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

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Outline

- Atomistic simulations in additive manufacturing
- Artificial Neural Networks (ANNs) in atomistic simulations
- Physically Informed Neural Networks (PINNs) potential
- Example for aluminum
- Computational implementation of PINN
- Conclusion

Atomistic Simulations in Additive Manufacturing

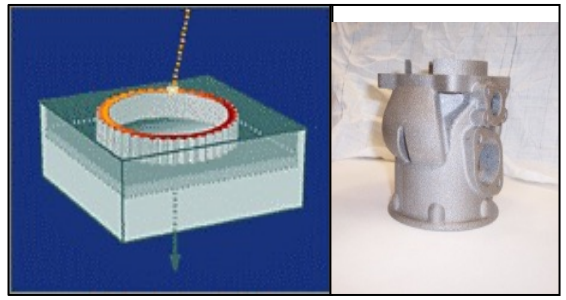
Role:

- Provides first-principles physics-based information on the highly dynamic Additive manufacturing (AM) processing during:
  - rapid heating and cooling (melt / solidification process)
  - strong thermal gradients (local heating)
  - high thermal stresses
- Complement other simulation methods at mesoscale by:
  - providing knowledge of microscopic mechanisms of key processes
  - obtaining material parameters not easily accessible experimentally

Objectives:

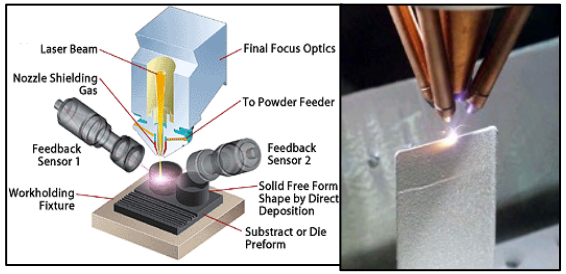
- Develop process parameter / microstructure relationships to guide process optimization
- Develop thermodynamics relationships to understand microstructure evolution and to guide design

Laser Sintering/E-beam Melting



Electron Beam Freeform Fabrication

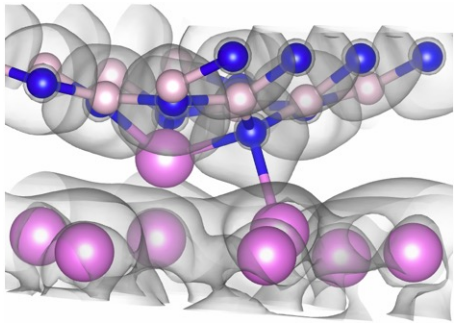
Laser Engineered Net Shaping



Why Machine Learning in Atomistic Simulations

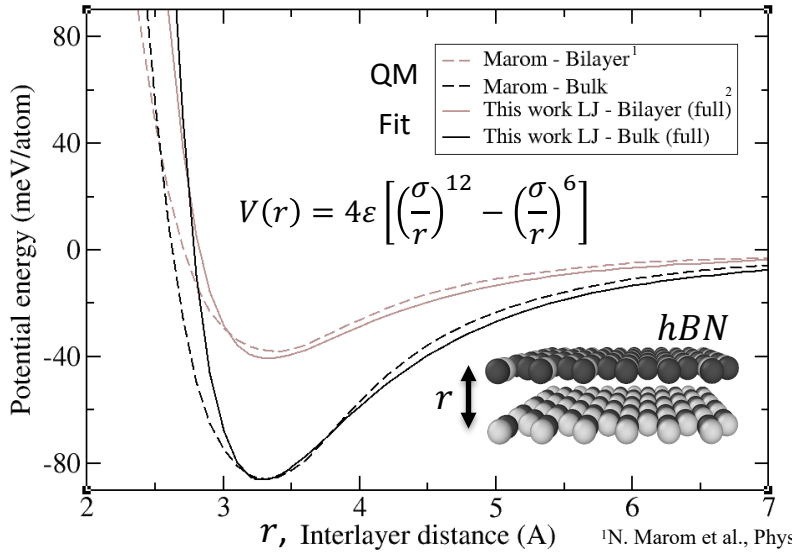
Atomic interactions in quantum mechanics (QM) are very complex and difficult to compute: central processing unit (cpu) time $\sim N^{3\div 8}$

Standard approach: replace the complex QM calculations with a simplified expression with empirically fitted parameters



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

QM in density functional theory (DFT) approximation



[1]N. Marom et al., Phys. Rev. Lett. 105 (2010) 046801.
[2]V. Yamakov et al., Comp. Mat. Sci. 135 (2017) 29.

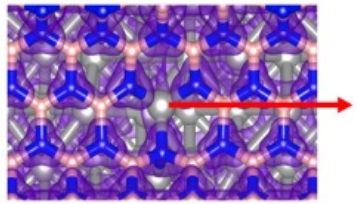
- Very accurate
- Generic to all known structures
- Very slow: cpu time ~$N^{3\text{-}8}$

- Very fast: ~10^{12} atoms
- Inaccurate
- Non-transferable (unique for each material)
- Difficult to create (expensive)

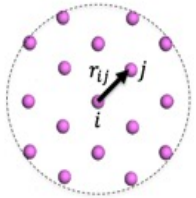
New approach is needed

Physically Informed Neural Network (PINN) Interatomic Potential

The universal approximation theorem: a neural network (NN) can approximate any f(x) NN universality



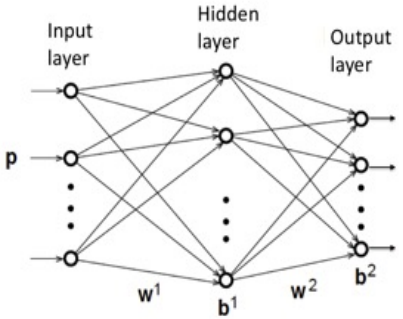
Material



Atomic environment

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

Structure coefficients



Neural Network

Contains the "knowledge" of the QM calculations

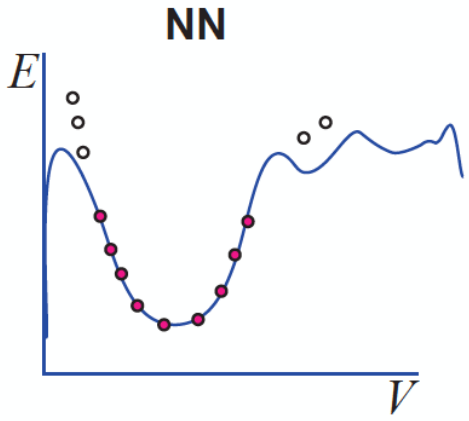
$$\begin{pmatrix} A_i \\ \alpha_{ij} \\ B_i \\ \beta_{ij} \\ \vdots \end{pmatrix}$$

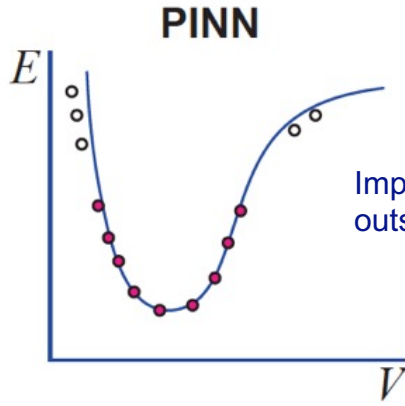
NN predicted parameters

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

NN parameterized potential energy function

Retains the physics of the atomic interactions





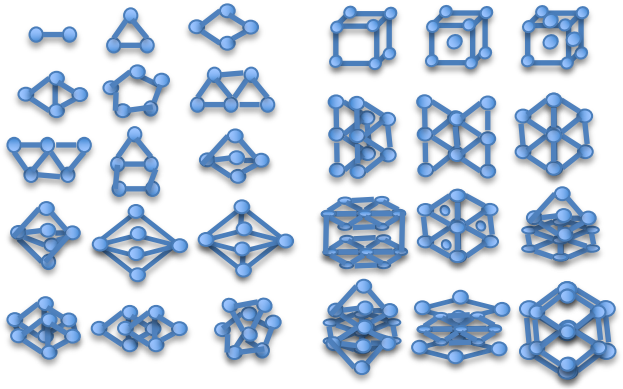
Improves transferability outside the training region

QM is replaced by a trained NN to parameterize a physics-based function for improved transferability

Implementation of PINN

Training Stage

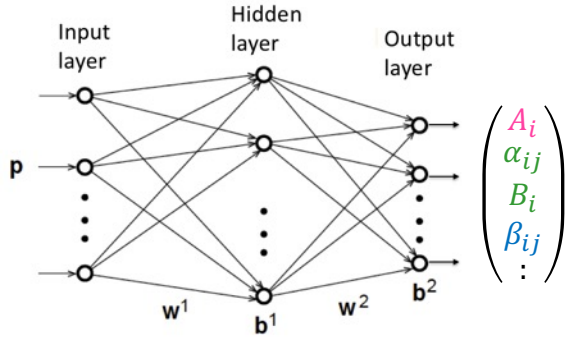
Use QM to calculate a large set of atomic structures



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

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

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



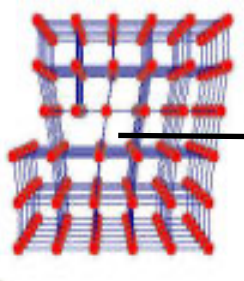
$$\begin{pmatrix} A_i \\ \alpha_{ij} \\ B_i \\ \beta_{ij} \\ \vdots \end{pmatrix} \rightarrow f(A_i, \dots, r_{ij}) = E_i$$

$$\varepsilon = \sum_n (\tilde{E}_i - E_i)^2$$

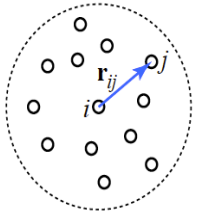
Objective function:

$\varepsilon \rightarrow 0$

Inference Stage



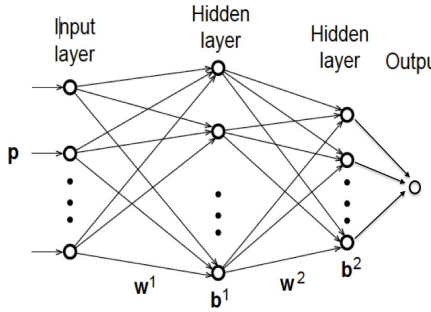
Material



Atomic environment

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

Structure parameters



Trained NN

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

Potential parameters

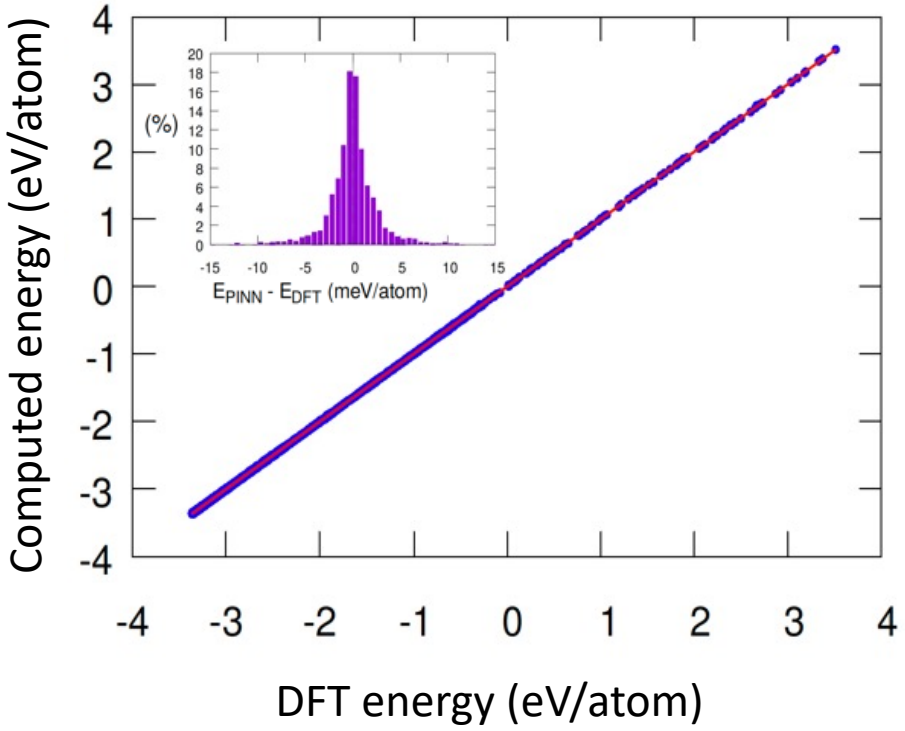
$$\frac{1}{2}\sum_{j\neq i}\left[e^{A_i-\alpha_{ij}r_{ij}} - S_{ij}b_{ij}e^{B_i-\beta_{ij}r_{ij}}\right]f_c(r_{ij}) = E_i$$

Approximate E_i of atom (i)

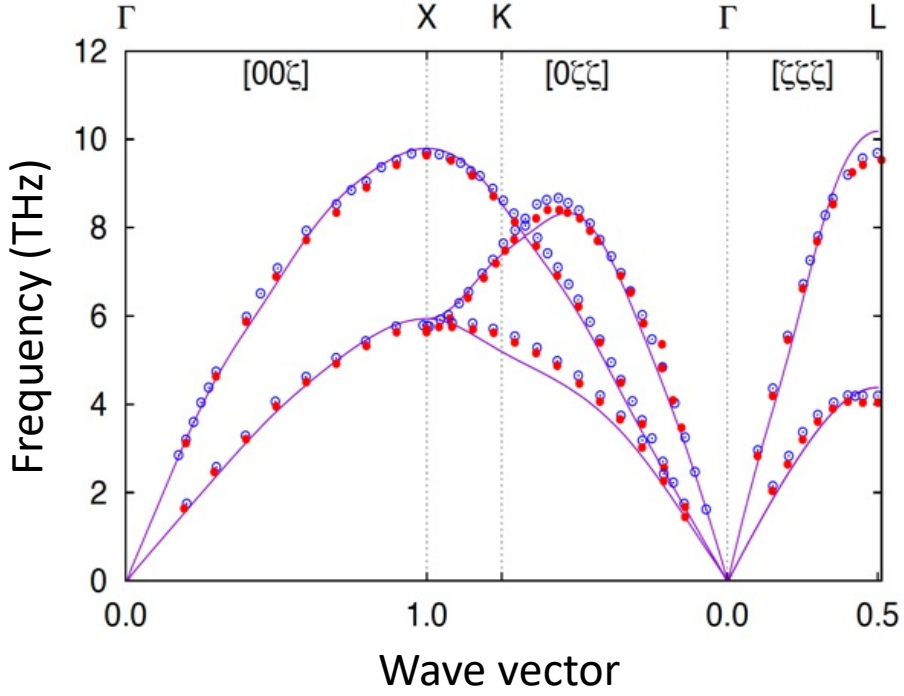
Retains the accuracy of QM while gaining in speed: cpu time ~ N

Example for Aluminum: Crystalline Phase

Energy



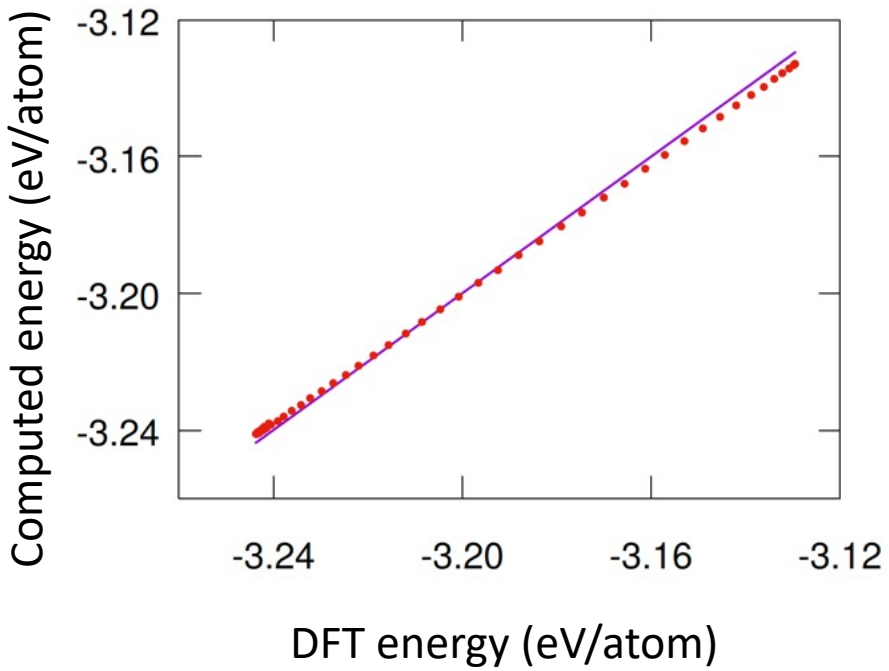
Phonon spectrum

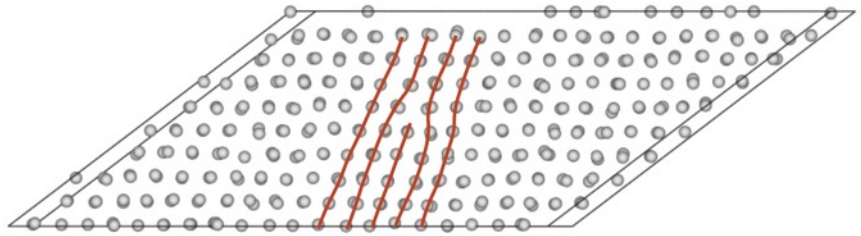


Excellent fit to DFT calculations

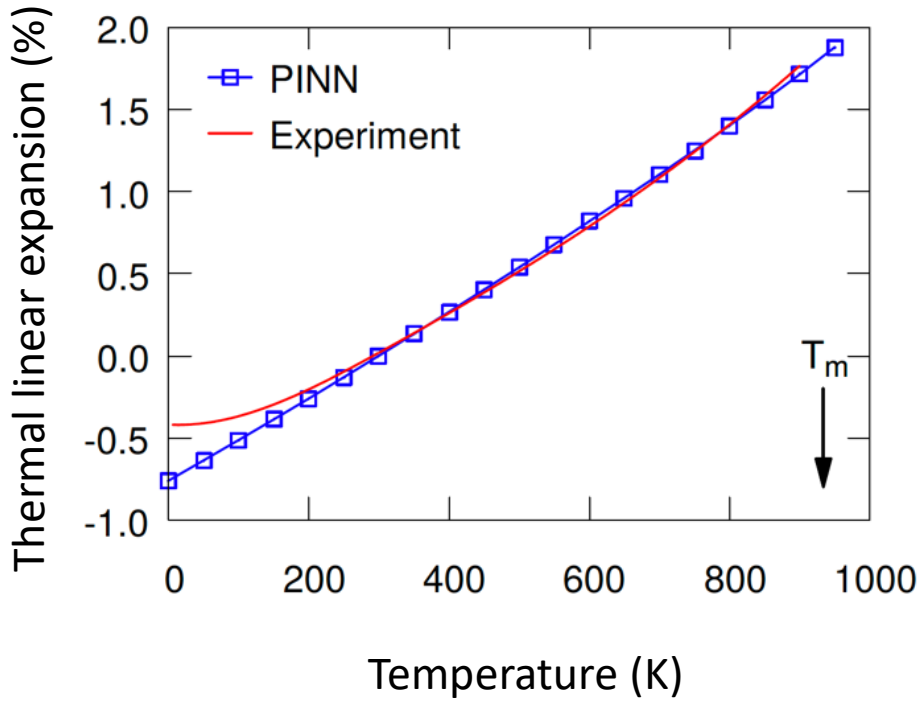
Example for Aluminum: Defect Structures

Edge dislocation





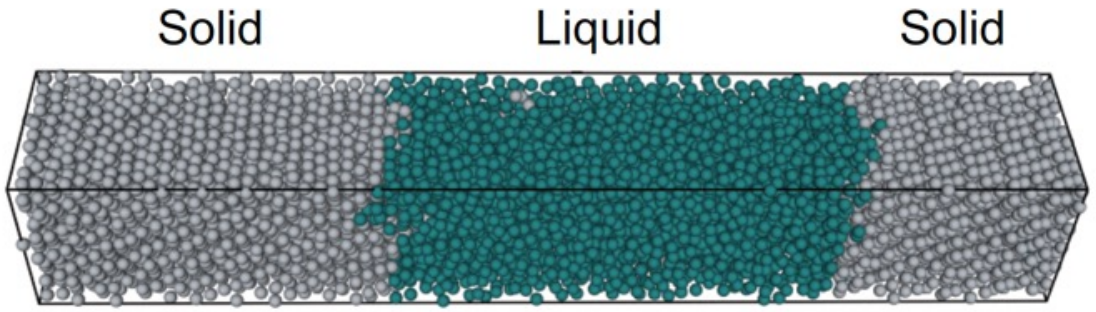
Thermal expansion

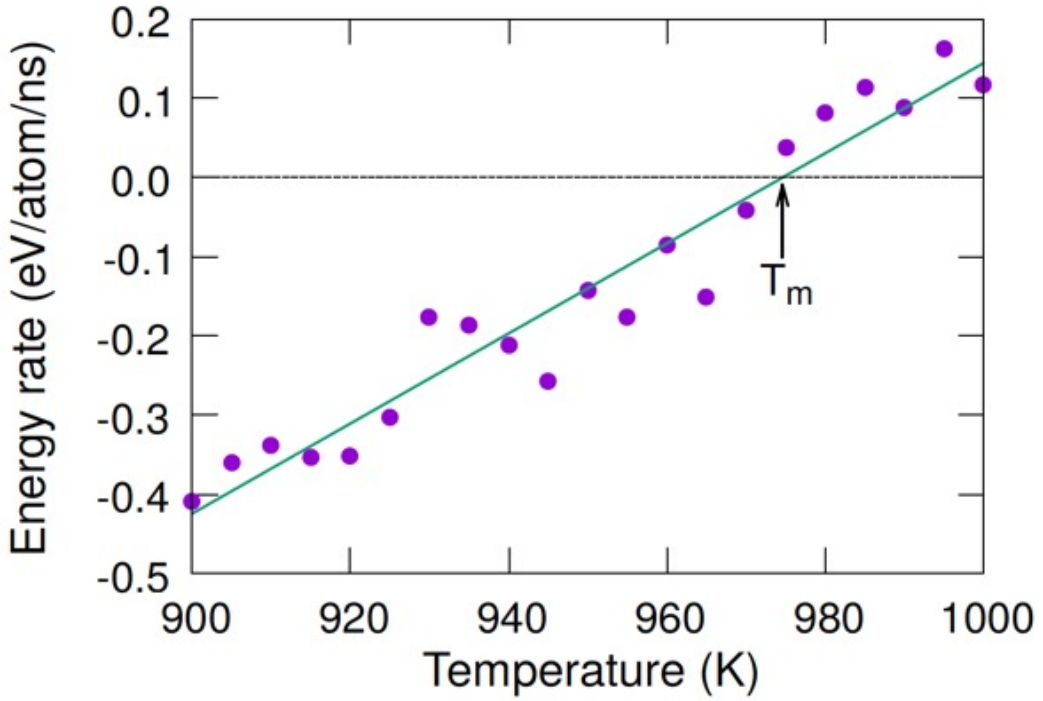


Excellent agreement with defect structures and thermal expansion

Example for Aluminum: Melt Properties

Melting temperature





$$T_{m\,(NN)} = 975\ K$$

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

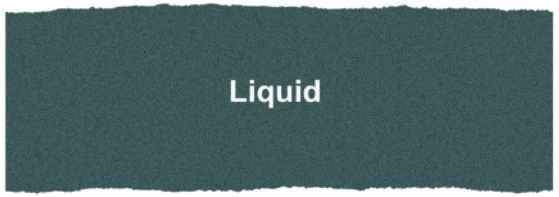
Reasonably good prediction of the melting temperature

Example for Aluminum: Melt Properties

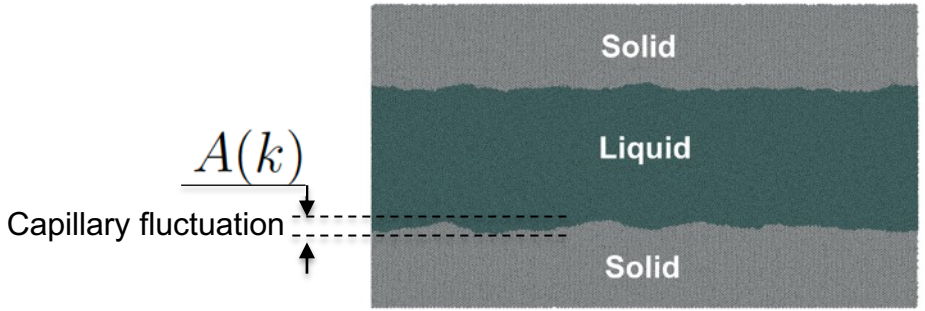
Liquid surface and liquid-solid interface energies

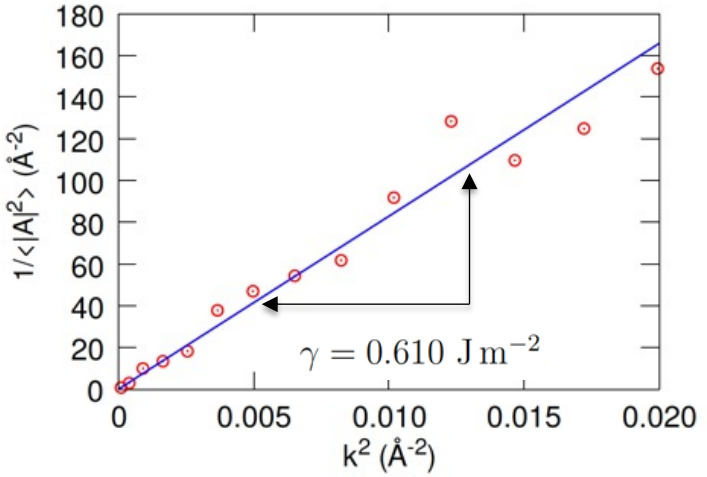
Capillary fluctuation method: $\langle |A(k)|^2 \rangle = \dfrac{k_B T}{lw\,(\gamma + \gamma'')\,k^2}$

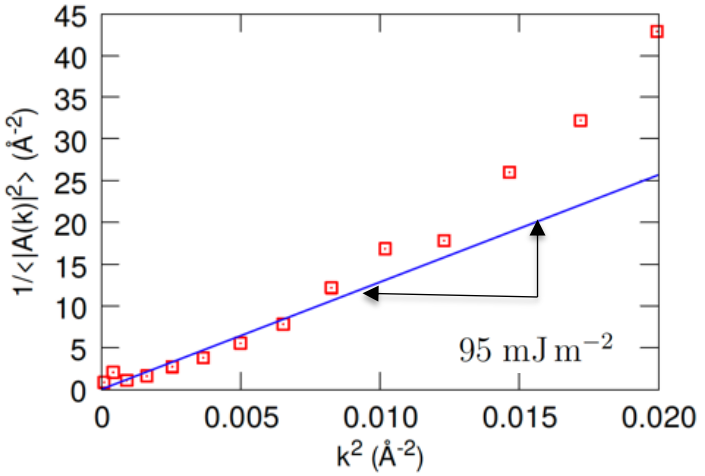
Surface tension, γ



Liquid-solid interface energy



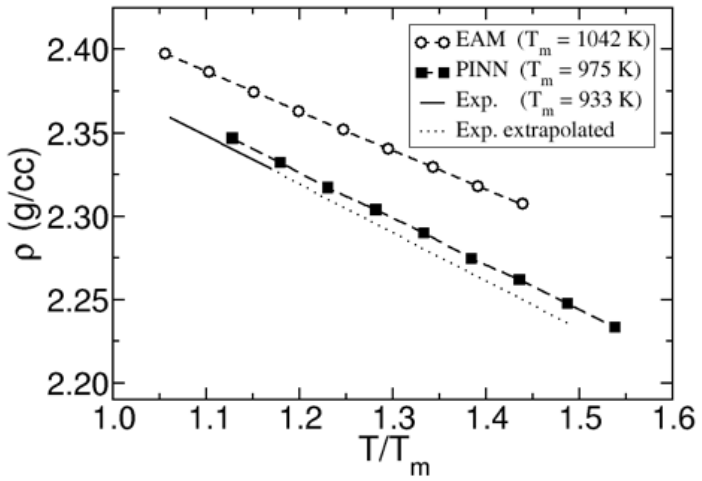




Prediction of difficult to calculate interface energies is essential of AM applications

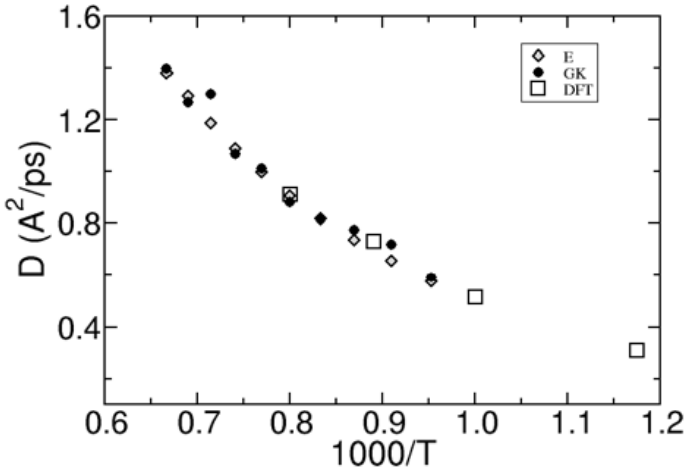
Example for Aluminum: Melt Properties

Density



EAM – Embedded Atom Method (Empirical) potential

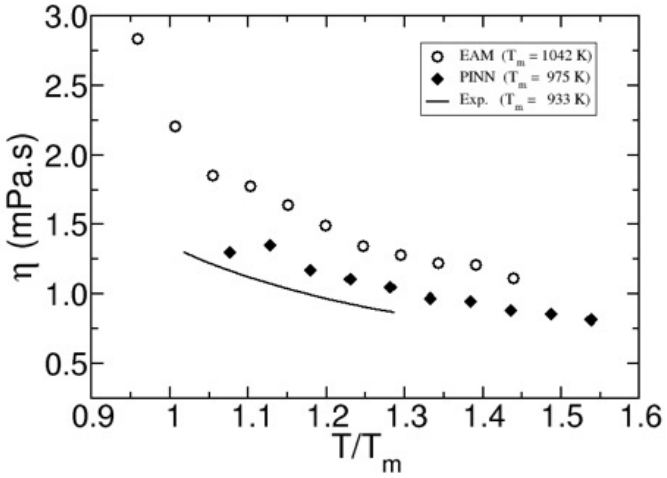
Diffusion



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

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

Viscosity



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

DFT: N. Jakse & A. Pasturel, Scientific Reports 3 (2013) 3135.

Accurate prediction of density, diffusivity, and viscosity is essential of AM applications

Computational Implementation of PINN

Exploring the recent advancements in supercomputer architectures

- PINN calculations are computationally highly demanding: ~ 3,000,000 floating point operations per atom
- High performance computing (HPC) implementation is strongly required
- ParaGrandMC code developed at NASA and National Institute of Aerospace provides massively parallel computational platform for PINN (https://software.nasa.gov/software/LAR-19893-1)

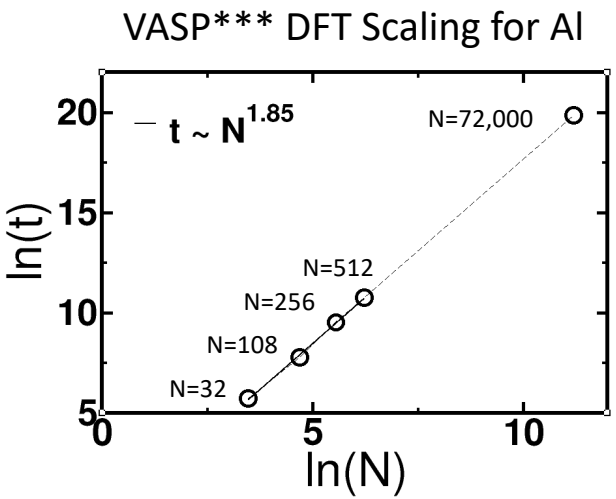
NASA Langley Research Center midrange supercomputing K-cluster

Empirical vs NN vs DFT Simulations

Test example on simulating aluminum crystal for 100 molecular dynamics steps (MDS)

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

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)	-



V100 – Volta 100 Nvidia graphic processing unit (GPU)

*Calculations performed by J. Hickman at National Institute of Standard and Technology (NIST) using VASP code

**Inhouse developed software: https://software.nasa.gov/search/software/ParagrandMC

***Specific vendor and manufacturer names are explicitly mentioned only to accurately describe the hardware used. This does not imply an endorsement by the U.S. Government.

Gain speed without losing accuracy

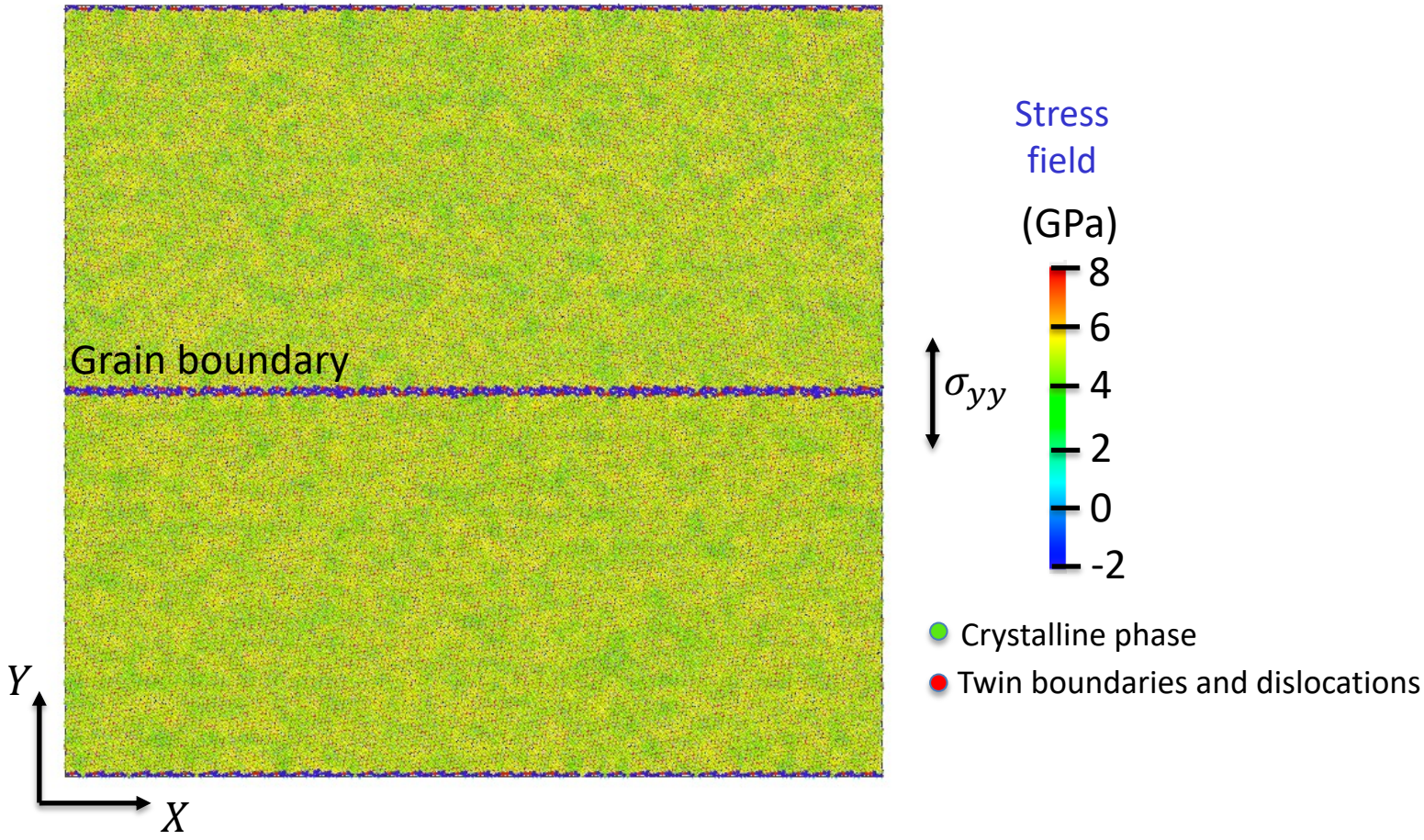
PINN: ParaGrandMC

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

Simulation of a central crack nucleation along a grain boundary in aluminum using PINN potential

Crack growth simulation with DFT precision

ParaGrandMC code developed at NASA (https://software.nasa.gov/software/LAR-19893-1)



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

Conclusions

- Machine learning in atomistic simulations reproduces atomic forces with quantum mechanics precision at orders of magnitude lower computational cost
- Applied in additive manufacturing ML based interatomic potential can accurately predict solid phase and melt properties of metallic alloys to guide process optimization
- Other PINN potentials under development for:
  - Additive manufacturing: Ti, Ti-Al, Ti-Al-V (Ti-6Al-4V aerospace alloy) – NASA Langley Research Center
  - Semiconductor industry: Si, Si-C – George Mason University, NIST
  - Other: Ta, Cu-Ta – in collaboration with George Mason University

Acknowledgements

- NASA Transformational Tools and Technologies (T3) Project
- High-End Computing Capability Project – NASA Advanced Supercomputing Division: Gabriele Jost and Daniel Kokron
- NASA Langley Research Center midrange supercomputing K-cluster
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