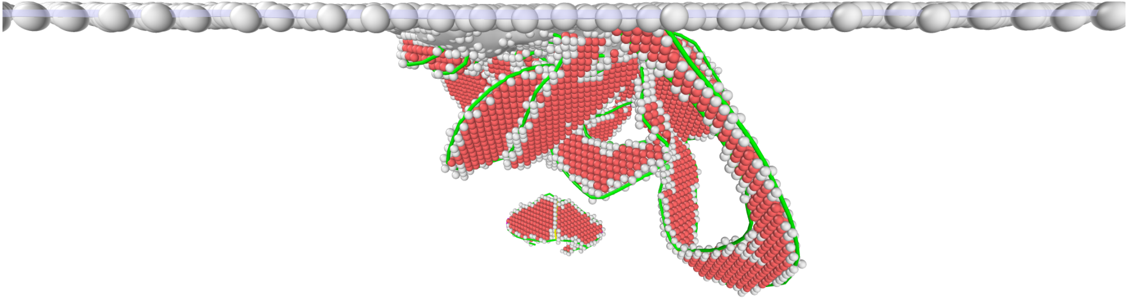

ADAPTIVE-PRECISION POTENTIALS FOR LARGE-SCALE ATOMISTIC SIMULATIONS

2024-03-18 | David Immel, Ralf Drautz, Godehard Sutmann |

ICAMS
INTERDISCIPLINARY CENTRE FOR ADVANCED MATERIALS SIMULATION

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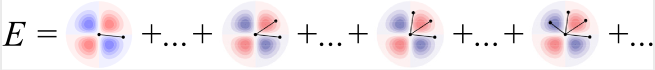
INTERATOMIC POTENTIALS

Atomic Cluster Expansion (ACE)[1]

modern and precise ML potential



Cu potential	nanoindentation core-h	nanoindentation cores	single force call[2] µs	single force call[2] cores
ACE[2]	66243	640	320.0	1
EAM[3]	83	128	1.5	1

EAM is 200-800 times faster than ACE

[1] Drautz, Ralf. Physical Review B. 2019
[2] Lysogorskiy, Yury et al. npj computational materials. 2021
[3] Mishin, Yuri et al. Physical Review B. 2001

Embedded Atom Model (EAM)

traditional and fast potential

$$E = \frac{1}{2}\sum_j V(r_{ij}) + F\left(\sum_{j\neq i}\rho(r_{ij})\right)$$

combine precise and fast

$$E = \lambda E_{\mathrm{EAM}} + (1-\lambda)E_{\mathrm{ACE}}$$

- ACE for most interesting atoms
- EAM for remaining atoms

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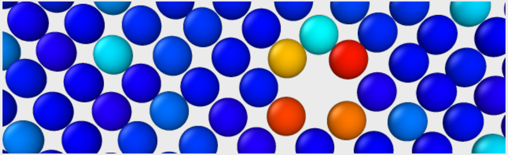
DETECTING INTERESTING ATOMS

centro-symmetry parameter[4] (CSP)

- detects defects, surfaces

⇒ interesting atoms

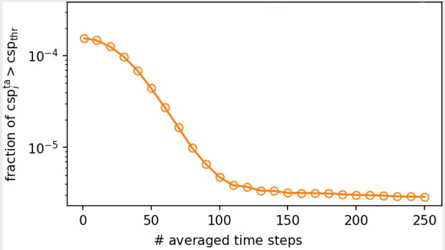
$$\mathrm{CSP}_i = \sum_{j=1}^{N/2} \left| \vec{r}_{i,j} + \vec{r}_{i,j+N/2} \right|^2$$



all atomistic visualisations with ovito[5]

time averaging

- slow change of CSP
- prevents detection of thermal fluctuations



[4] Kelchner, Cynthia L, Plimpton, SJ, and Hamilton, JC. Physical review B. 1998
[5] Stukowski, Alexander. Modelling and simulation in materials science and engineering. 2009

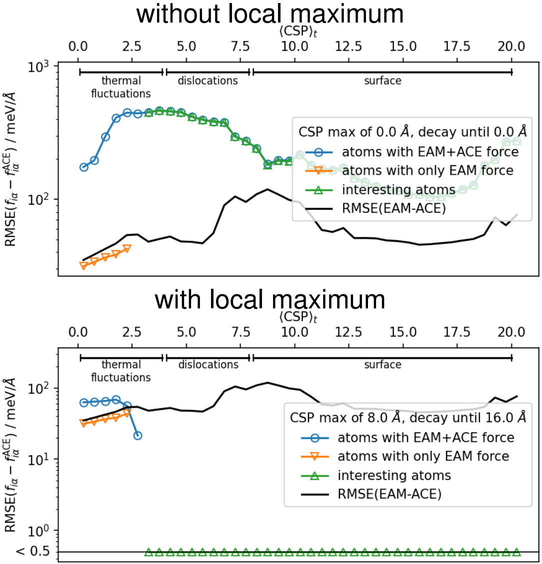
FORCES IN (100) COPPER

$$F_i = \sum_k \Bigg(\underbrace{\cancel{-(\nabla_i \lambda_k)(E_k^{\mathrm{EAM}} - E_k^{\mathrm{ACE}})}}_{\text{next slide}} \underbrace{- \lambda_k (\nabla_i E_k^{\mathrm{EAM}}) - (1 - \lambda_k)(\nabla_i E_k^{\mathrm{ACE}})}_{\text{all } \lambda_k \text{ influence } F_i} \Bigg)$$

local maximum of CSP

- use $\max\left(\{\langle \mathrm{CSP}_j \rangle_t f(r_{ij})\}\right)$ to calculate λ_i

$\Rightarrow$ less EAM influence on interesting atoms



ENERGY CONSERVATION

- one cannot calculate $\nabla_i \lambda_k$
- potential is conservative for constant $\{\lambda_k\}$

local thermostat per atom

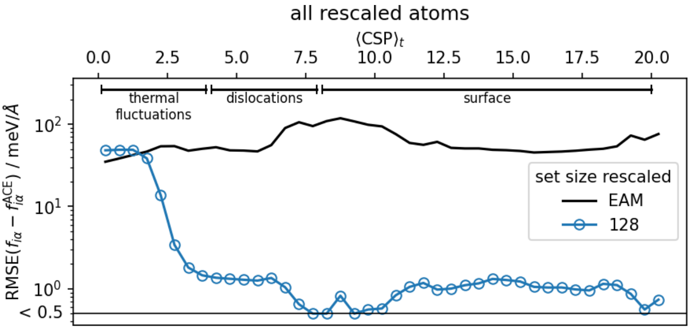
1. calculate energy difference compared to constant $\{\lambda_k\}$ case
2. rescale velocities of random local atoms

$\Rightarrow$ energy & momentum conservation

velocity change by integrator

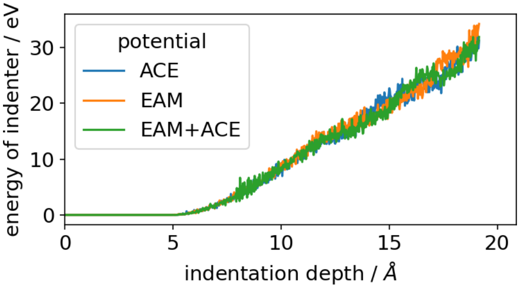
$$\Delta v = \frac{F}{m} \Delta t$$

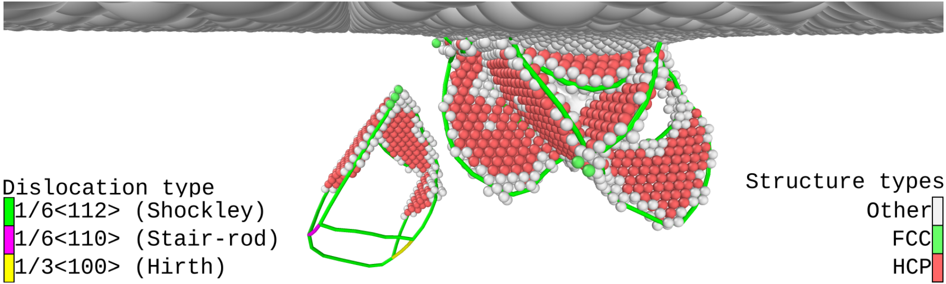
$\Rightarrow$ comparison with forces possible



NANOINDENTATION

- simulated with LAMMPS[6]
- 68^3 unit cells $\approx$ 1.25 million atoms
- temperature: 292 K
- velocity controlled nanoindentation
- imaginary, spherical, repulsive indenter





[6]Thompson, Aidan P et al. Computer Physics Communications. 2022

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ADAPTIVE-PRECISION POTENTIALS

Summary

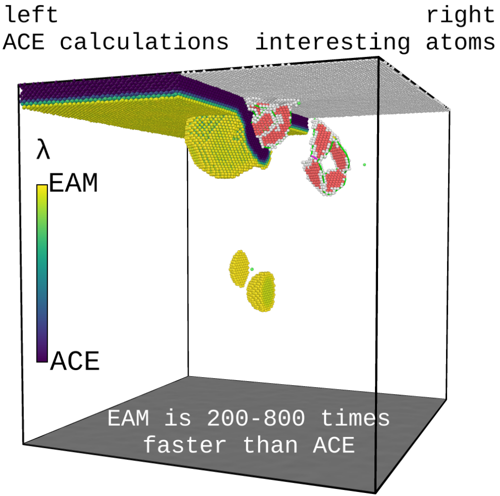
$$E_i = \lambda_i E_{i,\mathrm{EAM}} + (1 - \lambda_i) E_{i,\mathrm{ACE}}$$

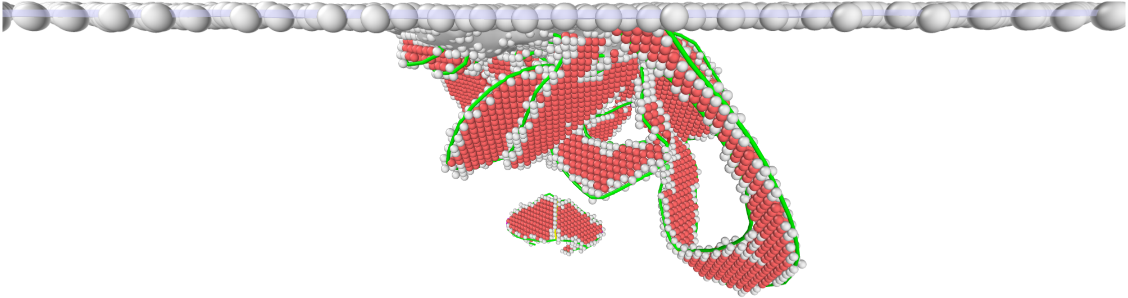
- detect interesting atoms with CSP

⇒ precise and fast potential

Outlook

- bcc metal: Tungsten





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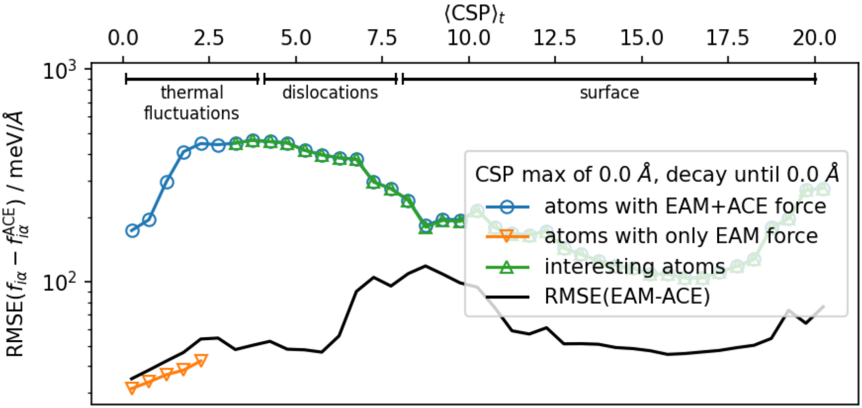
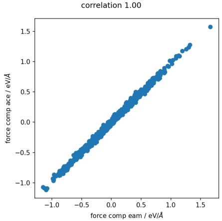
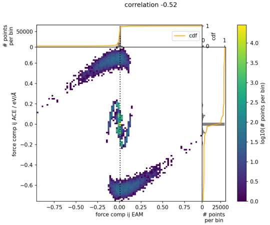
EAM + ACE FORCES



$F_i^{EAM} \approx F_i^{ACE}$



$F_{i\to j}^{EAM} \not\approx F_{i\to j}^{ACE}$



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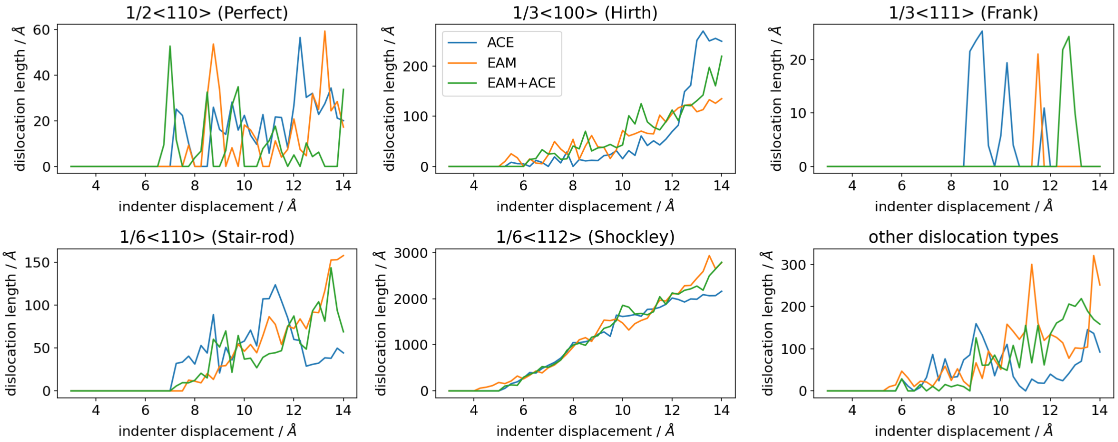
DISLOCATIONS



EAM+ACE generates the same dislocations types like ACE.

DYNAMIC LOAD BALANCING

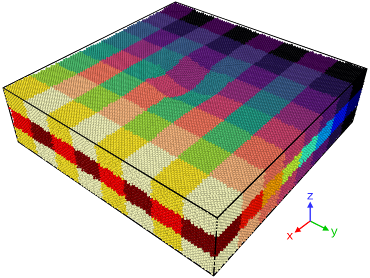
load per domain

- load = force calculation time τ_p
- one potential: $\tau_p = \tau_p^{\text{pot}}$
- EAM+ACE: $\tau_p = n_p^{\text{EAM}} \tau_p^{\text{EAM}} + n_p^{\text{ACE}} \tau_p^{\text{ACE}} + n_p^{\text{CSP}} \tau^{\text{CSP}}$

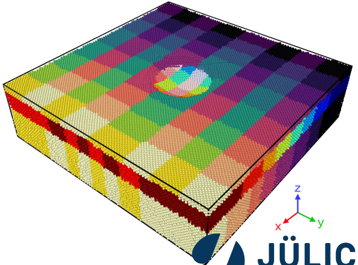
staggered grid

- cut box into layers, cut layer into rows, cut row into cells
- calculate domain boundaries with ALL[a]

[a] R. Halver, S. Schulz, and G. Sutmann. https://gitlab.version.fz-juelich.de/SLMS/loadbalancing/-/releases. 2023.



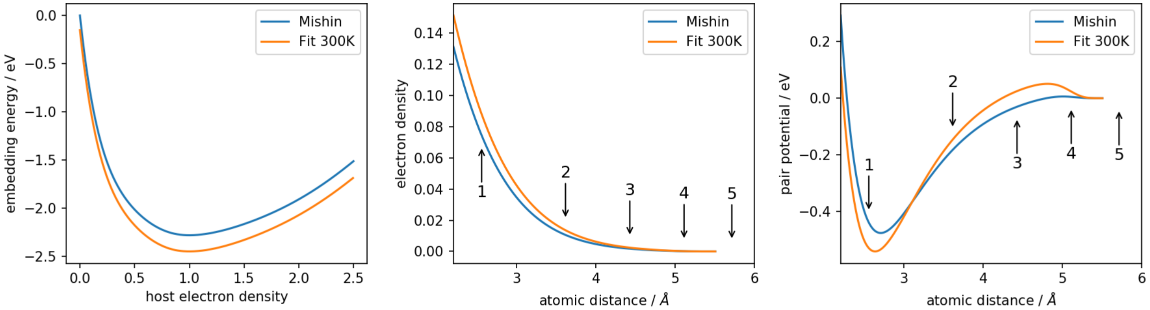
adjust domains to balance load



UPFITTING EAM WITH ATOMICREX[7]

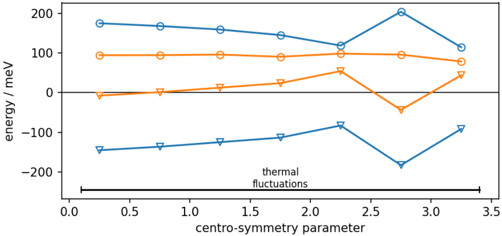
$$\mathcal{L}(A) = \sum_{o\in\mathcal{O}} \left(\frac{A_o^{\text{targ}} - A_o^{\text{pred}}}{\delta_o^{\text{tol}}} \right)^2 + \sum_{s\in\mathcal{S}} \frac{1}{N_s} \left(\sum_{i=1}^{N_s} \left(\frac{E_{s,i}^{\text{targ}} - E_{s,i}^{\text{pred}}}{\delta_{E_{\text{md}}}^{\text{tol}}} \right)^2 + \sum_{i=1}^{N_s} \left(\frac{\| F_{s,i}^{\text{targ}} - F_{s,i}^{\text{pred}} i \|_{L_2}}{\delta_{F_{\text{md}}}^{\text{tol}}} \right)^2 \right)$$

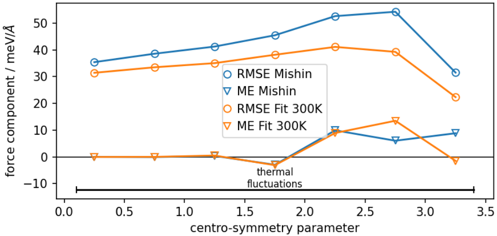
- fitted scalar properties $\mathcal{O}$: a_0^{FCC}, E_{coh}, B, C_{11}, C_{12}, C_{44}
- fitted structures $\mathcal{S}$: snapshots of MD simulation of bulk with ACE at T

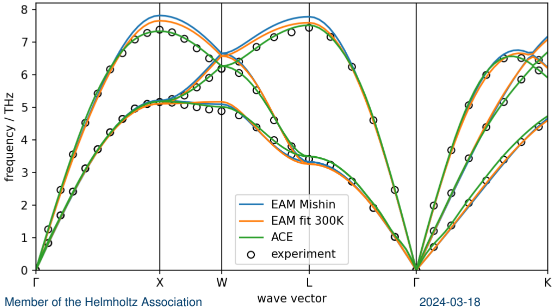


[7]Stukowski, Alexander et al. Modelling and Simulation in Materials Science and Engineering. 2017.

UPFITTED EAM PROPERTIES







	ACE	EAM fit	EAM ref
E_{coh} / eV	-3.6994	-3.6956	-3.5579
a_0^{FCC} / Å	3.6309	3.6304	3.6149
C_{11} / GPa	173	171	171
C_{12} / GPa	120	120	124
C_{44} / GPa	77	80	76
B / GPa	138	137	139