Application of Phase Field and CALPHAD Methods to Additive Manufacturing in IN625

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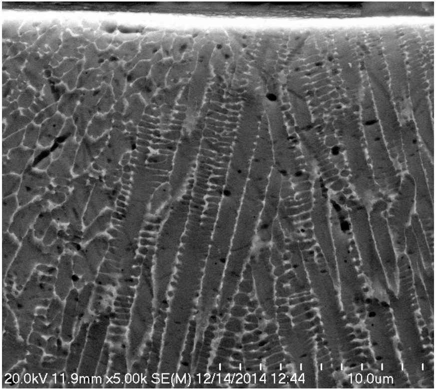
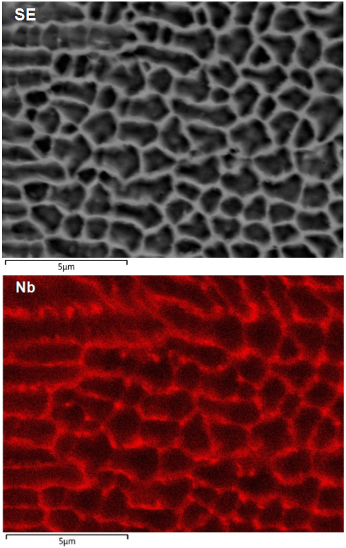
AM Inconel 625 As-Built Microstructure

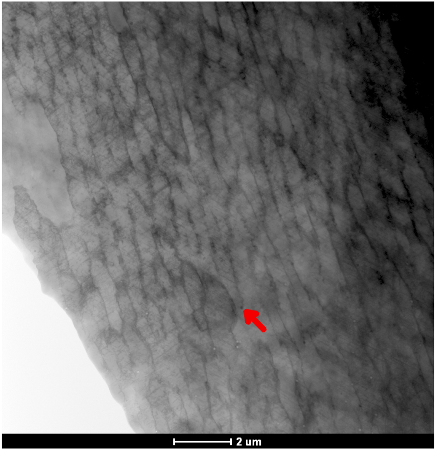


S. Cheruvathur (NIST)

Partitioning is expected.

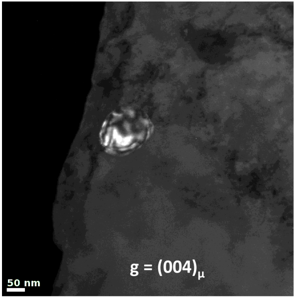


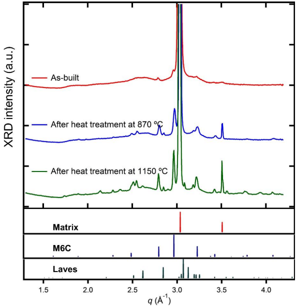
AM Inconel 625 Stress-Relieved Microstructure



Y. Idell and F. Zhang (NIST)

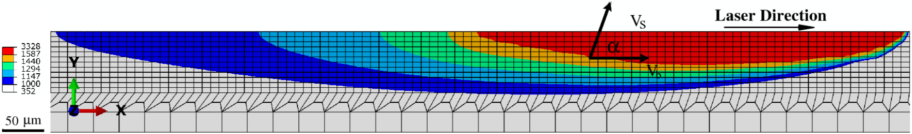
Precipitates are unwelcome.

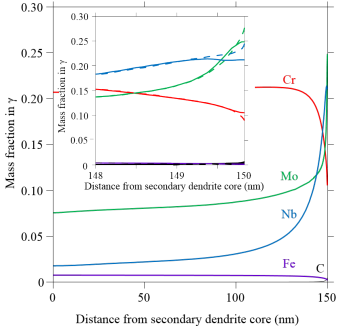


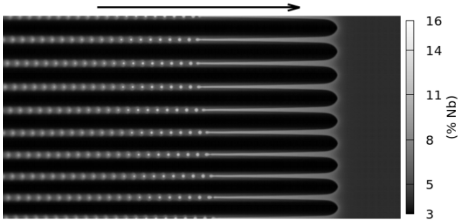


Modeling Microsegregation in AM Inconel 625

T. Keller, G. Lindwall, S. Ghosh, L. Ma, *et al.*,
"Application of Finite Element, Phase-field, and CALPHAD-based Methods to Additive Manufacturing of Ni-based Superalloys."
Acta Materialia (2017), DOI: 10.1016/j.actamat.2017.05.003.







Modeling Microsegregation in AM Inconel 625

T. Keller, G. Lindwall, S. Ghosh, L. Ma, *et al.*, "Application of Finite Element, Phase-field, and CALPHAD-based Methods to Additive Manufacturing of Ni-based Superalloys." *Acta Materialia* (2017), DOI: 10.1016/j.actamat.2017.05.003.

Thermodynamic driving force for nucleation of secondary phases from γ for the enriched (interdendritic) composition, Ni–0.13 % C–13.6 % Cr–0.35 % Fe–13.9 % Mo–23.5 % Nb, at the stress relief treatment temperature.

Interdendritic composition favors precipitation. Carbides are inevitable, but intermetallics?

1143 K	
Phase	$-\Delta G^{nuc}$
$\underline{MC}$	20.5 kJ/mol
M_2C	15.6 kJ/mol
$\underline{\mu}$	8.0 kJ/mol
M_6C	7.9 kJ/mol
BCC	6.3 kJ/mol
$\underline{\sigma}$	5.2 kJ/mol
Laves	4.1 kJ/mol
$\underline{\delta}$	3.5 kJ/mol
γ''	3.5 kJ/mol
$M_{23}C_6$	3.4 kJ/mol

Phase-field Model: Unary Solidification

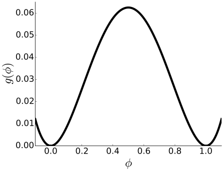
Model free energy:

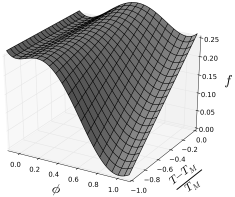
$$\mathcal{F} = \int_V \left[f_{\text{bulk}} + f_{\text{bias}} + f_{\text{grad}} \right] \mathrm{d}V$$

$$f_{\text{bulk}} = W\phi^2(1-\phi)^2$$

$$f_{\text{bias}} = L\frac{T_M - T}{T_M}p(\phi)$$

$$f_{\text{grad}} = \frac{1}{2}\epsilon^2|\nabla\phi|^2$$

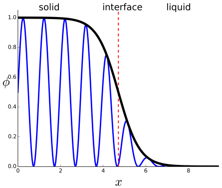




Non-conserved dynamics (Allen-Cahn):

$$\frac{\delta\mathcal{F}}{\delta\phi} = \frac{\partial f_{\text{bulk}}}{\partial\phi} - \epsilon^2\nabla^2\phi = 0$$

$$\frac{\partial\phi}{\partial t} = -M\frac{\delta\mathcal{F}}{\delta\phi}$$



Boettinger, *Ann. Rev. Mater. Res.* **32** (2002) 163.

Multicomponent Multiphase Model

Represent Inconel 625 as Cr–Nb–Ni with γ, δ, and Laves phases:

$$f_{\mathrm{bulk}} = \sum W_i \phi_i^2 (1 - |\phi_i|)^2 + \alpha \sum \sum \phi_i^2 \phi_j^2$$

$$f_{\mathrm{bias}} = n_\gamma f_\gamma(x_{\mathrm{Cr}}^\gamma, x_{\mathrm{Nb}}^\gamma) + n_\delta f_\delta(x_{\mathrm{Cr}}^\delta, x_{\mathrm{Nb}}^\delta) + n_{\mathrm{L}} f_{\mathrm{L}}(x_{\mathrm{Cr}}^{\mathrm{L}}, x_{\mathrm{Nb}}^{\mathrm{L}})$$

$$f_{\mathrm{grad}} = \sum \kappa_i (\nabla \phi_i)^2$$

$$i \in \delta, \mathrm{Laves}$$

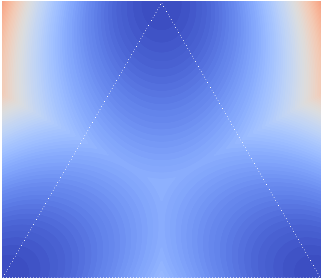
$$\frac{\partial x_j}{\partial t} = V_m^2 M_j \nabla^2 \left[\frac{\partial f_\gamma(x_{\mathrm{Cr}}^\gamma, x_{\mathrm{Nb}}^\gamma)}{\partial x_j^\gamma} \right]$$

$$j \in \mathrm{Cr}, \mathrm{Nb}$$

$$\frac{\partial \phi_i}{\partial t} = -M_i \left(\frac{\partial f_{\mathrm{bulk}}}{\partial \phi_i} - 2\kappa \nabla^2 \phi_i \right)$$

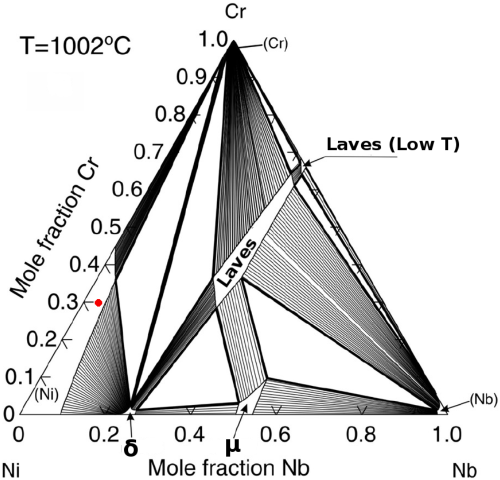
After Zhou *et al.*, *Acta Mater.* **65** (2014) 270.

$f_{\mathrm{bulk}}(\phi_1, \phi_2, 1 - \phi_1 - \phi_2)$



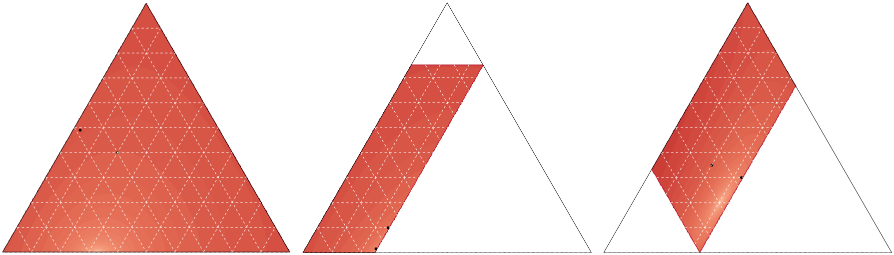
https://github.com/tkphd/multiphase-interface-planarization

Ternary Analogue to Inconel 625: Cr–Nb–Ni



Du *et al.* *Calphad* **29** (2005) 140–148.

CALPHAD Free Energy Domain Restrictions

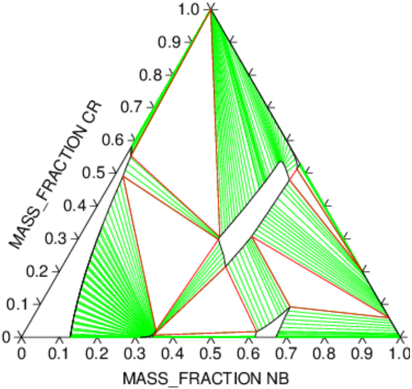


γ landscape | δ landscape | Laves landscape

Physically reasonable, but numerically unforgiving.

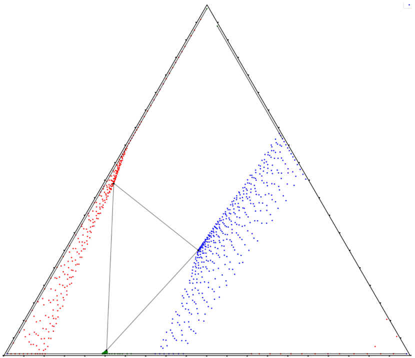
Cr–Nb–Ni Phase Diagrams

γ-δ-μ-Laves



Sublattices:
Physically reasonable

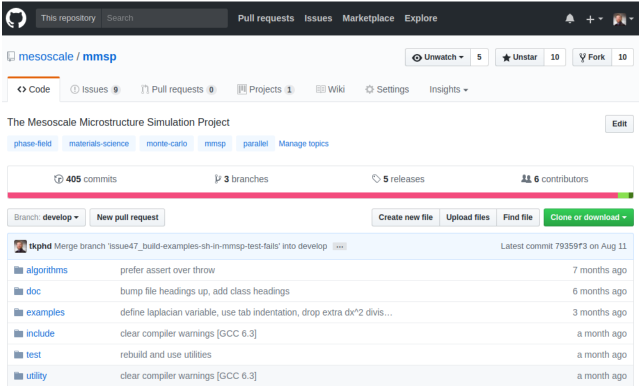
γ-δ-Laves



Paraboloids:
Numerically forgiving

Simulation Software

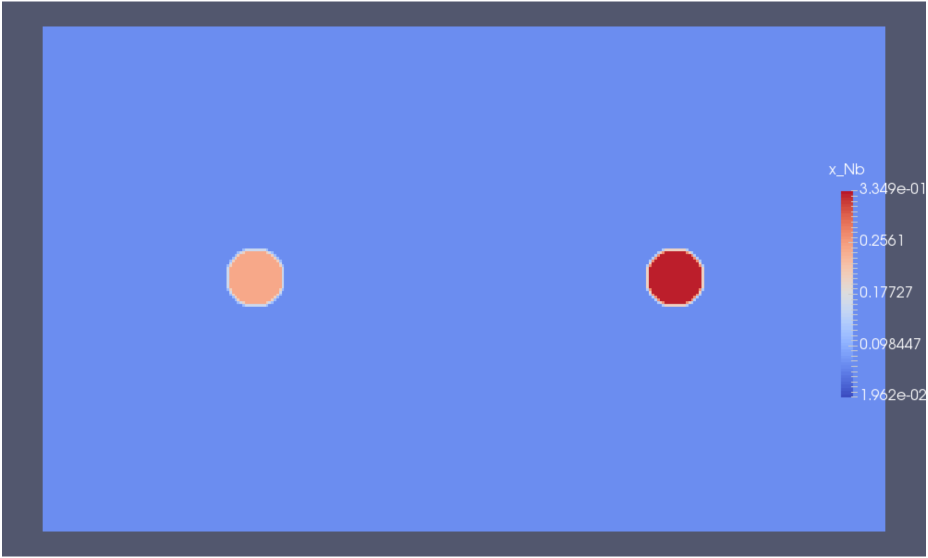
MMSP



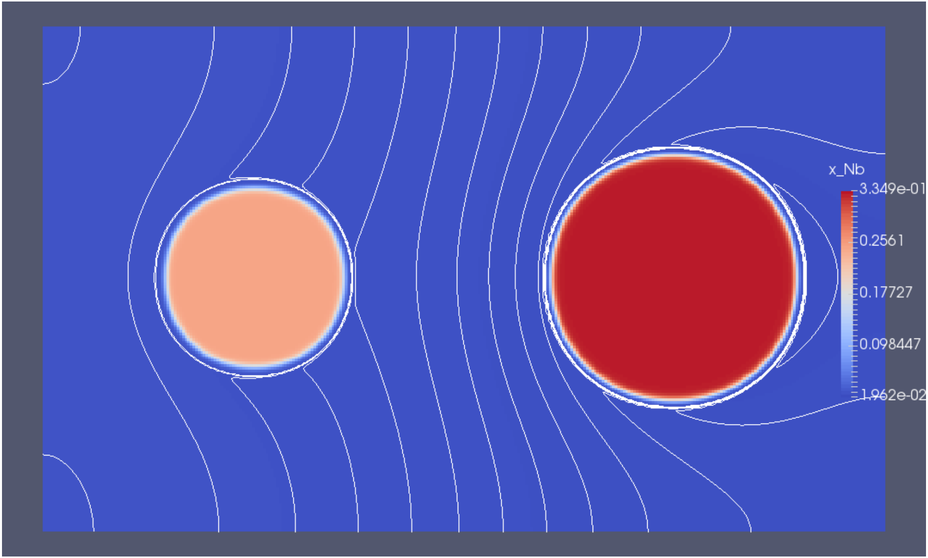
`github.com/mesoscale/mmsp`

- parallel grid (MPI)
- C++, templated by type & dimension
- user supplies kernel code
- 20+ examples: phase-field & Monte Carlo, finite difference

2D Simulation: Nb composition, no-flux boundaries

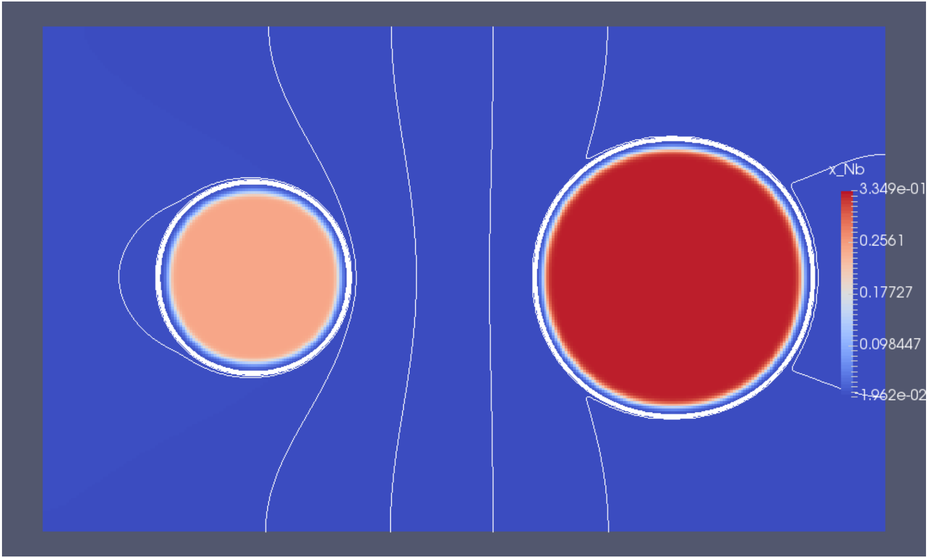


2D Simulation: Nb composition, no-flux boundaries



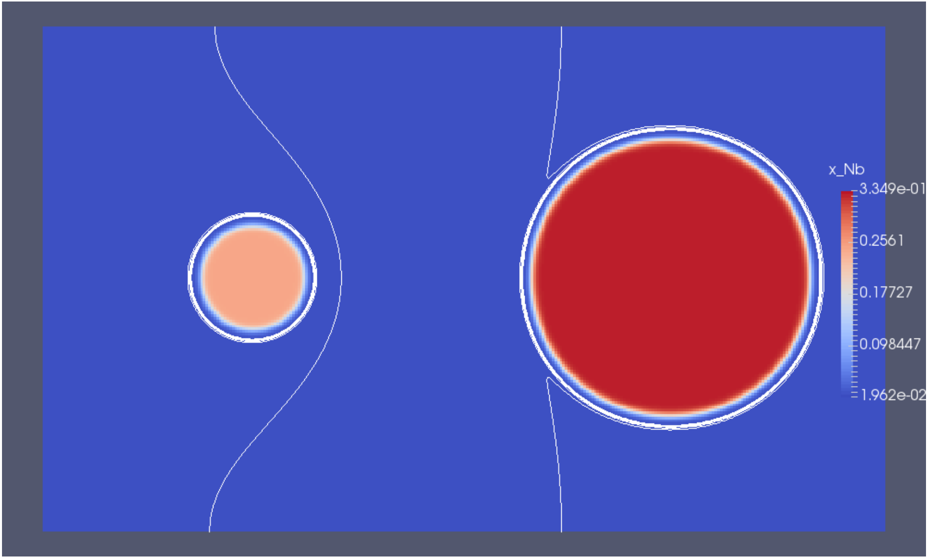
Early: flux from γ toward particles

2D Simulation: Nb composition, no-flux boundaries



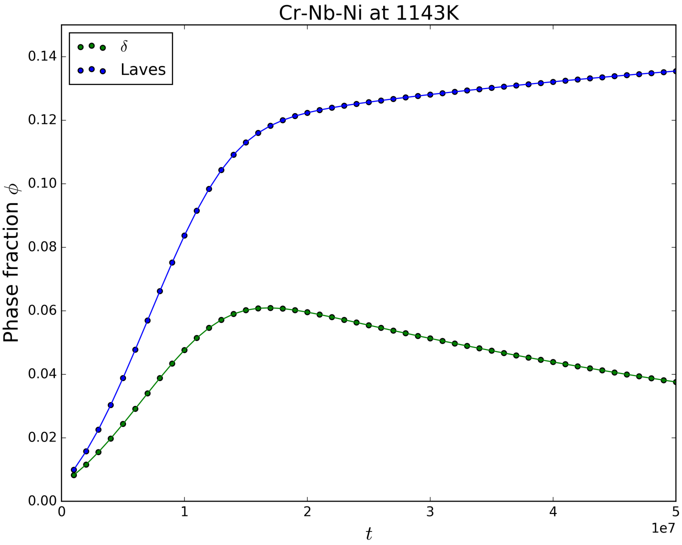
Middle: flux from γ and δ toward Laves

2D Simulation: Nb composition, no-flux boundaries



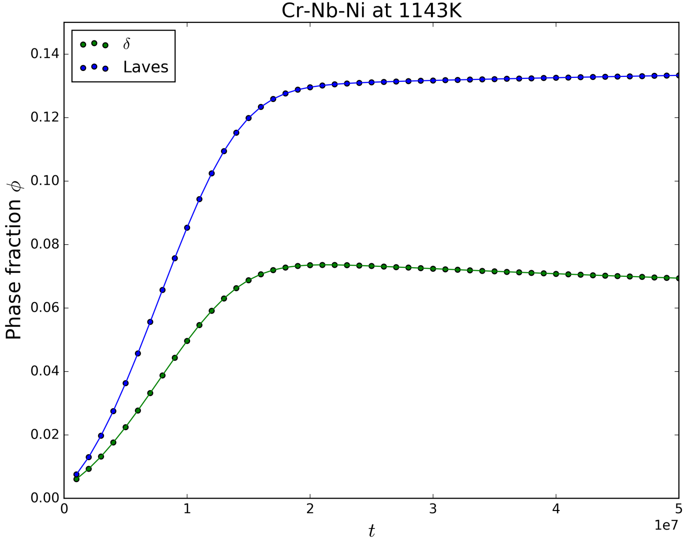
Late: flux from δ toward Laves

2D Simulation: Nb composition, no-flux boundaries



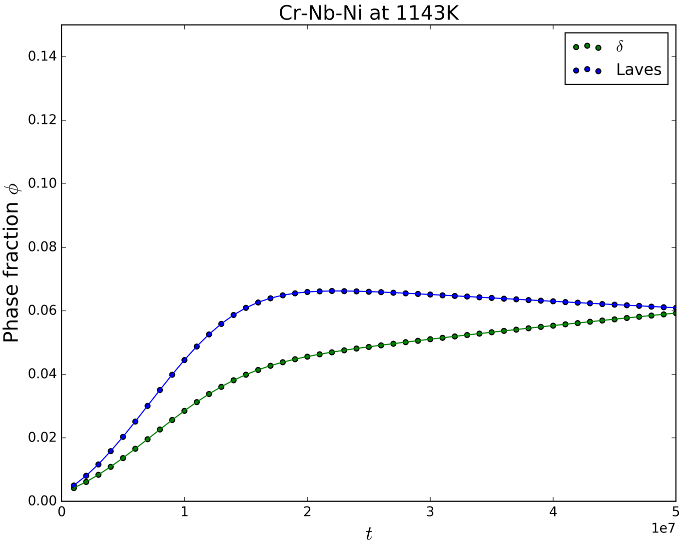
Laves consuming δ

2D Simulation: Nb composition, no-flux boundaries



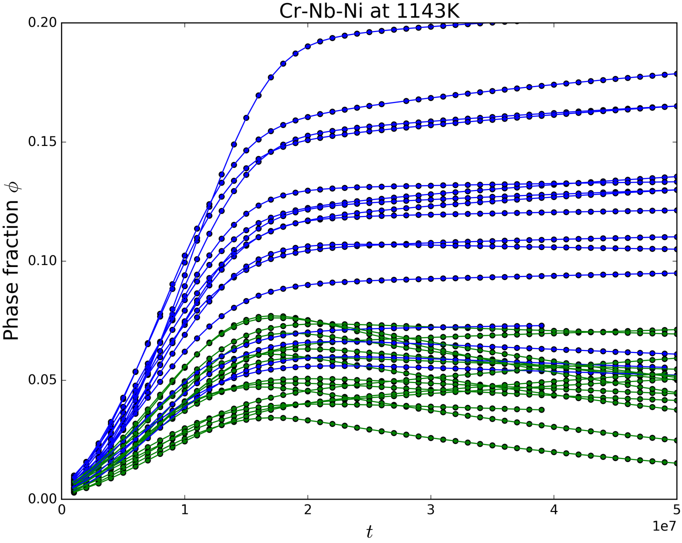
Laves coexists with δ

2D Simulation: Nb composition, no-flux boundaries



δ consuming Laves

2D Evolution Trajectories



Small sample of ternary coexistence field, small domains

Hardware and Software Changes

HiPerC

Navigation

Contents:

High Performance Computing Strategies for Boundary Value Problems

Ever wonder if a GPU or Xeon Phi accelerator card would make your code faster? Fast enough to justify the expense to your manager, adviser, or funding agency? This project can help answer your questions!

docs passing chat on gitter

The example codes in this repository implement the same basic algorithm using whichever of the mainstream accelerator programming methods apply. Running the code on different parallel hardware configurations — CPU threading, GPU offloading, and CPU coprocessing — provides a benchmark of these tools using common computational materials science workloads.

`hiperc.readthedocs.io`

Goals

- Explore
- Compare
- Share

CPU

- Serial
- OpenMP
- TBB

GPU

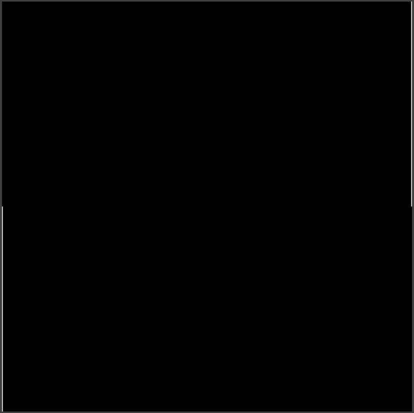
- CUDA
- OpenACC
- OpenCL

KNL

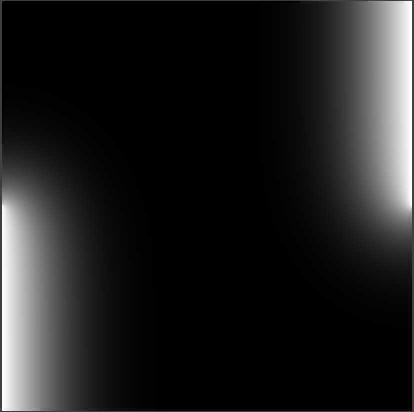
Hybrid

HiPerC Diffusion: Carburizing Process

$t = 0$



$t = 100000\Delta t$

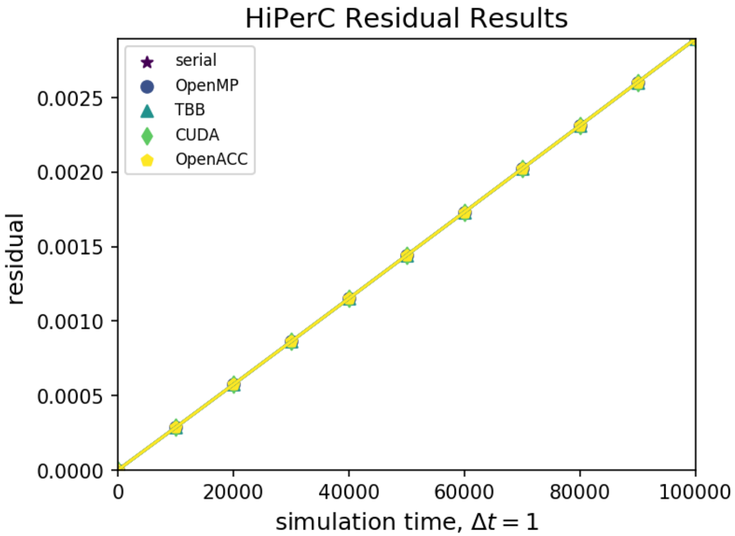


$$D = 6.25 \times 10^{-3}$$
$$\Delta x = 0.5$$
$$\Delta t = 1$$

$$c(x,t) \approx \text{erfc}\left(\frac{\vec{r}_L}{\sqrt{4Dt}}\right) + \text{erfc}\left(\frac{\vec{r}_R}{\sqrt{4Dt}}\right)$$

hiperc.readthedocs.io

Preliminary HiPerC Diffusion Results



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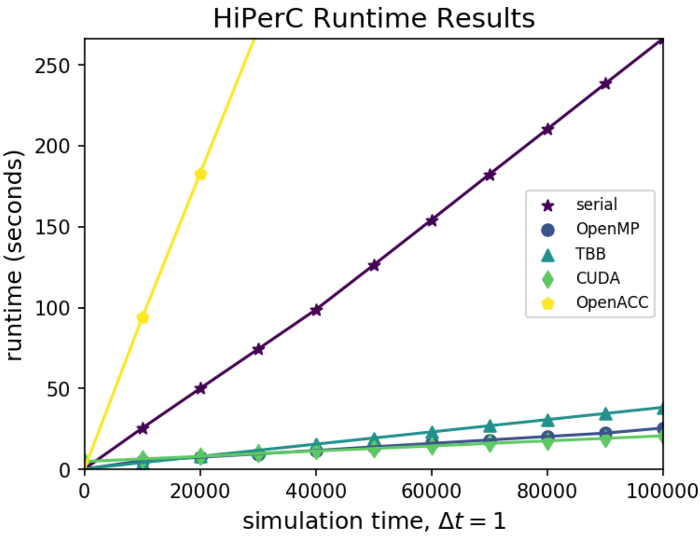
Preliminary HiPerC Diffusion Results



hiperc.readthedocs.io

Benchmarks Codes

CHiMaD Phase Field

Integrating the phase field community

In January 2015 a group of phase field theorists and code developers met at Northwestern University to discuss ways for the community to improve code collaboration efforts. Everyone agreed that the community needs to become more open and work in a more collaborative manner.

A key factor to improving community code collaboration is to develop resources to compare and contrast phase field codes and libraries. This site aims to provide some of these resources and become a useful web service for phase field practitioners.

`pages.nist.gov/chimad-phase-field`

Benchmarks:

- Spinodal decomposition
- Ostwald ripening
- Dendritic growth
- Precipitation & elasticity
- Stokes flow
- Cahn-Hilliard with electrostatics

Thank You For Your Attention

Conclusions & Future Work:

- Phase-field modeling shows competition between δ and Laves particles in a ternary analogue to Inconel 625
- Further analysis needed to distinguish ripening from reversion (interfacial vs. bulk thermodynamics), finite size effects
- Extension to larger systems with more accurate free energy requires changes to
  - Model formulation: Kim-Kim-Suzuki $\rightarrow$ grand potential
  - Computer architecture: CPU $\rightarrow$ GPU
  - Sublattice description or ternary system

Refactoring code for new architectures is worthwhile.
It can also be easy. Contact me if you're curious:
`trevor.keller@nist.gov`