Phase field modelling

Current challenges and opportunities for high performance computing

P G Tennyson†, D Mohan‡, G Phanikumar‡, M P Gururajan[1]

Department of Metallurgical Engineering and Materials Science,
Indian Institute of Technology Bombay, Mumbai 400076 INDIA
†: Tata Research Development and Design Center (TRDDC), Pune
‡: Department of Metallurgical and Materials Engineering, IIT Madras, Chennai

December, 2018

[1]guru.mp@iitb.ac.in,gururajan.mp@gmail.com

Acknowledgements

- Funding: IRCC, IIT Bombay, DST, Government of India, DRDO and SASE, Ministry of Defence, Government of India, DST-DAAD, Tata Steel, GE India
- Computational resources: Spinode, Dendrite, Nebula / Space-Time, Param Yuva (C-DAC, Pune)
- Organisers, specifically, Dr. Shenoy, C-DAC, Pune
- Teachers, collaborators, students

Outline

- Microstructure and its evolution
- Phase field modelling
- Examples: Six-fold anisotropy on morphology / Solidification
- Way forward!

Computational Materials Engineering Group

Figure: CMEG: part of materials and process modelling lab

The problem

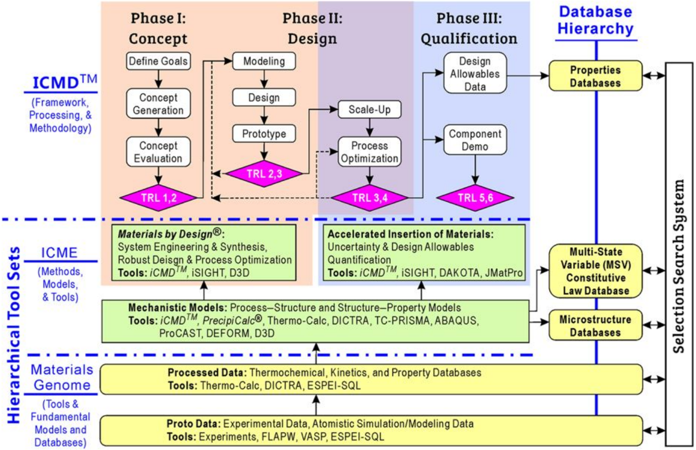


Figure: New material development cycle: 10 to 20 years. Can we bring it down to less than 5 years? Xiong and Olson, npj Computational Materials, 2016

ICME

Figure: ICME: The minerals, metals and materials society (TMS) study, 2013

Tools and techniques

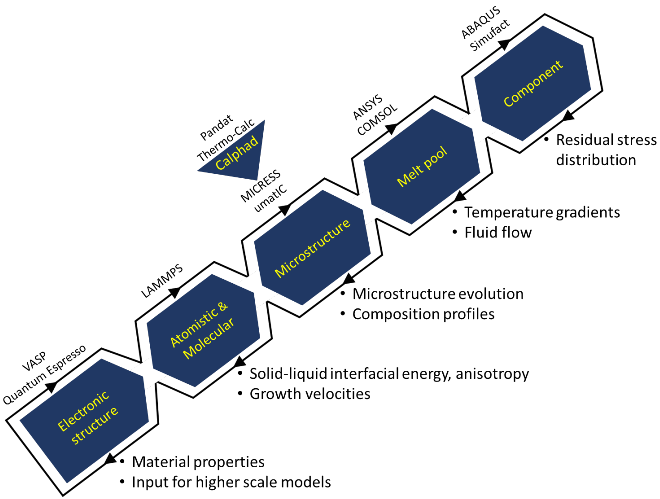


Figure: Computational materials science: tools and techniques

What is microstructure?

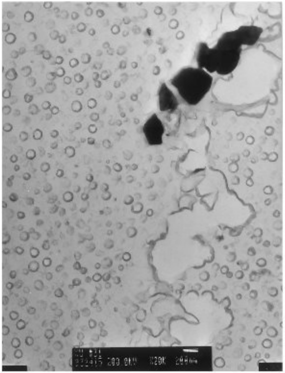


Figure: Microstructure (a Ni-base superalloy). Xu et al, Met. Mat. Trans. A, 1998

Structure, shapes, sizes and distribution of interfaces

Microstructural evolution

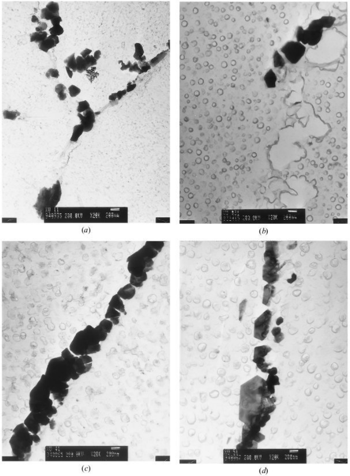


Fig. 11—Replica TEM micrographs of specimens aged for the indicated time at 900 °C after the 1135 °C solution treatment: (a) 40 min, (b) 24 h, (c) 48 h, and (d) 90 hours (×20 K).

Figure: Effect of heat treatment. Xu et al, Met. Mat. Trans. A, 1998

Microstructural evolution

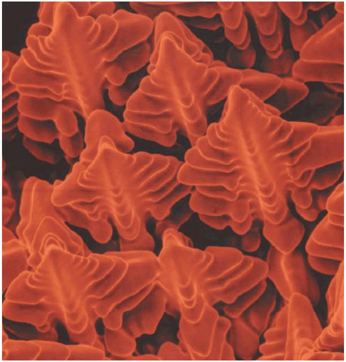


Figure: Dendrites during solidification. David et al, JOM, 2003

Spinodal decomposition

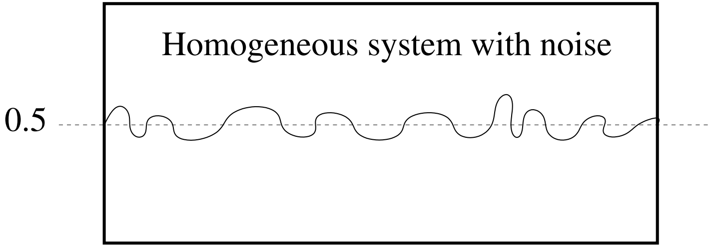


Figure: A homogeneous alloy with a slighlty noisy composition profile

Pure material solidification

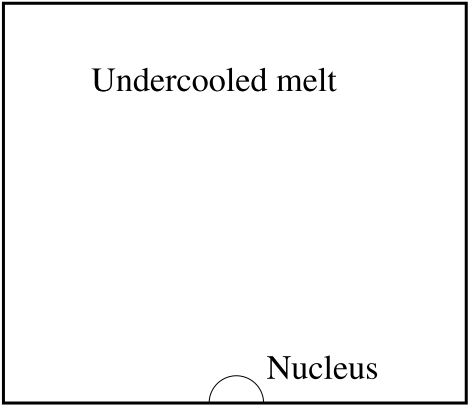


Figure: An undercooled melt with insulated sides and nucleus on one of the walls. The interfacial energy is 4-fold anisotropic.

Six-fold dendrites

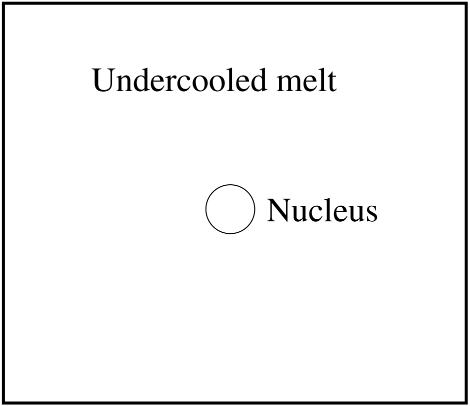


Figure: An undercooled melt with insulated sides and nucleus at the centre. The interfacial energy is 6-fold anisotropic.

Spinodal decomposition

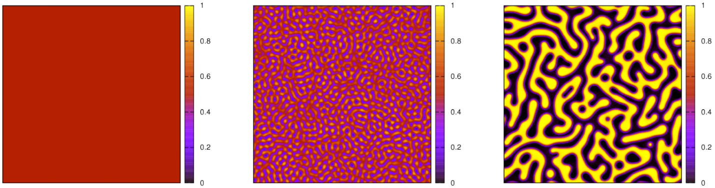


Figure: Regions rich in A (B) become richer in A (B) with time. Microstructures at times 0, 100 and 1000 units.

Issue 1

The phase field method, like many other modeling approaches, is practically limited by the computational expense entailed in running large simulations. The challenge stems from the need to resolve a diffuse interface that has a diffuseness that is on a much smaller length scale than a typical microstructural evolution length scale.

–Modeling Across Scales: A Roadmapping Study for Connecting Materials Models and Simulations Across Length and Time Scales, TMS study report, 2015

Issue 2

Common software: Micress$^{\mathrm{TM}}$, FiPy$^{\mathrm{TM}}$, OpenPhase$^{\mathrm{TM}}$, and MOOSE (Marmot)$^{\mathrm{TM}}$
Compare with VASP, LAMMPS, ParaDIS, ...
Phase field: an approach and not a set methodology (like FEM)
pfHUB: maintained by NIST

Phase field models

$$\frac{\partial c}{\partial t} = \nabla M \nabla \mu = \nabla M \nabla [g(c) - \kappa \nabla^2 c] \tag{1}$$

$$\frac{\partial \phi}{\partial t} = -L\mu = L[\kappa \nabla^2 \phi - g(\phi)] \tag{2}$$

Ginzburg-Landau, Alan Turing (Chemical morphogenesis), ...

Characteristics of phase field models

- Interfaces are not sharp; diffuse interface model
- No tracking of interface: numerical solutions are easier
- Gradient energy coefficient: interfacial energy contributions (Gibbs-Thomson, for example) are automatically accounted for
- Topological singularities (splitting or disappearance of interfaces): naturally taken care of
- Elastic stress, magnetic and electric field: can be coupled by adding the relevant free energy term!

What is phase field modelling?

Some representative viewpoints:

- An approach to obtain solutions of PDEs that are hard to solve – by introducing artificial regions of continuity where there are discontinuities (Mathematical)
- Non-linear partial differential equations that lead to solutions which are interesting patterns (Biology)
- Continuum equations derived from statistical mechanics that lead (as solution) to interesting patterns (Physics)
- Partial differential equations that describe diffusion (of atoms and heat) as well as phase transformations (Materials science)

Spectral technique

$$\frac{\partial c}{\partial t} = D\nabla^2 c \tag{3}$$

Spatial Fourier transform of c: $\tilde{c} = \int c(x) \exp\left[-i\mathbf{k}\cdot\mathbf{r}\right] dV$
Turns the PDE into ODE:

$$\frac{d\tilde{c}}{dt} = -Dk^2\tilde{c} \tag{4}$$

Semi-implicit Fourier spectral technique

$$\frac{\partial c}{\partial t} = \nabla M \nabla \mu = \nabla M \nabla [g(c) - \kappa \nabla^2 c] \tag{5}$$

$$\frac{\partial \phi}{\partial t} = -L\mu = L[\kappa \nabla^2 \phi - g(\phi)] \tag{6}$$

Advantages of FFT

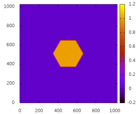
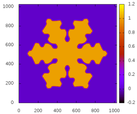
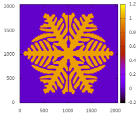
- Periodic boundary conditions: representative volume elements
- Semi-implicit Fourier spectral technique
- Good, fast, open source FFT codes: FFTW

Extended Cahn-Hilliard free energy: anisotropic interfacial energy

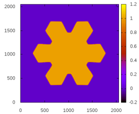
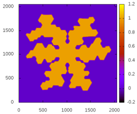
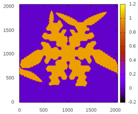
$$\begin{aligned} \mu &= g(c) \\ &- 2\kappa^{I}_{ij} c_{ij} \\ &- 12\beta^{I}_{ijkl} c_{ij} c_k c_l + 2\beta^{III}_{ijkl} c_{ijkl} \\ &- 30\alpha^{I}_{ijklmn} c_{ij} c_k c_l c_m c_n - 2\alpha^{VII}_{ijklmn} c_{ijklmn} \end{aligned} \quad (7)$$

For details: E S Nani and M P Gururajan, Philosophical Magazine Letters (2014)

Six fold anisotropy

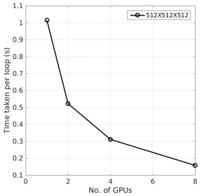
Interfacial energy anisotropy / Point effect of diffusion / FG to CG

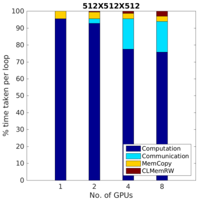




Att. kinetics anisotropy / SG to CG / Noise and Point Effect of Diff
From unpublished M Tech thesis of Mr. Abhinav Soni

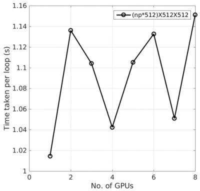
Profiling on NIVIDIA® - K40C GPUs (Ternary alloy code)

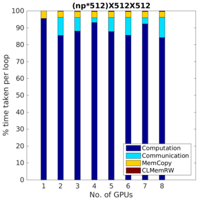
- Strong scaling





- Weak scaling





Profiling

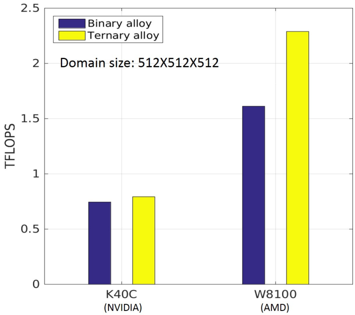


Figure: Profiling of 3D phase-field code

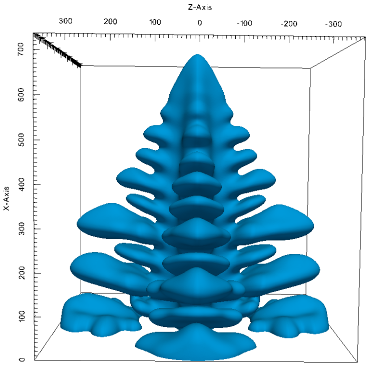
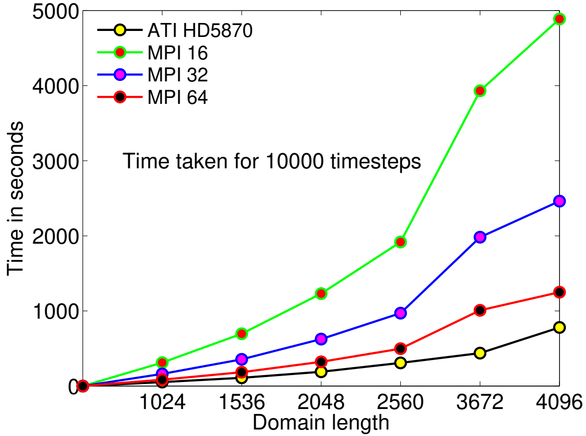


Figure: Ni - 19 Cr - 5 Nb (wt.%) alloy - 3D isothermal dendrite at $\Delta T = 8.0$ K, $\Delta t = 58.0$ ns for $\Delta x = 50.0$ nm. ($384 \times 384 \times 1024$)

Mohan and Phanikumar, Unpublished

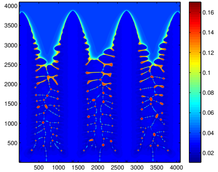
Performance

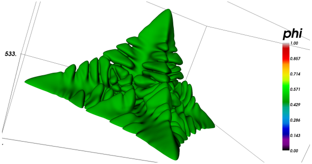


P G Tennyson, G M Karthik, and G Phanikumar, Computer Physics Communications, 2015.

Data Visualization

- Data files from each processor written at specific time intervals as unformatted .bin files
- Data files collated and converted to .mat files by Mat I/O library by Christopher Hulbert
- Visualization of data output was done in Matlab®
- MayaVi, created by Prabhu Ramachandran, was used for 3- D data visualization





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Summary

- Phase field models: highly nonlinear, stiff PDEs
- Large scale computations solving phase field models: important from an applications point of view
- There is plenty to explore: including developing standard, open source code and its parallel implementation

THANK YOU!