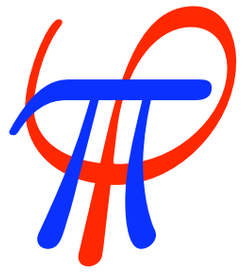

Modeling of Materials with Python

J. E. Guyer, D. Wheeler & J. A. Warren

www.ctcms.nist.gov/fipy

Metallurgy Division &
Center for Theoretical and Computational Materials Science
Materials Science and Engineering Laboratory

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NIST: Origins

"Uniformity in the currency, weights, and measures of the United States is an object of great importance, and will, I am persuaded, be duly attended to."

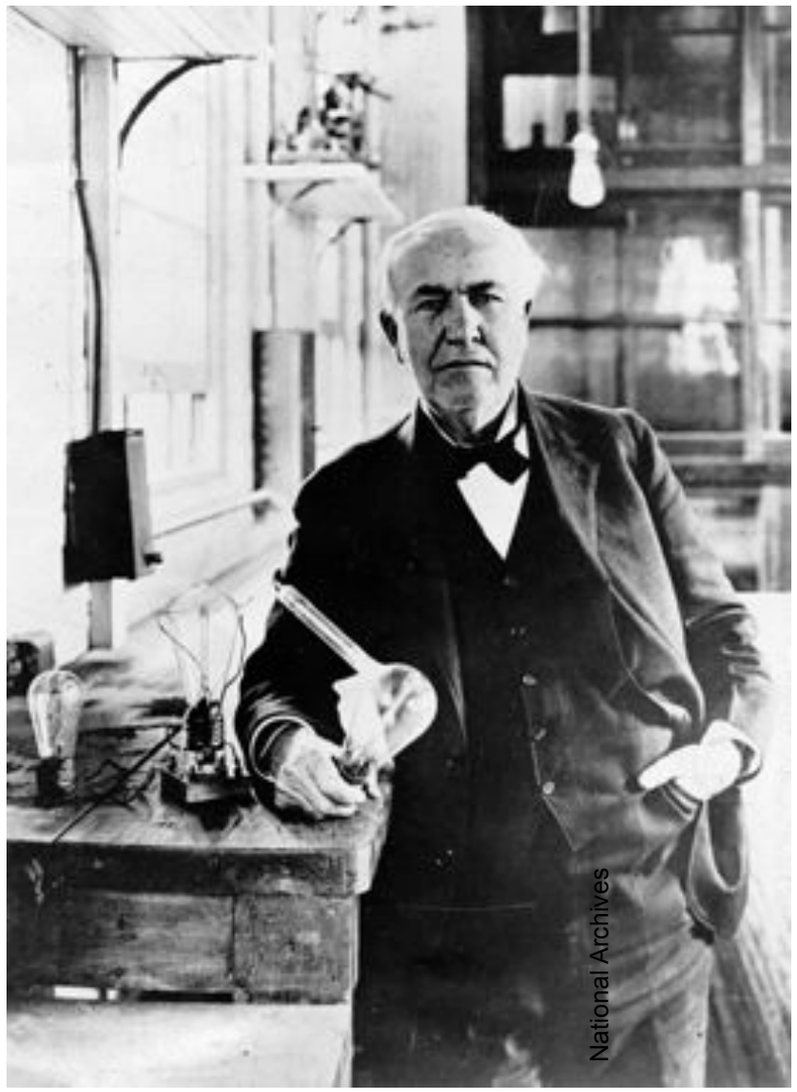
George Washington, State of the Union Address, 1790

U. S. Constitution, Article I, Section 8

NIST: Origins

National Bureau of Standards
Established by Congress in 1901

- Eight different "authoritative' values for the gallon
- Nascent electrical industry needed standards
- American instruments sent abroad for calibration
- Consumer products and construction materials uneven in quality and unreliable



NIST: Rigorous and Objective

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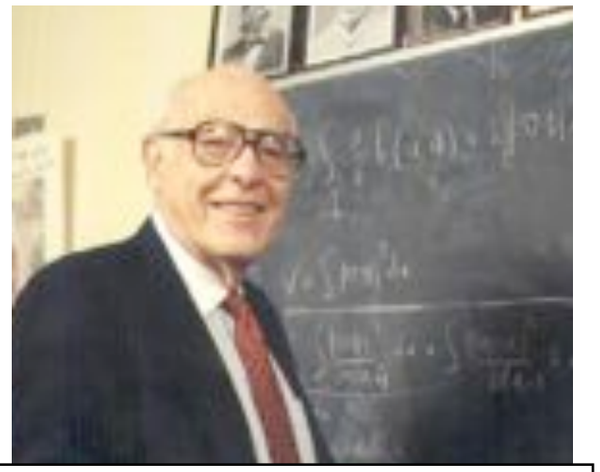
NIST: World-Class Staff

Jan Hall
2005 Nobel Prize
in Physics

Eric Cornell
2001 Nobel Prize
in Physics

Bill Phillips
1997 Nobel Prize
in Physics



John Cahn
1998 National Medal of
Science

Anneke Sengers
2003 L'Oréal-UNESCO
Women in Science Award

Debbie Jin
2003 MacArthur Fellowship

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NIST: Trusted Investigator

Great Baltimore Fire, 1904

World Trade Center Collapse
9/11/2001

Silver Bridge Collapse, 1967

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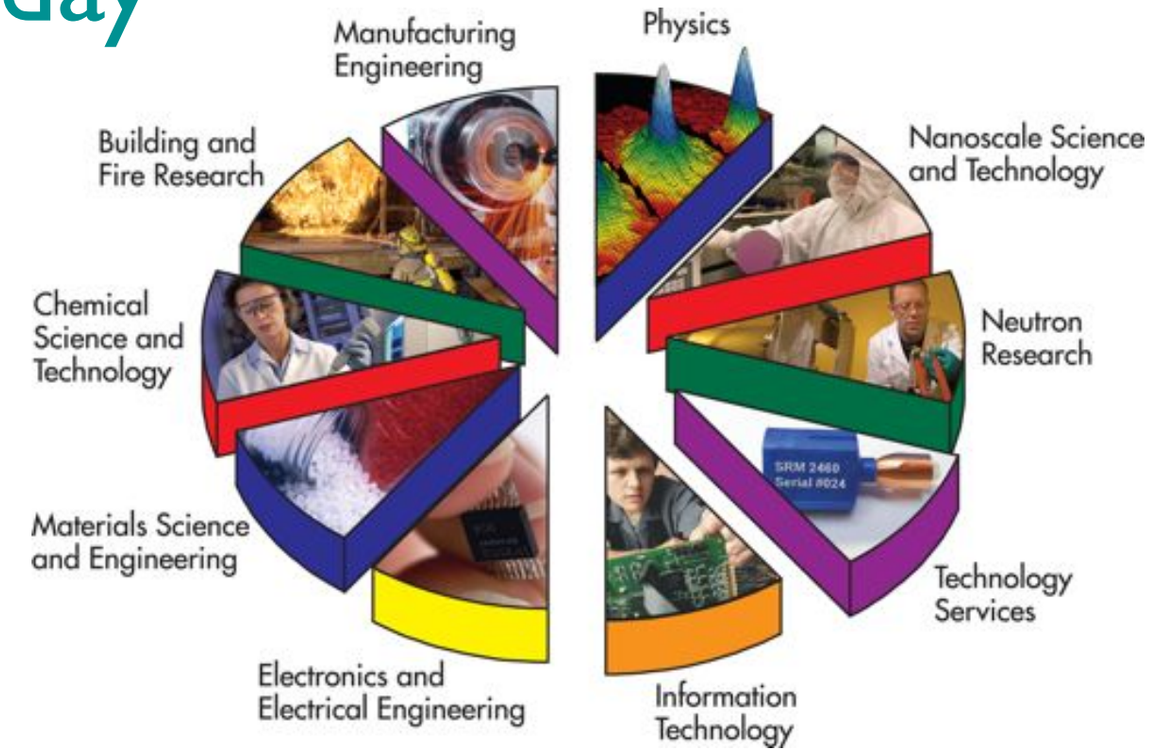
NIST: Today

≈2900 employees

≈2600 associates and facilities users

≈1600 field staff in partner organizations

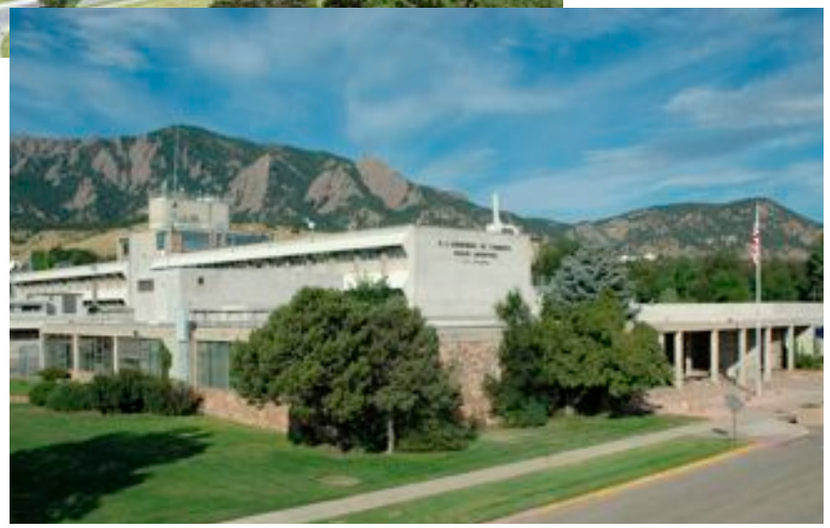
≈400 NIST staff serving on 1000 national and international standards committees



Gaithersburg, MD

Courtesy HDR Architecture, Inc./Steve Hall ©Hedrich Blessing

Boulder, CO



©Geoffrey Wheeler

≈100 Standard Reference Data sets

≈1300 Standard Reference Materials

≈16000 calibration tests per year

≈800 accreditations per year

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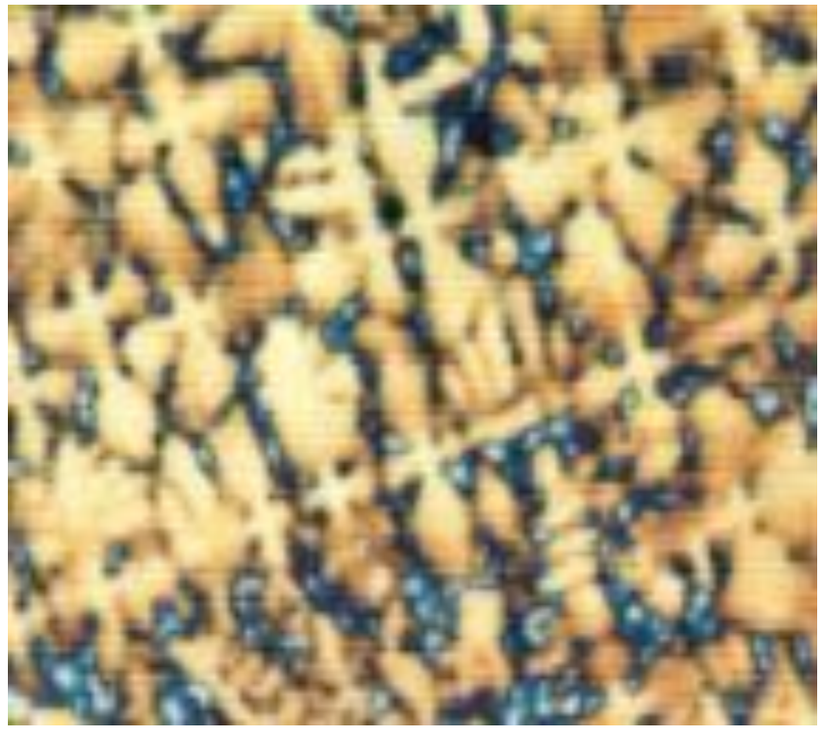
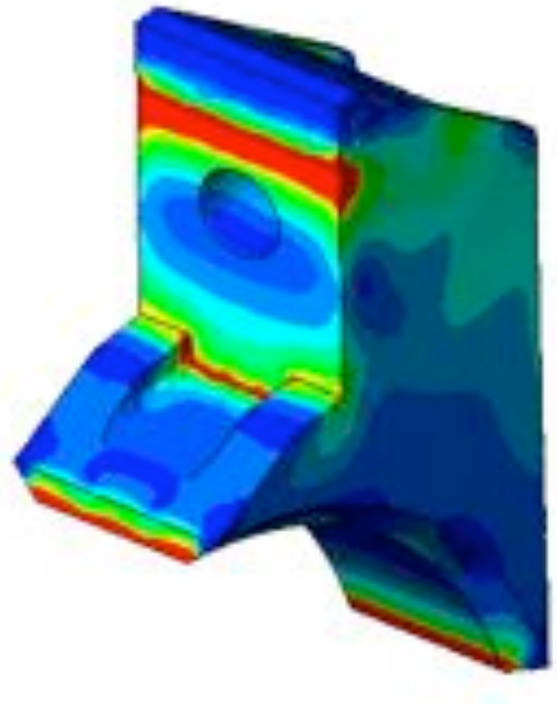
Materials Science

Processing



Structure



Properties

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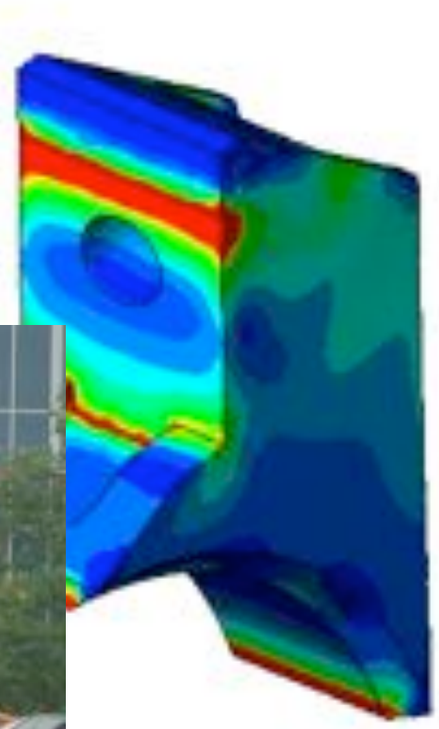
Materials Science



Processing

perties

Performance

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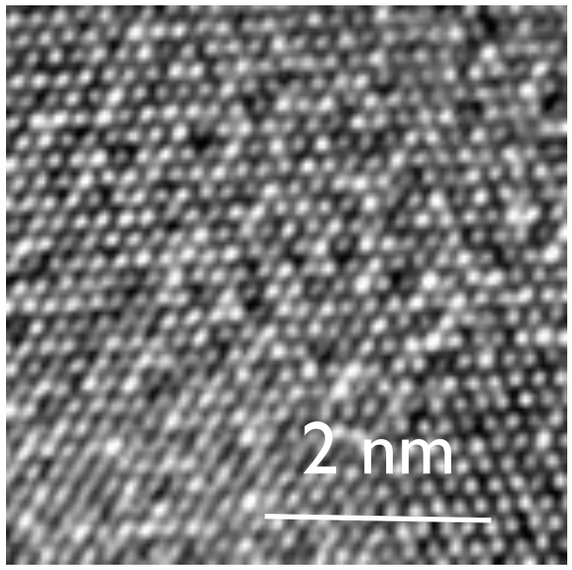
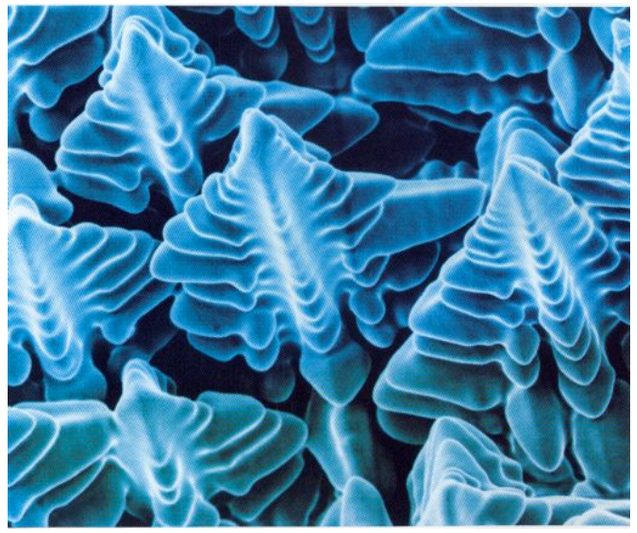
Materials And Models



Atomic scale



Micro scale

Millimeter scale

Component scale

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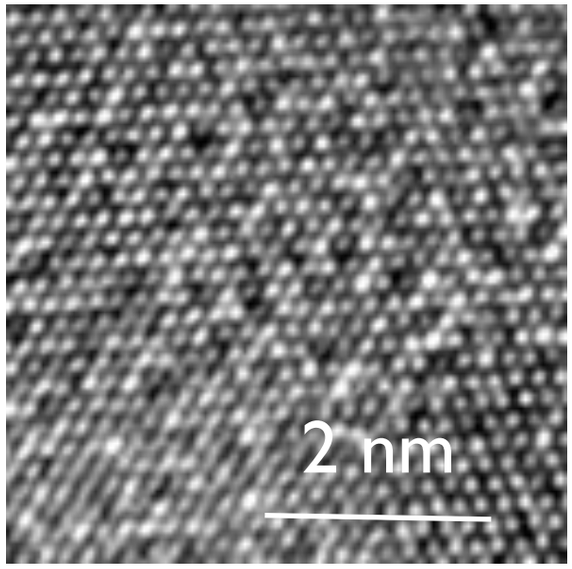
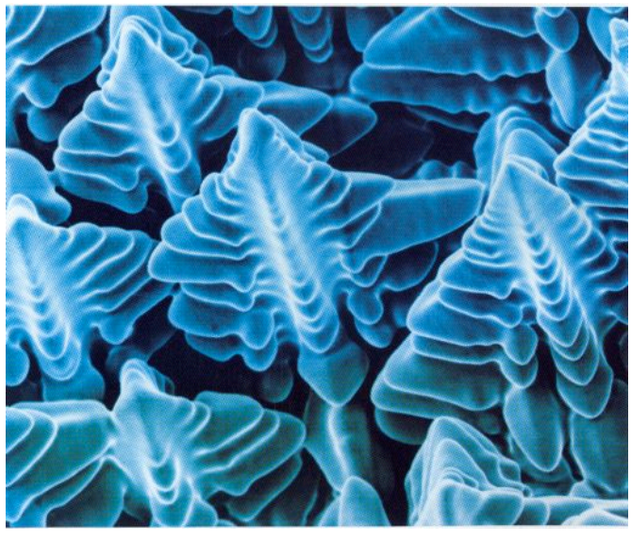
Materials And Models



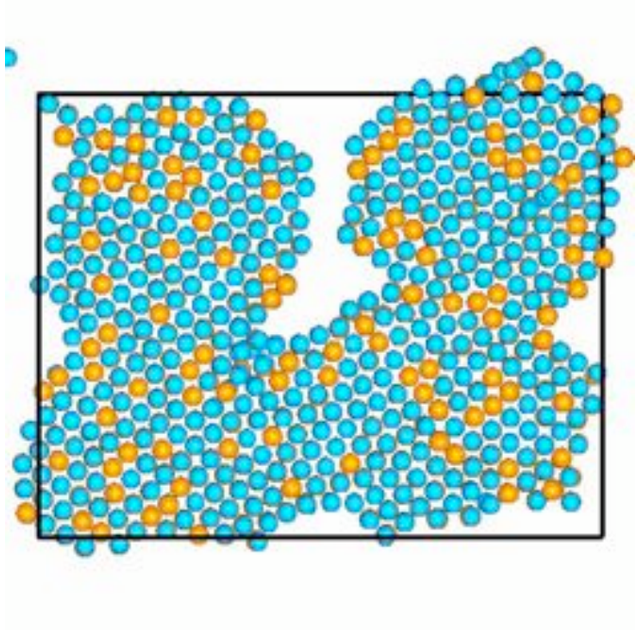
Atomic scale

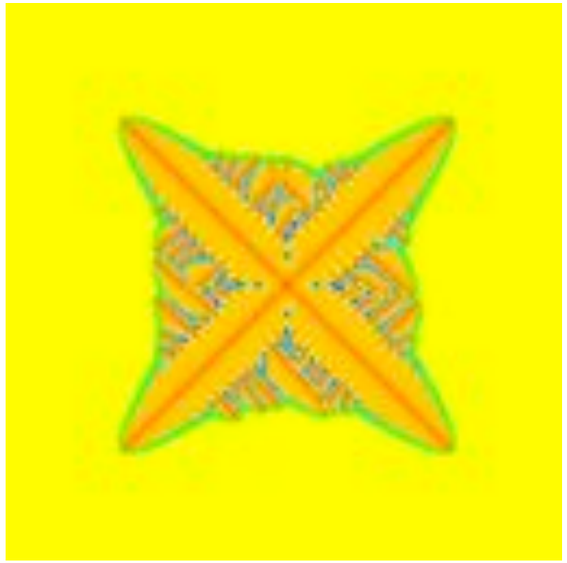


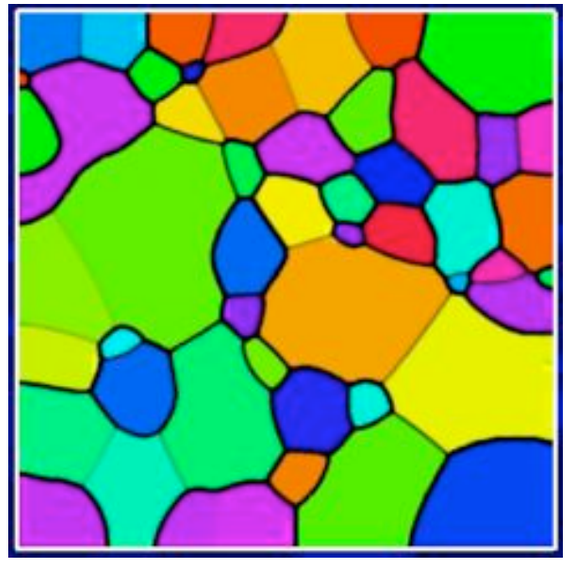
Micro scale

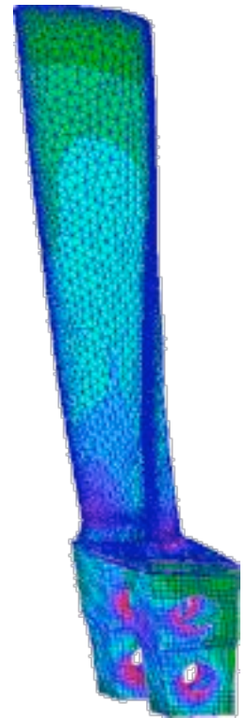
Millimeter scale

Component scale









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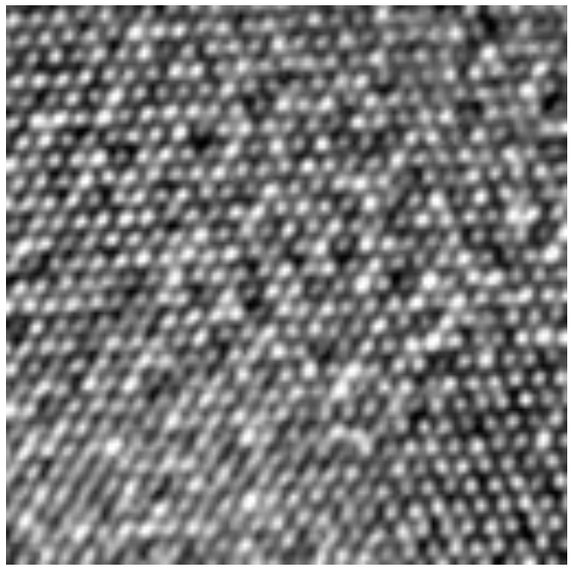
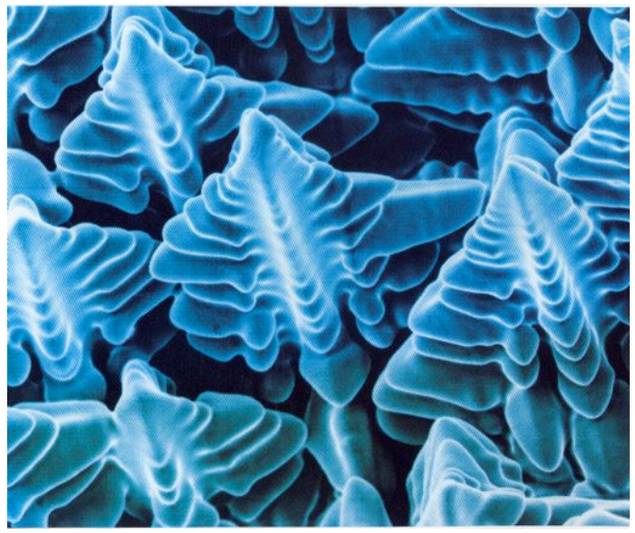
Modeling is the basis of Measurement Science



Electronic Properties



Heat and Energy

Strength

Diffusion

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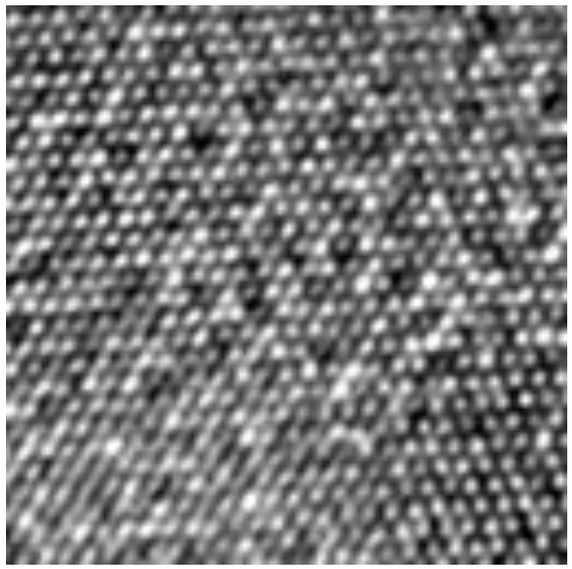
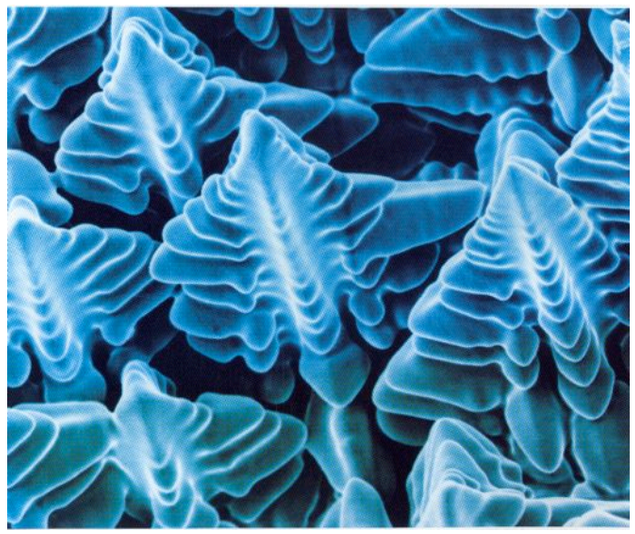
Modeling is the basis of Measurement Science



Electronic Properties

$$V = IR$$



Heat and Energy

$$dE = TdS - PdV + \mu dN$$

Strength

$$\sigma_{ij} = C_{ijkl}\epsilon_{kl}$$

Diffusion

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2}$$

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Center for Theoretical and Computational Materials Science

Provides the infrastructure for Theory, Modeling and Simulation in MSEL

- By providing hardware, and a collaborative work environment (space)
- By developing new measurement paradigms using simulation and theory
- By encouraging the development of software tools, both for internal use and to aid in the dissemination of existing results

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Why a common code?

- PDEs are ubiquitous in materials science
- Many codes for solving materials science problems at NIST
- Dissemination to other researchers is "difficult"

Why a common code?

- PDEs are ubiquitous in ~~materials~~ science
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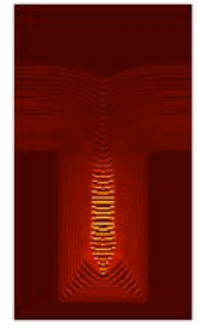

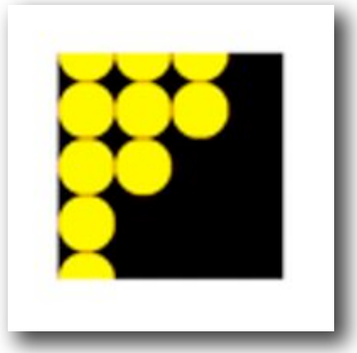

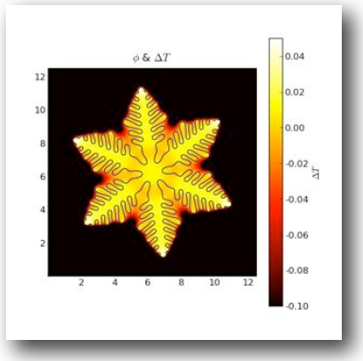

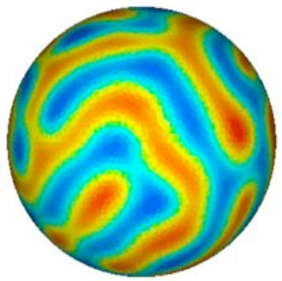

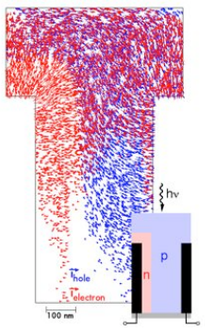

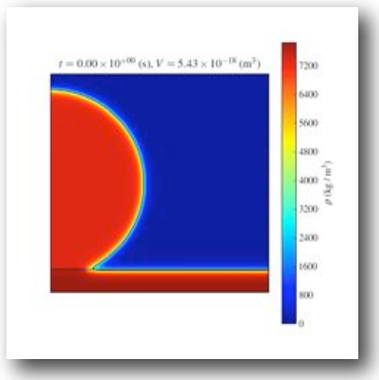

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Why Scripting?

- hard-code

```
  :
  :
common /params/temperature,steps,tolerance,...

data temperature,steps,tolerance/273.15,10000,1.d-3,.../
  :
  :
```

Why Scripting?

- hard-code

```
  :
  :
common /params/temperature,steps,tolerance,...

data temperature,steps,tolerance/273.15,10000,1.d-3,.../
  :
  :
```

- batch file

```
273.15
10000
1.d-3
  :
  :
```

Why Scripting?

- hard-code

```
  :
  :
common /params/temperature,steps,tolerance,...

data temperature,steps,tolerance/273.15,10000,1.d-3,.../
  :
  :
```

- batch file

```
273.15
10000
1.d-3
  :
  :
```

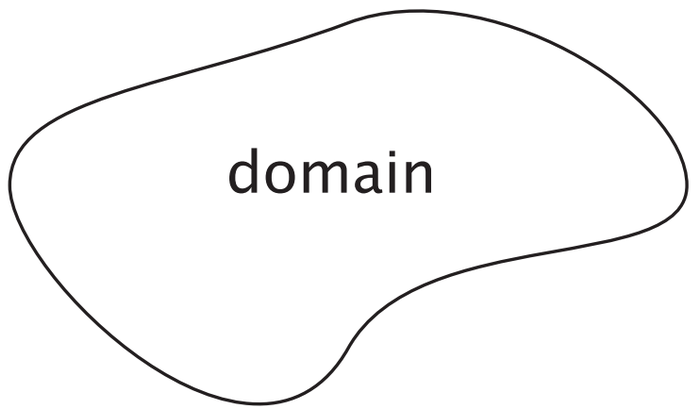
- comment character

```
273.15 # temperature (K)
10000  # steps
1.d-3    # tolerance
  :
  :
```

Finite Volume Method

- Solve a general PDE on a given domain for a field ϕ

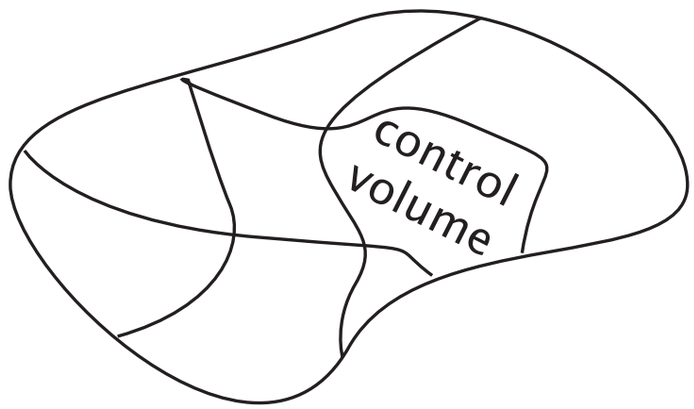
$$\underbrace{\frac{\partial(\rho\phi)}{\partial t}}_{\text{transient}} - \underbrace{[\nabla\cdot(\Gamma_i\nabla)]^n\phi}_{\text{diffusion}} - \underbrace{\nabla\cdot(\vec{u}\phi)}_{\text{convection}} - \underbrace{S_\phi}_{\text{source}} = 0$$



Finite Volume Method

- Solve a general PDE on a given domain for a field ϕ
- Integrate PDE over arbitrary control volumes

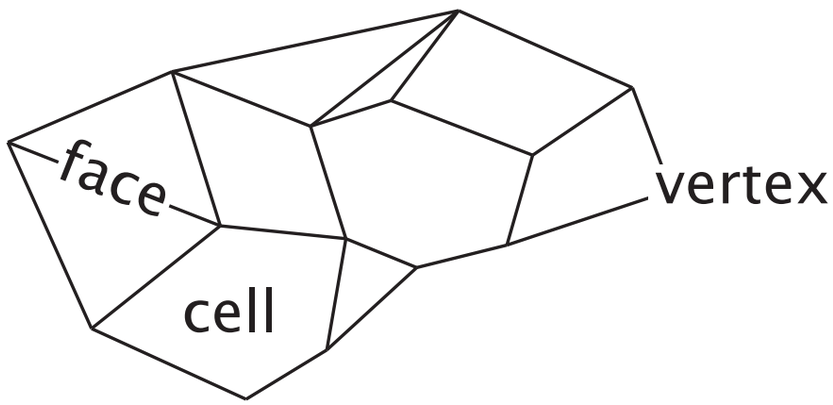
$$\underbrace{\int_V \frac{\partial(\rho\phi)}{\partial t}\,dV}_{\text{transient}} - \underbrace{\int_S \Gamma_n(\vec{n}\cdot\nabla\{\cdots\})\,dS}_{\text{diffusion}} - \underbrace{\int_S (\vec{n}\cdot\vec{u})\phi\,dS}_{\text{convection}} - \underbrace{\int_V S_\phi\,dV}_{\text{source}} = 0$$



Finite Volume Method

- Solve a general PDE on a given domain for a field ϕ
- Integrate PDE over arbitrary control volumes
- Evaluate PDE over polyhedral control volumes

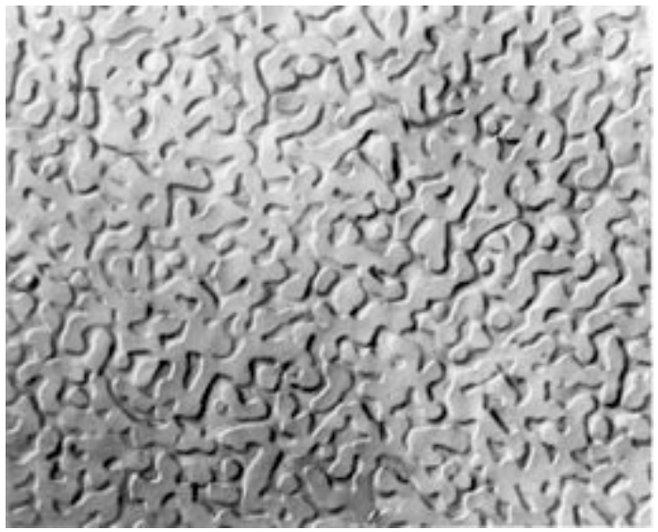
$$\underbrace{\frac{\rho\phi V - (\rho\phi V)^{\text{old}}}{\Delta t}}_{\text{transient}} - \underbrace{\sum_{\text{face}} [\Gamma_n A\vec{n} \cdot \nabla \{\cdots\}]_{\text{face}}}_{\text{diffusion}} - \underbrace{\sum_{\text{face}} [(\vec{n} \cdot \vec{u}) A\phi]_{\text{face}}}_{\text{convection}} - \underbrace{V S_\phi}_{\text{source}} = 0$$



Finite Volume Method

- Solve a general PDE on a given domain for a field ϕ
- Integrate PDE over arbitrary control volumes
- Evaluate PDE over polyhedral control volumes
- Obtain a large coupled set of linear equations in ϕ

$$\begin{pmatrix} a_{11} & a_{12} & & \\ a_{21} & a_{22} & \ddots & \\ & \ddots & \ddots & \ddots \\ & & \ddots & a_{nn} \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$



Cahn-Hilliard Example

$$\frac{\partial \phi}{\partial t} = \nabla \cdot D \nabla \left(\frac{\partial f}{\partial \phi} - \epsilon^2 \nabla^2 \phi \right)$$

$$f = \frac{a^2}{2} \phi^2 (1 - \phi)^2$$

Cahn-Hilliard Example

$$\underbrace{\frac{\partial \phi}{\partial t}}_{\text{transient}} = \underbrace{\nabla \cdot D a^2 \left[1 - 6\phi\left(1 - \phi\right)\right] \nabla \phi}_{2^{\text{nd}}\text{ order diffusion}} - \underbrace{\nabla \cdot D \nabla \epsilon^2 \nabla^2 \phi}_{4^{\text{th}}\text{ order diffusion}}$$

```
from fipy import *
mesh = Grid2D(nx=1000, ny=1000, dx=0.25, dy=0.25)

phi = CellVariable(name=r"$\phi$", mesh=mesh)
phi.setValue(GaussianNoiseVariable(mesh=mesh,
                                   mean=0.5,
                                   variance=0.01))

PHI = phi.getArithmeticFaceValue()
D = a = epsilon = 1.
eq = (TransientTerm()
      == DiffusionTerm(coeff=D * a**2 * (1 - 6 * PHI * (1 - PHI)))
      - DiffusionTerm(coeff=(D, epsilon**2)))

viewer = Viewer(vars=(phi,), datamin=0., datamax=1.)

dexp = -5
elapsed = 0.
while elapsed < 1000.:
    dt = min(100, exp(dexp))
    elapsed += dt
    dexp += 0.01
    eq.solve(phi, dt=dt)
    viewer.plot()
```

Cahn-Hilliard Example

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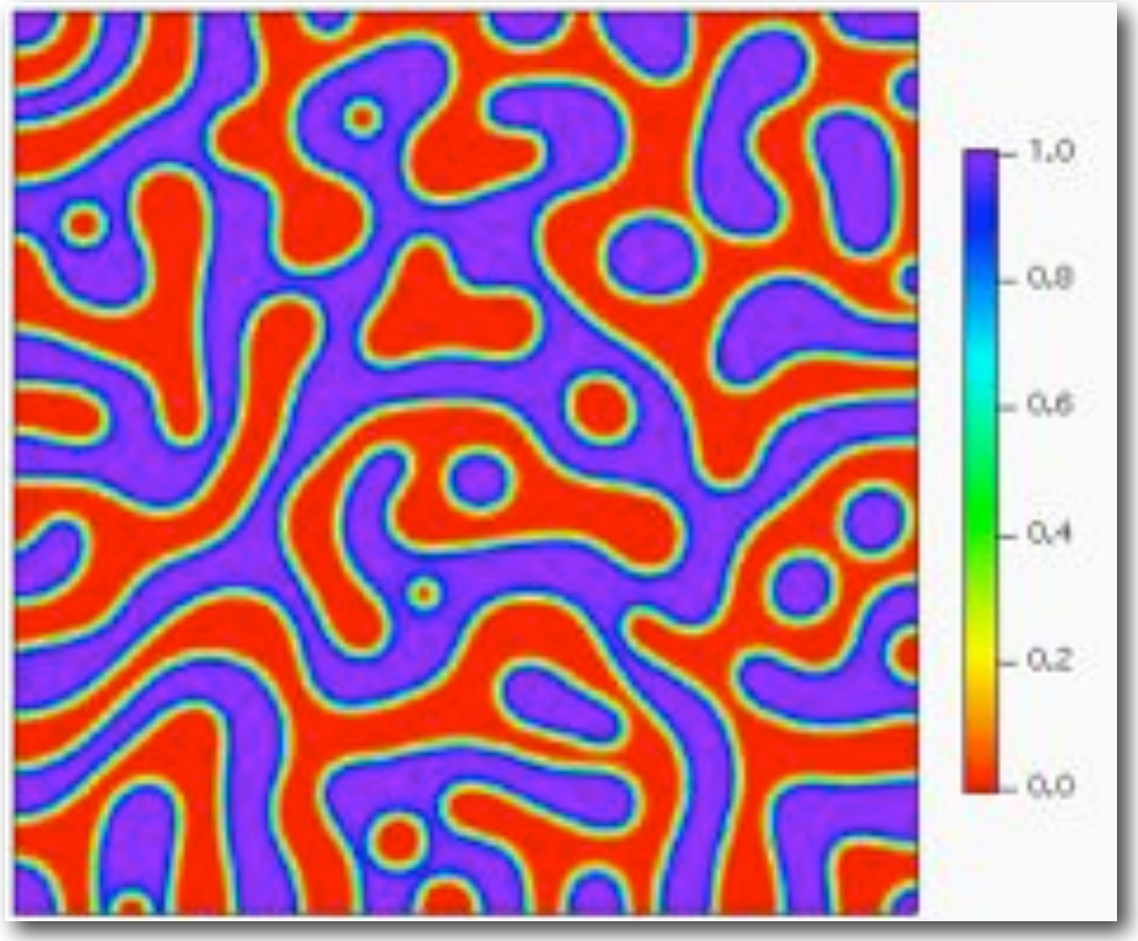
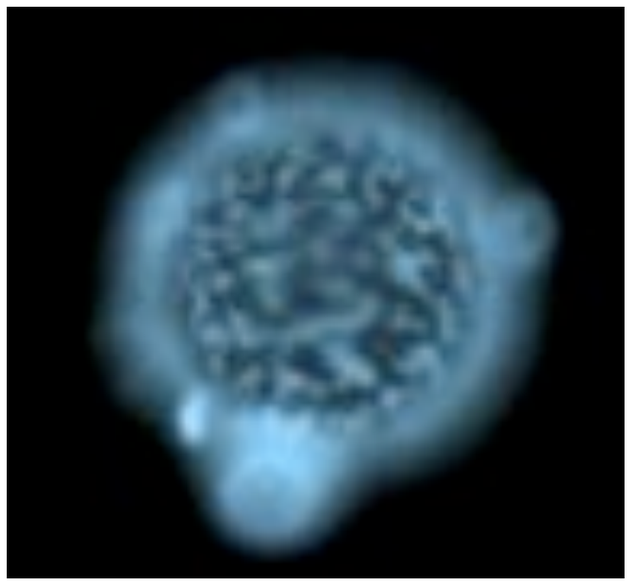
```





Cahn-Hilliard Example

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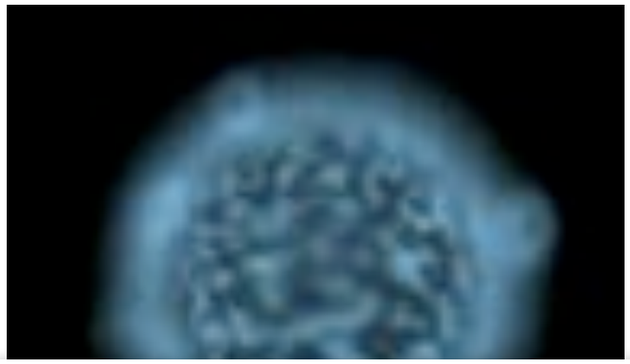
Cahn-Hilliard Example



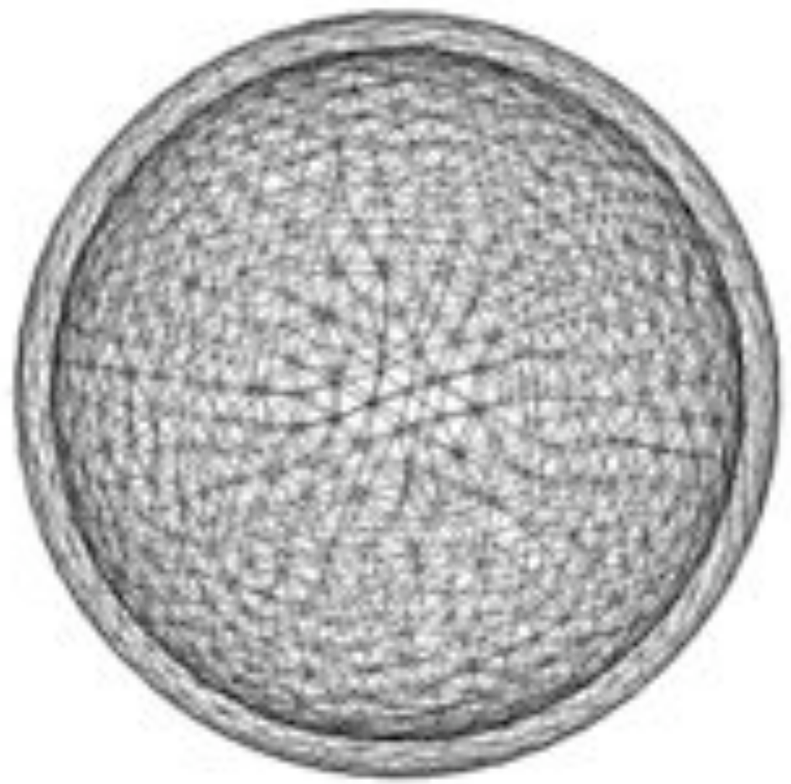
$$\underbrace{\frac{\partial \phi}{\partial t}}_{\text{transient}} = \underbrace{\nabla \cdot D a^2 \left[1 - 6\phi\left(1-\phi\right)\right] \nabla \phi}_{2^{\text{nd}}\text{ order diffusion}} - \underbrace{\nabla \cdot D \nabla \epsilon^2 \nabla^2 \phi}_{4^{\text{th}}\text{ order diffusion}}$$

```
mesh = Grid2D(nx=1000, ny=1000, dx=0.25, dy=0.25)
mesh = GmshImporter2DIn3DSpace("""
    radius = 5.0;
    cellSize = 0.3;

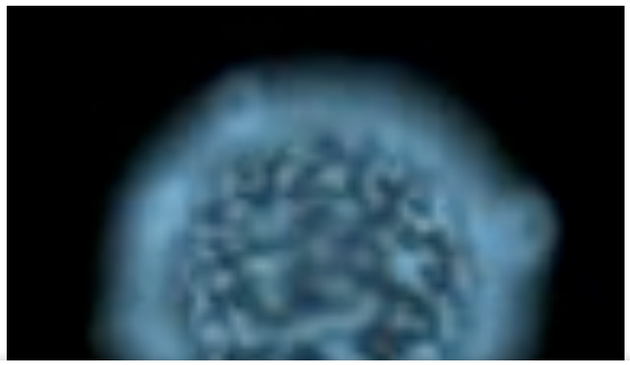
    // create inner 1/8 shell
    Point(1) = {0, 0, 0, cellSize};
    Point(2) = {-radius, 0, 0, cellSize};
    Point(3) = {0, radius, 0, cellSize};
    Point(4) = {0, 0, radius, cellSize};
    Circle(1) = {2, 1, 3};
    Circle(2) = {4, 1, 2};
    Circle(3) = {4, 1, 3};
    Line Loop(1) = {1, -3, 2} ;
    Ruled Surface(1) = {1};

    // create remaining 7/8 inner shells
    t1[] = Rotate {{0,0,1},{0,0,0},Pi/2} {Duplicata{Surface{1};}};
    t2[] = Rotate {{0,0,1},{0,0,0},Pi} {Duplicata{Surface{1};}};
    t3[] = Rotate {{0,0,1},{0,0,0},Pi*3/2} {Duplicata{Surface{1};}};
    t4[] = Rotate {{0,1,0},{0,0,0},-Pi/2} {Duplicata{Surface{1};}};
    t5[] = Rotate {{0,0,1},{0,0,0},Pi/2} {Duplicata{Surface{t4[0]};}};
    t6[] = Rotate {{0,0,1},{0,0,0},Pi} {Duplicata{Surface{t4[0]};}};
    t7[] = Rotate {{0,0,1},{0,0,0},Pi*3/2} {Duplicata{Surface{t4[0]};}};

    // create entire inner and outer shell
    Surface Loop(100)={1,t1[0],t2[0],t3[0],t7[0],t4[0],t5[0],t6[0]};
""").extrude(extrudeFunc=lambda r: 1.1 * r)
```



Cahn-Hilliard Example



$$\underbrace{\frac{\partial \phi}{\partial t}}_{\text{transient}} = \underbrace{\nabla \cdot Da^2 \left[1 - 6\phi\left(1-\phi\right)\right] \nabla \phi}_{2^{\text{nd}}\text{ order diffusion}} - \underbrace{\nabla \cdot D \nabla \epsilon^2 \nabla^2 \phi}_{4^{\text{th}}\text{ order diffusion}}$$

```
mesh = Grid2D(nx=1000, ny=1000, dx=0.25, dy=0.25)
mesh = GmshImporter2DIn3DSpace("""
    radius = 5.0;
    cellSize = 0.3;

    // create inner 1/8 shell
    Point(1) = {0, 0, 0, cellSize};
    Point(2) = {-radius, 0, 0, cellSize};
    Point(3) = {0, radius, 0, cellSize};
    Point(4) = {0, 0, radius, cellSize};
    Circle(1) = {2, 1, 3};
    Circle(2) = {4, 1, 2};
    Circle(3) = {4, 1, 3};
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    // create remaining 7/8 inner shells
    t1[] = Rotate {{0,0,1},{0,0,0},Pi/2} {Duplicata{Surface{1};}};
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    t3[] = Rotate {{0,0,1},{0,0,0},Pi*3/2} {Duplicata{Surface{1};}};
    t4[] = Rotate {{0,1,0},{0,0,0},-Pi/2} {Duplicata{Surface{1};}};
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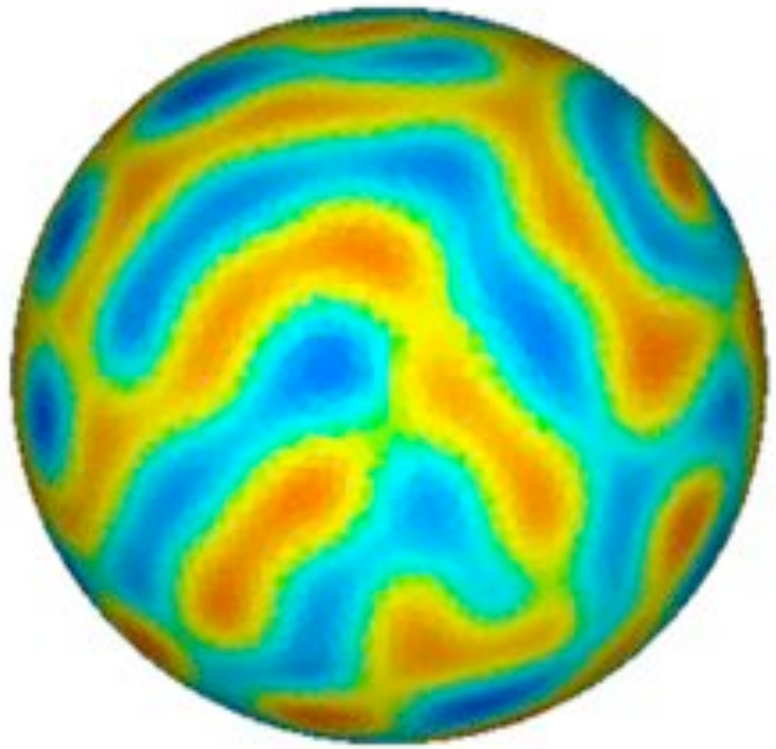
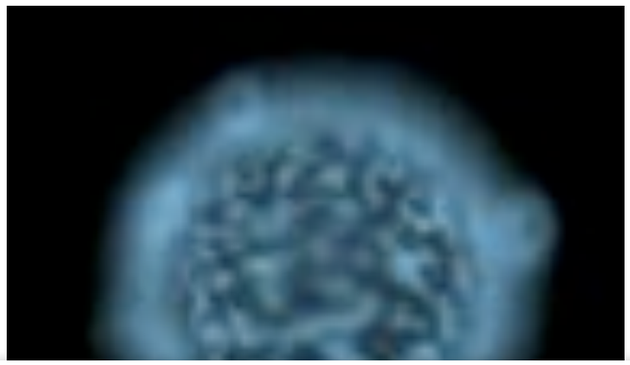
    t6[] = Rotate {{0,0,1},{0,0,0},Pi} {Duplicata{Surface{t4[0]};}};
    t7[] = Rotate {{0,0,1},{0,0,0},Pi*3/2} {Duplicata{Surface{t4[0]};}};

    // create entire inner and outer shell
    Surface Loop(100)={1,t1[0],t2[0],t3[0],t7[0],t4[0],t5[0],t6[0]};
""").extrude(extrudeFunc=lambda r: 1.1 * r)
```



Cahn-Hilliard Example



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```
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    radius = 5.0;
    cellSize = 0.3;

    // create inner 1/8 shell
    Point(1) = {0, 0, 0, cellSize};
    Point(2) = {-radius, 0, 0, cellSize};
    Point(3) = {0, radius, 0, cellSize};
    Point(4) = {0, 0, radius, cellSize};
    Circle(1) = {2, 1, 3};
    Circle(2) = {4, 1, 2};
    Circle(3) = {4, 1, 3};
    Line Loop(1) = {1, -3, 2} ;
    Ruled Surface(1) = {1};

    // create remaining 7/8 inner shells
    t1[] = Rotate {{0,0,1},{0,0,0},Pi/2} {Duplicata{Surface{1};}};
    t2[] = Rotate {{0,0,1},{0,0,0},Pi} {Duplicata{Surface{1};}};
    t3[] = Rotate {{0,0,1},{0,0,0},Pi*3/2} {Duplicata{Surface{1};}};
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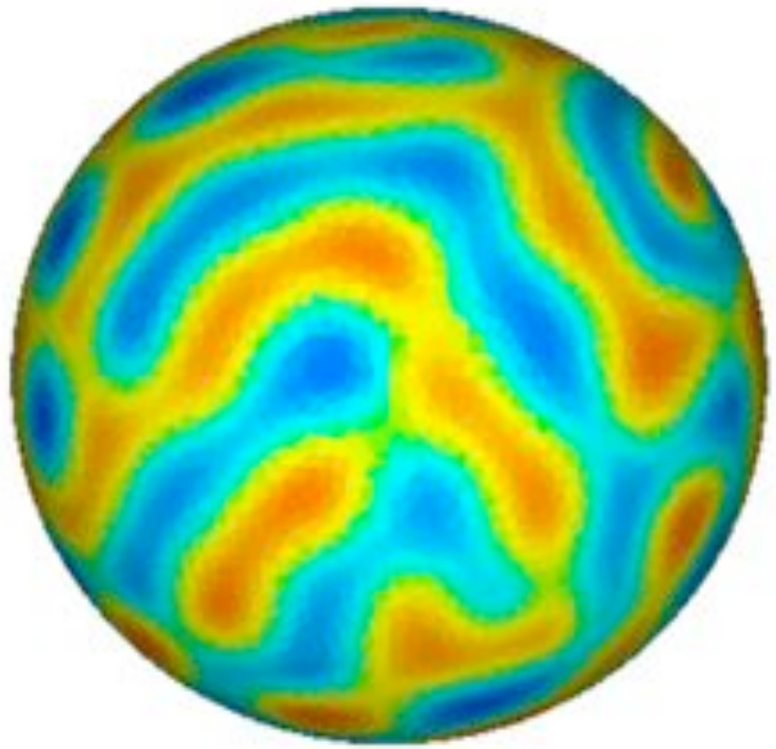
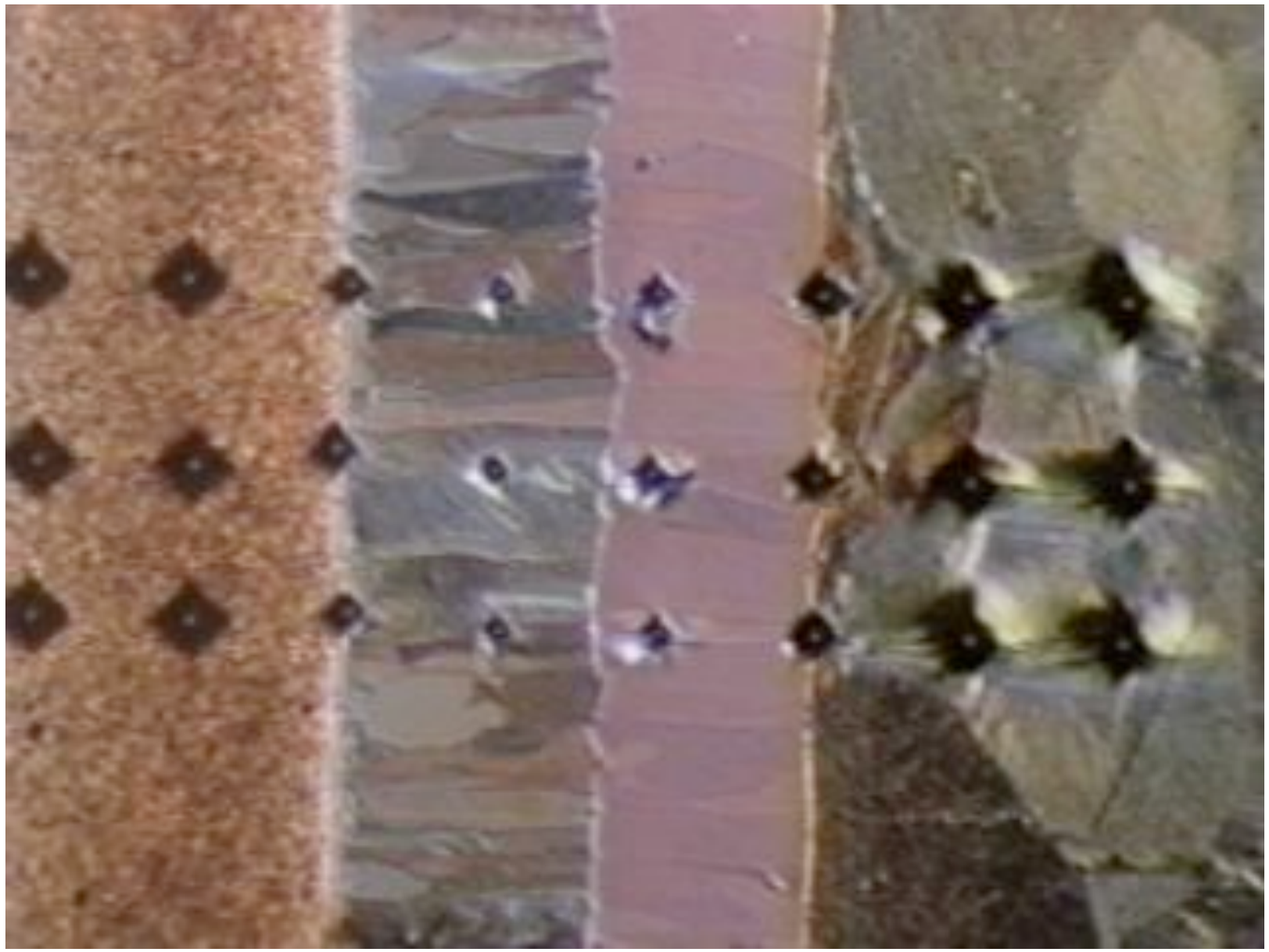
""").extrude(extrudeFunc=lambda r: 1.1 * r)
```



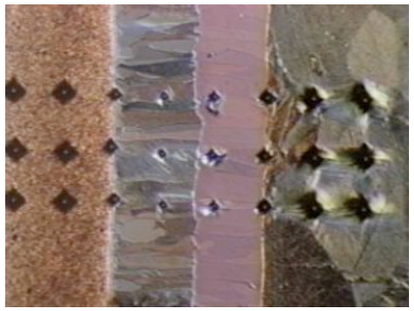
compare, e.g.,
youtube.com/watch?v=kDsFP67_ZSE

Kirkendall effect

Cu  Sb

Heumann & Ruth © IWF, Göttingen 1986

Kirkendall effect



W. J. Boettinger, J. E. Guyer,
C. E. Campbell & G. B. McFadden,
Proceedings of the Royal Society A: Mathematical
463 (2007) 3347–3373

Cahn-Hilliard treatment

$$\frac{\partial X_B}{\partial t} = \frac{\partial}{\partial z}\left\{\tilde{M}(X_B)\frac{\partial}{\partial z}\left[-\Omega(X_B - X_A) + RT(\ln X_B - \ln X_A) - 2K\frac{\partial^2 X_B}{\partial z^2}\right]\right\}$$

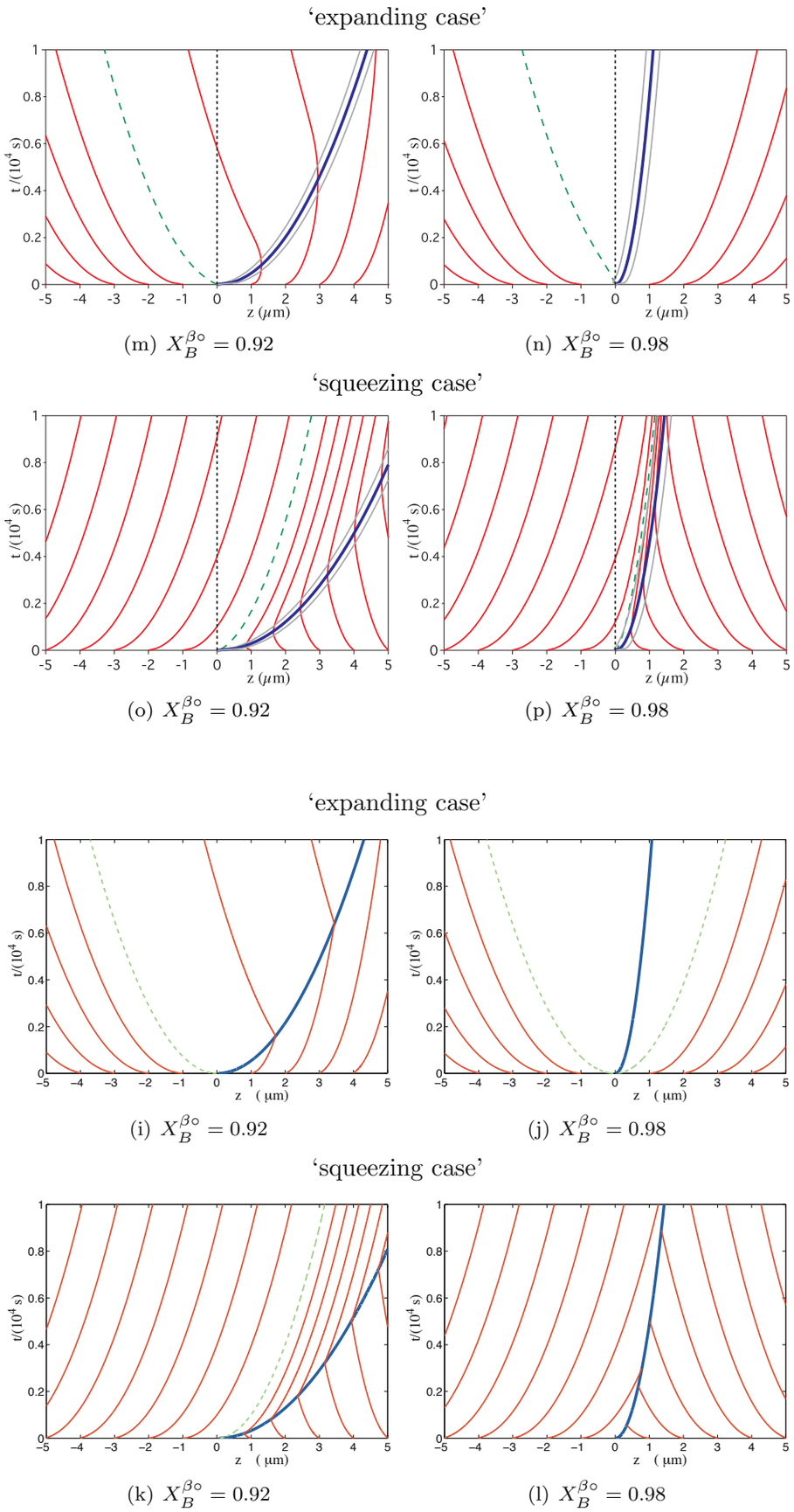
$$\begin{aligned}\tilde{M} &= X_A X_B[X_B M_A + X_A M_B] \\ M_A &= M_0[\beta_1(1 - X_B) + \beta_2 X_B] \\ M_B &= M_0[\beta_2(1 - X_B) + \beta_1 X_B]\end{aligned}$$

$$v(z,t) = X_A X_B[M_B - M_A]\frac{\partial}{\partial z}\left(-\Omega(X_B - X_A) + RT(\ln X_B - \ln X_A) - 2K\frac{\partial^2 X_B}{\partial z^2}\right)$$

$$\frac{\partial Z(z,t)}{\partial t} = -v\frac{\partial Z(z,t)}{\partial z}$$

both Eulerian and Lagrangian

compared with
sharp interface similarity solution
and DICTRA calculations



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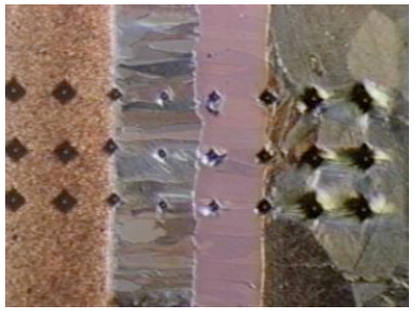
Kirkendall effect



W. J. Boettinger, J. E
C. E. Campbell & G. B. McFadden,
Proceedings of the Royal So
463 (2007) 33

Cahn-Hilliard t

$$\frac{\partial X_B}{\partial t} = \frac{\partial}{\partial z}\left\{\tilde{M}(X_B)\frac{\partial}{\partial z}\left[-\Omega(X_B - X_A) + \right.\right.$$

$$\begin{aligned}
\tilde{M} &= X_A X_B[X_B M \\
M_A &= M_0[\beta_1(1 - X \\
M_B &= M_0[\beta_2(1 - X
\end{aligned}$$

$$v(z,t) = X_A X_B[M_B - M_A]\frac{\partial}{\partial z}\left(-\Omega(X_B - X_A\right.$$

$$\frac{\partial Z(z,t)}{\partial t} = -v\frac{\partial}{}$$

both Eulerian and

compared

sharp interface simi

and DICTRA calculations

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PROCEEDINGS OF THE ROYAL SOCIETY A

Proc. R. Soc. A (2007) **463**, 3347–3373
doi:10.1098/rspa.2007.1904
Published online 9 October 2007

Computation of the Kirkendall velocity and displacement fields in a one-dimensional binary diffusion couple with a moving interface

By W. J. Boettinger[1], J. E. Guyer[1,*], C. E. Campbell[1]

FiPy implementation of Cahn-Hilliard model for
"Computation of the Kirkendall Velocity and Displacement Field in a 1-D
Binary Diffusion Couple with a Moving Interface"

W. J. Boettinger[1], J. E. Guyer[1], C. E. Campbell[1], and G. B. McFadden[2]

[1]Metallurgy Division, Materials Science and Engineering Laboratory,
and
[2]Mathematical and Computational Sciences Division, Information Technology Laboratory,

National Institute of Standards and Technology, Gaithersburg, MD 20899, USA

September 11, 2007

Module `kirkendall`

Attention!

This software was developed at the National Institute of Standards and Technology by employees of the Federal Government in the course of their official duties. Pursuant to title 17 Section 105 of the United States Code this software is not subject to copyright protection and is in the public domain. `kirkendall.py` is an experimental system. NIST assumes no responsibility whatsoever for its use by other parties, and makes no guarantees, expressed or implied, about its quality, reliability, or any other characteristic. We would appreciate acknowledgement if the software is used.
This software can be redistributed and/or modified freely provided that any derivative works bear some notice that they are derived from it, and any modified versions bear some notice that they have been modified.

FiPy implementation of Cahn-Hilliard model for Kirkendall diffusion.

Note

Information about FiPy can be found at http://www.ctcms.nist.gov/fipy
This script was tested with revision 2108 of the FiPy source code, available from
https://www.matforge.org/fipy/browser/trunk

We solve for the concentration X_B on a 1D domain of length $L = 10$ with 2000 evenly spaced mesh points.

```
>>> from fipy import *

>>> L = 10.
>>> nx = 2000

>>> mesh = Grid1D(nx=nx, dx=L / nx)

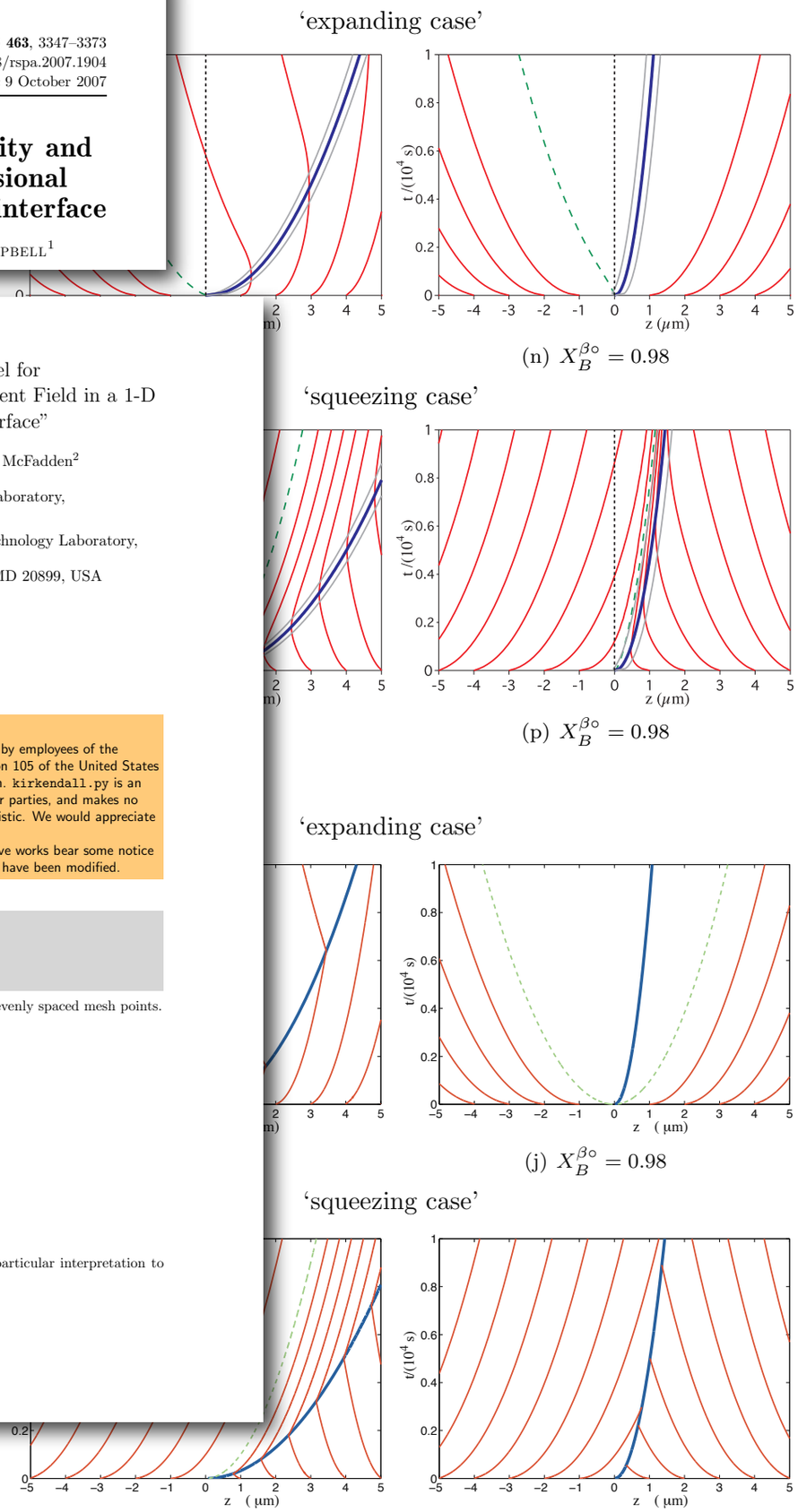
>>> xB = CellVariable(name="X_B", mesh=mesh, hasOld=1)
>>> xA = 1. - xB
```

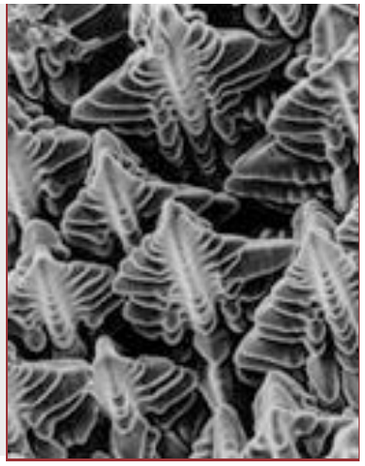
We set the initial conditions of

$$X_B = \begin{cases} 0 & \text{for } \zeta \le L/2 \\ 0.92 & \text{for } \zeta > L/2 \end{cases}$$

where ζ is the position within the domain (at this stage, we don't attach any particular interpretation to the frame of ζ):

1





Phase Field Example

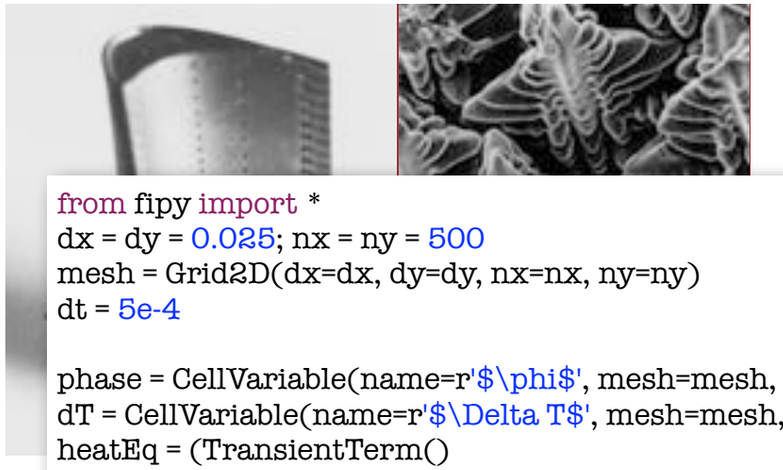
$$\frac{\partial \Delta T}{\partial t} = D_T \nabla^2 \Delta T + \frac{\partial \phi}{\partial t}$$

$$\tau_\phi \frac{\partial \phi}{\partial t} = \nabla \cdot \mathsf{D} \nabla \phi + \phi(1-\phi)\left[\phi - \frac{1}{2} - \frac{\kappa_1}{\pi}\arctan\left(\kappa_2 \Delta T\right)\right]$$

$$\beta = \frac{1-\Phi^2}{1+\Phi^2}$$

$$\mathsf{D} = \alpha^2 (1+c\beta) \begin{bmatrix} 1+c\beta & -c\frac{\partial \beta}{\partial \psi} \\ c\frac{\partial \beta}{\partial \psi} & 1+c\beta \end{bmatrix} \qquad \Phi = \tan\left(\frac{N}{2}\psi\right)$$

$$\psi = \theta + \arctan \frac{\partial \phi / \partial y}{\partial \phi / \partial x}$$



Phase Field Example

```
from fipy import *
dx = dy = 0.025; nx = ny = 500
mesh = Grid2D(dx=dx, dy=dy, nx=nx, ny=ny)
dt = 5e-4

phase = CellVariable(name=r'$\phi$', mesh=mesh, hasOld=True)
dT = CellVariable(name=r'$\Delta T$', mesh=mesh, hasOld=True)
heatEq = (TransientTerm()
          == DiffusionTerm(2.25)
          + (phase - phase.getOld()) / dt)

alpha = 0.015; c = 0.02; N = 6.; theta = pi / 8.
psi = theta + arctan2(phase.getFaceGrad()[1],
                      phase.getFaceGrad()[0])
Phi = tan(N * psi / 2)
PhiSq = Phi**2
beta = (1. - PhiSq) / (1. + PhiSq)
DbetaDpsi = -N * 2 * Phi / (1 + PhiSq)
Ddia = (1.+ c * beta)
Doff = c * DbetaDpsi
D = alpha**2 * (1.+ c * beta) * (Ddia * (( 1, 0),
                                         ( 0, 1)) + Doff * (( 0,-1),
                                                            ( 1, 0)))
tau = 3e-4; kappa1 = 0.9; kappa2 = 20.
phaseEq = (TransientTerm(tau)
           == DiffusionTerm(D)
           + ImplicitSourceTerm((phase - 0.5 - kappa1 / pi * arctan(kapp
                                 * (1 - phase)))
radius = dx * 5.
C = (nx * dx / 2, ny * dy / 2)
x, y = mesh.getCellCenters()
phase.setValue(1., where=((x - C[0])**2 + (y - C[1])**2 < radius**2)
dT.setValue(-0.5)

viewer = DendriteViewer(phase=phase, dT=dT,
                        title=r"%s & %s" % (phase.name, dT.name),
                        datamin=-0.1, datamax=0.05)
for i in range(10000):
    phase.updateOld()
    dT.updateOld()
    phaseEq.solve(phase, dt=dt)
    heatEq.solve(dT, dt=dt)
    if i % 10 == 0:
        viewer.plot()
```

$$\frac{\partial \Delta T}{\partial t} = D_T \nabla^2 \Delta T + \frac{\partial \phi}{\partial t}$$

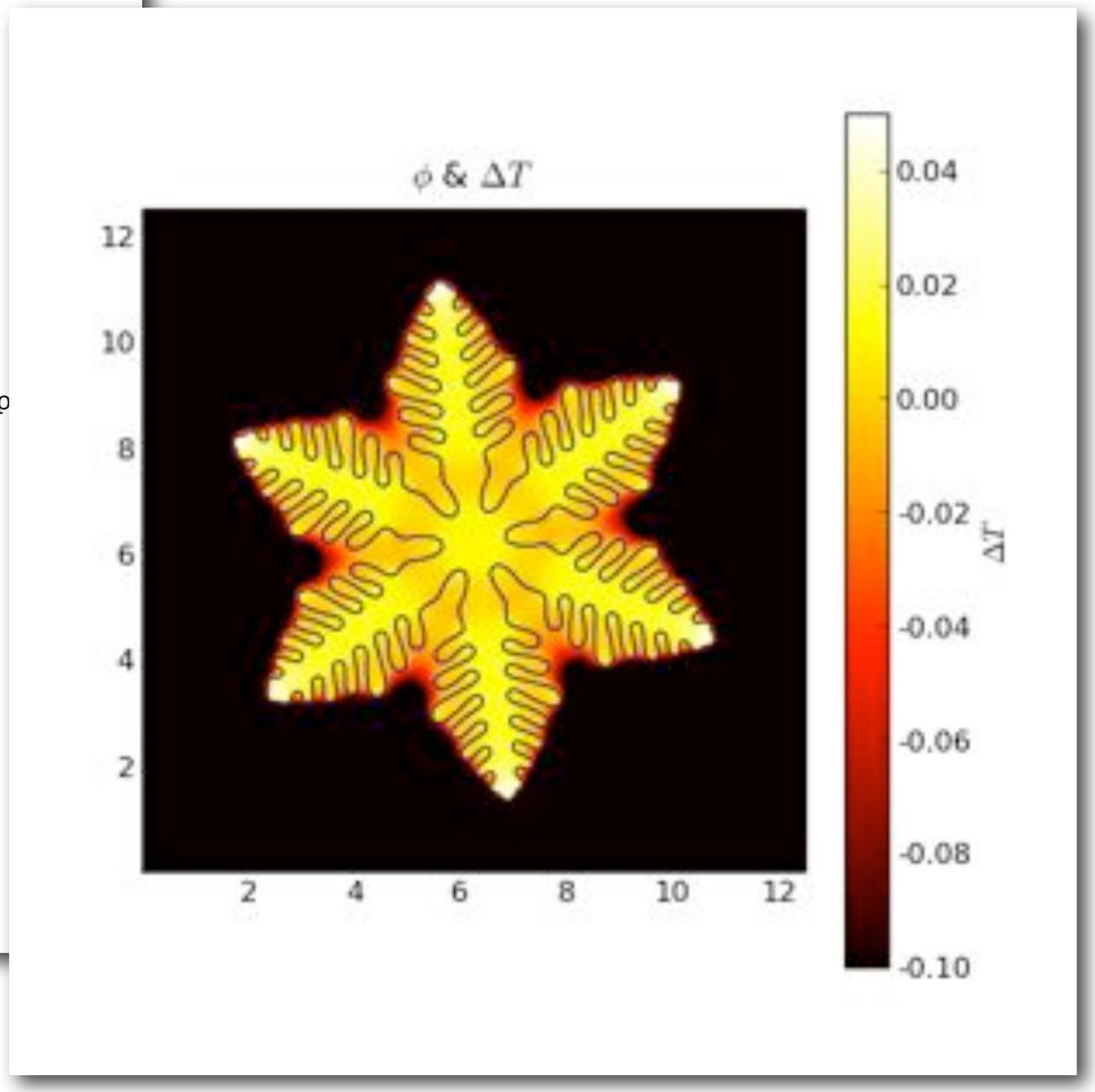
$$\tau_\phi \frac{\partial \phi}{\partial t} = \nabla \cdot \mathsf{D} \nabla \phi + \phi(1-\phi)\left[\phi - \frac{1}{2} - \frac{\kappa_1}{\pi}\arctan\left(\kappa_2 \Delta T\right)\right]$$

$$\mathsf{D} = \alpha^2 (1 + c\beta) \begin{bmatrix} 1 + c\beta & -c\frac{\partial \beta}{\partial \psi} \\ c\frac{\partial \beta}{\partial \psi} & 1 + c\beta \end{bmatrix}$$

$$\beta = \frac{1 - \Phi^2}{1 + \Phi^2}$$

$$\Phi = \tan\left(\frac{N}{2}\psi\right)$$

$$\psi = \theta + \arctan \frac{\partial \phi / \partial y}{\partial \phi / \partial x}$$



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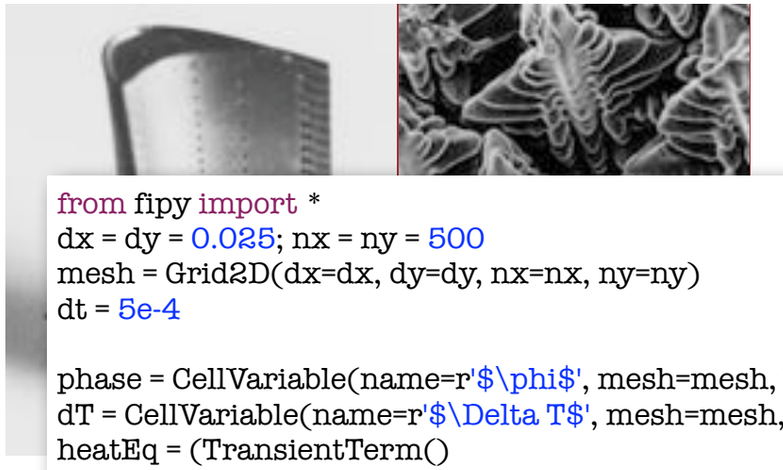

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```
from fipy import *
dx = dy = 0.025; nx = ny = 500
mesh = Grid2D(dx=dx, dy=dy, nx=nx, ny=ny)
dt = 5e-4

phase = CellVariable(name=r'$\phi$', mesh=mesh, hasOld=True)
dT = CellVariable(name=r'$\Delta T$', mesh=mesh, hasOld=True)
heatEq = (TransientTerm()
          == DiffusionTerm(2.25)
          + (phase - phase.getOld()) / dt)

alpha = 0.015; c = 0.02; N = 6.; theta = pi / 8.
psi = theta + arctan2(phase.getFaceGrad()[1],
                      phase.getFaceGrad()[0])
Phi = tan(N * psi / 2)
PhiSq = Phi**2
beta = (1
DbetaDp
Ddia = (
Doff = c
D = alph

tau = 3e-
phaseEq

radius =
C = (nx *
x, y = me
phase.se
dT.setVa

viewer =

for i in r
    phase
    dT.upd
    phaseEq.solve(phase, dt=dt)
    heatEq.solve(dT, dt=dt)
    if i % 10 == 0:
        viewer.plot()
```

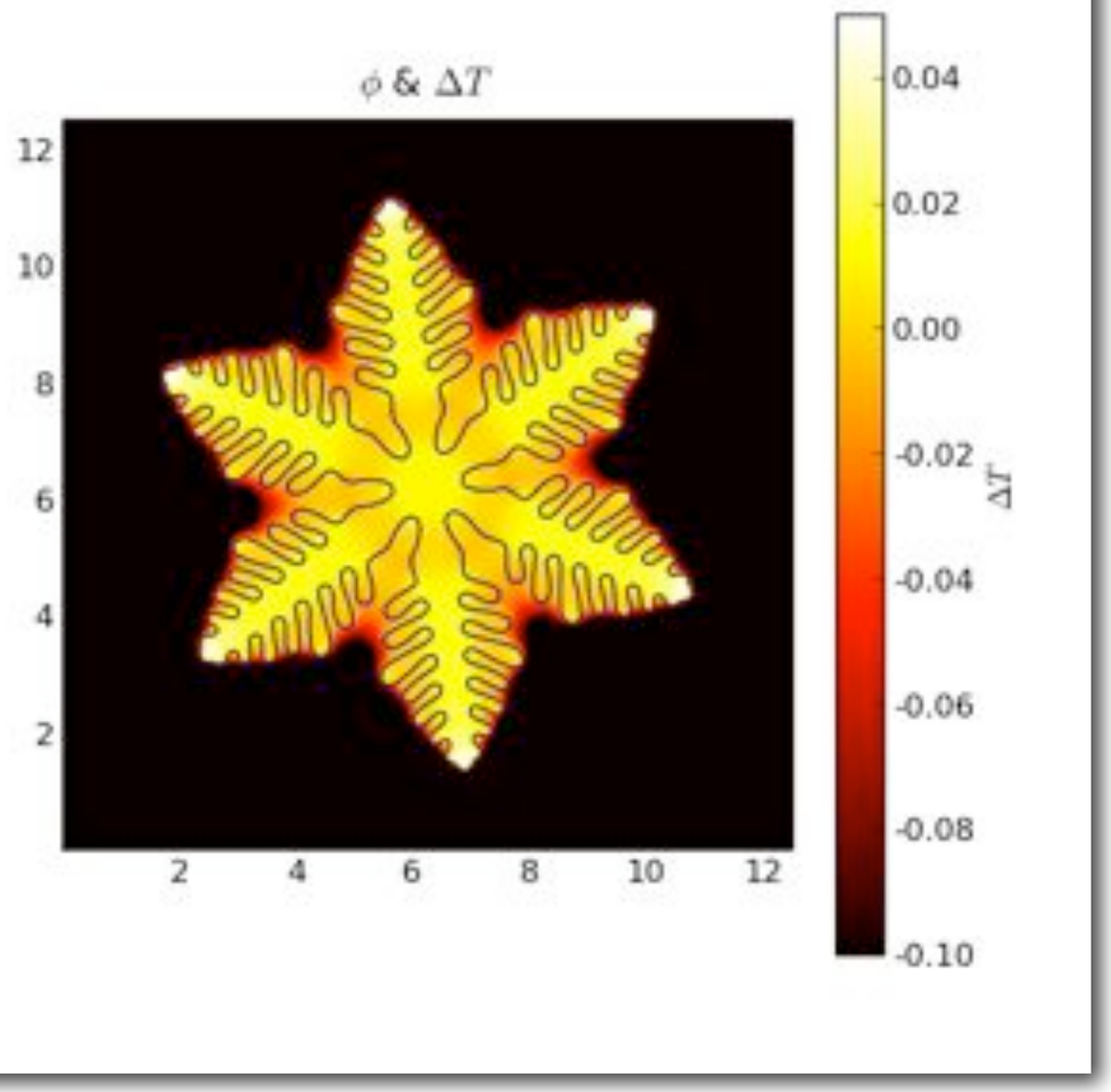
```
import pylab
class DendriteViewer(Matplotlib2DGridViewer):
    def __init__(self, phase, dT, title=None, limits={}, **kwlimits):
        self.phase = phase
        self.contour = None
        Matplotlib2DGridViewer.__init__(self, vars=(dT,), title=title,
                                        cmap=pylab.cm.hot,
                                        limits=limits, **kwlimits)

    def _plot(self):
        Matplotlib2DGridViewer._plot(self)

        if self.contour is not None:
            for c in self.contour.collections:
                c.remove()

        mesh = self.phase.getMesh()
        shape = mesh.getShape()
        x, y = mesh.getCellCenters()
        z = self.phase.getValue()
        x, y, z = [a.reshape(shape, order="FORTRAN") for a in (x, y, z)]

        self.contour = pylab.contour(x, y, z, (0.5,))
```



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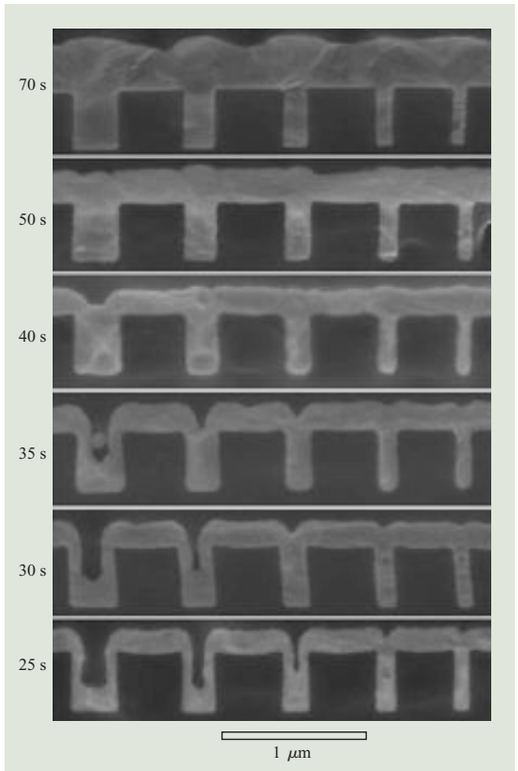
"Superfill"

D. Josell, D. Wheeler, W. H. Huber & T. P. Moffat
Physical Review Letters **87**(1) (2001) 016102



$$v = \frac{\Omega}{nF}(b_0 + b_1\theta)\frac{c_m^i}{c_m^\infty}\exp\left(\frac{-\alpha F}{RT}\eta\right)$$

$$\frac{\partial\phi}{\partial t} + v_{\text{ext}}|\nabla\phi| = 0$$

$$\frac{\partial\theta}{\partial t} - Jv\theta - k_\theta c_\theta^i(1-\theta) = 0$$

$$\frac{\partial c_m}{\partial t} - \nabla\cdot D_m\nabla c_m = 0$$

$$D_m\hat{n}\cdot\nabla c_m = \frac{v}{\Omega} \quad \text{on } \phi = 0$$

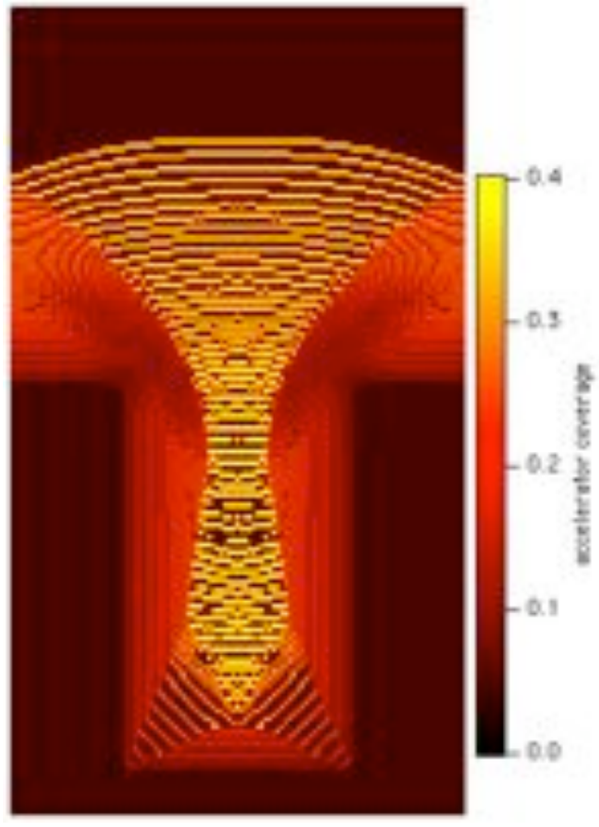
$$\frac{\partial c_\theta}{\partial t} - \nabla\cdot D_\theta\nabla c_\theta = 0$$

$$D_\theta\hat{n}\cdot\nabla c_\theta = -k_\theta c_\theta\Gamma(1-\theta) \quad \text{on } \phi = 0$$

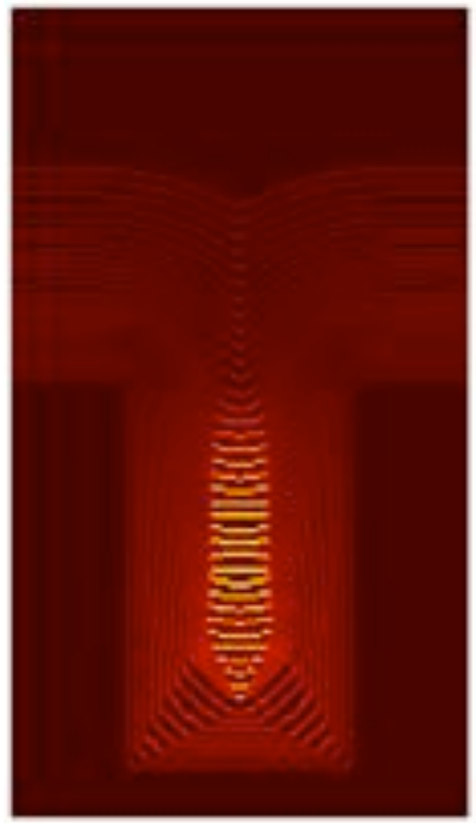
$$|\nabla\phi| = 1$$

Level Set method
(combination of PDE
and algorithmic solution)

no "leveler"



with "leveler"



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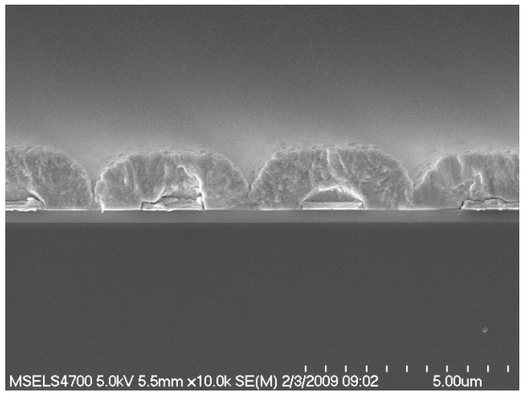
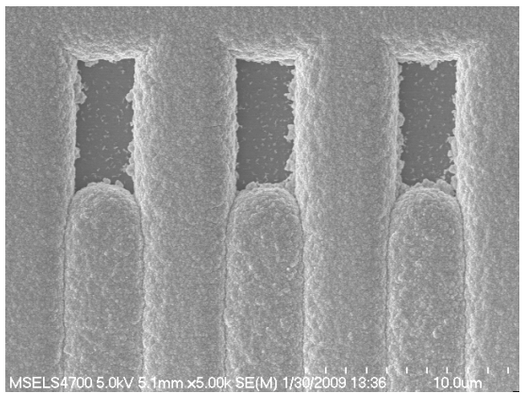
Photovoltaics





J. E. Guyer & D. Josell

$$0 = \nabla \cdot \epsilon \nabla V + p - n + N_D^+ - N_A^-$$

$$0 = -\nabla \cdot (\mu_n n \nabla \phi_n) + G - U$$

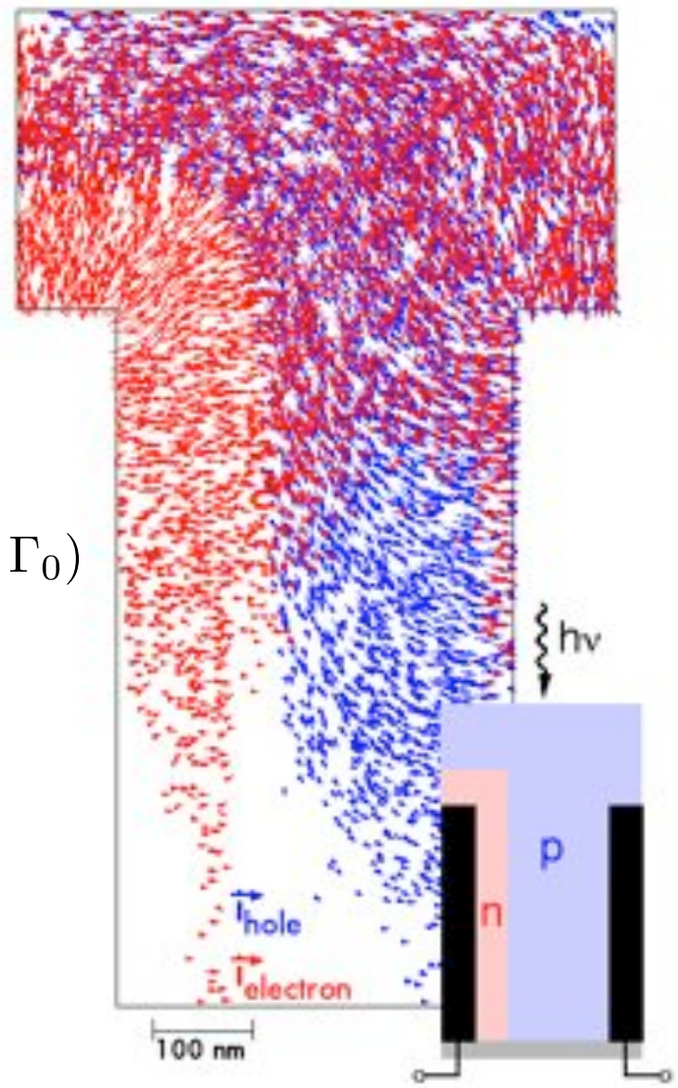
$$0 = \quad \nabla \cdot (\mu_p p \nabla \phi_p) + G - U$$

$$G = \alpha \Gamma \qquad (0 = \nabla \cdot \Gamma \vec{c} + \alpha c \Gamma, \quad \Gamma|_{z=0} = \Gamma_0)$$

$$U = \frac{pn - n_i^2}{\tau_{p0}(n + n') + \tau_{n0}(p + p')}$$

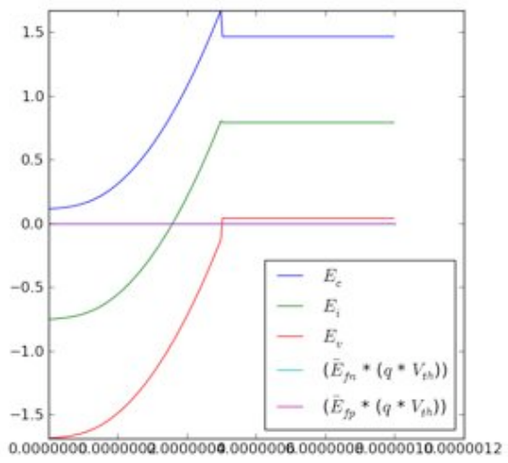
$$n = n_i \exp\left(\frac{V - \phi_n}{kT}\right)$$

$$p = n_i \exp\left(\frac{\phi_p - V}{kT}\right)$$

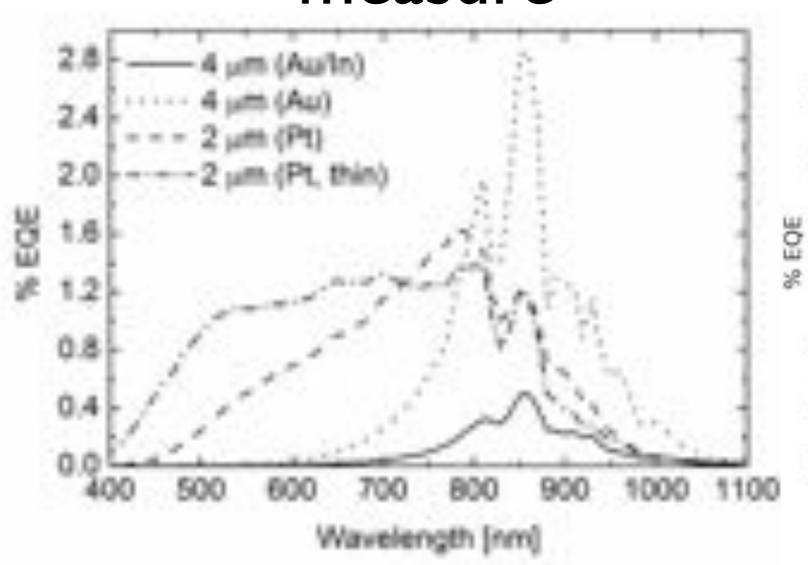


Scharfetter-Gummel discretization

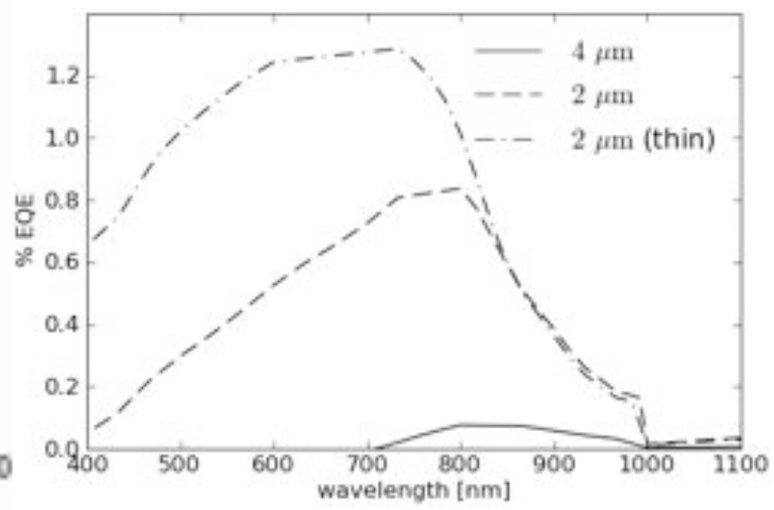
Newton-Block SOR sweeping



measure



model



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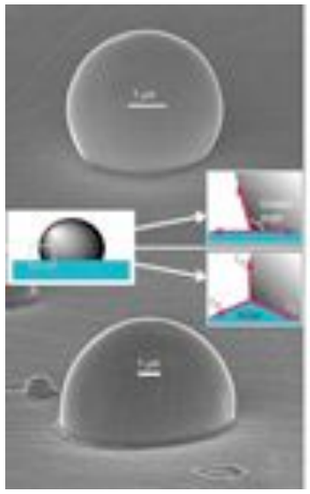
Reactive Wetting



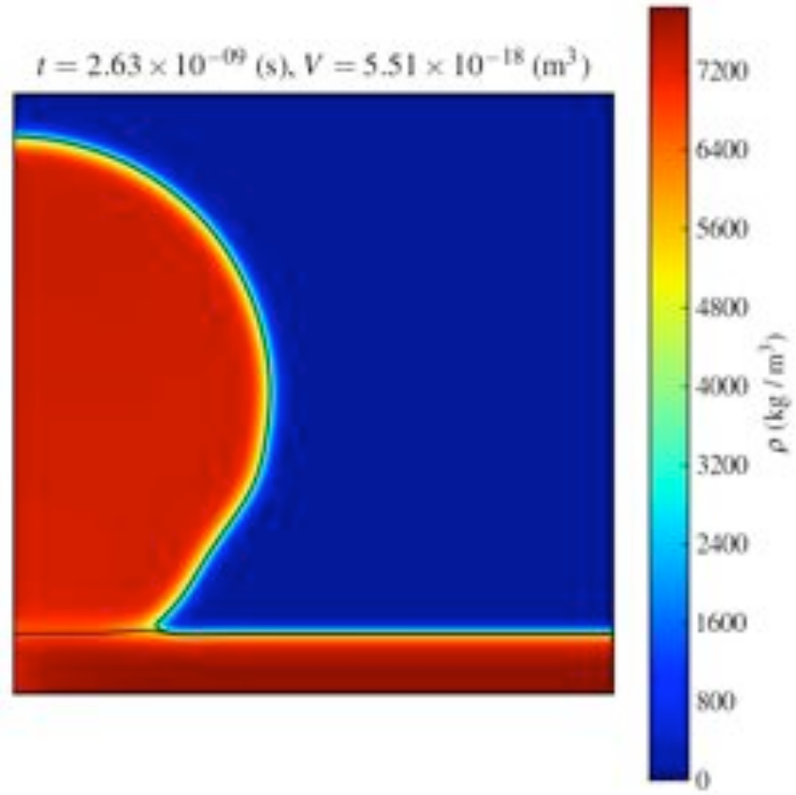
D. Wheeler, J. A. Warren & W. J. Boettinger

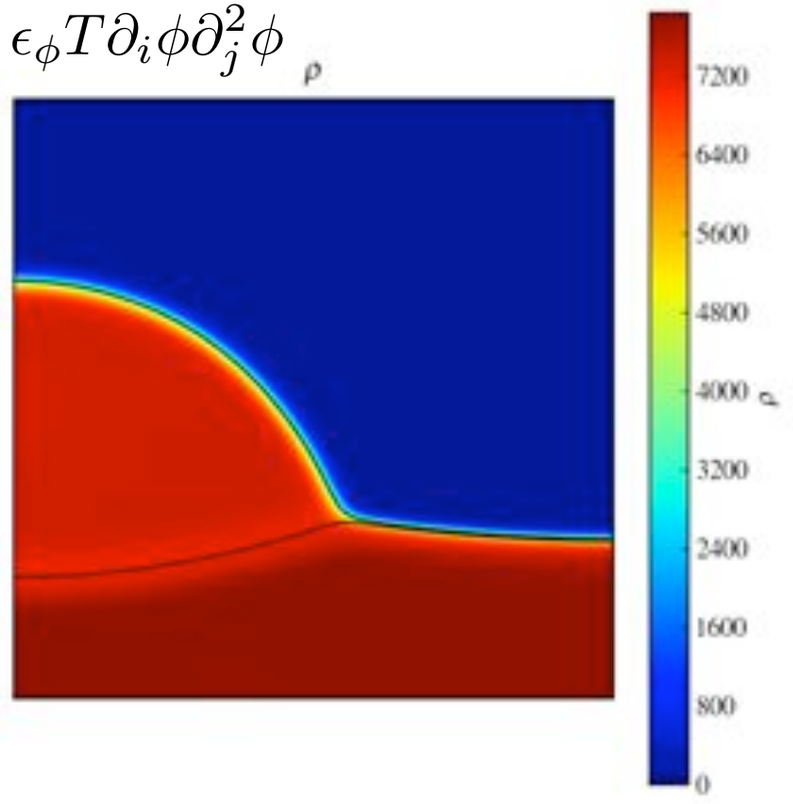
$$\frac{\partial \rho_1}{\partial t} + \partial_j \left(\rho_1 u_j\right) = \partial_j \left(\frac{M}{T} \partial_j \left[\mu_1^{NC} - \mu_2^{NC} \right] \right)$$

$$\frac{\partial \rho_2}{\partial t} + \partial_j \left(\rho_2 u_j\right) = \partial_j \left(\frac{M}{T} \partial_j \left[\mu_2^{NC} - \mu_1^{NC} \right] \right)$$

$$\frac{\partial \left(\rho u_i\right)}{\partial t} + \partial_j \left(\rho u_i u_j\right) = \partial_j \left(\eta \left[\partial_j u_i + \partial_i u_j\right]\right) - \partial_i P + \epsilon_1 T \rho_1 \partial_i \partial_j^2 \rho_1 + \epsilon_2 T \rho_2 \partial_i \partial_j^2 \rho_2 - \epsilon_\phi T \partial_i \phi \partial_j^2 \phi$$

$$\frac{\partial \phi}{\partial t} + u_j \partial_j \phi = \epsilon_\phi M_\phi \partial_j^2 \phi - \frac{M_\phi}{T} \frac{\partial F}{\partial \phi}$$





Coupled solution
Parallel

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don't invent when you can steal

NumPy

SciPy

matplotlib

Mayavi

python

Gmsh

Pysparse

The Trilinos Project

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Variable

```
>>> A = Variable(value=3)
>>> B = Variable(value=4)
>>> C = A * B**2
>>> C
(Variable(value=array(3)) * (pow(Variable(value=array(4)), 2)))
>>> print C
48
>>> B.setValue(5)
>>> print C
75
```

- Contains, but doesn't inherit from, NumPy array
- MeshVariable holds field of values; Mesh holds geometry and topology
- units (mostly stolen from Konrad Hinsen)

```
>>> (Variable("1 ft*lb*gn") / "2 wk").inUnitsOf('N*m/s')
PhysicalField(1.12088124035e-06,'m*N/s')
```

- supports automatic weave inlining

```
>>> C._getCstring()
'(var0 * (pow(var10, var11)))'
```

Design: test-based development

- hundreds of major tests, comprising thousands of low-level tests
- Tests *are* documentation (and vice versa)

__**ge**__(*self*, *other*)

Test if a Variable is greater than or equal to another quantity

```
>>> a = Variable(value = 3)
>>> b = (a >= 4)
>>> b
(Variable(value = 3) >= 4)
>>> b()
0
>>> a.setValue(4)
>>> b()
1
>>> a.setValue(5)
>>> b()
1
```

Design: test-based development

- hundreds of major tests, comprising thousands of low-level tests
- Tests *are* documentation (and vice versa)

to the top-left and bottom-right corners. Neumann boundary conditions are automatically applied to the top-right and bottom-left corners.

```
>>> x, y = mesh.getFaceCenters()
>>> facesTopLeft = ((mesh.getFacesLeft() & (y > L / 2))
...                 | (mesh.getFacesTop() & (x < L / 2)))
>>> facesBottomRight = ((mesh.getFacesRight() & (y < L / 2))
...                     | (mesh.getFacesBottom() & (x > L / 2)))

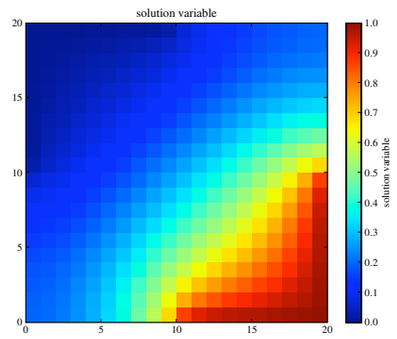
>>> BCs = (FixedValue(faces=facesTopLeft, value=valueTopLeft),
...        FixedValue(faces=facesBottomRight, value=valueBottomRight))
```

We create a viewer to see the results

```
>>> if __name__ == '__main__':
...     viewer = Viewer(vars=phi, datamin=0., datamax=1.)
...     viewer.plot()
```

and solve the equation by repeatedly looping in time:

```
>>> timeStepDuration = 10 * 0.9 * dx**2 / (2 * D)
>>> steps = 10
>>> for step in range(steps):
...     eq.solve(var=phi,
...              boundaryConditions=BCs,
...              dt=timeStepDuration)
...     if __name__ == '__main__':
...         viewer.plot()
```



We can test the value of the bottom-right corner cell.

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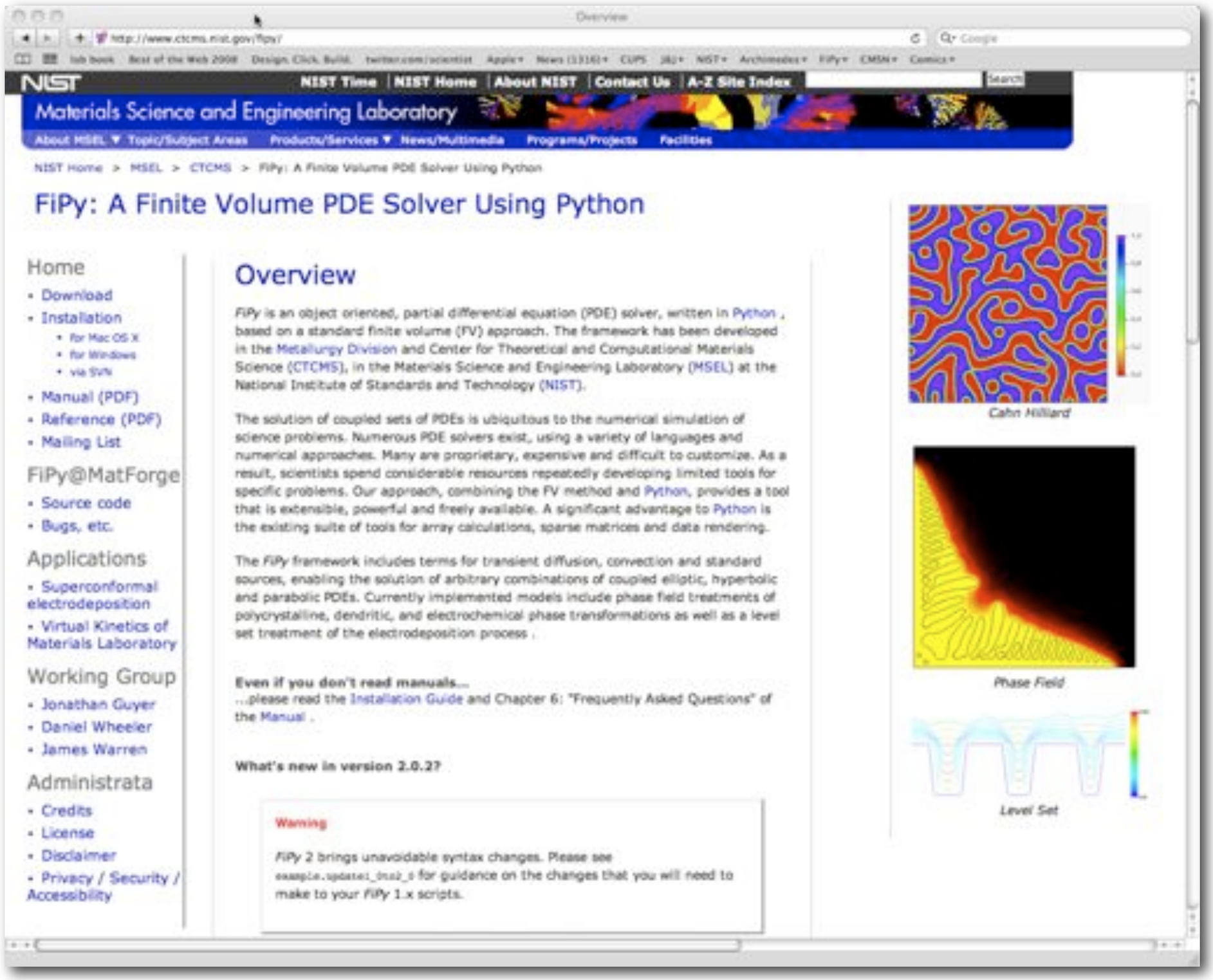
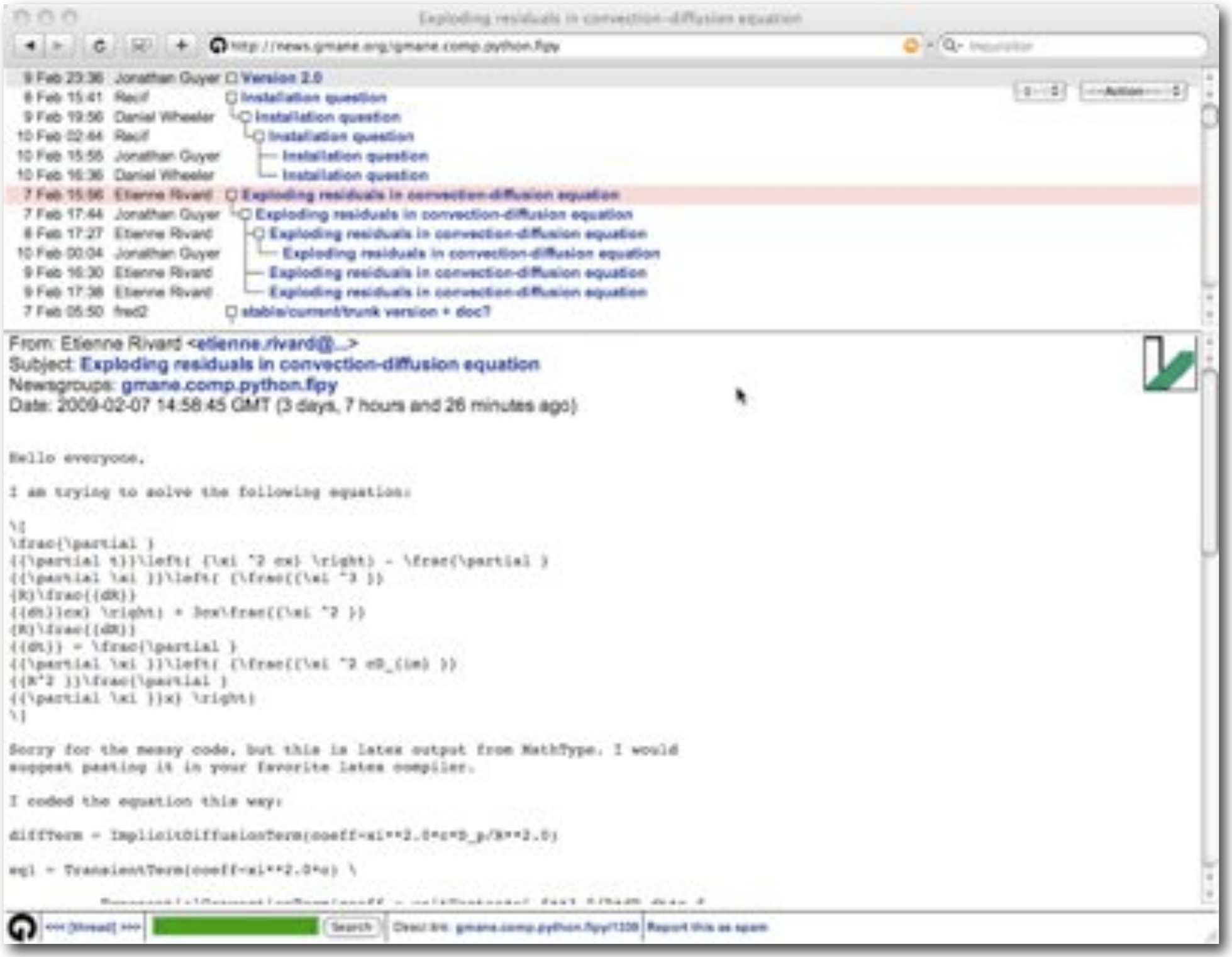
www.ctcms.nist.gov/fipy



fipy@nist.gov



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bitten
continuous integration rethought

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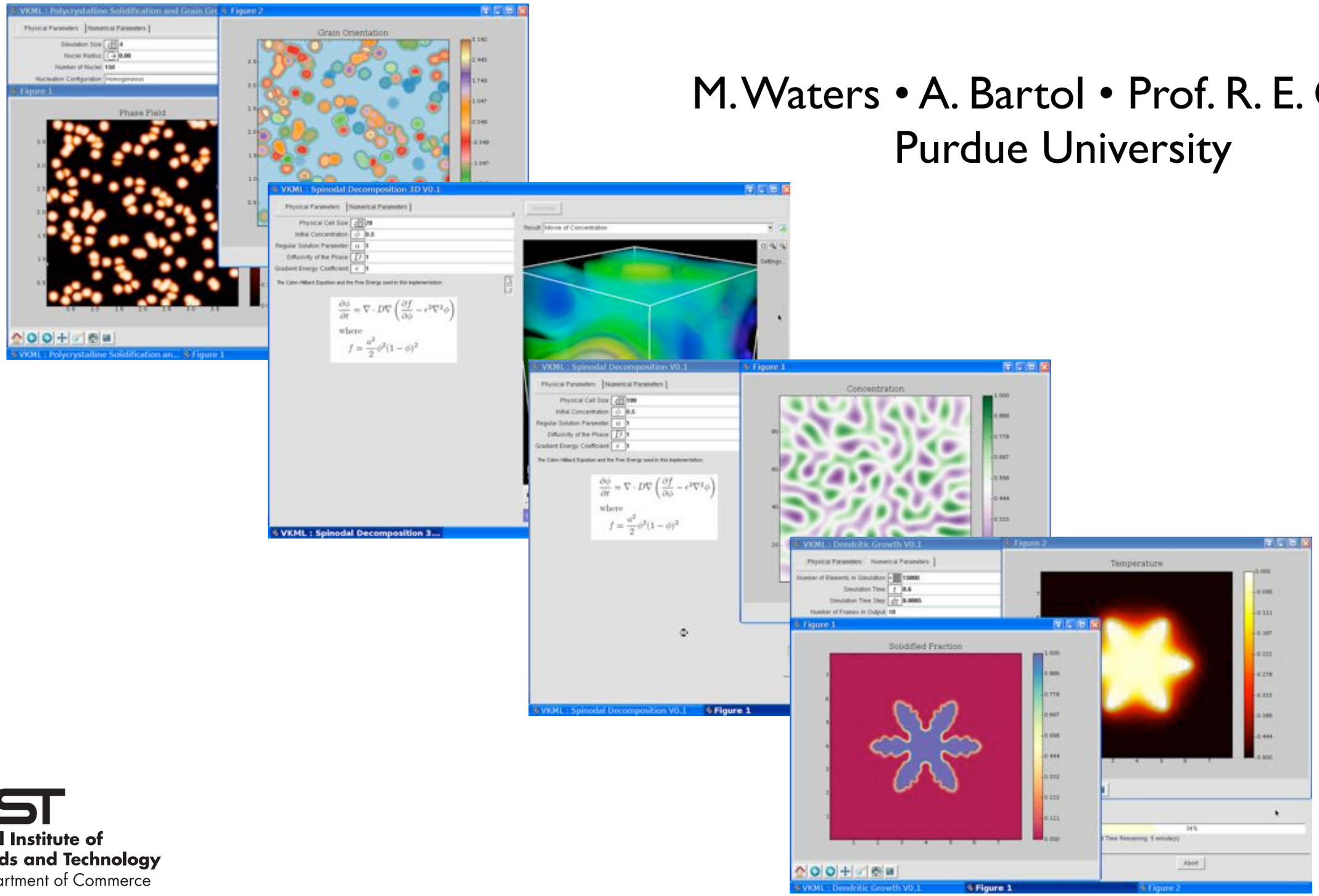
A Sampling of External Users

- NIST – gold nanoparticle hyperthermia
- U. of Central Florida – thermomigration and precipitate growth
- U. of Maine – water percolation through peat bogs
- Silesian University of Technology – solar irradiation of soil
- U. C. Berkeley – mRNA reaction-diffusion in fruitfly embryos
- Seagate Technologies – heat conduction in magnetic devices
- Princeton Satellite Systems – wind turbine development
- Rensselaer Polytechnic Institute – fuel cells
- Purdue University – stresses in photodiodes

Virtual Kinetics of Materials Library

nanohub.org/tools/vkmlggs
nanohub.org/tools/vkmlpsgg

nanohub.org/tools/vkmlsd
nanohub.org/tools/vkmlsd3d



M. Waters • A. Bartol • Prof. R. E. García
Purdue University

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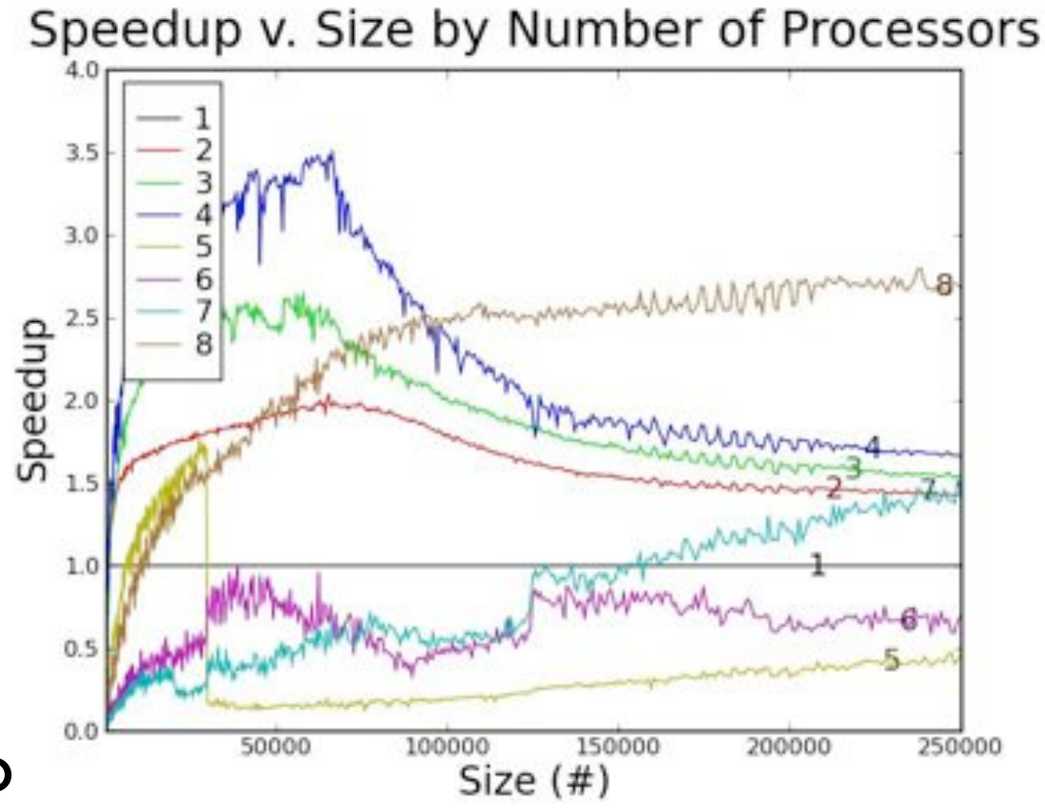
Parallel



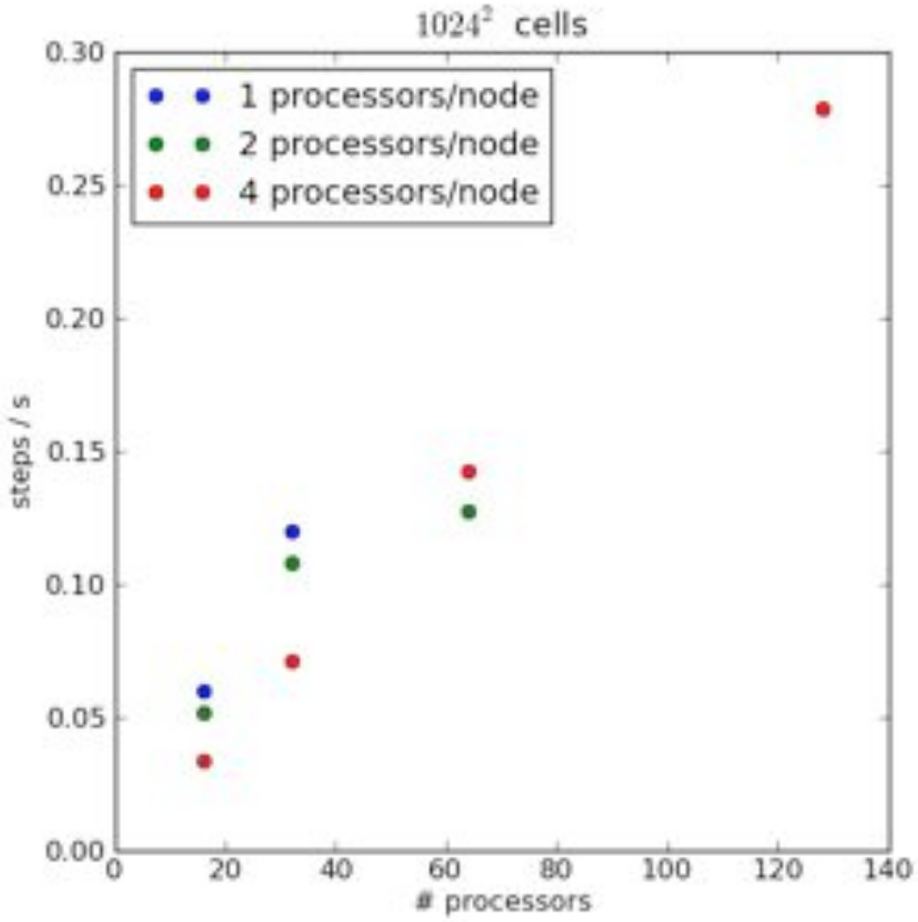
- 2007 Max Gibiansky - Harvey Mudd - SURF student
  - Integrate FiPy with PyTrilinos
    Matrix solves in parallel…
    …but builds in serial
- 2008 Olivia Buzek - U of Maryland - SURF student
  Daniel Stiles - Montgomery Blair High School
  - Build matrix in parallel with PyTrilinos, too
  - Pervasive changes to every FiPy data type to make "parallel aware"
  - Fragile and poor scaling performance
- Presently
  - Leave FiPy alone (mostly)
  - Break processes into separate FiPy problems with limited overlap
  - PyTrilinos (and a little mpi4py) for communication and parallel solution

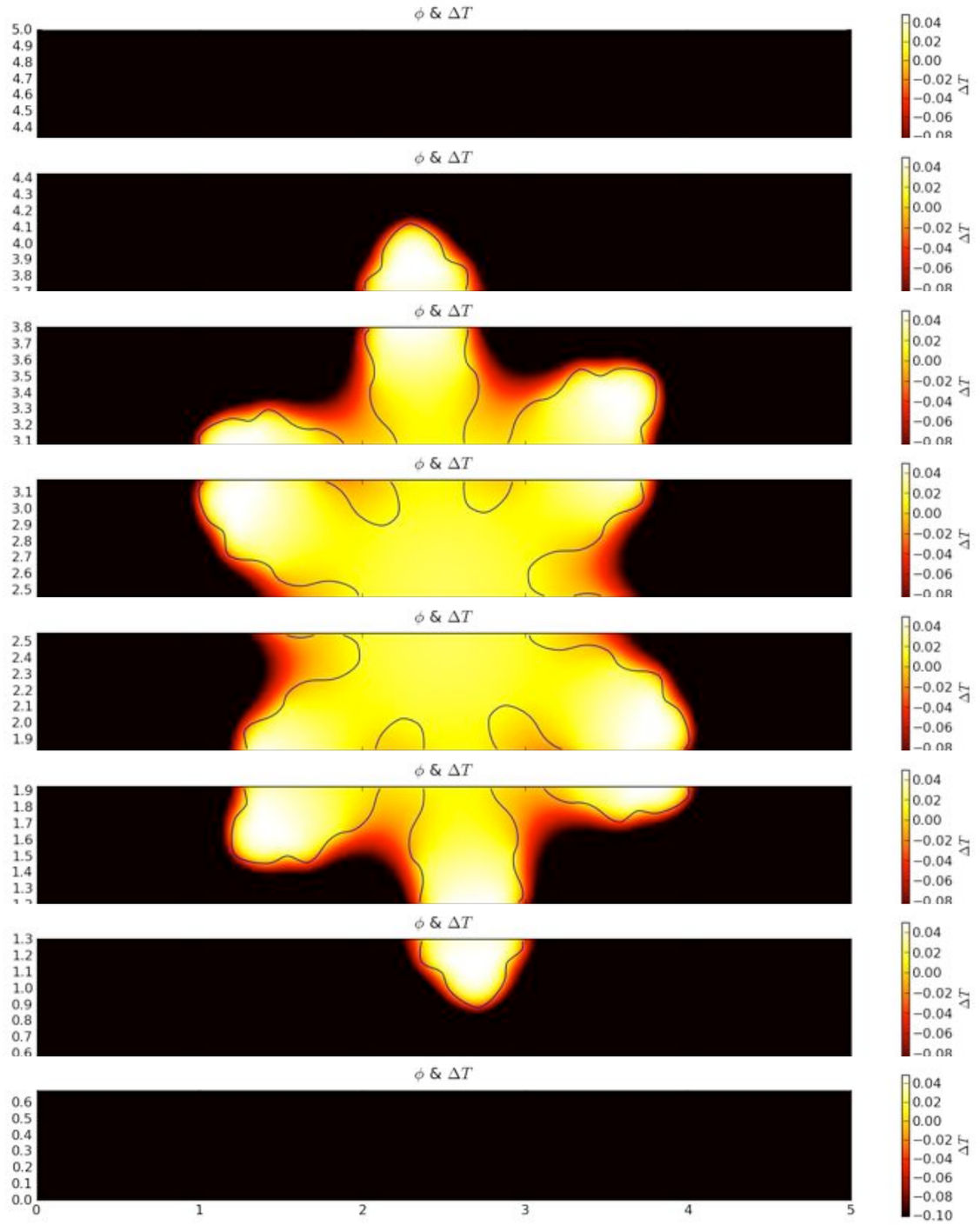
Parallel

mpirun -np 8 python examples/phase/anisotropy.py

- presently a Trilinos & PySparse hybrid
- doctests
  - conditional tests?
- zero-element arrays

  numpy:ticket:1171





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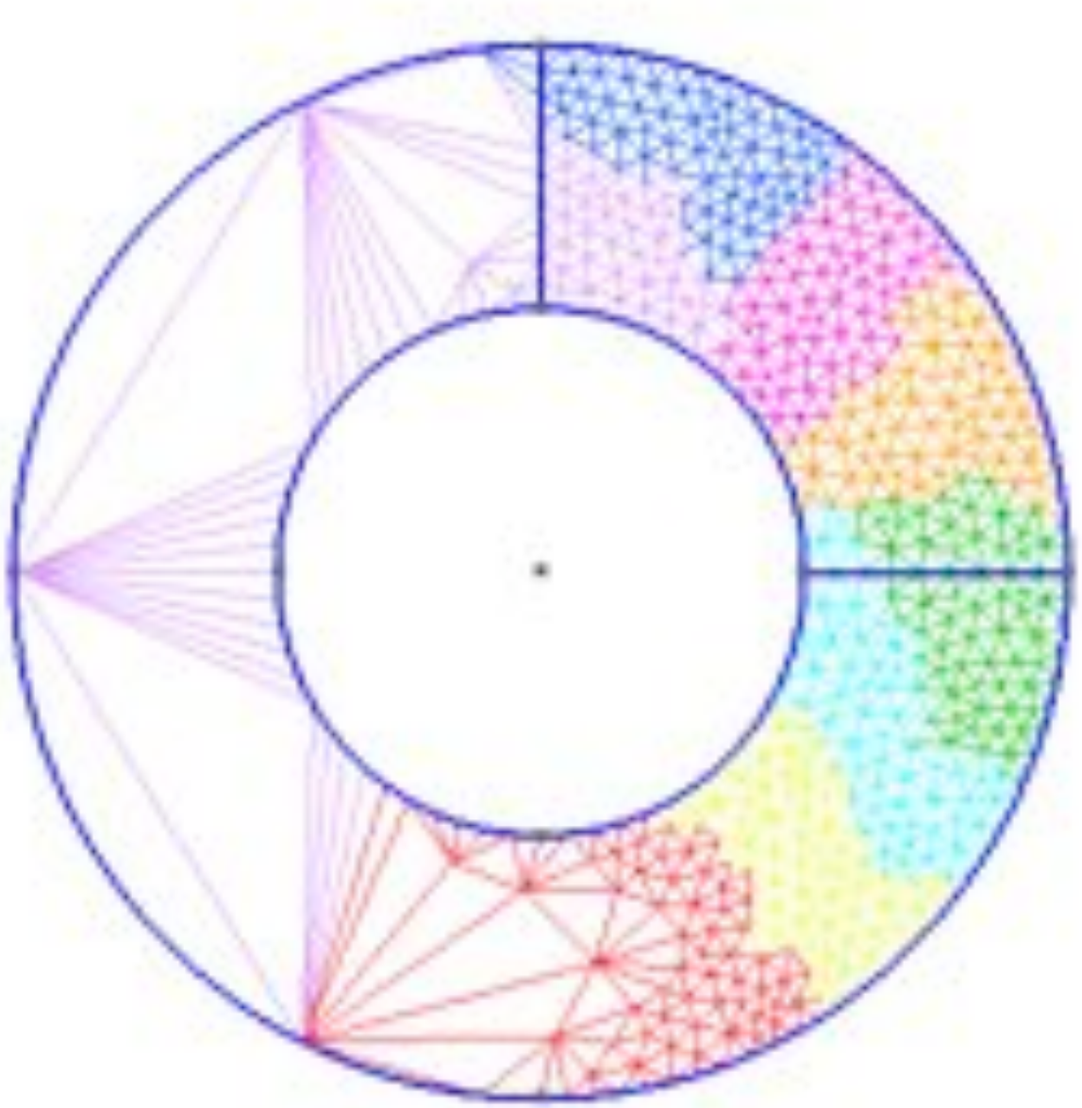
Parallel: Partitioning

- Presently only support primitive slices of Grid meshes
- PyMetis - “hard to install”
- Zoltan (Trilinos) - no Python wrapper
- Gmsh (uses Metis) - easy to install and use, but how to efficiently obtain overlaps?
- NetworkX?



Future Work: Coupled Equations

$$\frac{\partial A}{\partial t} = \nabla \cdot D_{AA} \nabla A + \nabla \cdot D_{AB} \nabla B$$

$$\frac{\partial B}{\partial t} = \nabla \cdot D_{BA} \nabla A + \nabla \cdot D_{BB} \nabla B$$

- Now

```
eqA = TransientTerm() == DiffusionTerm(coeff=DAA) + (DAB * B.getFaceGrad()).getDivergence()
eqB = TransientTerm() == (DBA * A.getFaceGrad()).getDivergence() DiffusionTerm(coeff=DBB)
for step in range(steps):
        resA = resB = 1e10
            while resA > 1e-3 or resB > 1e-3:
                resA = eqA.sweep(var=A)
                resB = eqB.sweep(var=B)
```

- Soon

```
eqA = TransientTerm()(A) == DiffusionTerm(coeff=DAA)(A) + DiffusionTerm(coeff=DAB)(B)
eqB = TransientTerm()(B) == DiffusionTerm(coeff=DBA)(A) + DiffusionTerm(coeff=DBB)(B)
eqs = CoupledEquations((eqA, eqB))
for step in range(steps):
        eqs.solve(vars=(A, B))
```

Future Work

- Solvers
  - SciPy sparse
  - PyAMG - they've already done it!
- FEMhub
- Sphinx
- VisIt
- Autonomous viewers
- CorePy? Cython?

Summary

- Cross-platform, Open Source code for phase transformation problems
- Capable of solving multivariate, coupled, non-linear PDEs
- Extensive documentation, dozens of examples, hundreds of tests
- Object-oriented structure easy to adapt to unique problems
- Slower to run than hand-tailored FORTRAN or C…
  - …but much faster to write

- Python is great, but…
  - …scientific Python community is our real enabling technology

FiPy 2.0 - released 2/9/2009
www.ctcms.nist.gov/fipy

"FiPy: PDEs with Python"
J. E. Guyer, D. Wheeler & J. A. Warren
Computing in Science and Engineering **May/June** (2009) 6

FiPy workshop, Winter 2009/2010

Major Contributers

- Alex Mont - Montgomery Blair High School
  - Gmsh import
- Katie Travis - Smith College
  - automated weave inlining
- Max Gibiansky - Harvey Mudd College
  - Trilinos solvers
- Andrew Reeve - U of Maine
  - anisotropic diffusion
- Olivia Buzek - U of Maryland
  - parallel
- Daniel Stiles - Montgomery Blair High School
  - parallel
  - Mayavi2
  - Gmsh partitioning

random thoughts on scientific Python

- Installation much easier, but…
- Be careful about licenses
- Don't just wrap
- Python is a great cross-platform equalizer, but…
  - GPUs are very platform specific
- Embrace 1.0!

- What becomes of SciPy if Python "dies"?
  - What if it's our fault?