Predicting Melt Properties using Atomistic Simulations with Highly Accurate Physically Informed Neural Network Interatomic Potential

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Outline

- The role of atomistic simulations in additive manufacturing
- Why machine learning in atomistic simulations
- Artificial Neural Networks (ANNs) in atomistic simulations
- Physically Informed Neural Network (PINN) potential
- Example for Aluminum
- Conclusions

Atomistic Simulations in Additive Manufacturing (AM)

Application of atomistic simulations in AM:

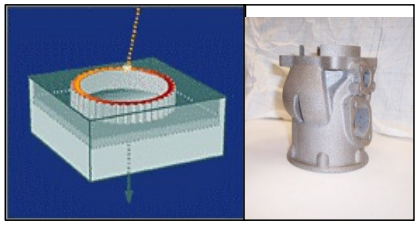
- Provide first-principles physics-based information on the highly dynamic AM processing
- Complementing other simulation methods at meso-scale by:
  - Providing knowledge of microscopic mechanisms of key processes
  - Obtaining material parameters that cannot be readily measured by experiment

Objectives:

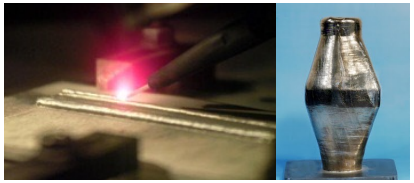
- Develop process parameter / microstructure relationships to guide process optimization
- Develop thermodynamics relationships to understand microstructure evolution
- Develop microstructure / behavior relationships to guide design

Benefits:

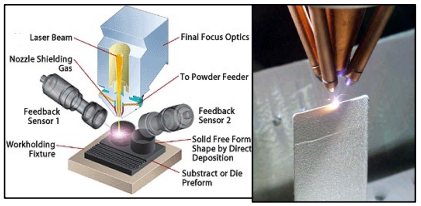
- Provide guidance to predict and tailor the high degree of variability in the microstructure of AM processing



Laser Sintering/E-beam Melting



Electron Beam Freeform Fabrication

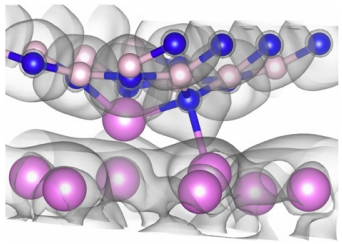


Laser Engineered Net Shaping

Why Neural Networks in Atomistic Simulations

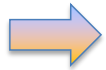
Atomic interactions governed by Quantum Mechanics (QM) are very complex and difficult to calculate:
cpu time $\sim N^{3-8}$

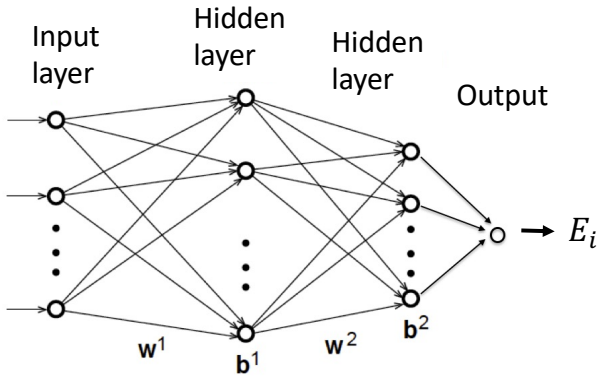
Replace QM calculations with an ANN



$$\hat{H}|\psi(t)\rangle = i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle$$

- CPU time ~N^{3-8} (for N atoms)
- System size, N ~10^2-10^3
- Accuracy: ~1 meV





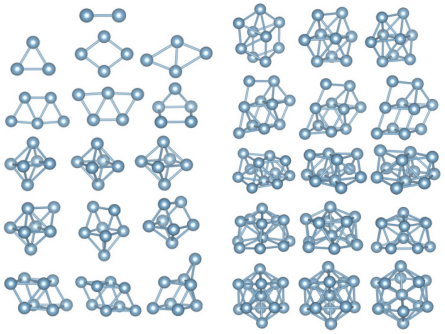
- CPU time ~N atoms
- System size, N ~10^4-10^6
- Accuracy: ~1 meV

Gain speed without losing accuracy

Neural Network Interatomic Potential

Training Stage

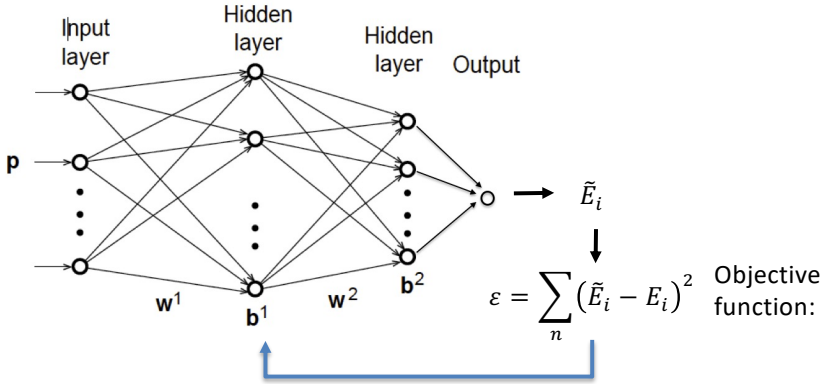
Use QM to calculate a large set of atomic structures



$$\begin{pmatrix} E_1 \\ E_2 \\ \vdots \\ E_n \end{pmatrix}$$

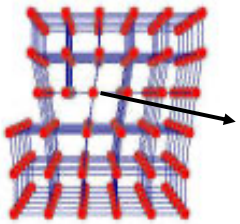
$$\hat{H}|\psi(t)\rangle = i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle$$

Train ANN against $\{w^1, b^1, w^2, b^2, \dots\}$ to minimize the objective function, ε



Inference Stage

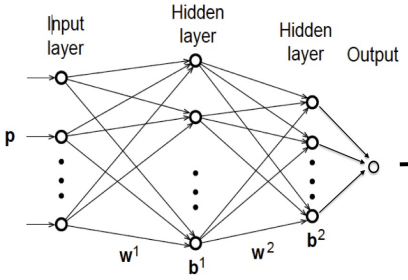
Use the trained ANN on the material of interest



Material

$$\begin{pmatrix} G_1 \\ G_2 \\ \vdots \\ G_n \end{pmatrix}$$

Structure parameters



Trained ANN

E_i

Atomic potential energy

$$U = \sum_i E_i$$

Total pot. energy

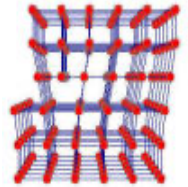
$$f_{x_i} = -\sum_{j \neq i} \frac{\partial U(x_{ij}, y_{ij}, \dots)}{\partial x_{ij}}$$

Atomic force

Physically Informed Neural Networks

ANN potential

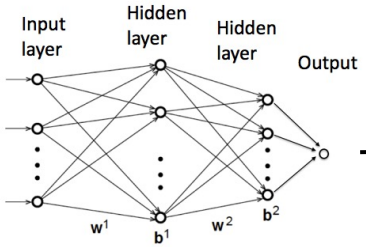
ANN gives atomic energy directly



Material

$$\begin{pmatrix} G_1 \\ G_2 \\ \vdots \\ G_n \end{pmatrix}$$

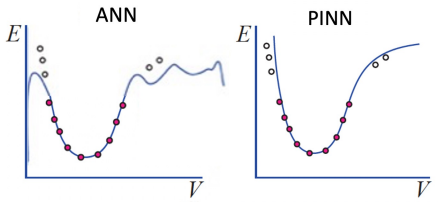
Structure coefficients



Trained ANN

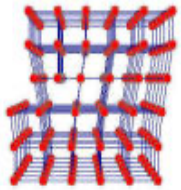
E_i

Atomic potential energy



Physically Informed NN potential (PINN): a symbiosis between ANN and functional potential*

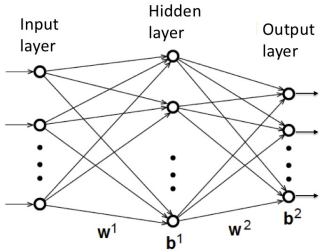
PINN gives customized potential parameters for each atom



Material

$$\begin{pmatrix} G_1 \\ G_2 \\ \vdots \\ G_n \end{pmatrix}$$

Structure coefficients



Contains the "knowledge" of the QM calculations

$$\begin{pmatrix} A_i \\ \alpha_{ij} \\ B_i \\ \beta_{ij} \\ \vdots \end{pmatrix}$$

Custom pot. parameters

Bond Order Potential (BOP)

$$\frac{1}{2}\sum_{j\neq i}\left[e^{A_i-\alpha_{ij}r_{ij}} - S_{ij}b_{ij}e^{B_i-\beta_{ij}r_{ij}}\right]f_c(r_{ij}) = E_i$$

ANN customizable potential energy function

Retains the physics of the atomic interactions

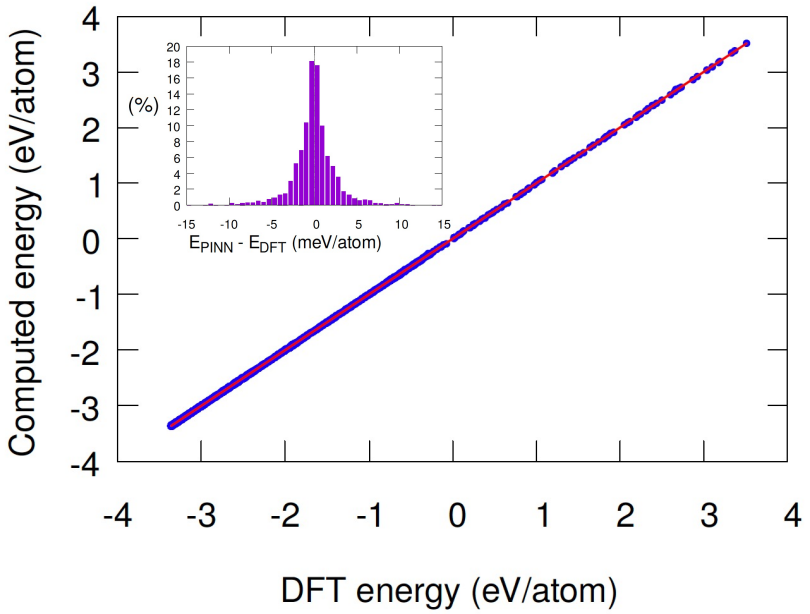
*G. P. Purja Pun et al., *Nature Communications* 10 (2019) 2339.

PINNs offers significantly improved transferability outside the training set

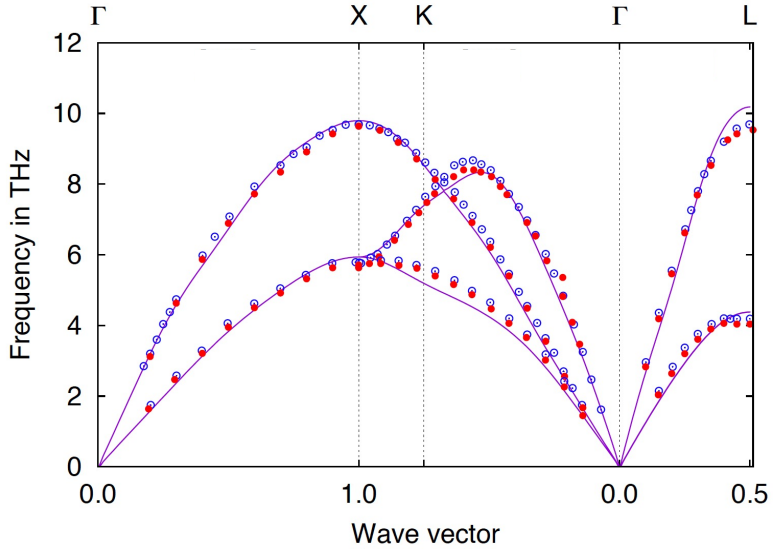
Example for Aluminum

Crystalline Phase

Energy



Phonon spectrum



DFT – Density Functional Theory calculations

ANN architecture: 40x16x16x8 -> 1064 fitting coefficients

Training set: 36,490 supercells of 2 to 79 atoms

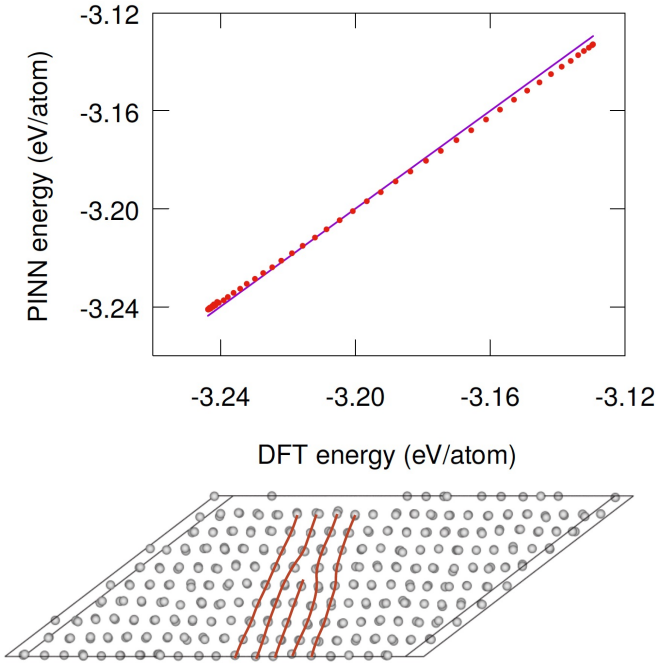
Excellent fit to DFT calculations

G. P. Purja Pun et al., *Physical Review Materials*, 4 (2020) 113807.

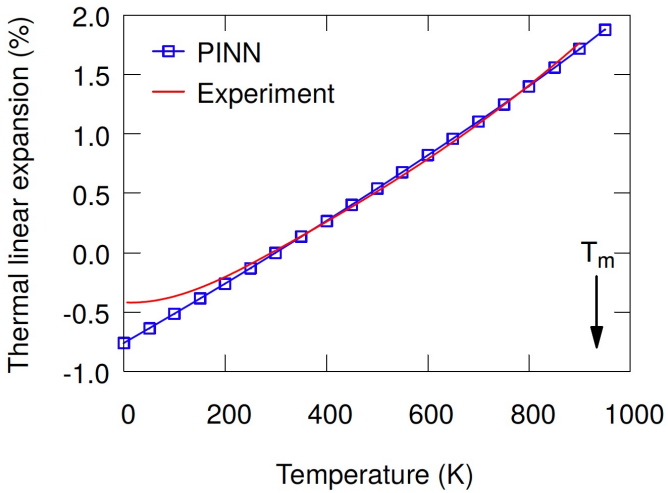
Example for Aluminum

Crystalline Phase

Edge dislocation



Thermal expansion

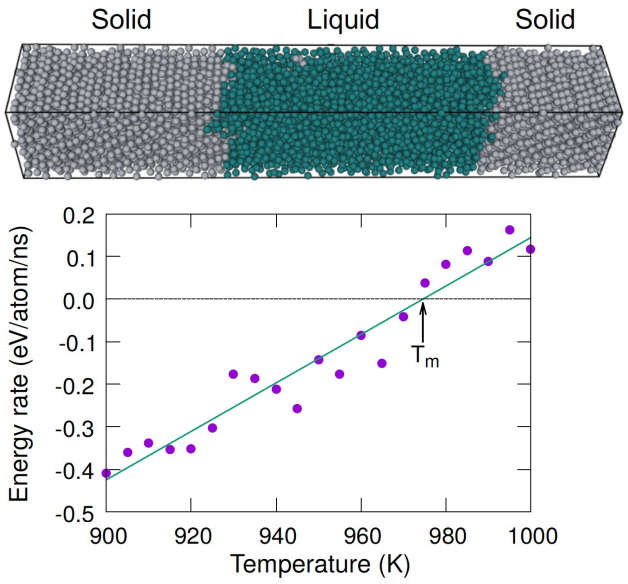


Excellent agreement with defect structures and thermal expansion

Example for Aluminum

Melt Properties

Melting temperature

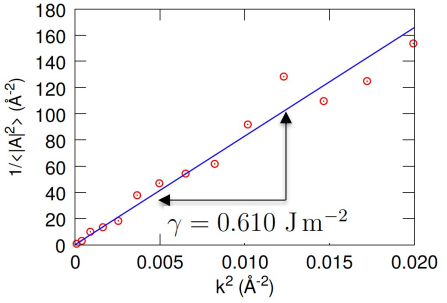


$T_{m\ (PINN)} = 975\ K$

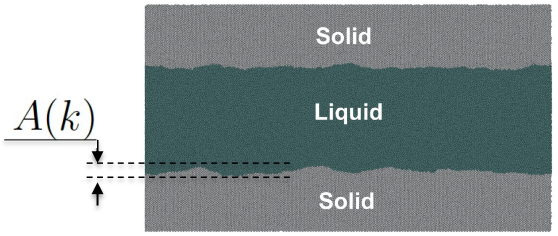
$T_{m\ (exp)} = 933\ K$

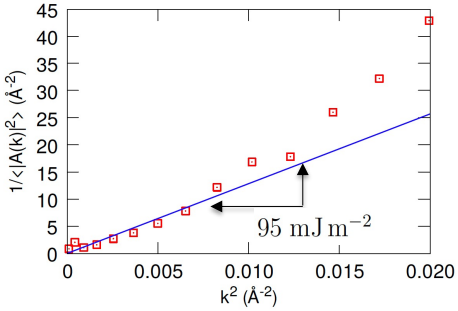
Capillary fluctuation method: $\langle |A(k)|^2 \rangle = \dfrac{k_B T}{lw\,(\gamma + \gamma'')\,k^2}$

Surface tension, γ



Liquid-solid interface energy, γ



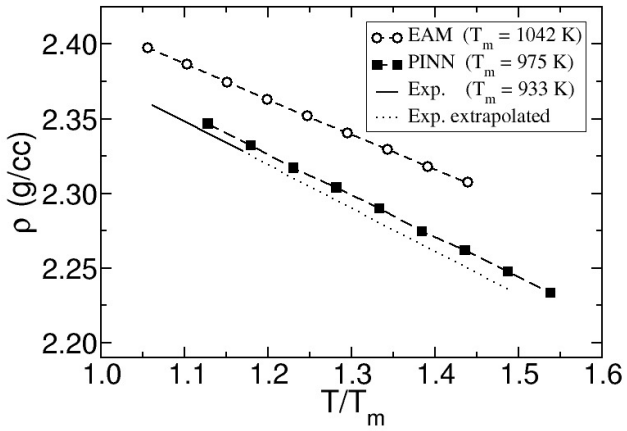


Prediction of difficult to measure interface energies is essential for AM applications

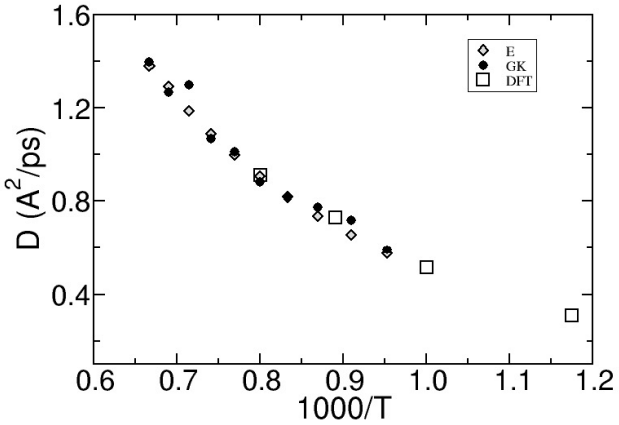
Example for Aluminum

Melt Properties

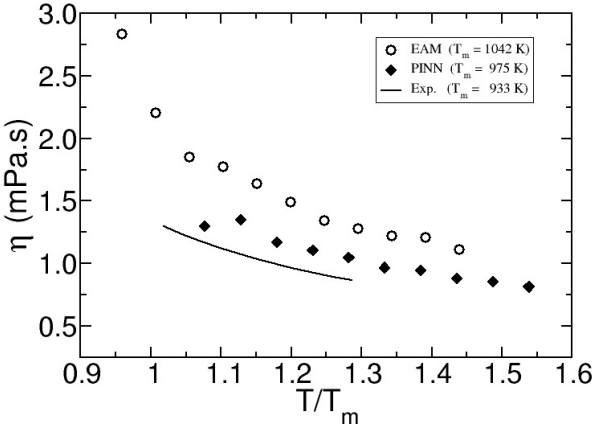
Density



Diffusion



Viscosity



EAM – Embedded Atom Method (Empirical) potential
PINN – Physically Informed Neural Network potential

Einstein: $D = \lim_{t\to\infty} \frac{1}{2t}\frac{1}{3N}\left\langle \sum_{i=1}^{N} [\vec{r}_i(t) - \vec{r}_i(0)]^2 \right\rangle$

Green-Kubo: $D = \frac{1}{3N}\int_0^{\infty} \left\langle \sum_{i=1}^{N} \vec{v}_i(t) * \vec{v}_i(0) \right\rangle dt$

$\eta_{xy} = \frac{1}{Vk_BT}\int_0^{\infty} \langle P_{xy}(t)P_{xy}(0)\rangle dt\,; \quad P_{xy}(t) = \frac{d\Psi_{xy,i}(t)}{dt}$

Accurate prediction of density, diffusivity, and viscosity is essential for melt pool calculations in AM

Computational Implementation of PINN

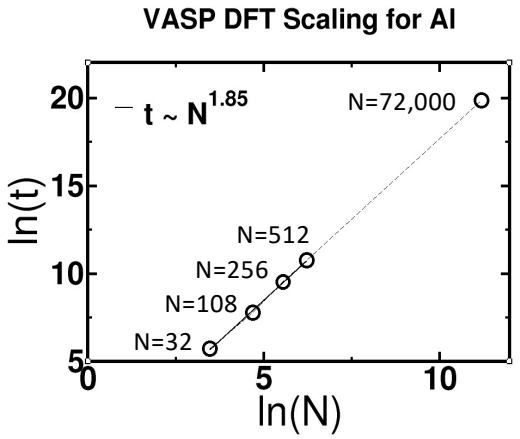
Test example on simulating aluminum crystal for 100 time-steps (MD steps)

Direct 1:1 comparison to DFT

N=500 100 MDS	EAM 16 cores	ANN 16 cores	PINN** 16 cores	DFT* 32 nodes
Time, t	0.39 s	14 s	35 s	46,688 s
t/t_{EAM}	1	38	89	119,107

Larger scale beyond DFT capabilities

N=72,000 100 MDS Time, t (t/t_{EAM})	EAM	ANN	PINN	DFT 32 nodes extrapolated
16 cores	3.5 s (1)	345 s (99)	528 s (151)	13.5 years
16 cores + V100	-	39 s (11)	115 s (33)	-



EAM – Embedded Atom Method (Empirical) potential
ANN – Artificial Neural Network potential
PINN – Physically Informed Neural Network potential
DFT – Density Functional Theory calculations

PINN gains speed without loss of accuracy

*VASP: J. Hickman (NIST)
**Inhouse developed software: https://software.nasa.gov/search/software/ParagrandMC

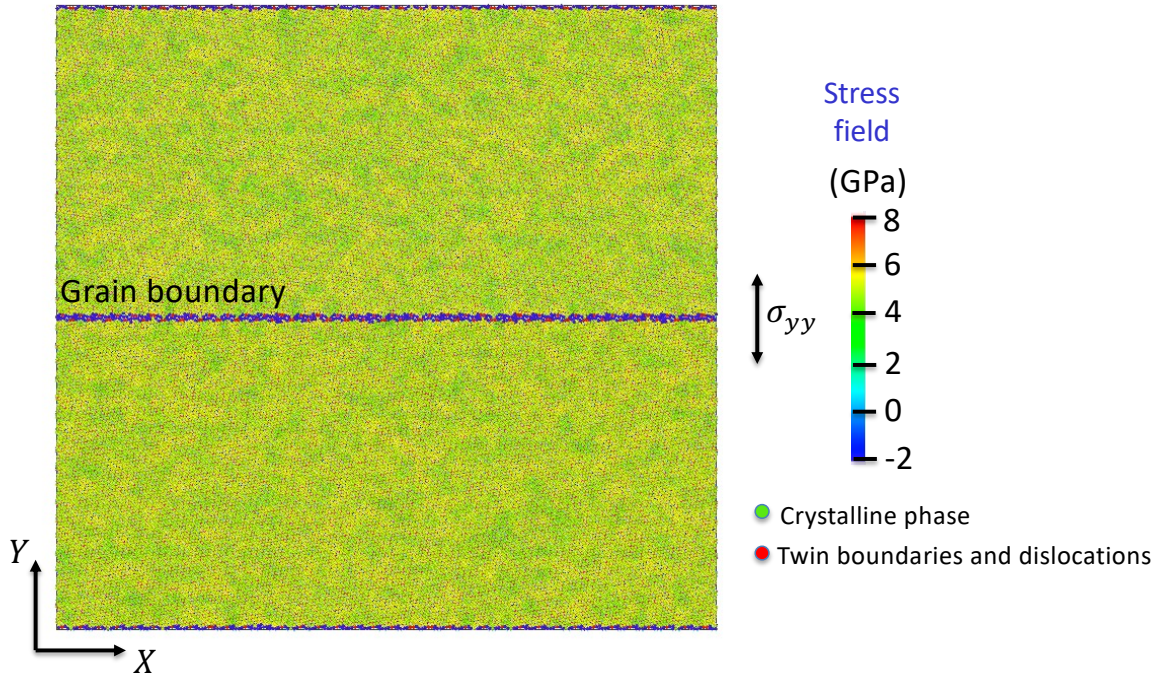
PINN: ParaGrandMC

https://software.nasa.gov/search/software/ParaGrandMC

Simulation of a central crack nucleation along a grain boundary in aluminum using Physically Informed Neural Network (PINN) potential

Crack growth simulation with DFT precision

433,000 atoms; 24 ps MD simulation (12,000 MD steps)
4 MPI nodes using (10 Skylake 6148 CPUs + V100 GPU) / node
14 cpu hours



PINN allows for large scale accurate physics-based simulations

Conclusions

- **Atomistic simulations provide first-principles physics-based information on highly dynamic AM processing**
- **Current atomistic modeling requires high precision interatomic force calculations**
  - ✓ QM – accurate but prohibitively slow
  - ✓ PINN provides transferability of the interatomic potential outside the training set
- **Machine learning strategies, such as ANNs, introduce new approaches (and new challenges) in atomistic simulations**
  - ✓ As accurate as QM and much faster
  - ✓ PINN allows for large scale accurate physics-based simulations