based on O. I. Imole, D. Krijgsman, T. Weinhart, V. Magnanimo, E. C. Montes, M. Ramaioli, and S. Luding.

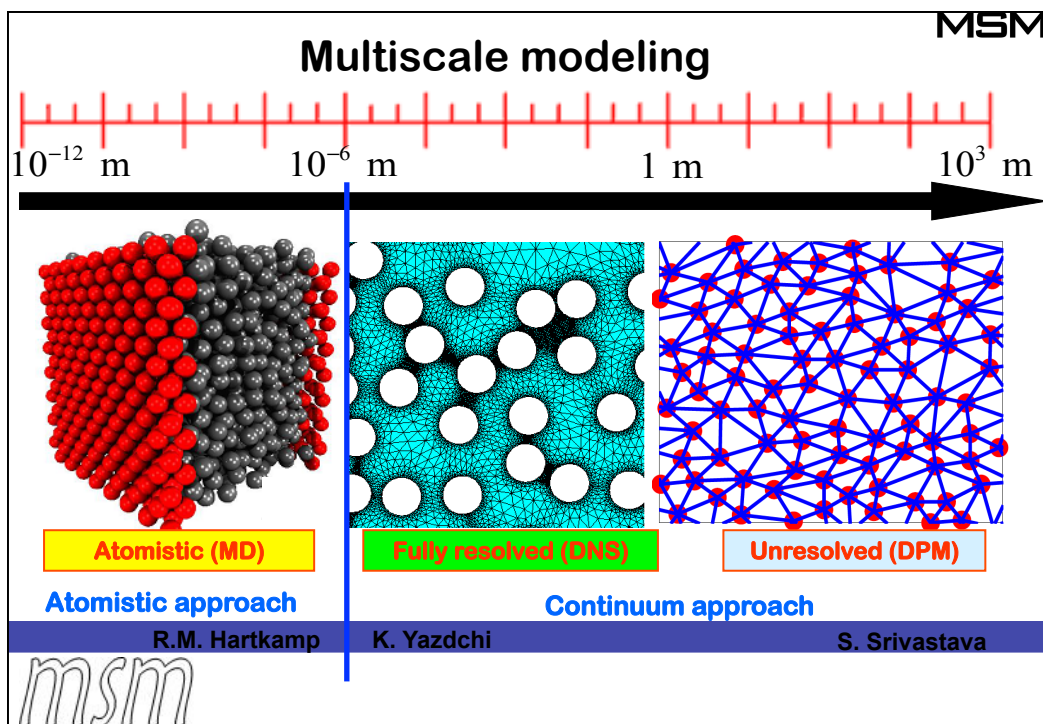
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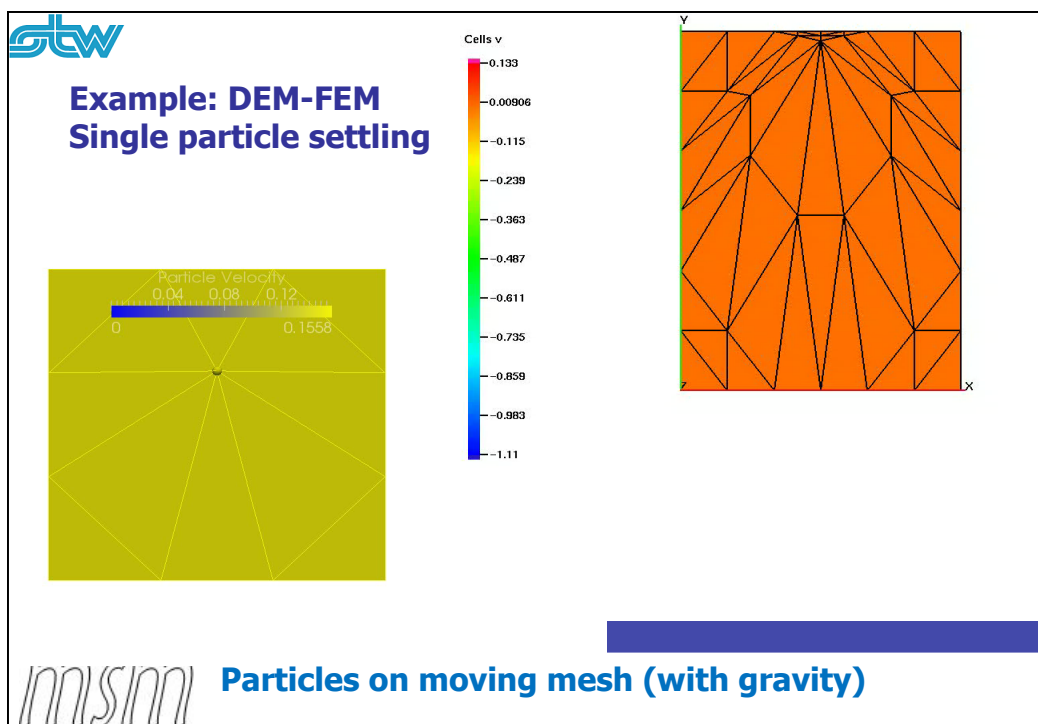
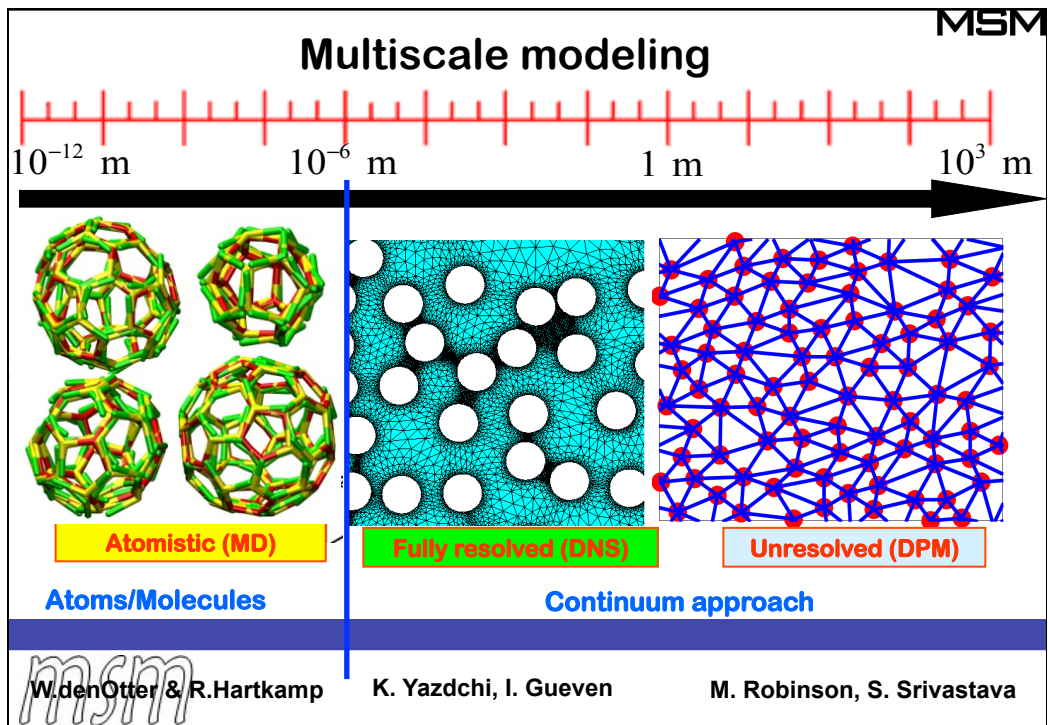
Dosing: DEM vs. experiment



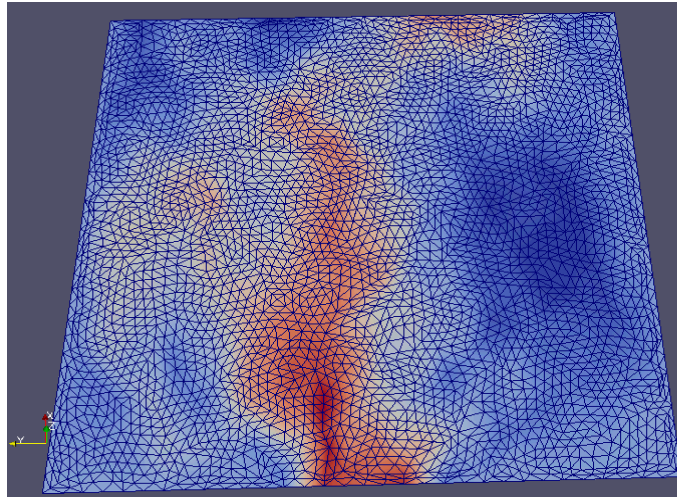
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Example: Fluidization DEM-FEM

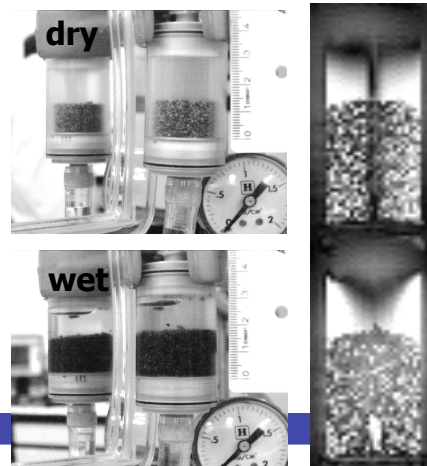


Fluidization on moving mesh with 800 particles (with gravity)

Realistic simulation of powder dispersion by a liquid jet

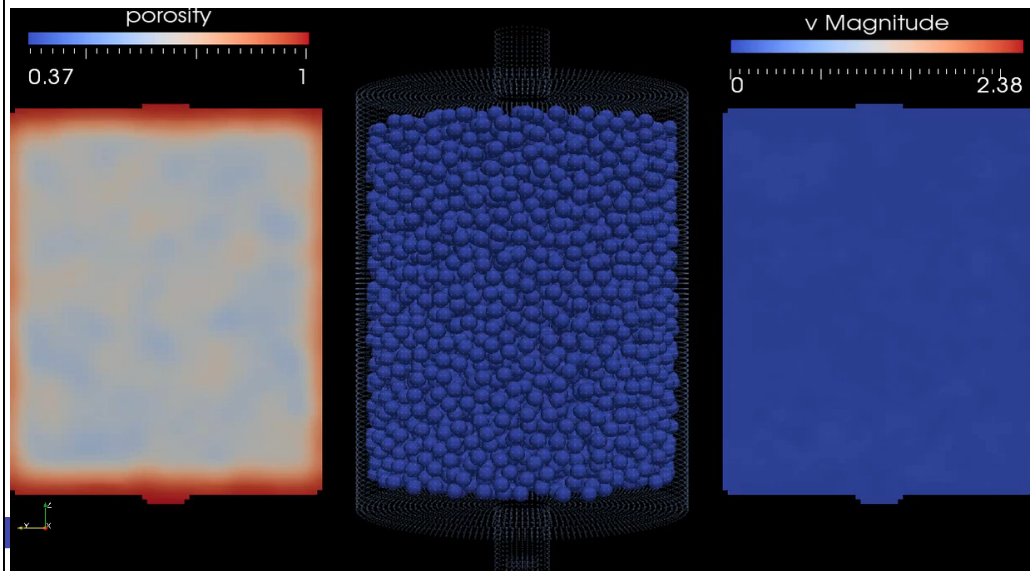
- **Dispersion** of grains by a liquid jet
=> food processing industry (Nestlé)
- **Controlled Lab-Experiment**
(camera, pressure sensor & MRI) data* for poppy seeds dispersed in water
- Goals:
 1. **Validate** SPH-DEM results to experiments
 2. Investigate dynamics of dispersed bed
 3. Map process parameters to different regimes
initial wet vs. initial dry particles

MRI

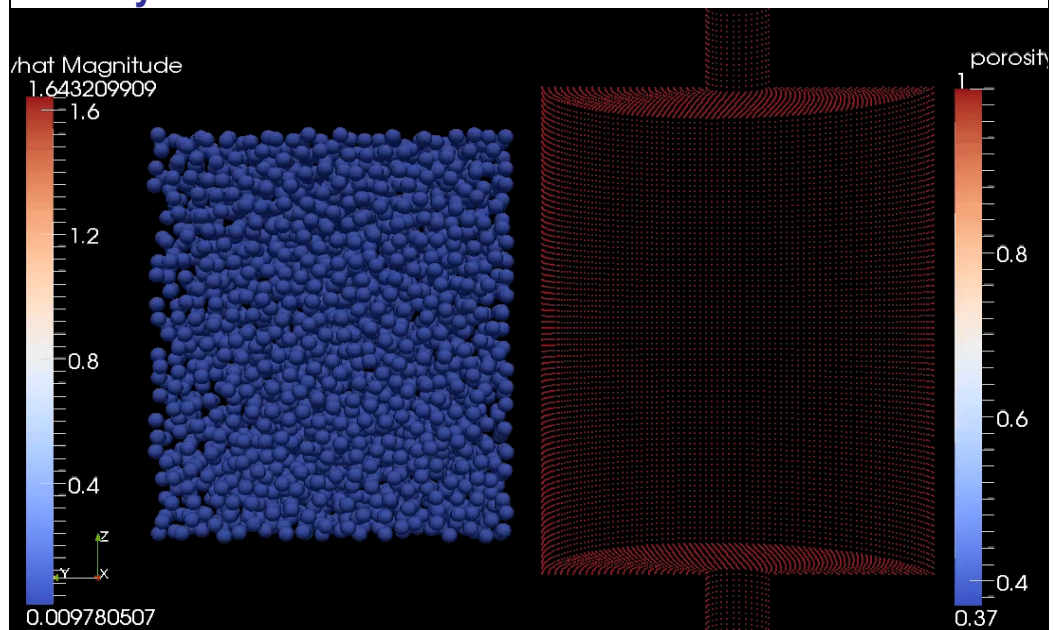


*Courtesy Dr Marco Ramaoli & Chloe Trarieux

Wet Start

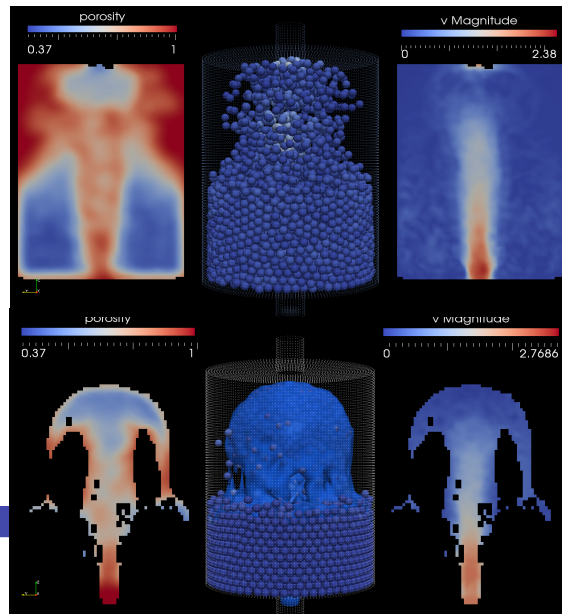


Dry Start



Experiment & Simulation of powder dispersion by a liquid jet

- Application: Particle dispersion
(collaboration with **Nestle**)
- Method: SPH-DEM
- Results:
 - **Wet** – Recovers qualitative features from experiment: Jet, dispersion ...
 - **Dry** – Fails to recover some major features (e.g. bed lift regime).
 - Surface tension not modeled yet.



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Multi Scale Mechanics

What can we do with the computer?

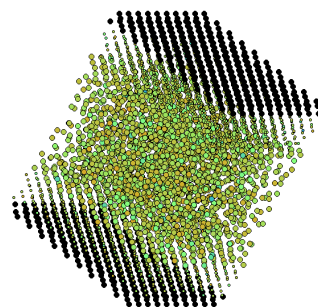
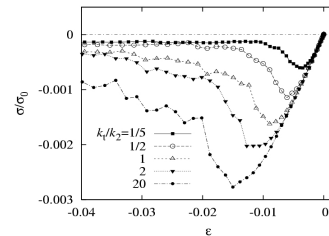
- Evaluation of (experimental) data
- Solving physical/engineering problems
- Numerical “experiments”

How do we do that?

- Compiler languages (C, **C++**, Fortran,...)
- Interpreter languages (**MATLAB**,...)

What do we learn?

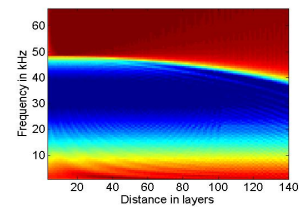
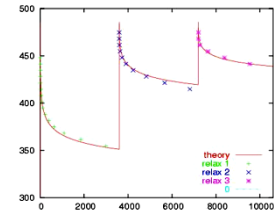
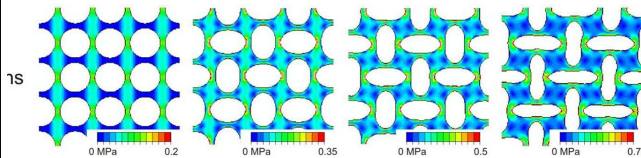
- Translate problems to algorithms
- Practical experiences (exercises, debugging...)



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Program:

- Algorithms to solve differential equations
- Finite differences (MD for solids 1D+2D)
- Finite element method (same solid)
- Molecular dynamics with Lennard-Jones for fluids
- Measuring pressure, temperature and diffusion in MD
- Random numbers & Fractals
- Monte-Carlo for solving integrals and (some) PDEs
- Finite Volume (e.g. shock problem)
- SPH (Fluids) and Lattice Boltzmann (Fluids)



When is the class?

From 10 November

Monday Morning ½	8.45-10.30	Theory
Monday Morning ¾	10.45-12.30	Practice

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Monday Morning ½	8.45-10.30	Theory
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10/11/13 - Introduction to APiE (Stefan Luding & Thomas Weinhart)

17/11/13 - ODE1 (Thomas Weinhart)

24/11/13 - ODE2 (Wouter den Otter)

01/12/13 -

08/12/13 -

15/12/13 -

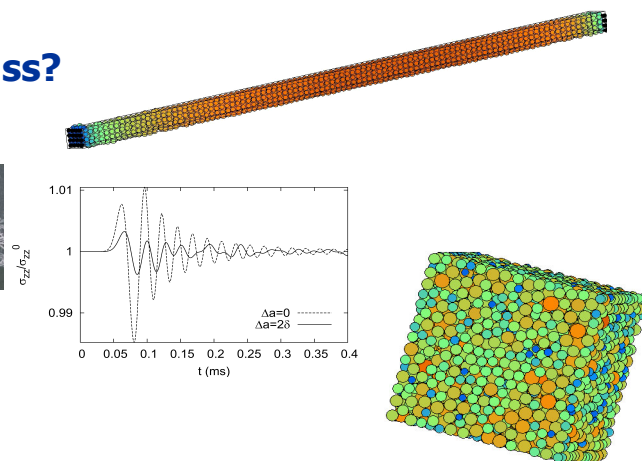
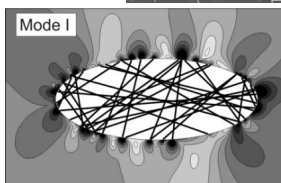
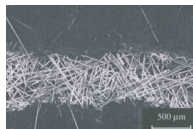
05/01/14 -

12/01/14 -

Where is the class?

see BB: default

OH 112



Questions?

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s.luding@utwente.nl

Contents

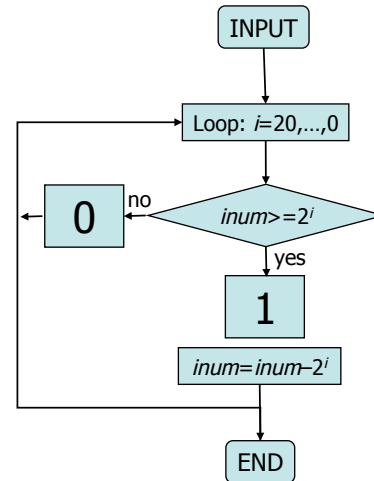
- Introduction – Examples 1&2
- 1st Goal: Debugging and Matlab Optimization
- 2nd Goal: Solve Differential Equations (ODE)
- 3rd Goal: ... 1D/2D Molecular Dynamics (ODE)
- Morning 3/4: Practical Exercises ...

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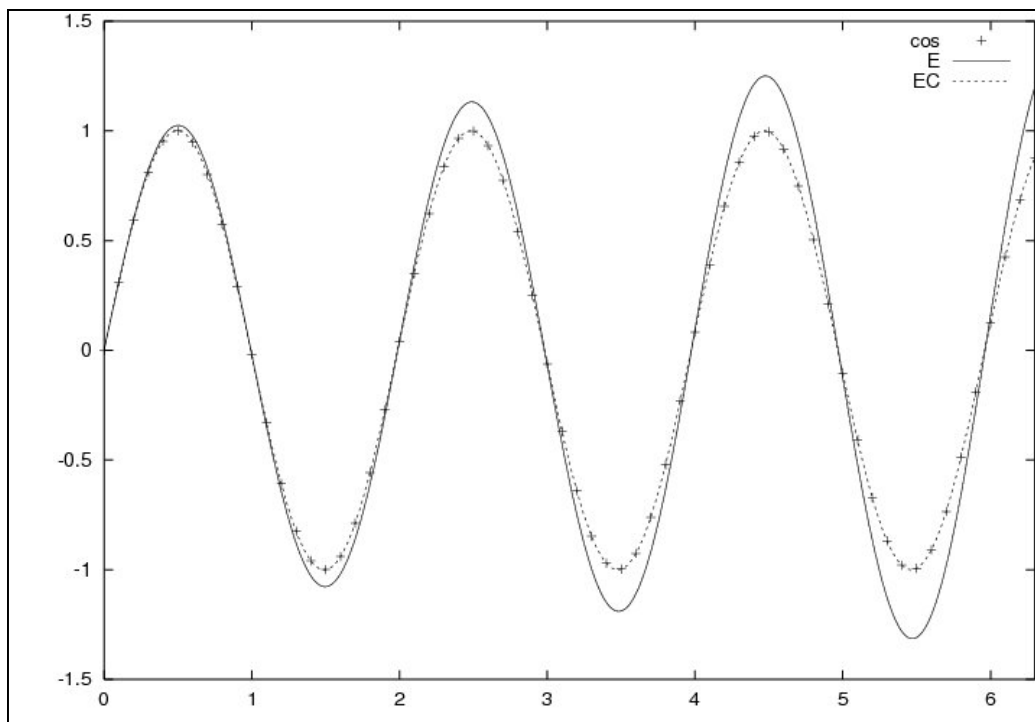
6. // main.cpp
7. {
8.     const int ipmax=20;
9.     int inum;
10.    cout << "Type number: ";
11.    cin >> inum;
12.    if(inum < pow(2.0,ipmax)) // check number
13.    {
14.        cout << "Base 10: " << inum << endl;
15.        cout << "Base 2: ";
16.
17.        // perform binary check for 2^ipmax
18.        for(int i=ipmax; i>=0; i--)
19.        {
20.            if(inum >= pow(2.0,i))
21.            {
22.                inum -= pow(2.0,i);
23.                cout << '1';
24.            }
25.            else
26.                cout << '0';
27.        }
28.        cout << endl;
29.    }
30.    else
31.    {
32.        cout << "ERROR: input-number " << inum << " > "
33.        << pow(2.0,ipmax) << " too large!" << endl;
34.    }
35.    system("PAUSE");
36.    return EXIT_SUCCESS;
37. }

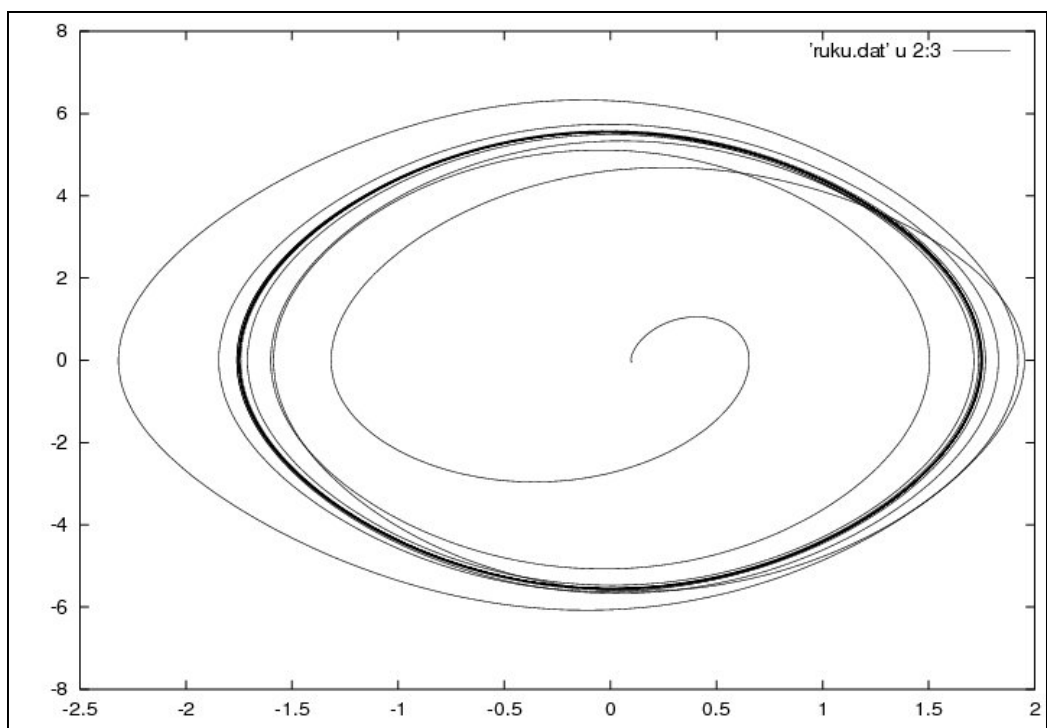
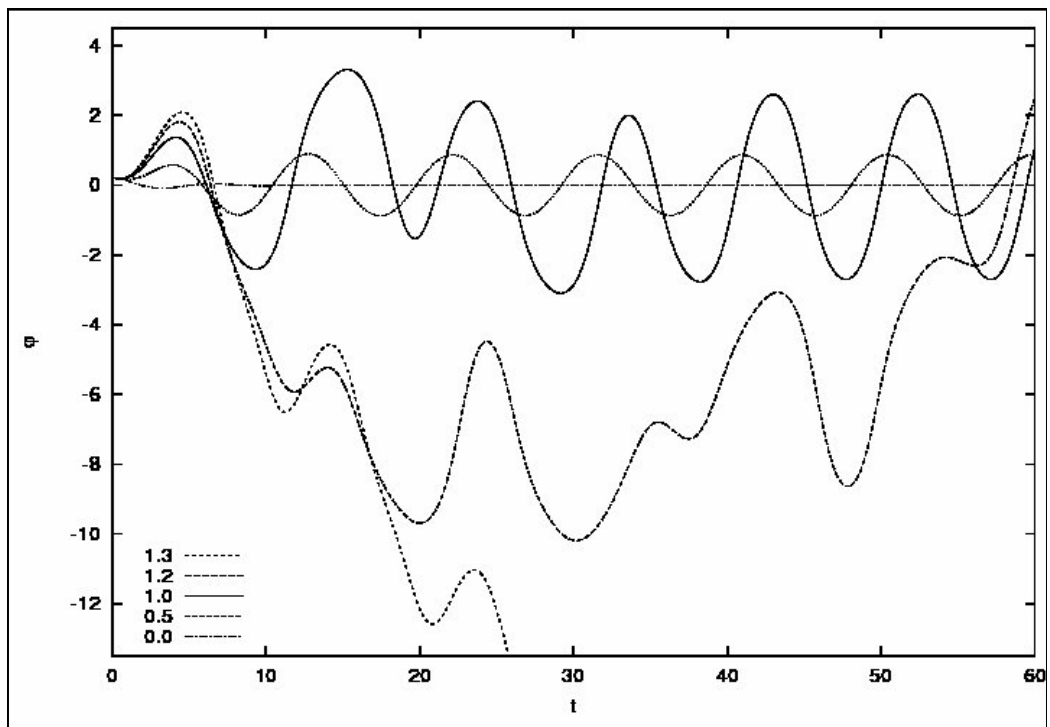
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Previous Course PiE: Exercises



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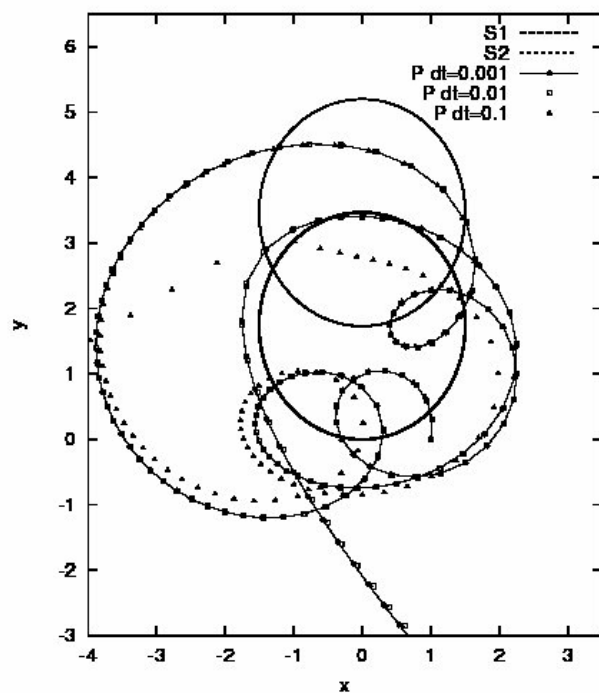
Differential Eqs

Poincare-cut

instead of x-t-plot

view: v-x-plot

attractors/chaos



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Questions?

08:45h – 10:30h
room: OH112

10:45h – 12:30h
room: OH112

Submission: Code+Support-files+PDF report

Advanced Programming in Engineering 191158500

**Vanessa Magnanimo, Thomas Weinhart, Wouter den Otter,
Nicolas Rivas, Marnix Schrojenstein Lantmann, Stefan Luding**

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