Modern Computational Tools in the Materials Science Curriculum

December 10th 2019

M.H.F. Sluiter

M.H.F.Sluiter@tudelft.nl

Conclusions

Materials Science education VERY relevant

is at the core of many societal “pain points”

Google ➔ need to be able to interpret/process data

➔ fundamental understanding & modern data tools (Python/Matlab)

Materials Science: Microstructure poorly suited for “calculus”: 3d fields

c(x,y,z,t) ➔ modern tools (Python/Matlab, Mathematica/Maple)

Materials Science and $20^{th} \Leftrightarrow 21^{st}$ century changes

Environmental impact (climate, pollution, scarcity) b/c

- technology and higher living standards
- world population growth

Accelerating tech/scientific development

- Wider & intensifying competition
- “globalization” of society

21^{st} century: what is needed?

Environment

energy (climate) / scarcity / pollution ➔ Materials Science

Accelerating tech/scientific development & competition

- increased importance of education (esp. techn/science)
- increased role of computation/modeling/prediction
- Increased role of data
    - Still need order-of-magnitude/common sense tests
    - Hard to think with data you need to look-up

Data & Modeling

Most important aspect of phone camera is software, fast processor & lots of fast memory.

Picture quality depends on image processing software, not on the lens!

A modern airplane (or drone) is not flown by the pilot, but through software. Pilot is "director of a software orchestra".

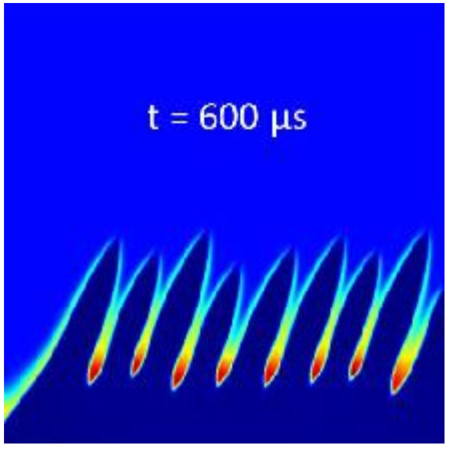
Bicycles with assisted steering!

Data & Modeling, past

Most models are analyzed using calculus: $f(x)$

$$\frac{df(x)}{dx} \qquad \int_{x_0}^{x_1} f(x)dx$$

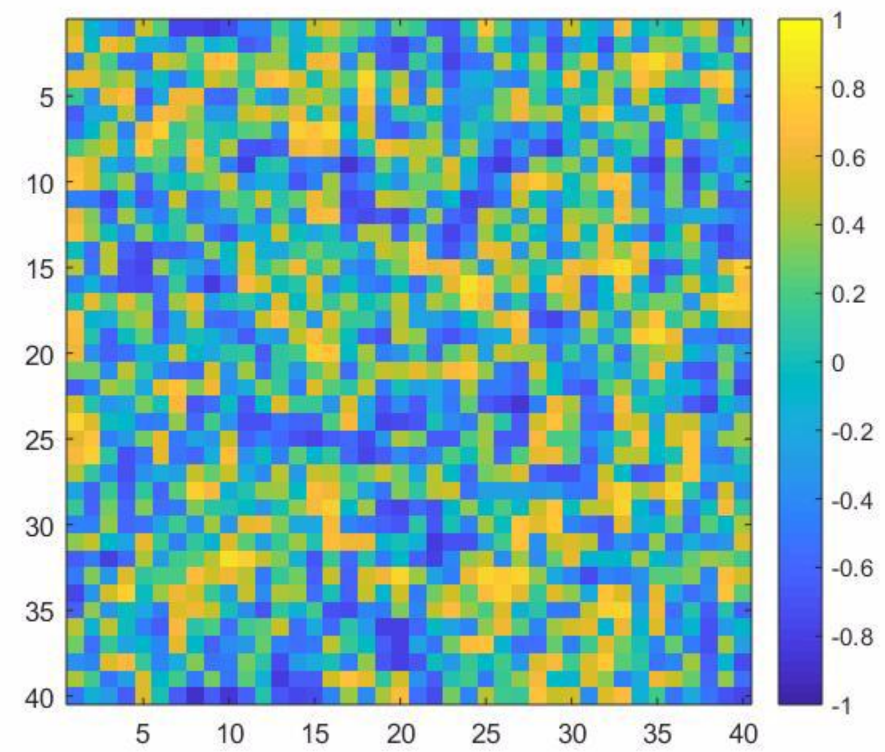
But reality is more like $\sum_{i,j,....p} f_{i,j,....p}(x, y, z, ..., t)$



Widmanstätten Ferrite Formation
composition(x,y,z,t), temperature(x,y,z,t), stress(x,y,z,t)

Phase field in 2D (or 3D) as a model for phase transformation

Colors indicate local order parameter



Phenomena in 2D (or 3D) as function of time …

Phase field with a single non-conserved order parameter (e.g. solidification) whole code! (a lot of comments + plotting)

Editor - D:\msluiter\My Documents\onderwijs\lesar\Chapter12_phasefield\phase_field_2d.m

enthalpy.m | catenary1.m | phase_field_2d.m

```matlab
function[] = phase_field_2d(nsize,ntime)
%simple model to play with solidification using the Allen-Cahn eqn
%Marcel Sluiter May16th 2017
%2D lattice with periodic boundary conditions
%p(x,y): order parameter at a given time t
%p=1 liquid
%p=-1 solid
%free energy function
%same free energy solid and liquid
%f = Delta*(p^4-2*p^2);
%derivative f wrt p
%df = 4*Delta*(p^3-p);
%initialize
p = 2*rand(nsize,nsize)-1; %values between -1 and 1
dpdt=zeros(nsize); %time derivative of order parameter, prealloc for speed
energy = zeros(ntime,1); %preallocation for speed
Delta=1;  %energy scale factor
L=1;      %mobility factor
alpha=1;  %gradient energy scale factor
a=1;      %distance between grid points
dt=0.1;   %time step
alphax=alpha/(a*a);
%updating "field"
for it = 1:ntime
    disp(['time step:',num2str(it)]);
    for ix=1:nsize
        ixl=1+mod(ix-2,nsize); %position to the left (periodic)
        ixr=1+mod(ix,nsize);   %position to the right (periodic)
    for iy=1:nsize
        iyl=1+mod(iy-2,nsize); %position to the "left" (periodic)
        iyr=1+mod(iy,nsize);   %position to the "right" (periodic)
        energy(it)=energy(it) + Delta*(p(ix,iy)^4-2*p(ix,iy)^2)+(alphax/8)*(
        dpdt(ix,iy)=-L*( 4*Delta*(p(ix,iy)^3-p(ix,iy)) - alphax*(p(ixr,iy)+p
    end
    end
```

enthalpy.m | catenary1.m | phase_field_2d.m

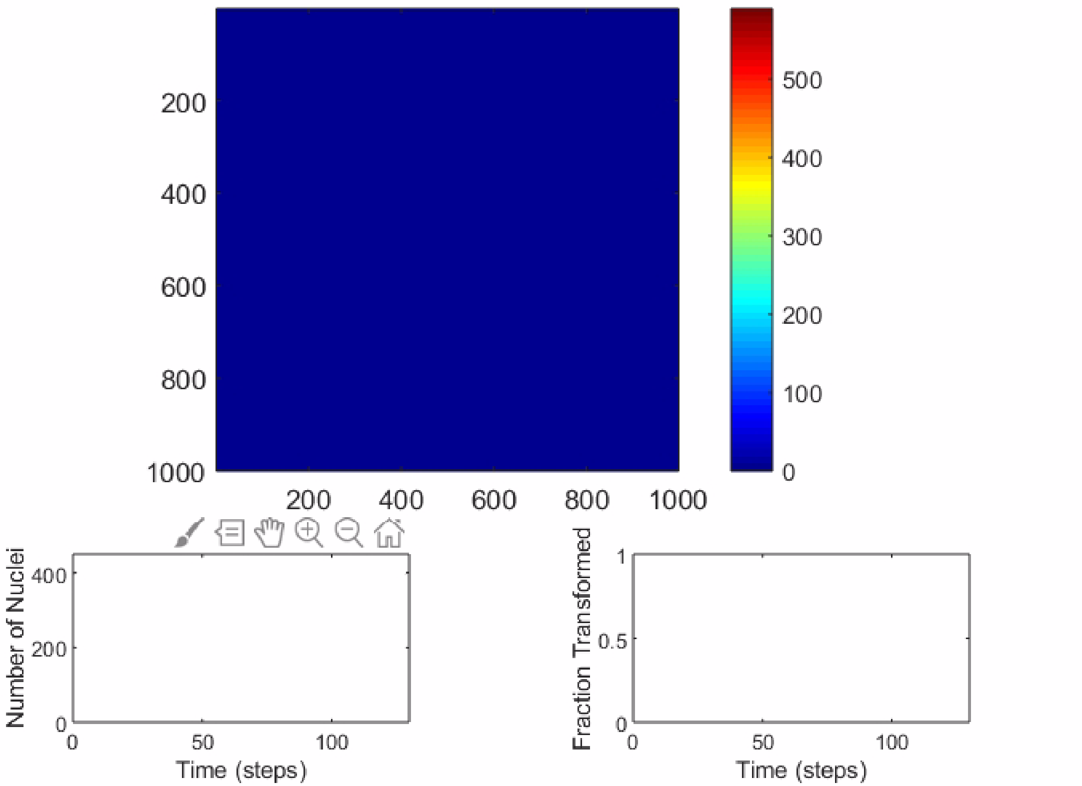
```matlab
    for iy=1:nsize
        p(ix,iy)=p(ix,iy)+dpdt(ix,iy)*dt;
    end
    end
% display microstructure
    imagesc(p)
    colorbar;
    set (gcf,'color','w');
    caxis([-1,1])
    axis equal;
    axis tight
    drawnow
end %it
%plot
figure;
plot((1:ntime),energy,'k')
set (gcf,'color','w');
xlabel('Time (steps)');
ylabel('Energy');
title(['solid-liquid on grid ',num2str(nsize),'x',num2str(nsize)]);
lnetp1 = log( energy + 1);
%more plots...
figure;
plot((1:ntime),lnetp1,'k')
set (gcf,'color','w');
xlabel('Time (steps)');
ylabel('ln(Energy(t)+1)');
title(['solid-liquid on grid ',num2str(nsize),'x',num2str(nsize)]);
lnt = log( (1:ntime) );
figure;
plot(lnt,lnetp1,'k')
set (gcf,'color','w');
xlabel('ln(Time) (steps)');
ylabel('ln(Energy(t)+1)');
title(['solid-liquid on grid ',num2str(nsize),'x',num2str(nsize)]);
```

teaching more visually

Avrami model (Johnson-Mehl-Avrami-Kolmogorov, JMAK)

Nucleation and growth model (one page computer code!)

Color indicates moment of nucleation (dark red: earliest, blue: latest, dark blue: not yet transformed)



power of Matlab & Python programming tools

Hanging chain problem (catenary) – classic problem of variational calculus (Maths by Leibniz, Huygens and Johann Bernoulli ~1691)

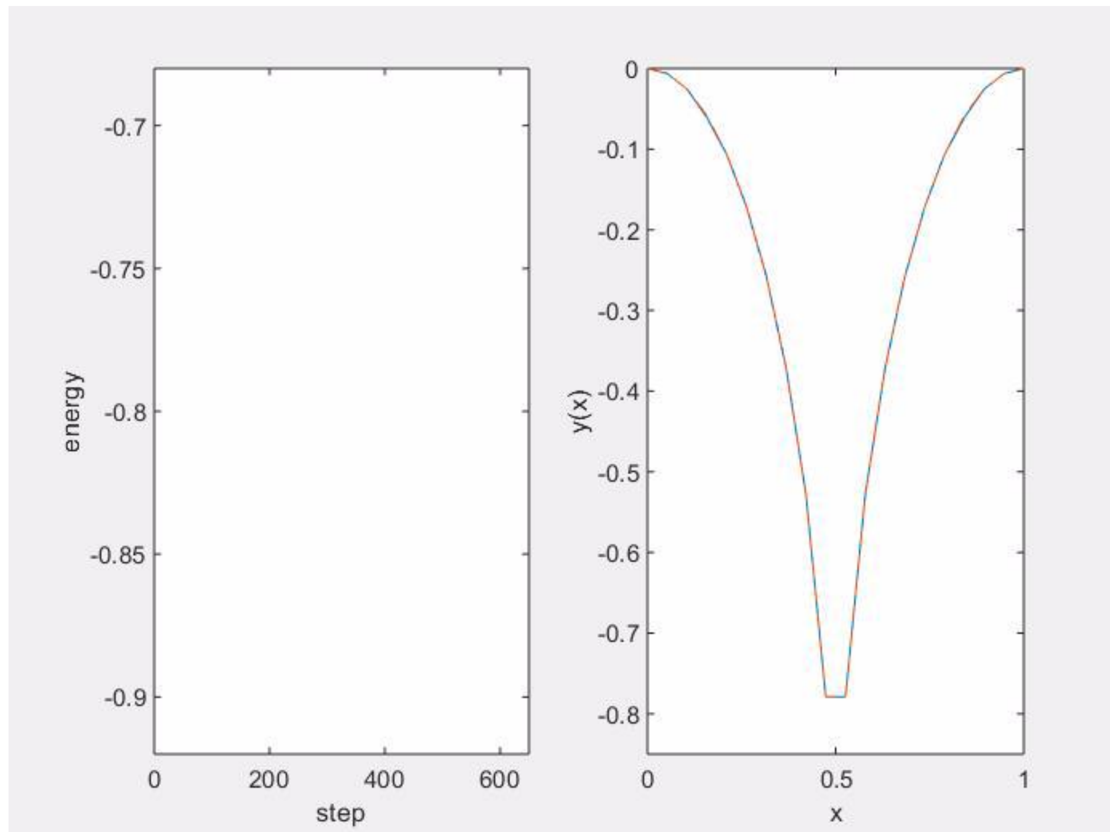
power of Matlab & Python programming tools

Editor - D:\msluiter\My Documents\onderwijs\lesar\chapter 4\catenary_optimizationprocess\cater

enthalpy.m | catenary1.m

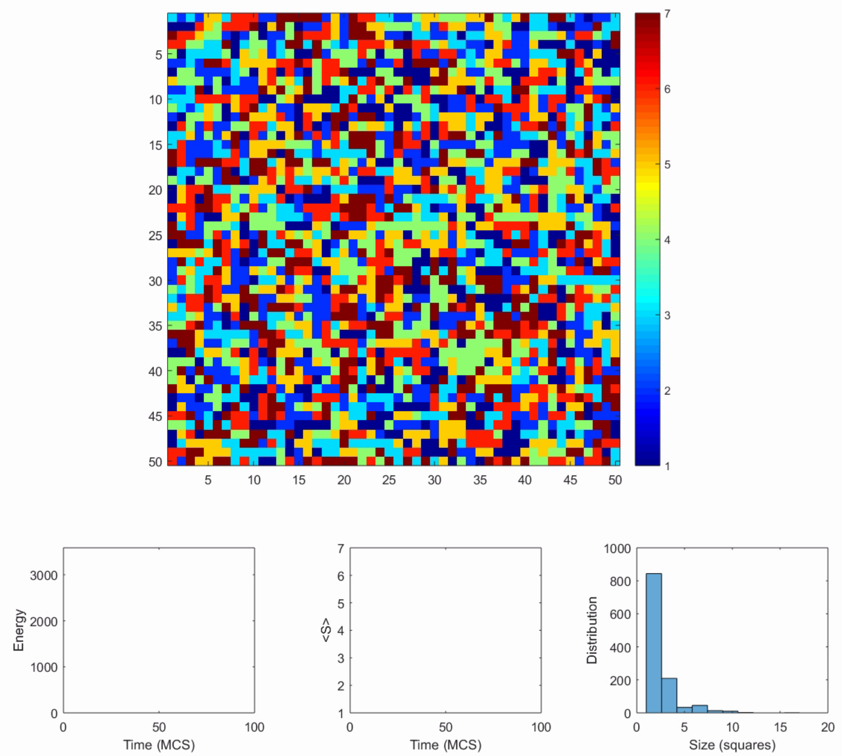
```
Estart = energy(x,yxstart,nx);
disp(['E_start:',num2str(Estart)]);
Eprev = Estart;

hvid = VideoWriter('./catenary.mp4','MPEG-4');
set(hvid,'Quality',100); % Full quality, because why not?
set(hvid,'FrameRate',30);% Set the frame rate
open(hvid);% Open the object for writing

iframe=0;
hfig = figure();
subplot(1,2,1)
  plot(Egy(1:1))
  xlabel('step')
  ylabel('energy')
  xlim([0 nframes])
  ylim([ymin1 inf]);
subplot(1,2,2)
  plot(x, yx, x, yxstart, '--')
  ylim([ymin2 inf])
  xlabel('x')
  ylabel('y(x)');
axis tight

%iteratively we try to improve on the trial solution
for it = 1:ntries
```

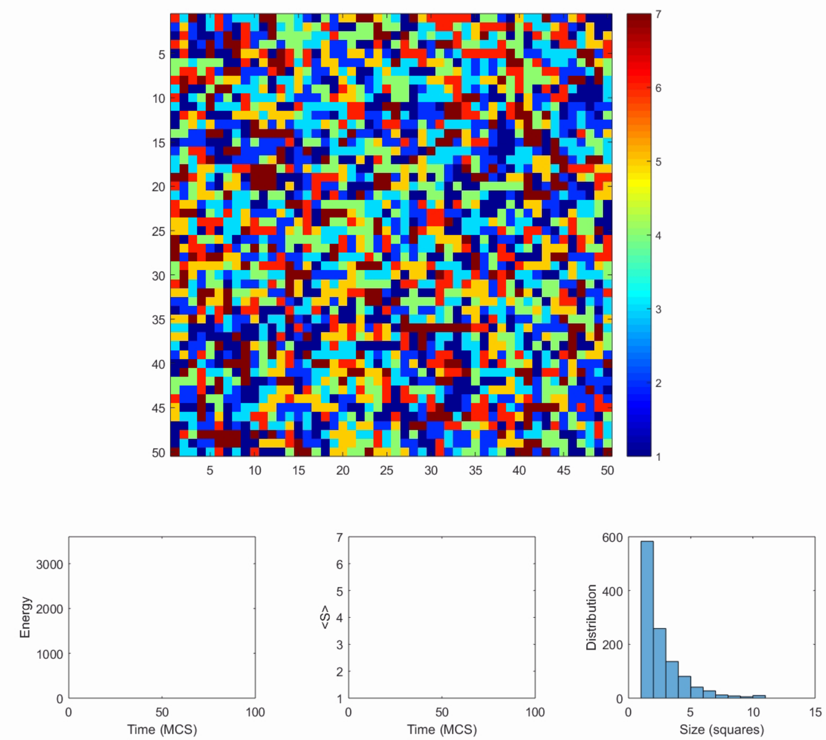
Make a movie with potential energy (left) and shape (right)



Grain growth through the Q-state Potts model

Colors indicate grains (left: no stored energy right: with stored energy)



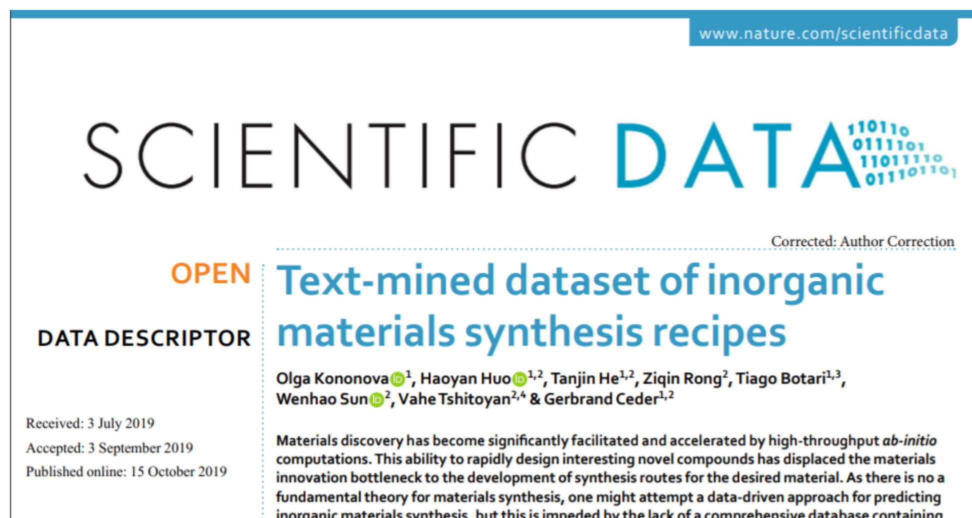


Future

Much more to come:
"Automatically" generated thermodynamic and kinetic databases (current!)

Gaming – computer plays games against itself and "discovers" rules
Computer "plays" with models – varying the input parameters, and then derives "simple rules of thumb" for us, or, gives immediate answers to lengthy simulation challenges by interpolating its database (machine learning)

Machine learning to facilitate the typical MSE relations
Composition & processing ⇔ microstructure ⇔ properties


www.nature.com/scientificdata

SCIENTIFIC DATA

Corrected: Author Correction

OPEN

DATA DESCRIPTOR

Text-mined dataset of inorganic materials synthesis recipes

Olga Kononova[1], Haoyan Huo[1,2], Tanjin He[1,2], Ziqin Rong[2], Tiago Botari[1,3], Wenhao Sun[2], Vahe Tshitoyan[2,4] & Gerbrand Ceder[1,2]

Received: 3 July 2019
Accepted: 3 September 2019
Published online: 15 October 2019

Materials discovery has become significantly facilitated and accelerated by high-throughput *ab-initio* computations. This ability to rapidly design interesting novel compounds has displaced the materials innovation bottleneck to the development of synthesis routes for the desired material. As there is no a fundamental theory for materials synthesis, one might attempt a data-driven approach for predicting inorganic materials synthesis, but this is impeded by the lack of a comprehensive database containing

Conclusions

Materials Science education VERY relevant

is at the core of many societal “pain points”

Google ➔ need to be able to interpret/process data

➔**fundamental understanding** & modern data tools (Python/Matlab)

Materials Science: Microstructure poorly suited for “calculus”: 3d fields $c(x,y,z,t)$ ➔ **modern tools (Python/Matlab, Mathematica/Maple)**

Teach modern data/programming tools as early as possible

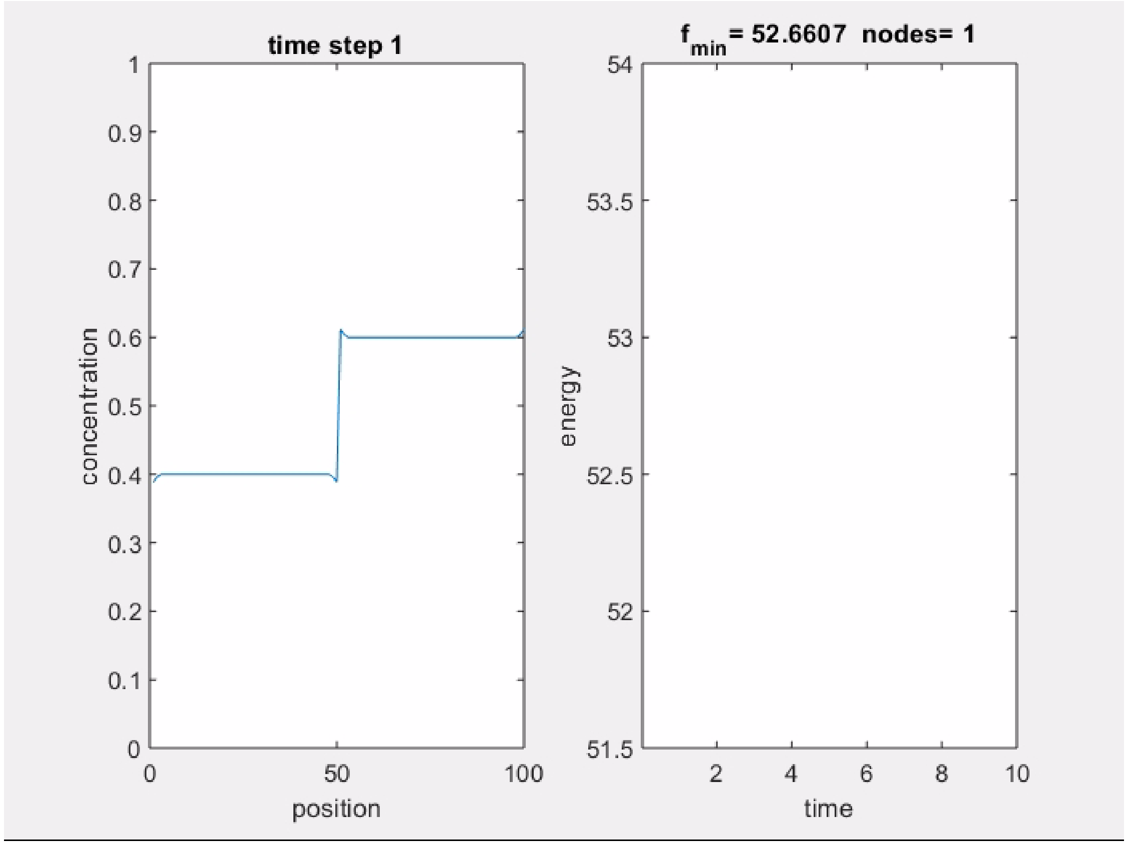
(and then use it “hands on”)

Extra slides

Computational experiments …

phase field with conserved order parameter, phase separating system

With a step in the composition profile …



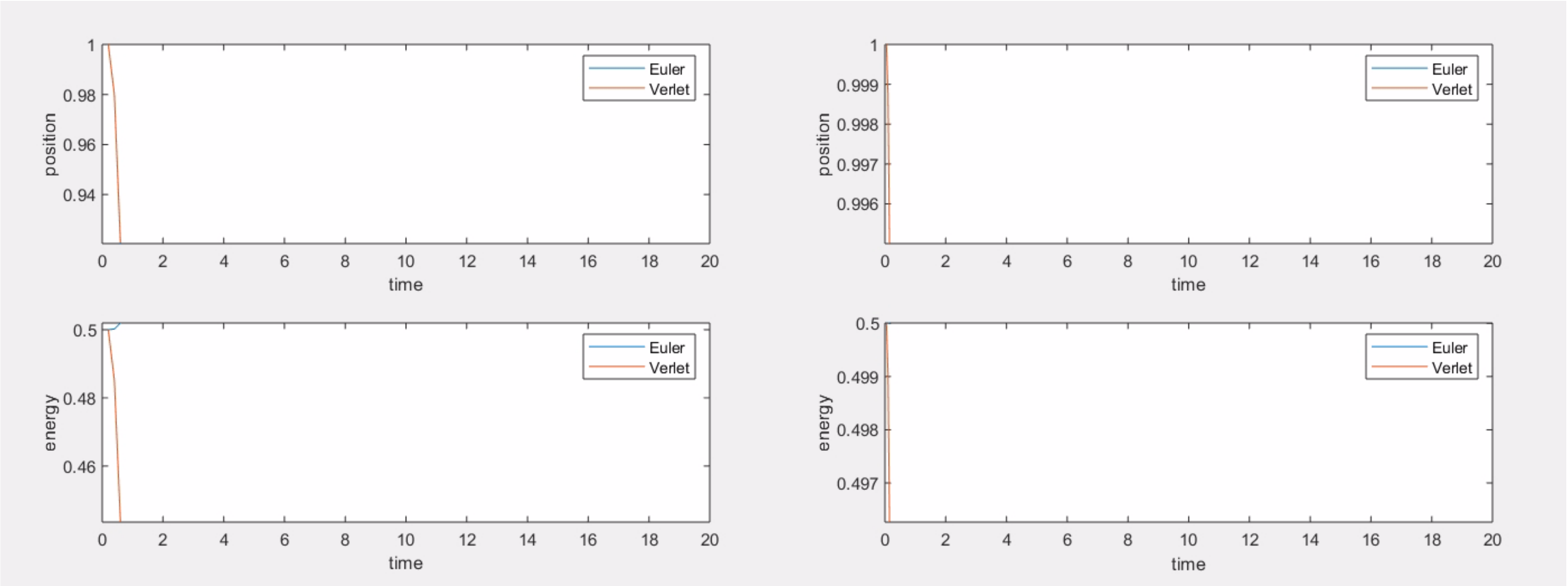
Or simply teaching more visually

Integrating Newtons equations of motion through Euler's or Verlet's (1st) method for a pendulum

Left: Δt=0.2   100 time steps
Top panel: position
Bottom panel: potential + kinetic energy

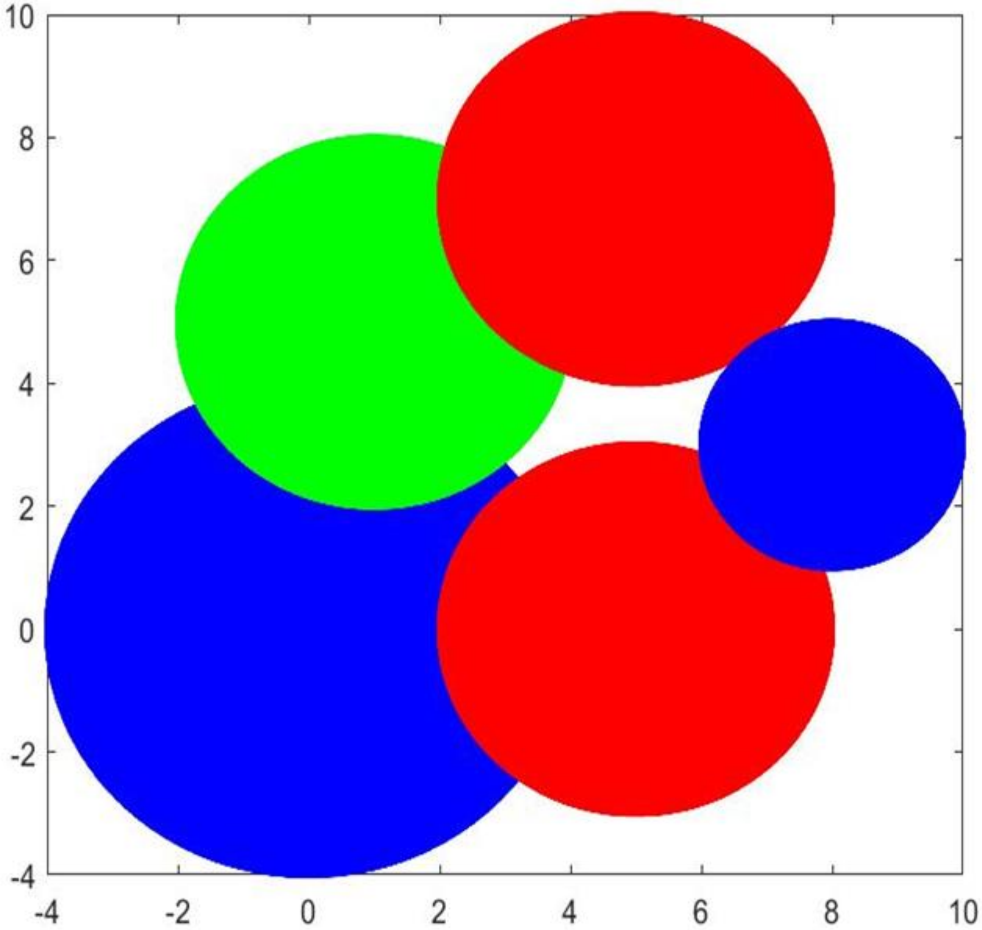
Right: Δt=0.05   400 time steps

Smaller time step but still NO energy conservation with Euler's



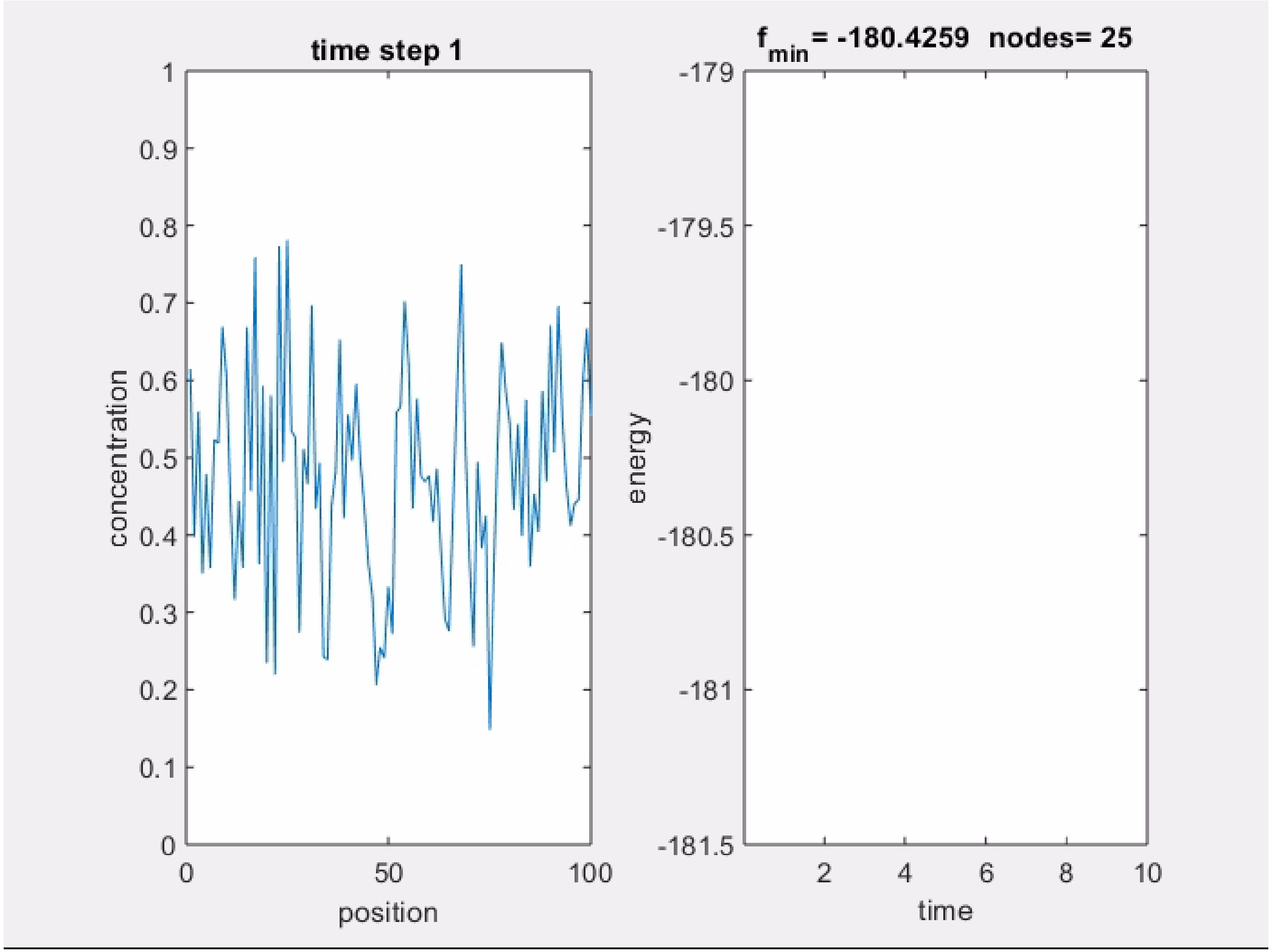
Monte Carlo Integration

Coverage of broadcasting towers



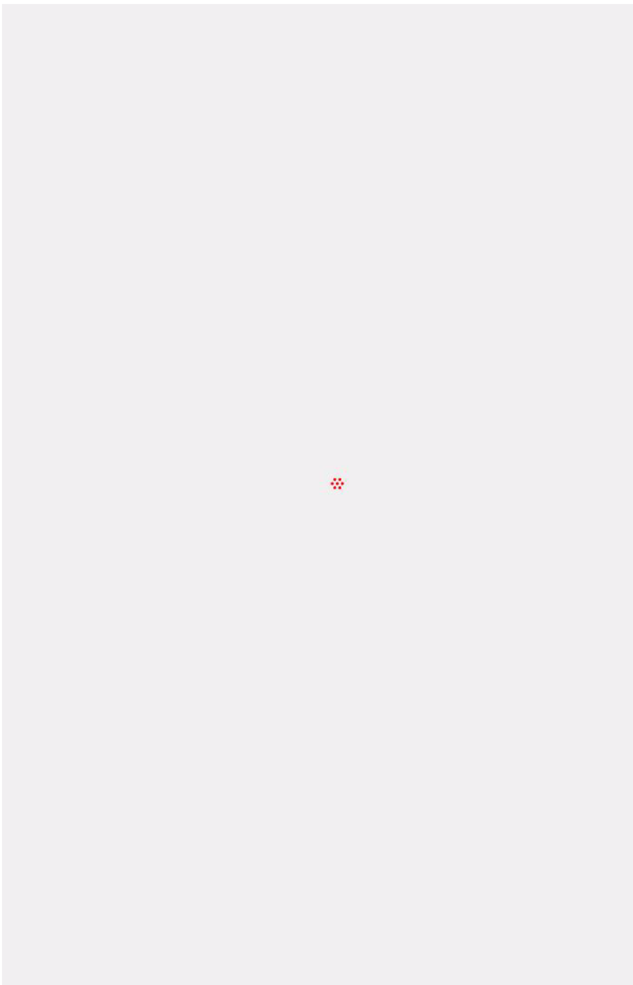
Homogenization

Phase field simulation



Cellular Automata

Phase transformation



Conclusions

Materials Science education VERY relevant

is at the core of many societal “pain points”

➔communication

Materials Science no bachelor in NL, diverse student population

limited background "in common“ ➔ core knowledge ⇔ specialization

Google ➔ need to be able to interpret/process data

➔ fundamental understanding & modern data tools (Python/Matlab)

Materials Science: Microstructure poorly suited for “calculus”: 3d fields

c(x,y,z,t) ➔ modern tools (Python/Matlab, Mathematica/Maple)