CANFSA

Center for Advanced Non-Ferrous Structural Alloys
An Industry/University Cooperative Research Center

# Project 36E-L: In-Situ Characterization of Microstructural Evolution During Simulated Additive Manufacturing in Model Alloys

## Semi-annual Spring Meeting

## April 2022


- Student: Brian Rodgers (Mines)
- Faculty: Amy Clarke (Mines)
- Industrial Mentors: Joe McKeown (LLNL), Saryu Fensin (LANL), Edwin Schwalbach (AFRL), Neil Carlson (LANL)
- Other Participants: Joe McKeown (LLNL), Alain Karma (Northeastern Univ.)


LRGF Laboratory Residency Graduate Fellowship

Office of Naval Research Science & Technology

U.S. Department of Energy | Office of Science

Colorado School of Mines

NSF

Iowa State University

# Project 36E-L: In-Situ Characterization of Microstructural Evolution During Simulated Additive Manufacturing in Model Alloys

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- Student: Brian Rodgers (Mines)
- Advisor(s): Amy Clarke (Mines)

**Project Duration**
PhD: September 2019 to Dec 2023

- Problem: Aerospace components are difficult to produce conventionally, but the effects of additive manufacturing (AM) on microstructural evolution are not understood enough to replace conventional manufacturing.
- Objective: Develop an understanding of solidification behavior in model alloys under AM conditions by *in-situ* characterization.
- Benefit: Microstructural control for additive manufacturing of aerospace components.

Recent Progress

- Completed residency at LANL for LRGF program
- TEM of Al-Ag DTEM samples

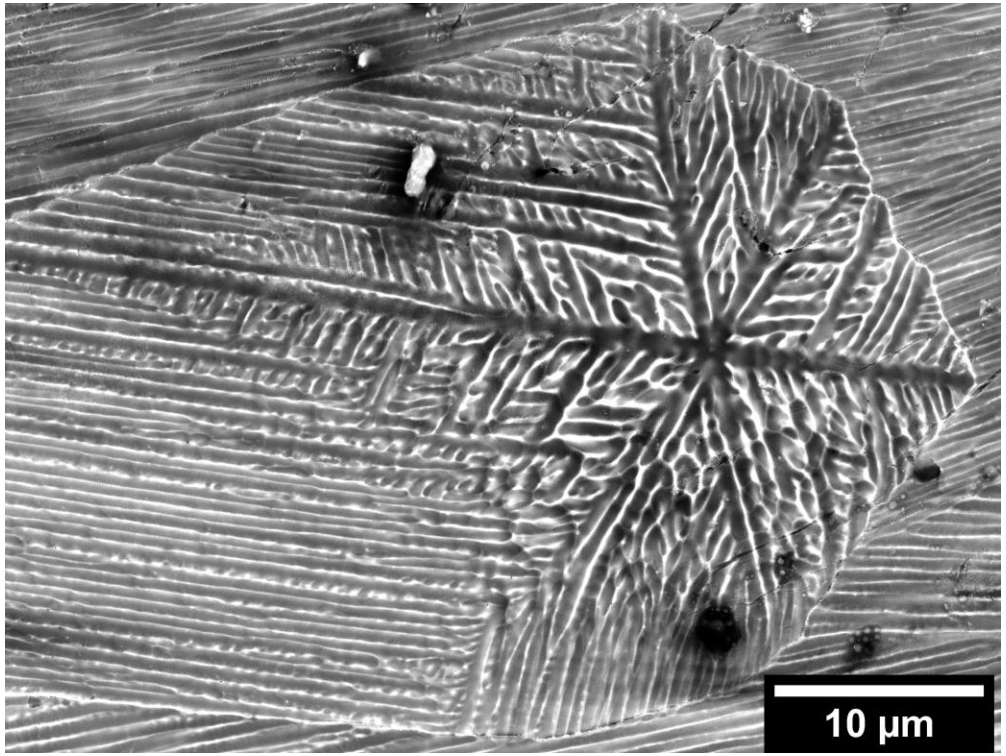
| Metrics | | |
|---|---|---|
| **Description** | **% Complete** | **Status** |
| 1. Literature review | 70% | ● |
| 2. Analysis of APS beam line data | 95% | ● |
| 3. Analysis of Dynamic Transmission Electron Microscopy (DTEM) of rapid solidification | 75% | ● |
| 4. Simulation of experimental conditions | 60% | ● |
| 5. Complementary *ex-situ* characterization | 70% | ● |

# Project overview

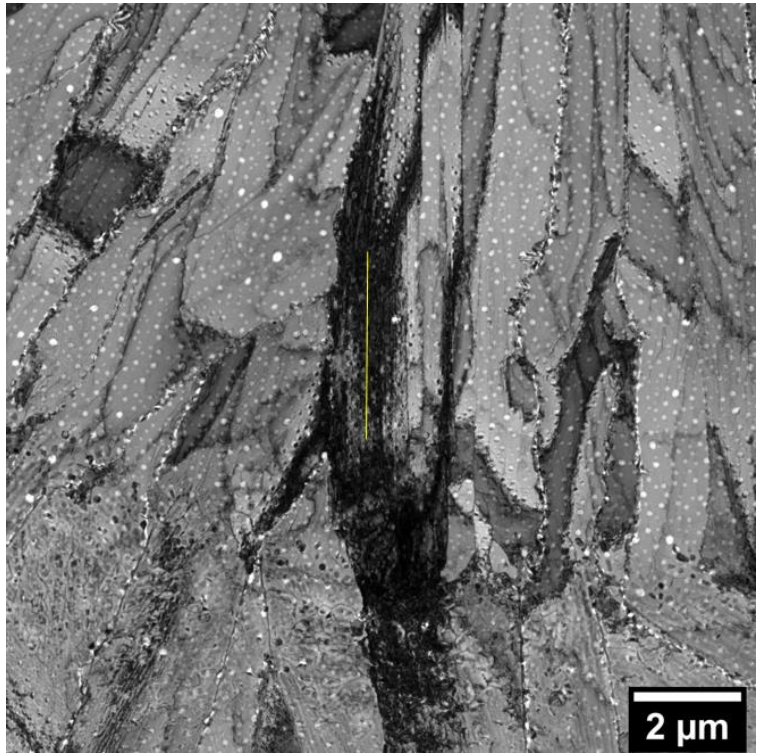
- Basic energy sciences funding to visualize microstructure development during rapid solidification
- Desire to predict microstructures formed during additive manufacturing
- Funding also provided by LRGF program, which requires two residencies

# Dendrite orientation transition (DOT)

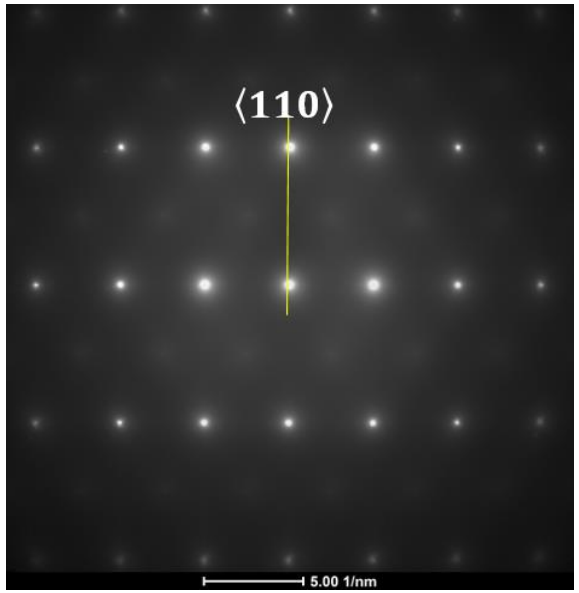
- Phenomena where preferred growth orientation changes with alloy composition
- Attributed to changes in anisotropy of solid-liquid interfacial energy
- Fundamental reasons for interfacial energy change not well understood yet




SEM backscatter



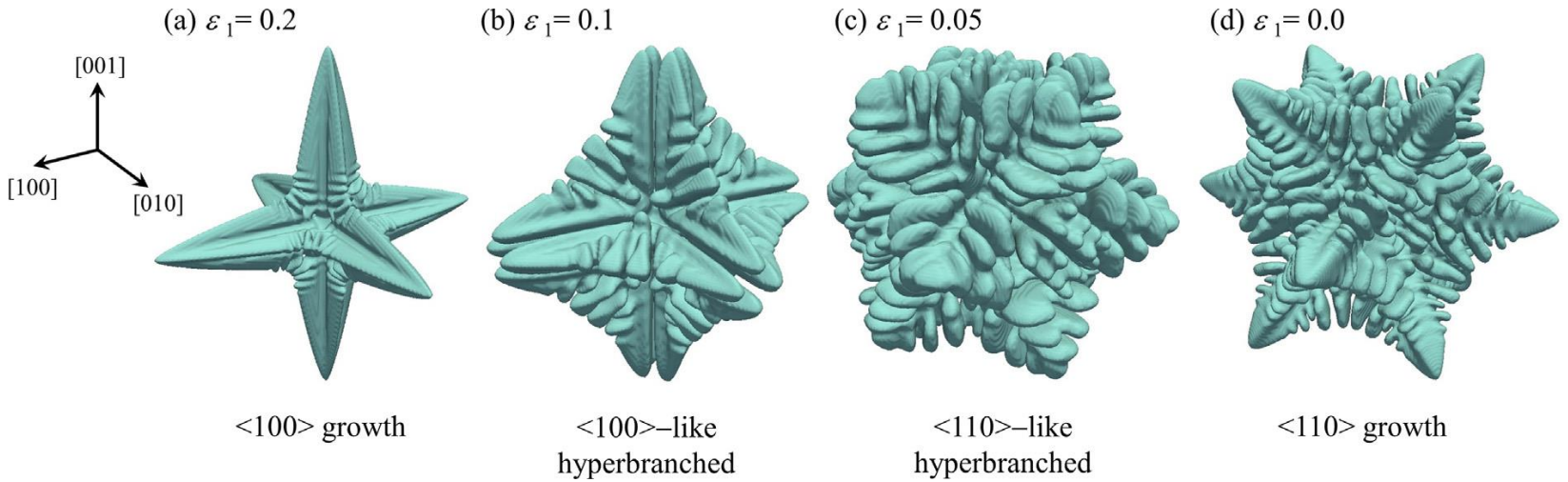

Down zone bright field




211 zone axis SADP

# Predicting DOT

- Desire to predict microstructure with phase field
- Requires knowing the values for the interfacial energy profile
- Extremely difficult to find experimentally, modeling is required




"A parametric study of morphology selection in equiaxed dendritic solidification", G. Kim, T. Takaki, Y. Shibuta, K. Matsuura, M. Ohno, *Comp. Mat. Sci.,* 2019

# Molecular Dynamics (MD) fundamentals

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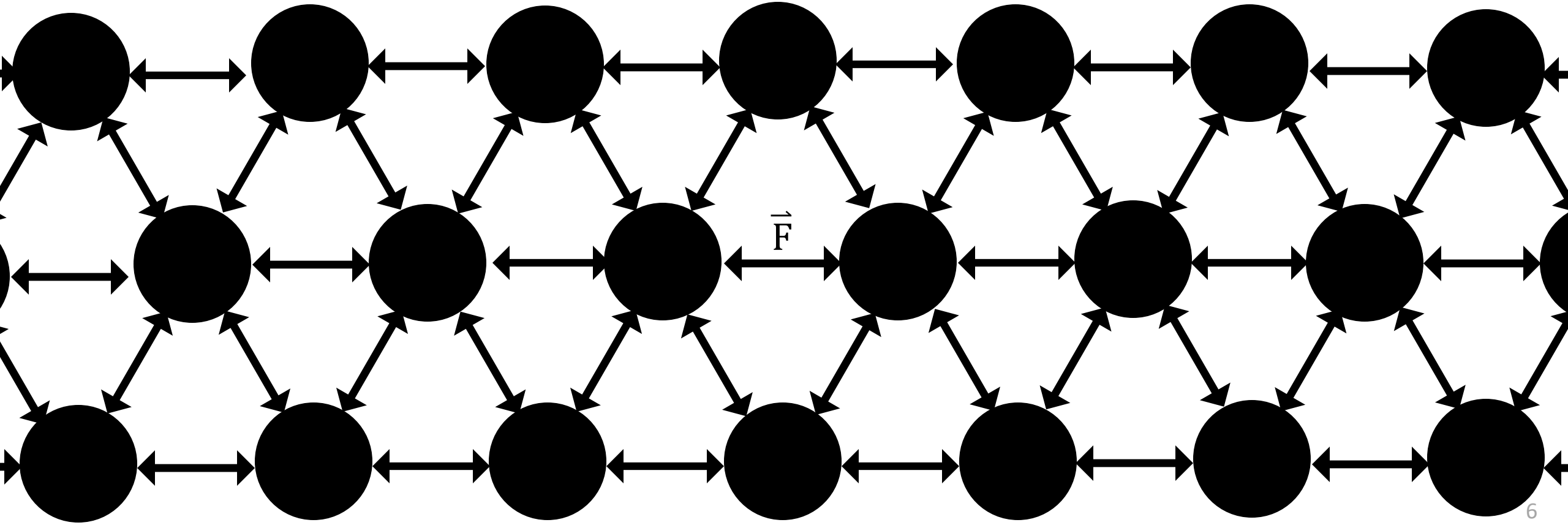
- Simulations handling ten of thousands to millions of individual atoms/molecules
- Not an atomistic method, quantum effects and electronic structure ignored
- Interaction between atoms approximated using potentials



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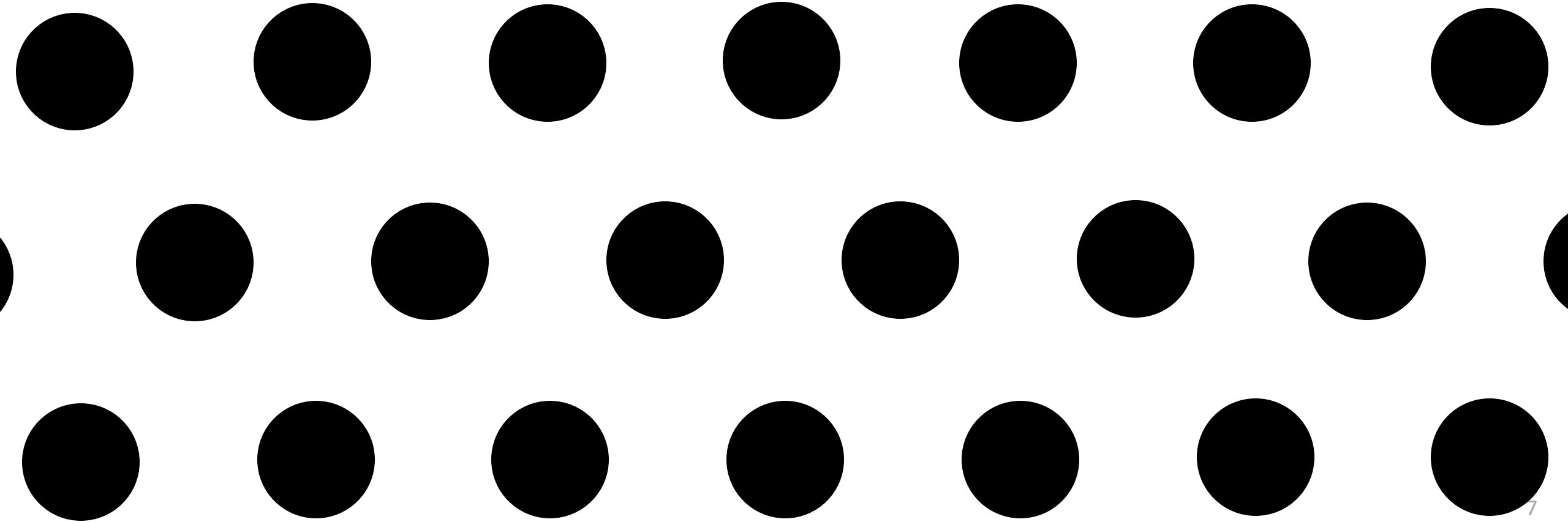
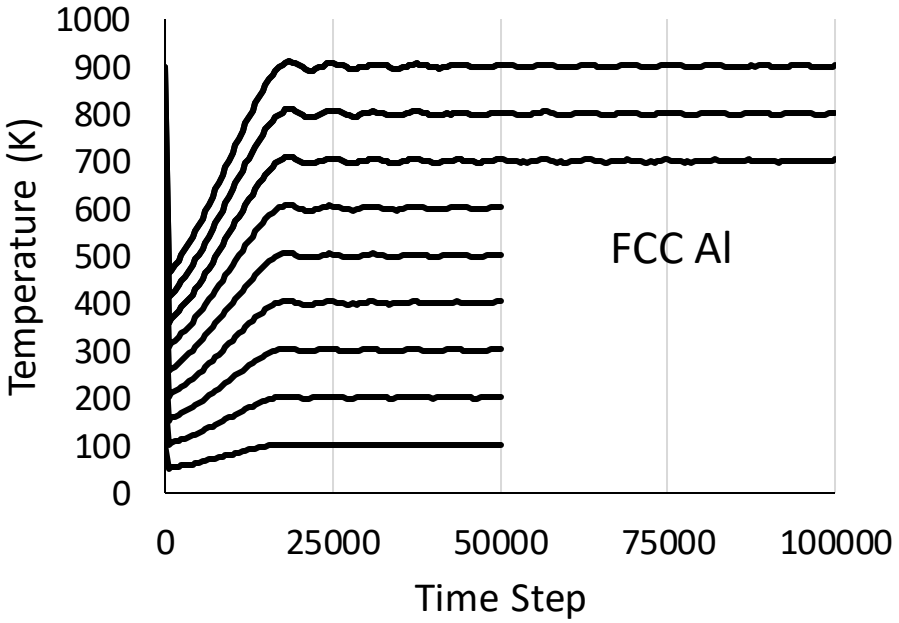
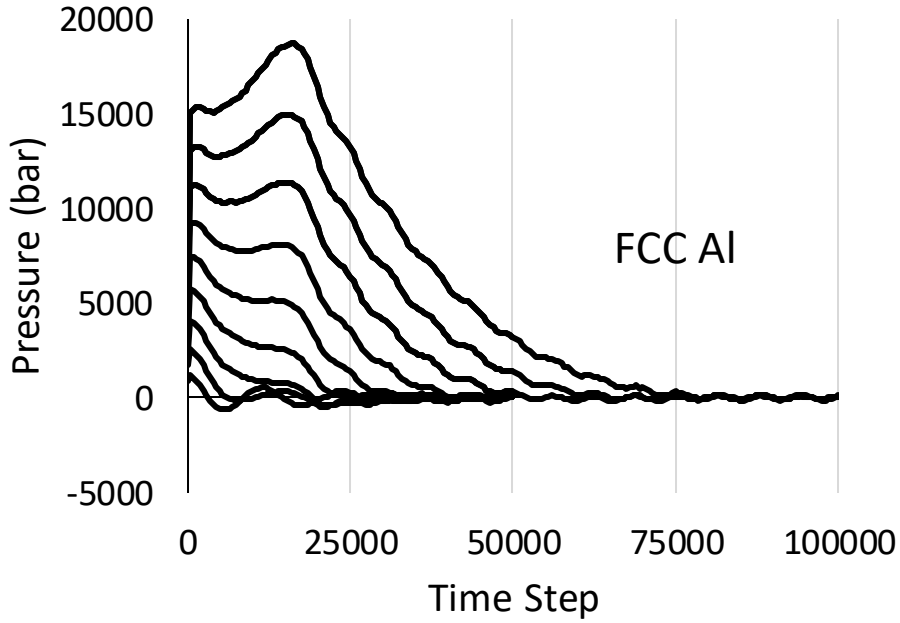


# Dynamic simulations

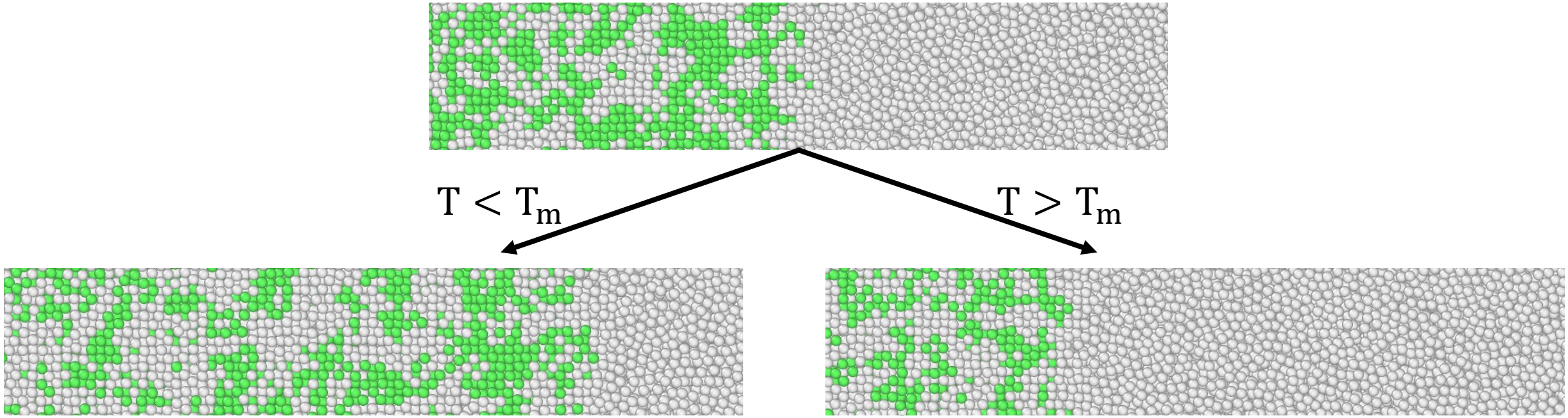
- Atoms are allowed to move
- Necessary for all simulations not taking place at absolute zero
- More computationally expensive
- Simulation needs time to equilibrate



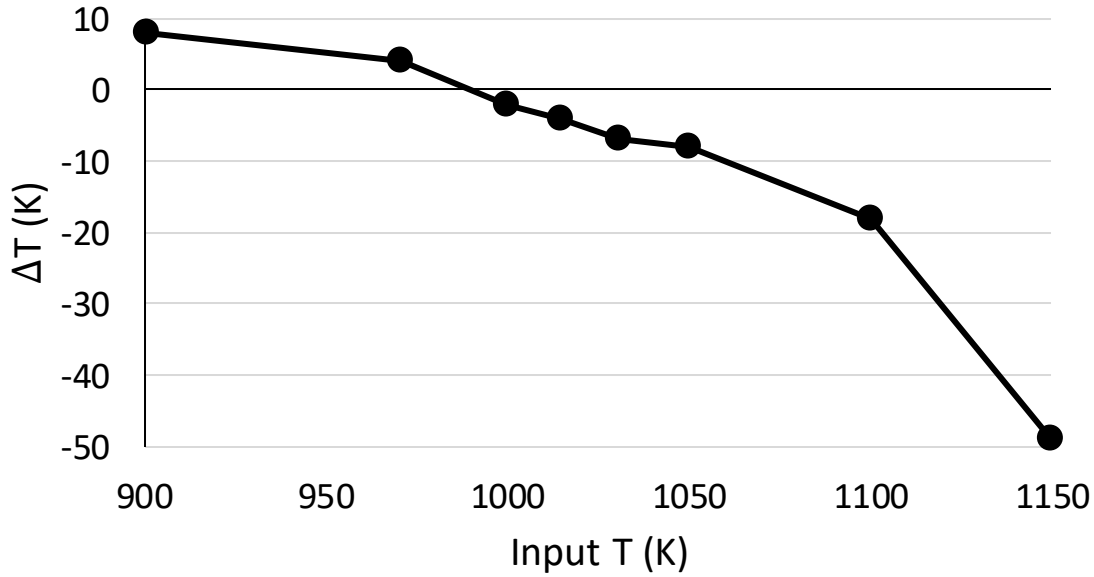
# Calculating melting point

- Multiple methods exist, two phase coexistence technique chosen
- Solid and liquid in contact equilibrated to some fixed temperature
- System then held under constant enthalpy
- Interface movement and temperature change serve as signals



# Iterative nature of melting point calculation

- An individual melting point simulation does not give the melting temperature
- Series of simulations required for guesses to converge on the actual value
- Can analyze as a response surface with y intercept being the melting point
- Determining the entire response surface is inefficient
- Want a method that produces low error bars with minimal iterations

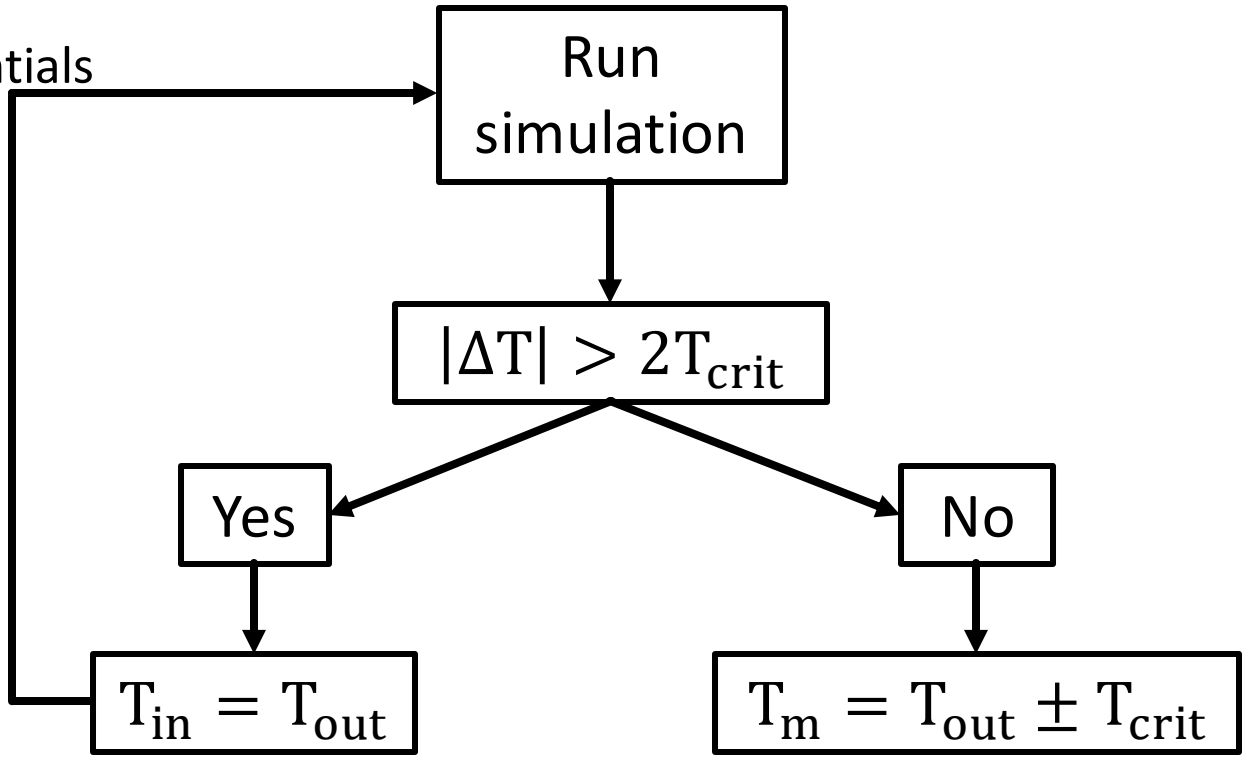


# LAVA

- Named after **LA**MMPS and **VA**SP
- Python based software made at LANL to semi-automate MD and atomistic simulations
- LAVA can do each of the simulation types shown thus far (and more!)
- Tested and validated each of those simulation types

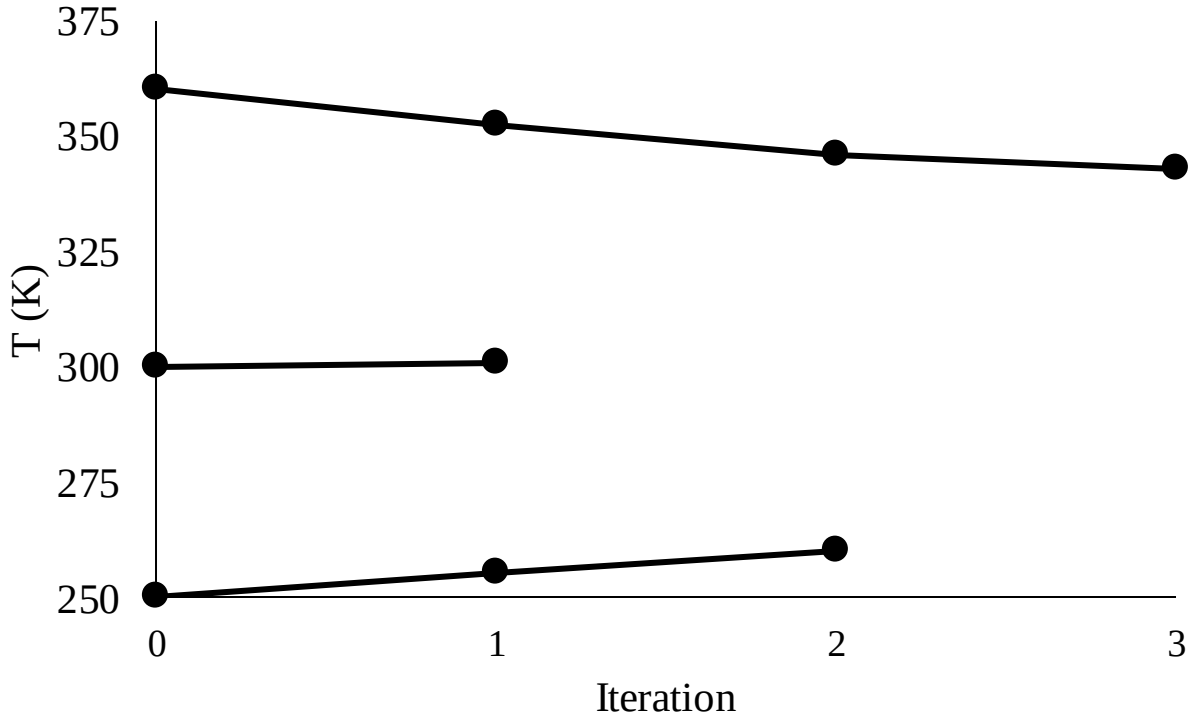
# LAVA melting point calculation

- Converge to melting point with a relative change based method
- Can be fast, but faces three issues
  - Error bars are not necessarily true
  - Failure to converge for some potentials
  - Noise affects convergence rate



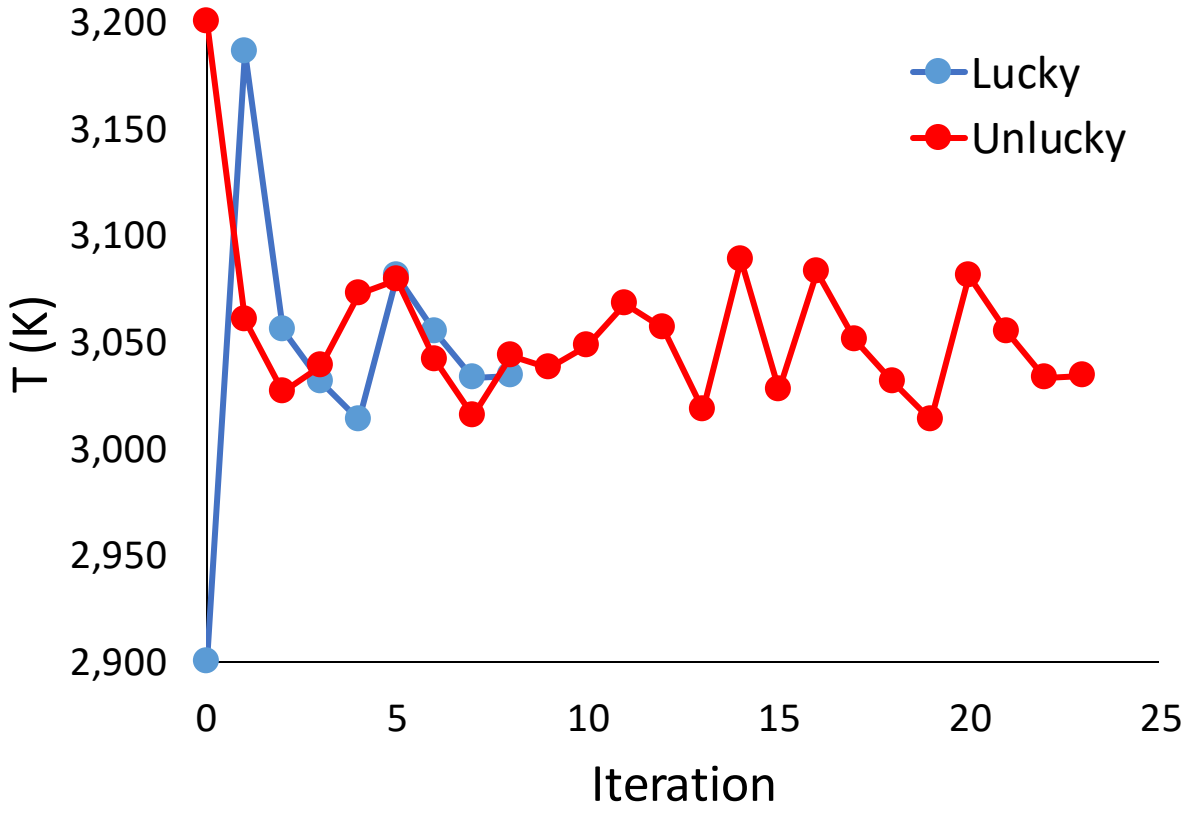
# Failure to converge

- Method relies on magnitude of changes
- Assumes size of change is always proportional to distance from melting point
- Some potentials have small changes between input and output temperature



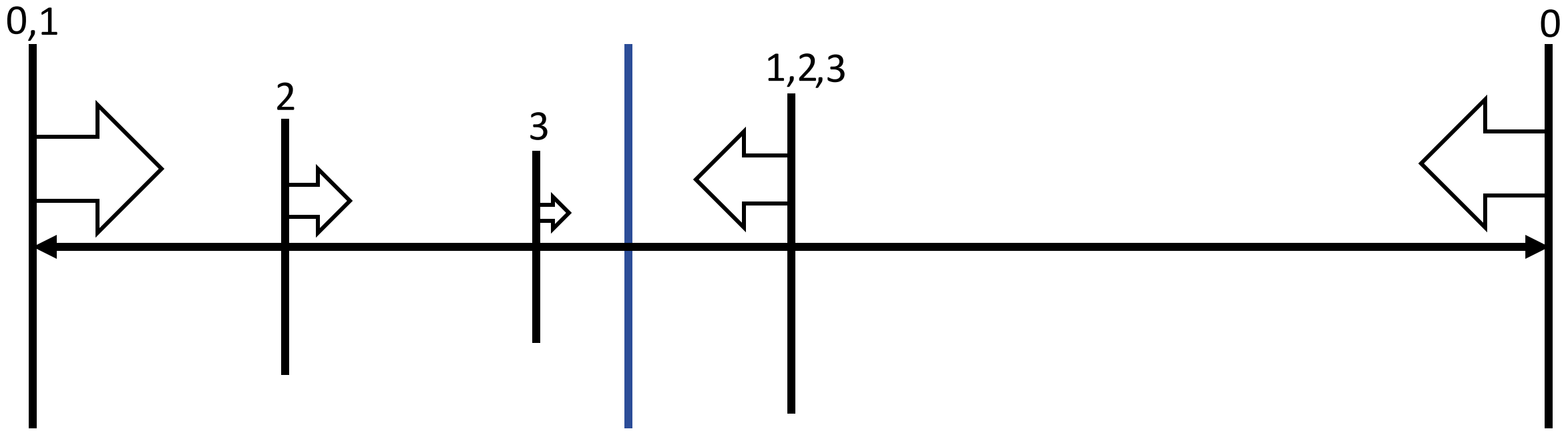
# Noise effect on convergence

- Thermal noise will always exist in MD simulations
- Magnitude of noise is inversely proportional to number of atoms
- Adding more atoms than needed to reduce noise is an expensive solution



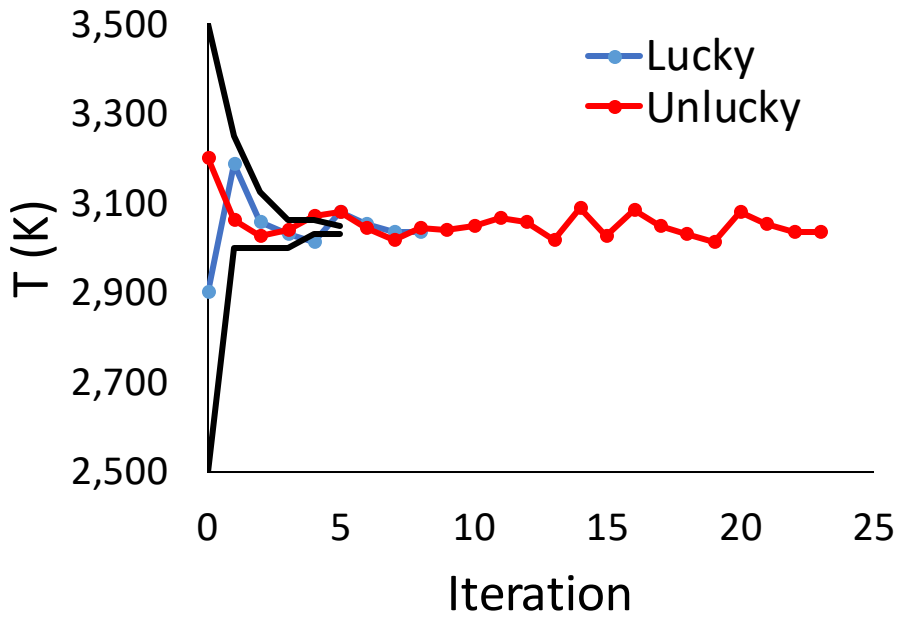
# Implementing bisection method

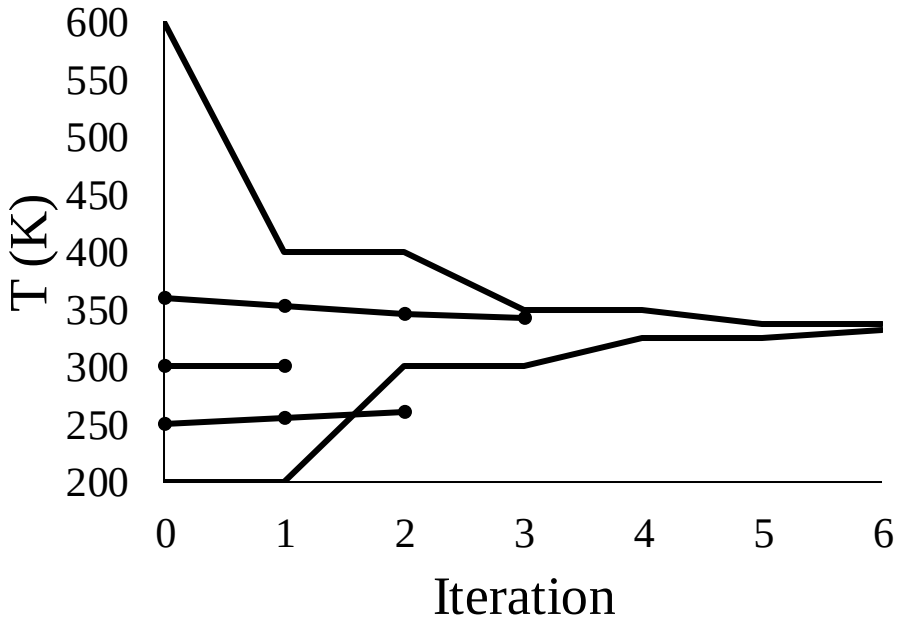
- Bisection method only depends on the sign of changes
- Number iterations controlled by starting interval and desired tolerance, and is consistent



# Improvement with bisection method

- Both cases with convergence issues function now
- Averaging out final ten temperature values to reduce noise effects as well

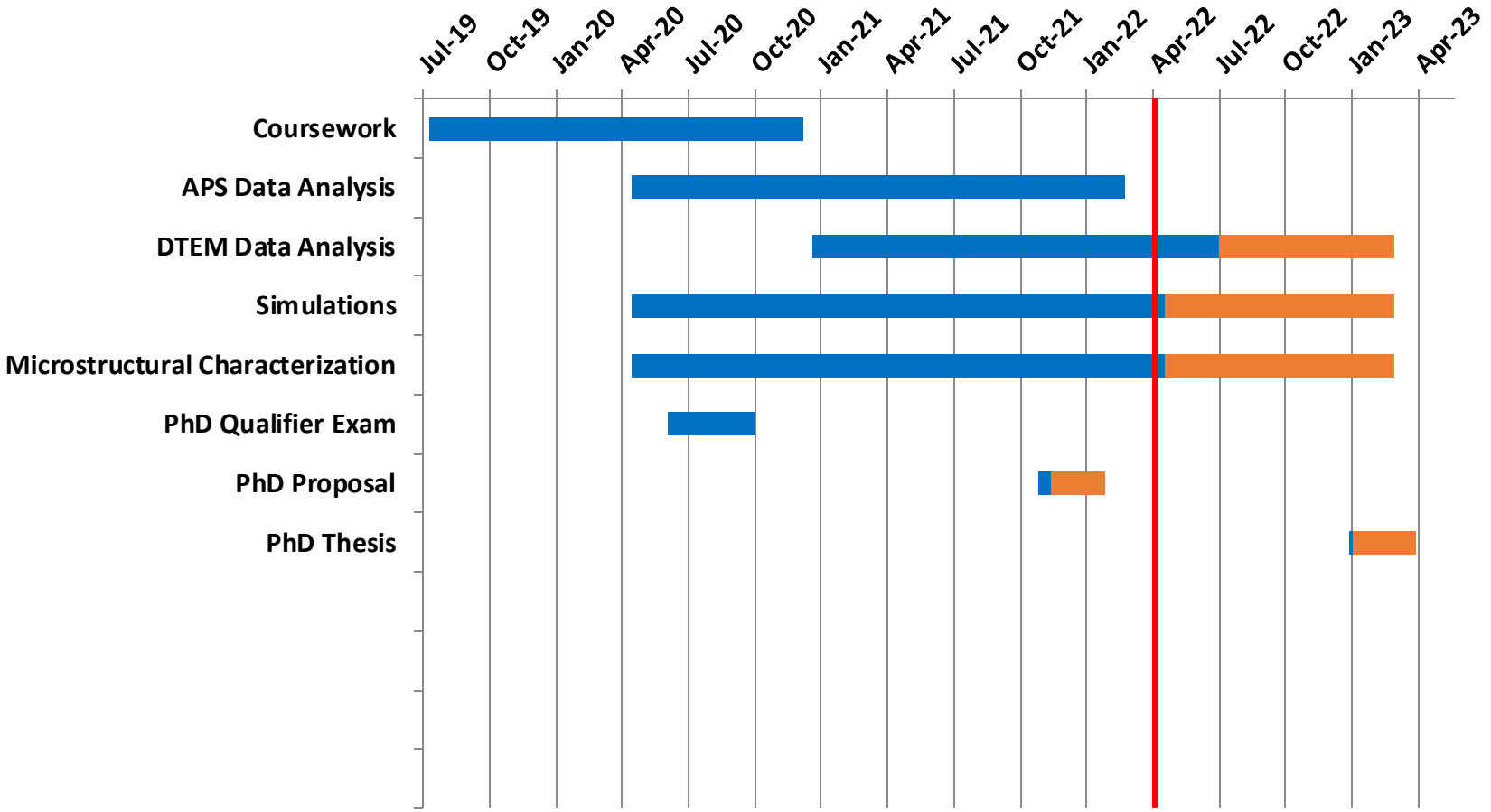


# Lava benefits to potential development

- Method to develop MD potentials with machine learning exists at LANL
- Can create the potential needed for the Al-Ag system
- Needs testing for training and validation, LAVA can help

# Gantt Chart



# Challenges & Opportunities

- Generate MD potential needed
- Predict DOT through interfacial energy anisotropy with phase field
- Further TEM analysis
- High quality publications

Thank you!

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