Accelerated Molecular Dynamics Simulations of Dislocation-Obstacle Interactions in Tungsten: Enabling Micro-Second Simulations

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LDRD
LABORATORY DIRECTED RESEARCH & DEVELOPMENT

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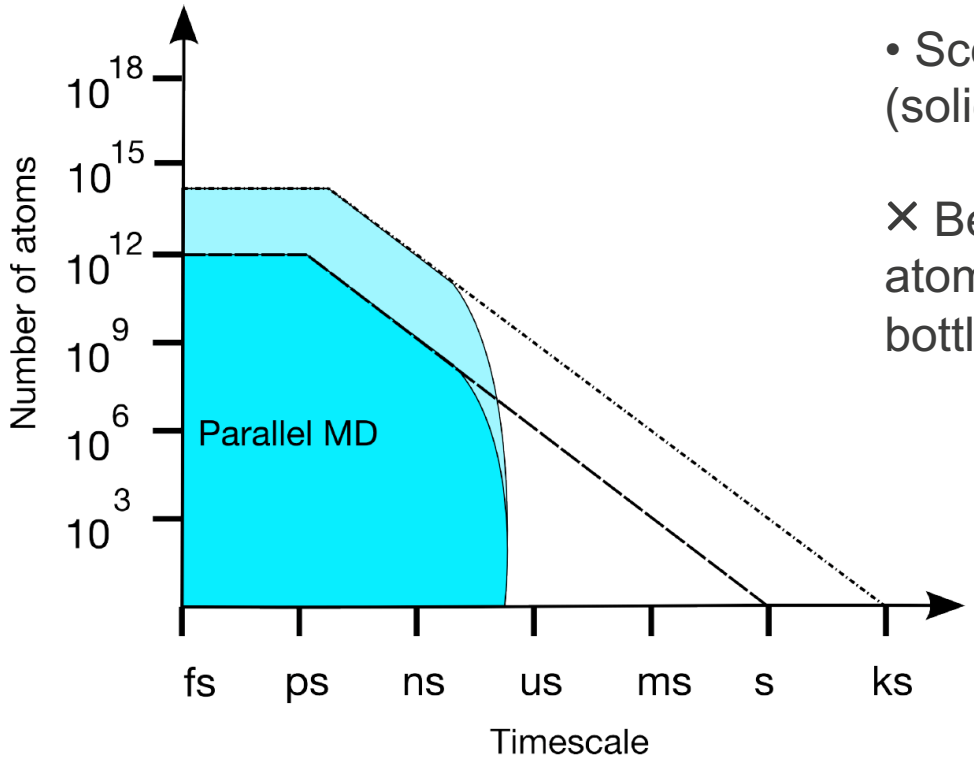
Molecular Dynamics

- Molecular Dynamics (MD) provides a detailed probe of thermodynamics and microstructural evolution

✓Given an accurate inter-atomic potential, MD is extremely predictive

✕ MD is computationally intensive



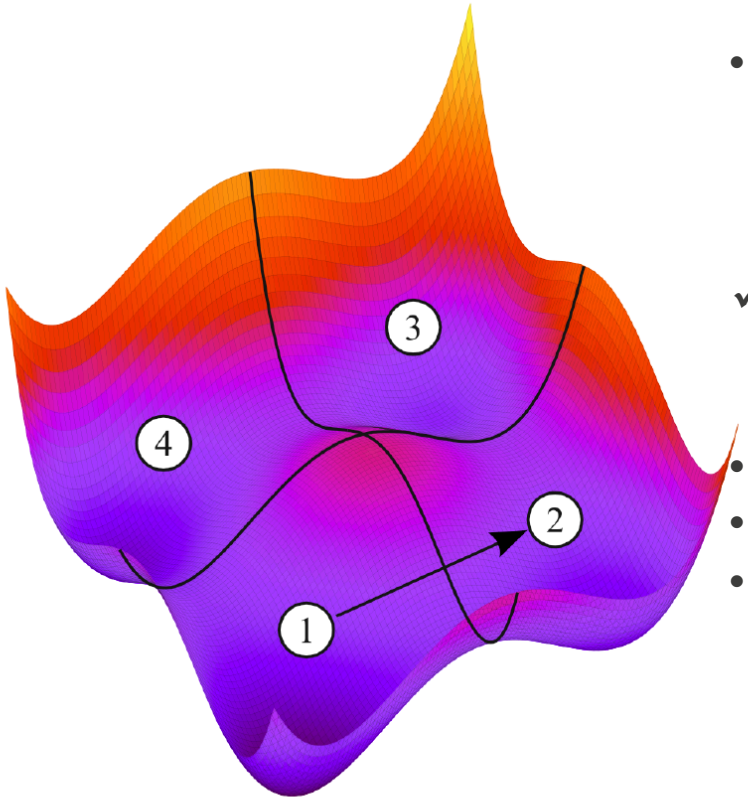
- Scope of direct-MD given a peta- (solid) or exa- (shaded) scale computer

✕ Beyond a lower-limit on number of atoms, direct-MD hits a communication bottle-neck and loses parallel efficiency

✓ Special techniques are needed to reach long time-scales

Accelerated Molecular Dynamics (AMD)

- In many problems of interest, long-time evolution consists of infrequent transitions



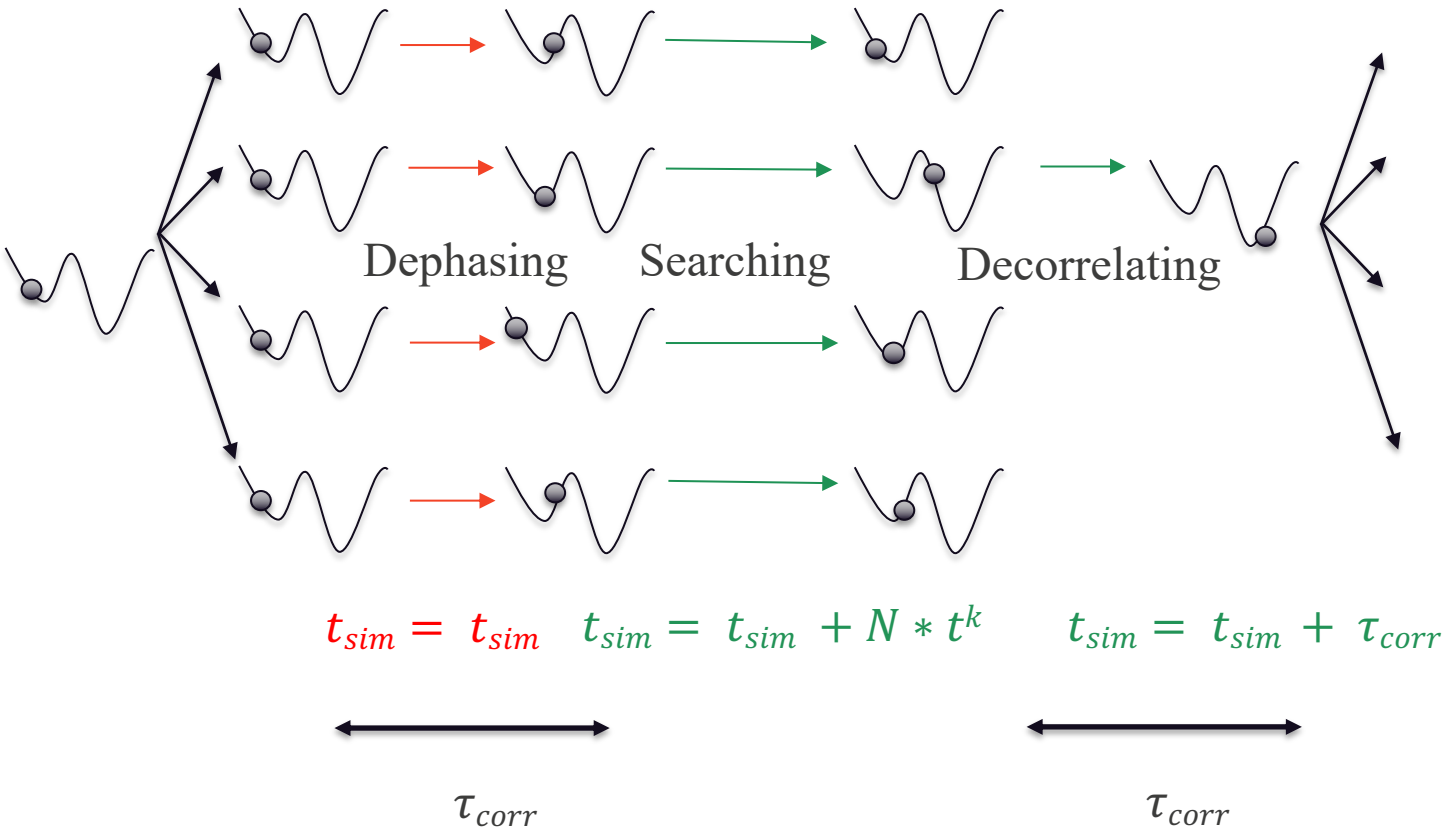
- Given a ***state***, we ask two questions:
  1. When will be the next transition?
  2. What will be the new ***state***?

✓ If we can answer these, we can accurately coarse-grain state-to-state dynamics

- Parallel Replica Dynamics (ParRep)[1]
- Preserves state-to-state dynamics
- Run many statistically-independent replicas to sample state-to-state transitions

1. A. F. Voter, Phys. Rev. B 57 (1998) 13985

Parallel Replica Dynamics (ParRep)

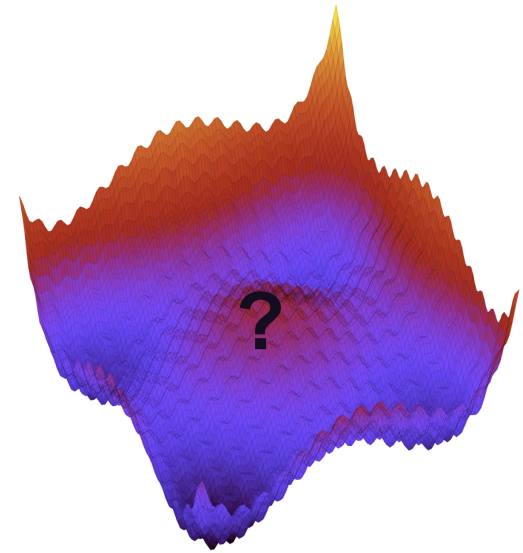


- ParRep is statistically exact for Markovian dynamics[1]
- ParRep errors $\propto exp(-(\lambda_2 - \lambda_1)\, \tau_{corr})$ for actual dynamics[2]
- $-\lambda_i$ are sorted eigenvalues that define the time-scales of the state

1. A. F. Voter, Phys. Rev. B 57 (1998) 13985 2. Le Bris *et al.*, Monte Carlo Meth. Appl. **18** (2012) 119

Koopman-ParRep

- To use ParRep, we need:
  - Definition of a state
  - Detect transitions out of a state
  - Estimate $\tau_{corr} > 1/(\lambda_2 - \lambda_1)$ for the state
  - Do all this ***on-the-fly***



- Conventional strategy:
  - Guess the states and use analytical approximations[1,2]
  - Works well on a smooth potential energy surface

- New strategy: Koopman-ParRep
  - States are defined as a function of τ_{corr}
  - Estimate τ_{corr} using the ***diffusion distance***[3] between two points in the trajectory

$$D_t^2(x,y) \simeq \sum_{j=2}^{\infty} \exp[-2(\lambda_j - \lambda_1)t] \left(\frac{\psi_j(x)}{\psi_1(x)} - \frac{\psi_j(y)}{\psi_1(y)} \right)^2$$

  - All points in the state should be diffusionally close to each other for τ_{corr}

1. Phys. Rev. B **57** (1998) 13985 2. Comp. Mat. Sci. **100** (2015) 90 3. Appl. Comp. Harm. Anal. **21** (2006) 113

Koopman-ParRep

- $\{\lambda_i, \psi_i\}$ are determined using the eigen-decomposition of the Koopman operator

$$\mathcal{K}_\tau f(x) = \mathbb{E}[f(x_{t+\tau})|x_t = x]$$

- We estimate K_τ using Extended Dynamic Mode Decomposition (EDMD)[1]
- EDMD is performed on a set of physically-motivated descriptors $\chi(x)$

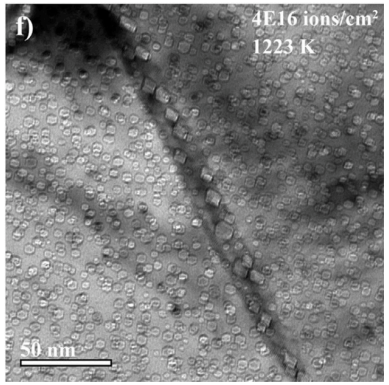
- **Defining a state:**
  - Run MD block
  - For each t_c in candidate τ_{corr} :
    - Estimate K_τ from $\{x_{t-wt_c}, \ldots\ldots, x_t\}$
    - Compute $D_{t_c}$from K_τ
    - If max $D < \epsilon$, define state with $x_{ref} = x_t$, τ_{corr}= t_c
- **Detecting transitions:**
  - Run MD block
  - Update K_τ
  - If $D_{\tau_{corr}}(x_{ref}, x_t) > \epsilon_t$: flag transition

✓ ***On-the-fly*** definition of states/transitions while ensuring accurate dynamics

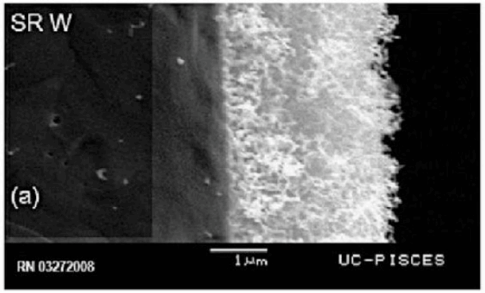
1. M. O. Williams et al., J. Nonlinear Sci. 25 (2015) 1307

Application: Dislocation-obstacle interactions in W

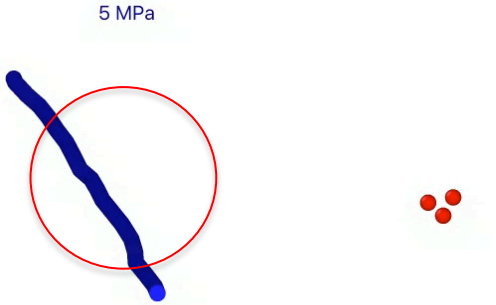
- Initial focus on He_nV_m clusters interacting with an edge dislocation
- He_nV_m clusters (bubbles) in W are formed under irradiation
- Influence fuzz formation, retention of Tritium, and results in hardening



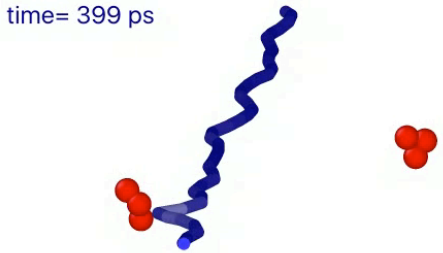
He bubbles in bulk/grain boundary[1]



Fuzz formation[2]



- 0 K, increasing stress
- Jog formation

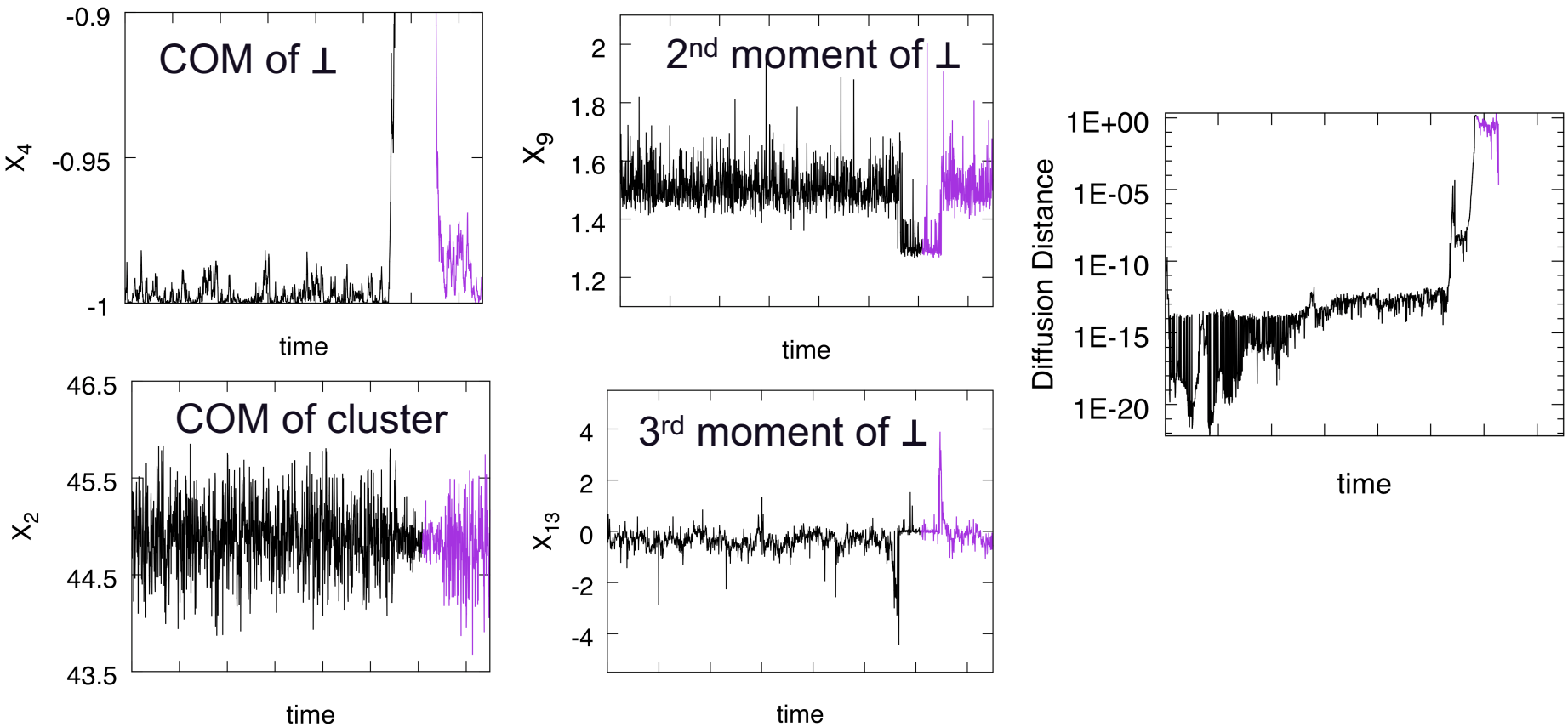


- 1000 K, 450 MPa
- No clear jog formation

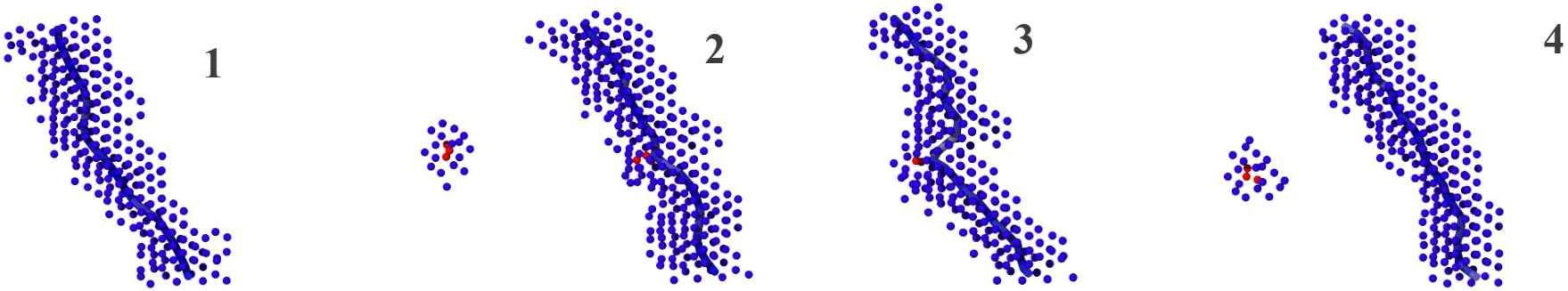
- Temperature/stress dependence of mechanisms/ activation energy

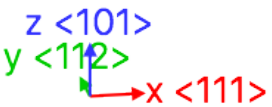
Dislocation-obstacle interactions in W

- User-defined descriptors: $\chi(\boldsymbol{x}) = \{\chi_1, \chi_2, \chi_3, \dots\dots, \chi_{22}\}$
- Up to 3rd moments of dislocation/cluster coordinates, cluster R_g
- All computations integrated with LAMMPS using Python bindings

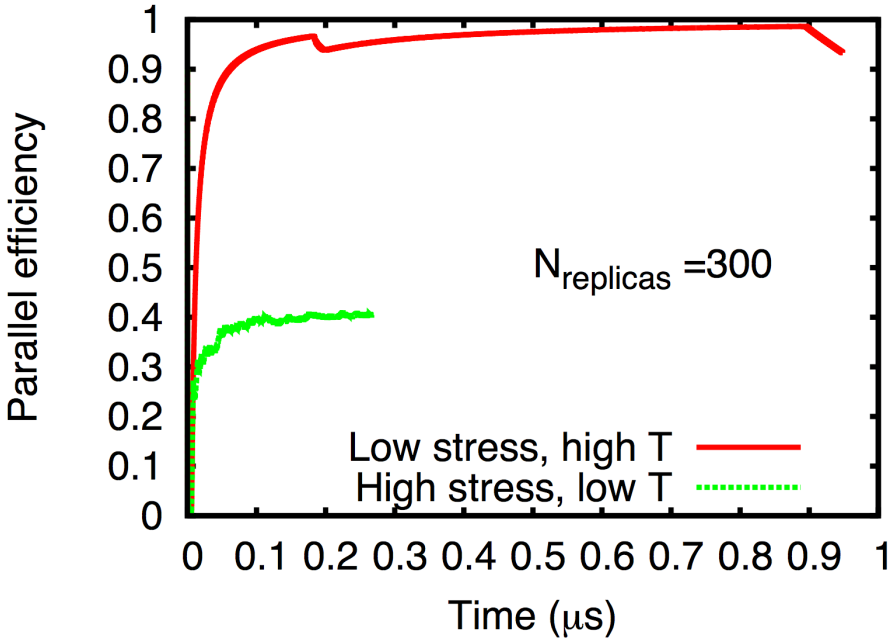


Speed-up obtained over direct MD





- States detected ***on-the-fly*** by Koopman-ParRep

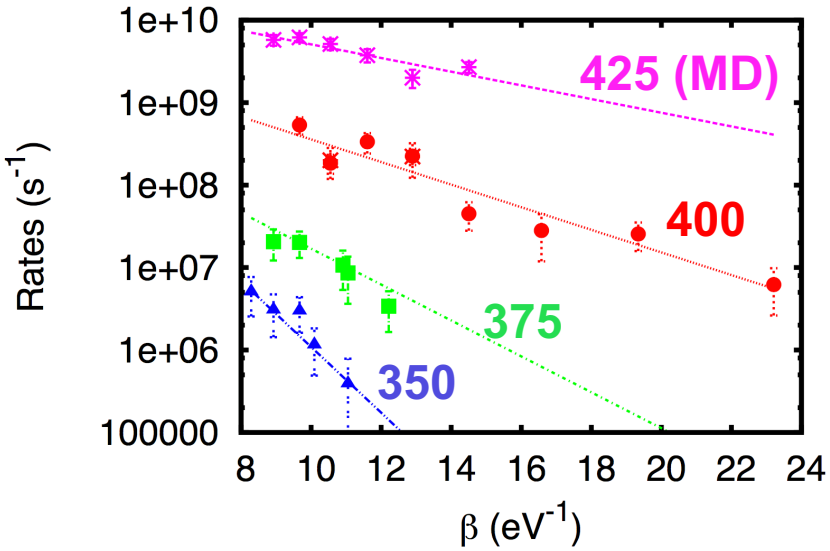


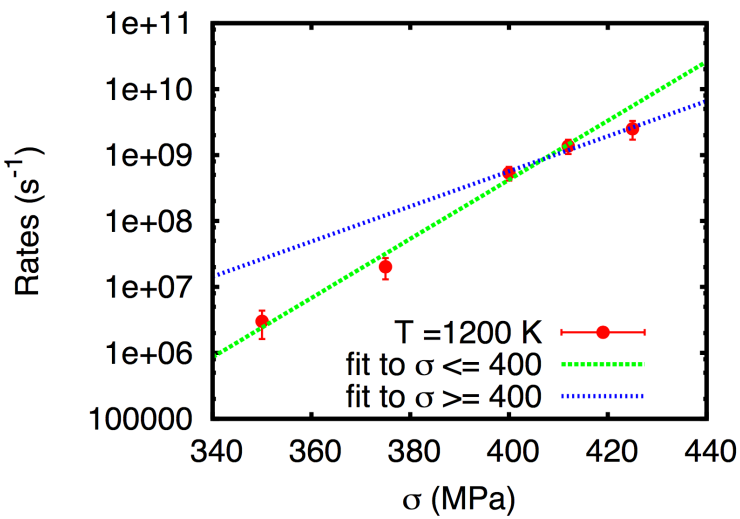
- Speed-up = Parallel efficiency × $N_{replicas}$

✓ Good parallel efficiency in these simulations (≈113,000 atoms, 1 fs timestep)

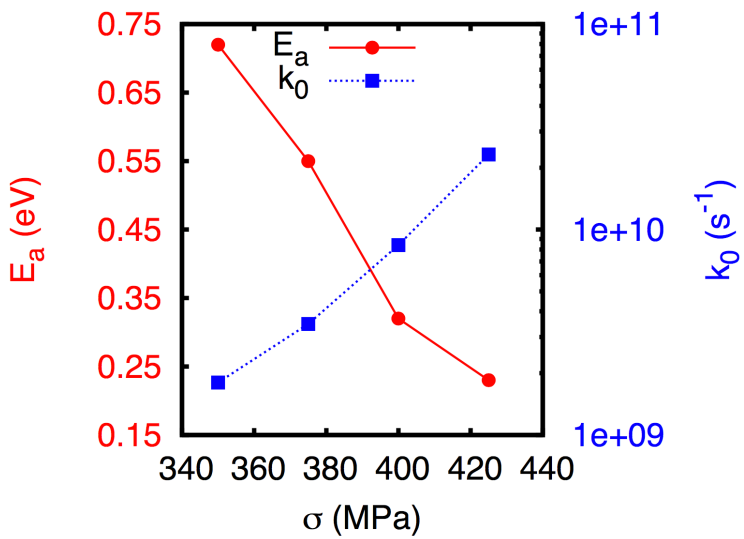
✓ Enable *μs* simulations

Bridging to meso-scale models





- ✓ Rates span over 4 orders of magnitude
- ✓ Strong dependence on the applied stress



- ✓ Stress-dependent activation energy/volume to inform meso-scale models

Thank you