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Hyperdynamics Method

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Collaborators: Danny Perez and Art Voter (LANL)

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Computation and Theory of Soft Matter
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CCR
Center for Computing Research

Sandia National Laboratories

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NNSA
National Nuclear Security Administration

What is hyperdynamics (HD)

- **Accelerated time method** for MD
  - *Voter, J Chem Phys, 106, 4665 (1997)*
  - bias the PE surface to enable more rapid transitions
  - time-accurate speed-up of a single trajectory
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  - variant: apply bias to only one pair of atoms (bond)
- **Local** hyperdynamics
  - *Kim, Perez, Voter, J Chem Phys 139, 144110 (2013)*
  - **global**: bias one bond in entire system each timestep
  - **local**: bias multiple bonds separated by $R_{cut} = 10$ Å
  - tested correctness for simple, small systems
  - accelerated event rates match theory and experiment
  - biasing pairs of atoms $\Rightarrow$ **multi-atom events**

What kind of systems can benefit from HD

- Key **requirements**:
  - system with distinct energy basins (solids, not soft matter)
  - equilibrium MD with rare transitions from one basin to another
- Effective speed-up can be **orders of magnitude**
  - especially for high barriers and low temperatures
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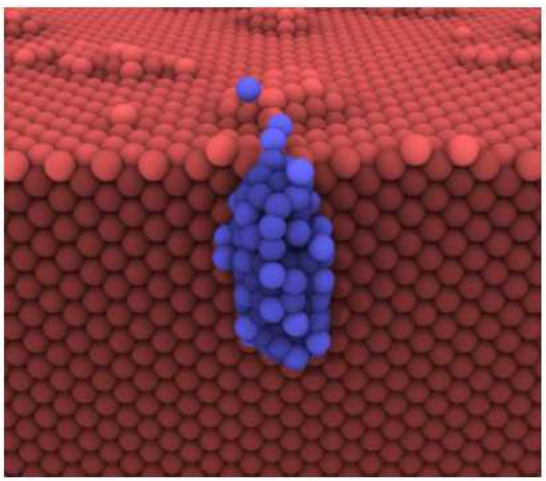
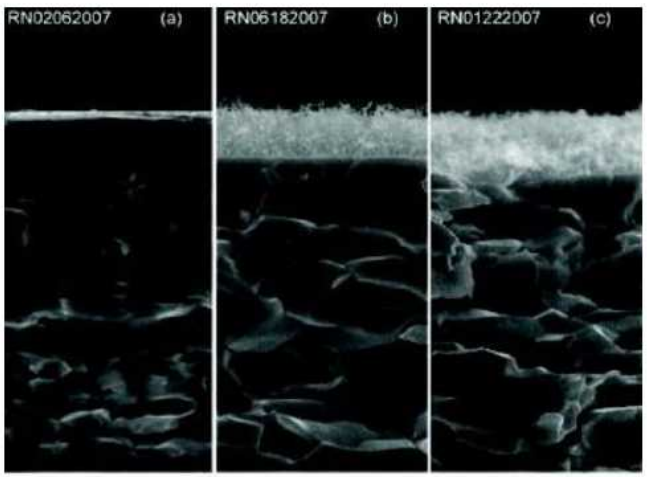
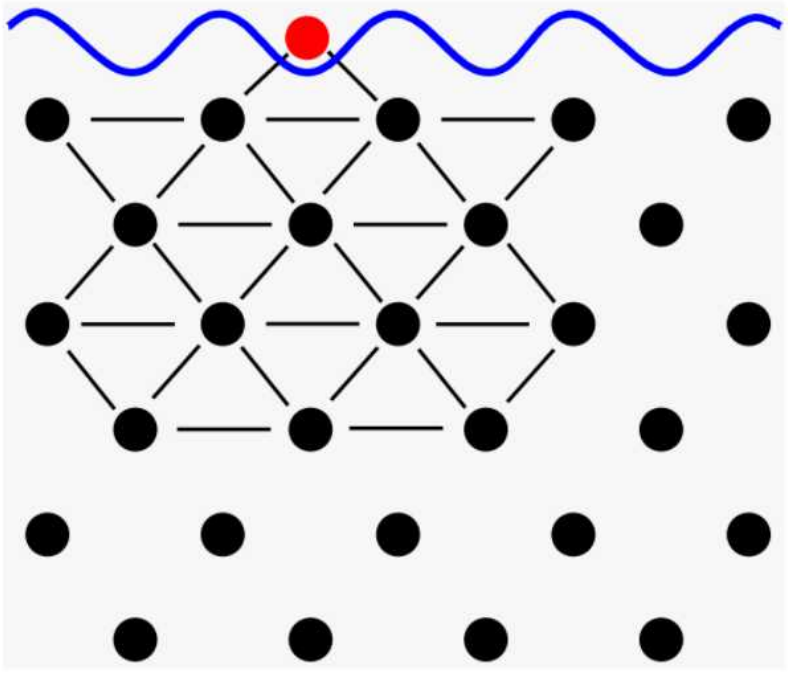




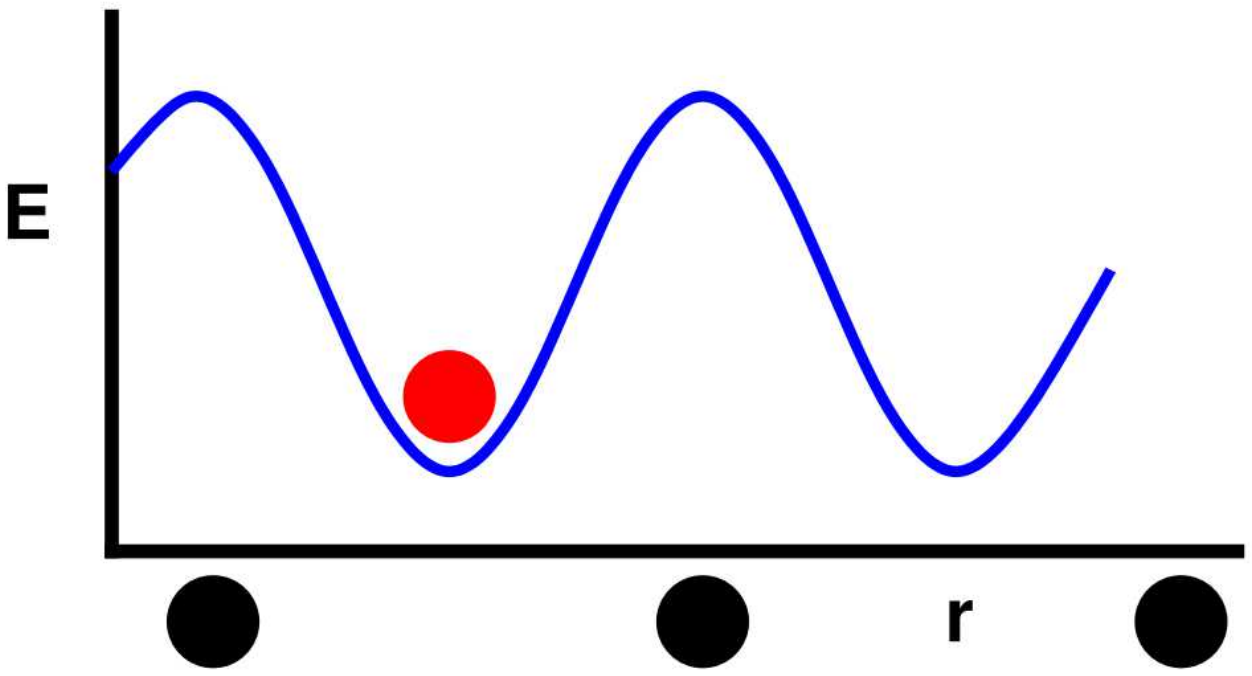
- DOE project to model materials in fission/fusion reactors
- **ITER**: degradation of W surfaces exposed to He plasma
- Due to sub-surface He bubbles producing nanoscale **fuzz**

Pictorial view of hyperdynamics

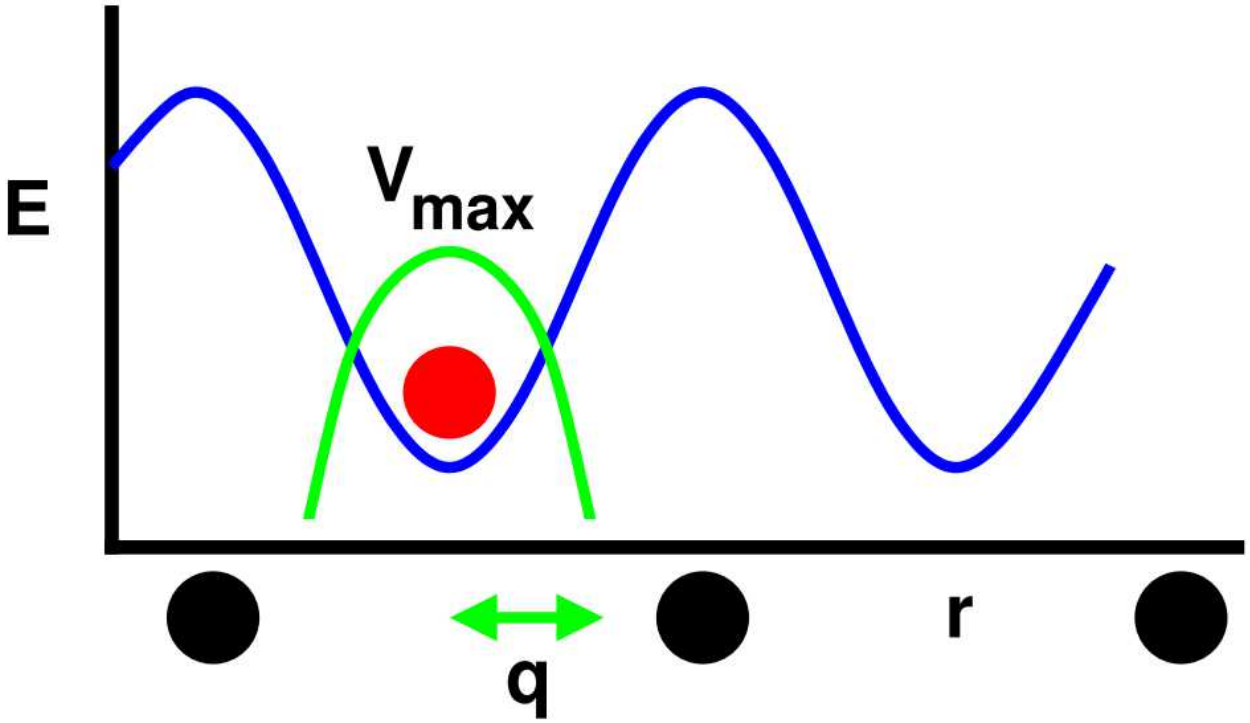


- Corrugated energy landscape for **adatom surface diffusion**
- Define (conceptual) **bonds** between all pairs of nearby atoms
  - e.g. $\sim$12 nearest neighbors per atom in fcc lattice

Zoom in to one adatom on surface

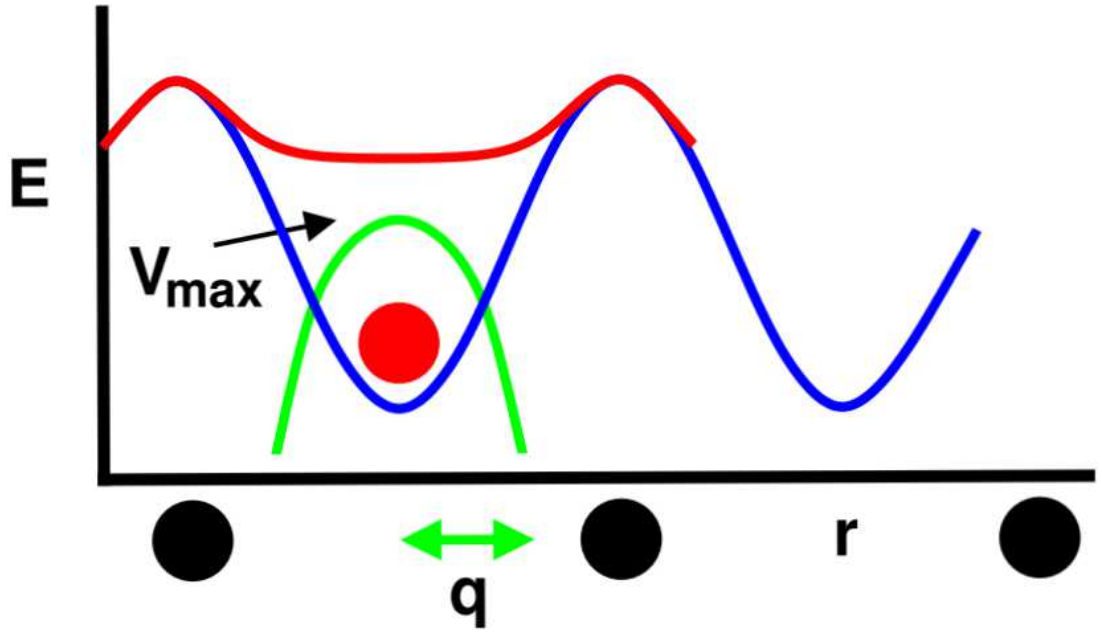


Added bias potential



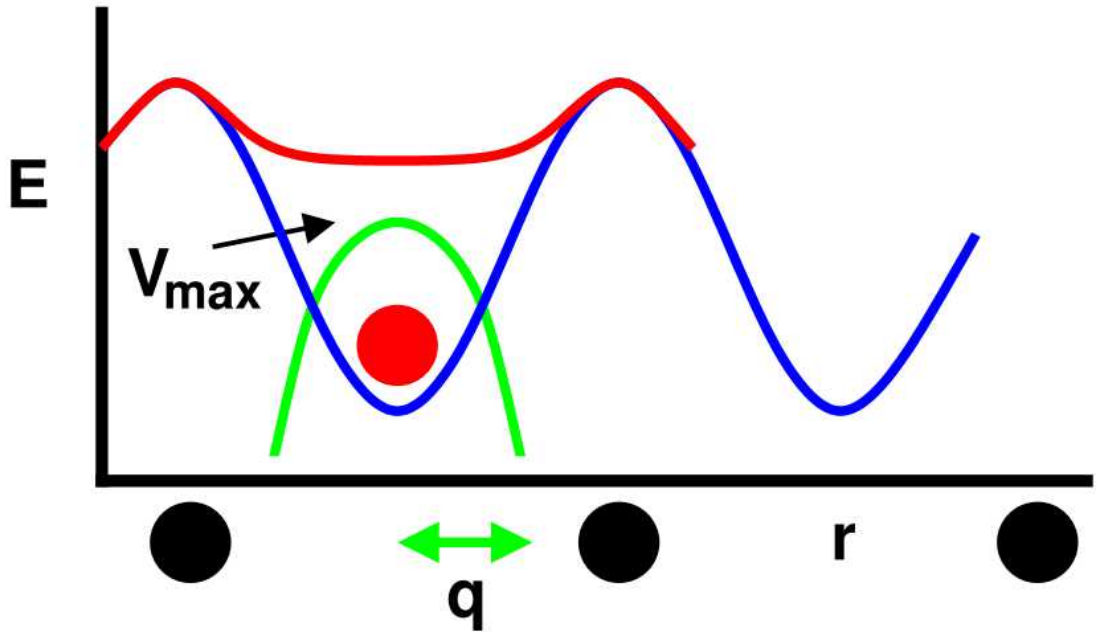
- Bond strain: $\epsilon_{ij} = (R_{ij} - Ro_{ij})/Ro_{ij}$
- Add **bias potential** to only the max-strain bond
- Bias: $V_{ij} = V_{max}[1 - (\epsilon_{ij}/q)^2], \quad |\epsilon_{ij}| < q, \quad \text{else} \quad$ **zero**
- **Different bond** may be biased at each timestep

Resulting potential energy surface



- Shallow well $\Rightarrow$ **faster transition** by I,J (and nearby) atoms

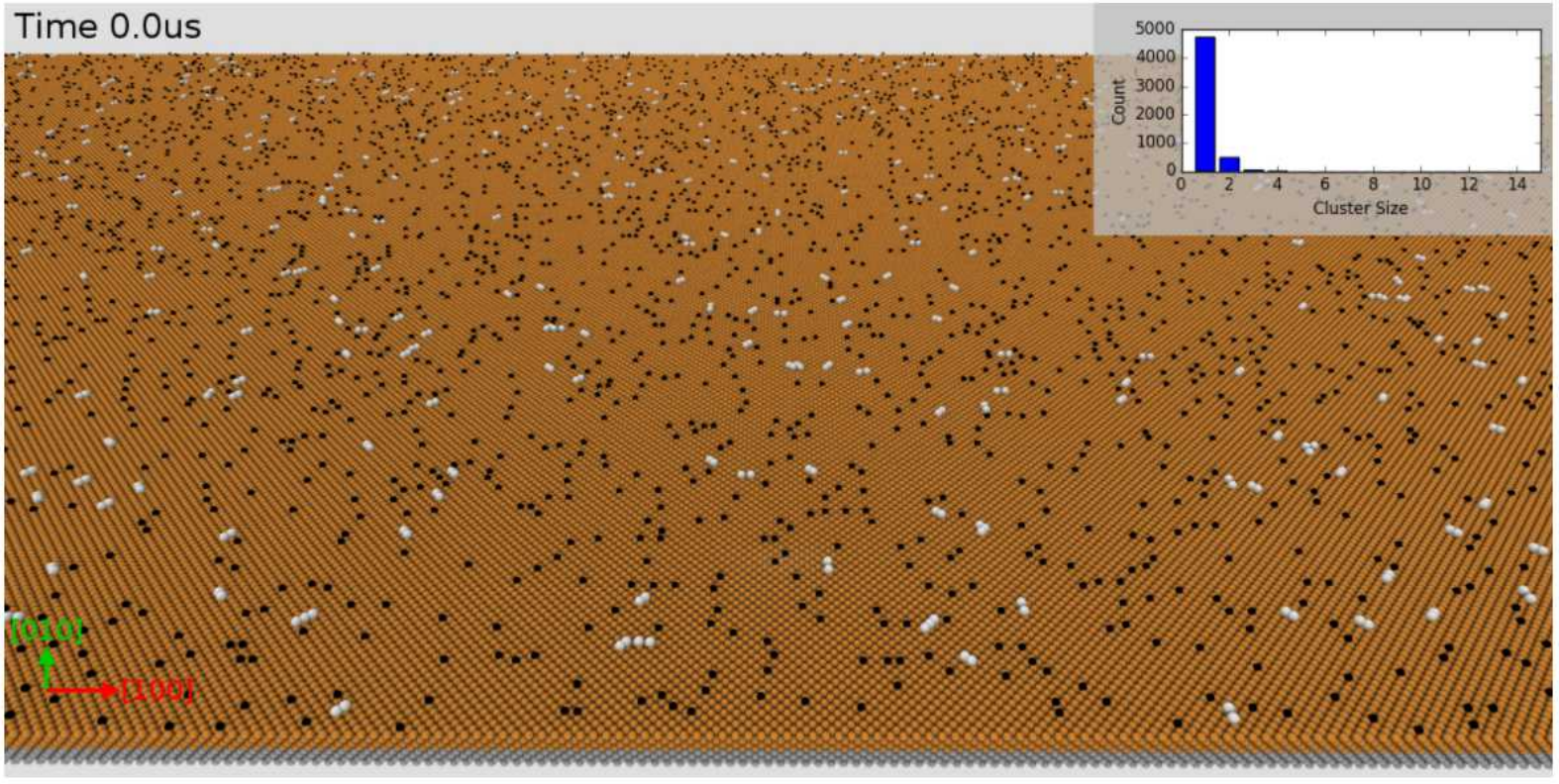
Resulting potential energy surface



- Shallow well $\Rightarrow$ **faster transition** by I,J (and nearby) atoms
- Must choose V_{max} and q carefully:
  - if: zero bias at dividing surfaces (Q), no local minima (V_{max})
  - if: do not induce correlated events that violate TST
  - then: relative transition rates not altered for competing events
  - then: trajectory is **time-accurate** (unlike enhanced sampling)
  - then: quantifiable **time boost factor** each timestep

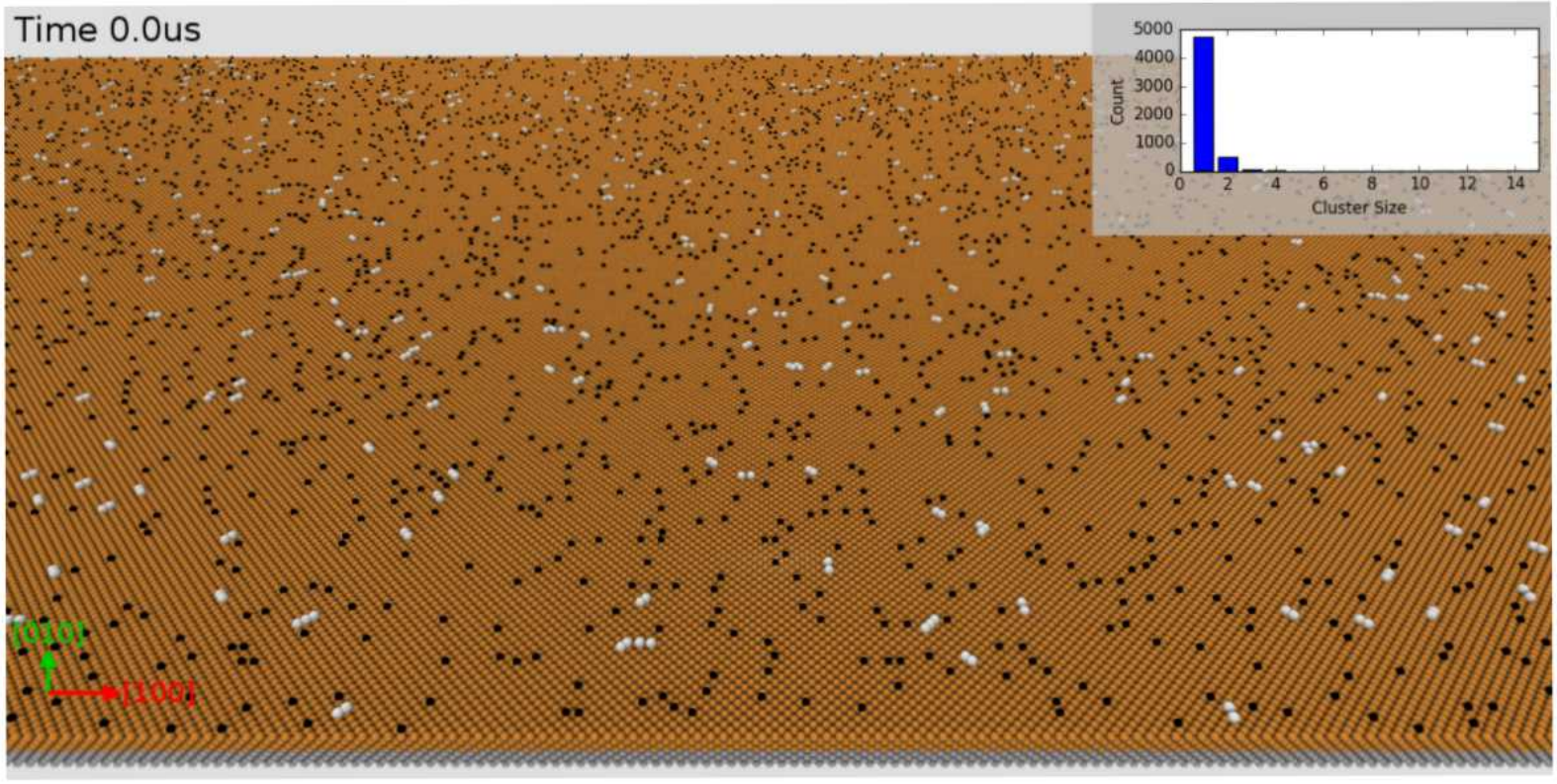
Surface diffusion modeling

- Pt (100) surface with 4% adatom coverage (random)
- EAM: hop barrier = 1.25 eV, exchange barrier = 0.64 eV
- HD: V_{max} = 0.4 eV, T = 400K ⇒ **4000x boost**
- **1.2M** atoms, 50M timesteps ⇒ **1 ms** of real time
- **48 hr run** on 128 Broadwell nodes (4K cores)



What movie will show

- Biasing ~**3000** bonds each timestep, ~**400K** diffusion events
- Versus 100 events with MD (one event per 60 adatoms)
- Rich variety of events occur naturally, no *a priori* insight
- **Cluster formation**, monitored by size histogram



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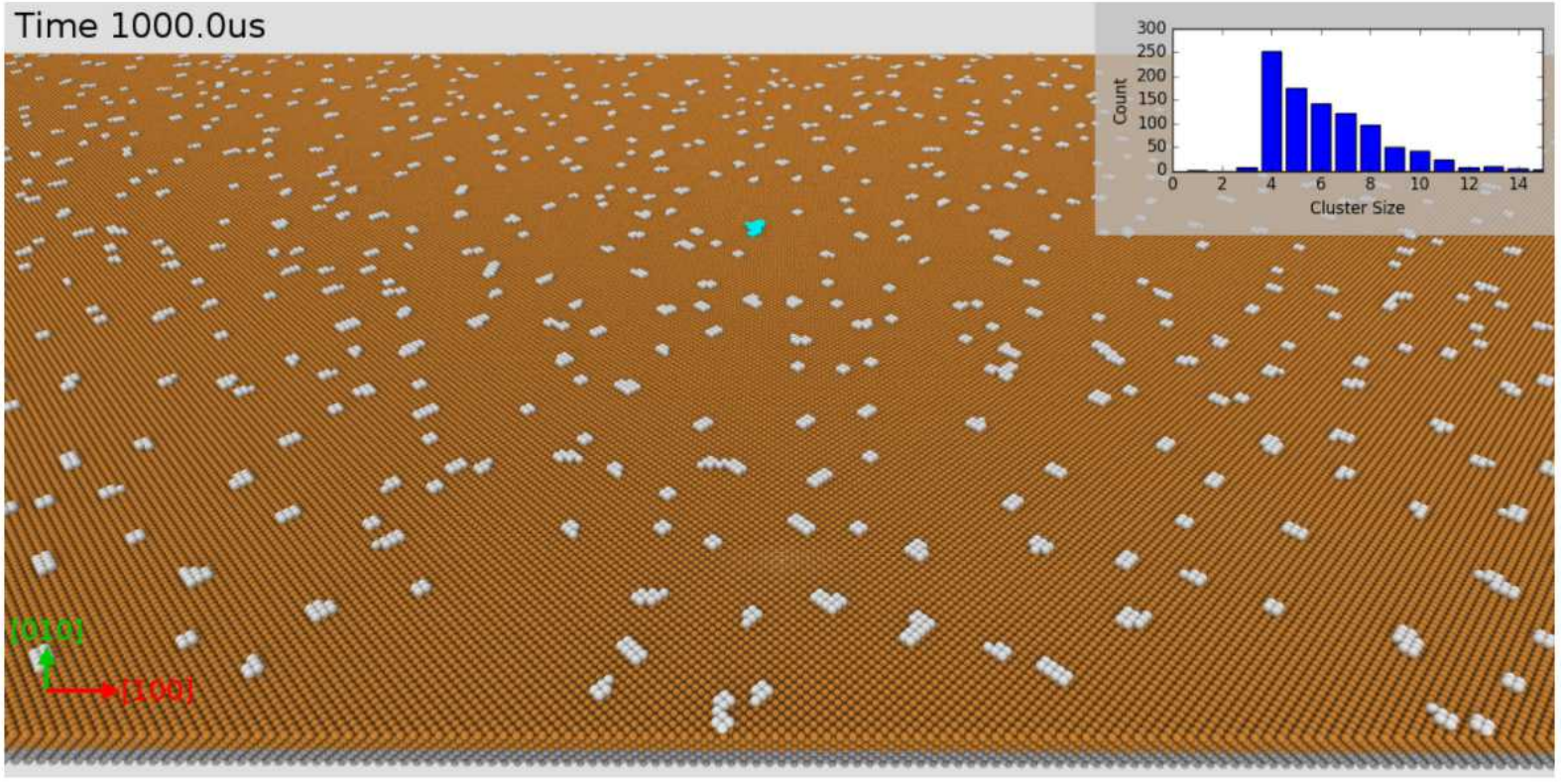
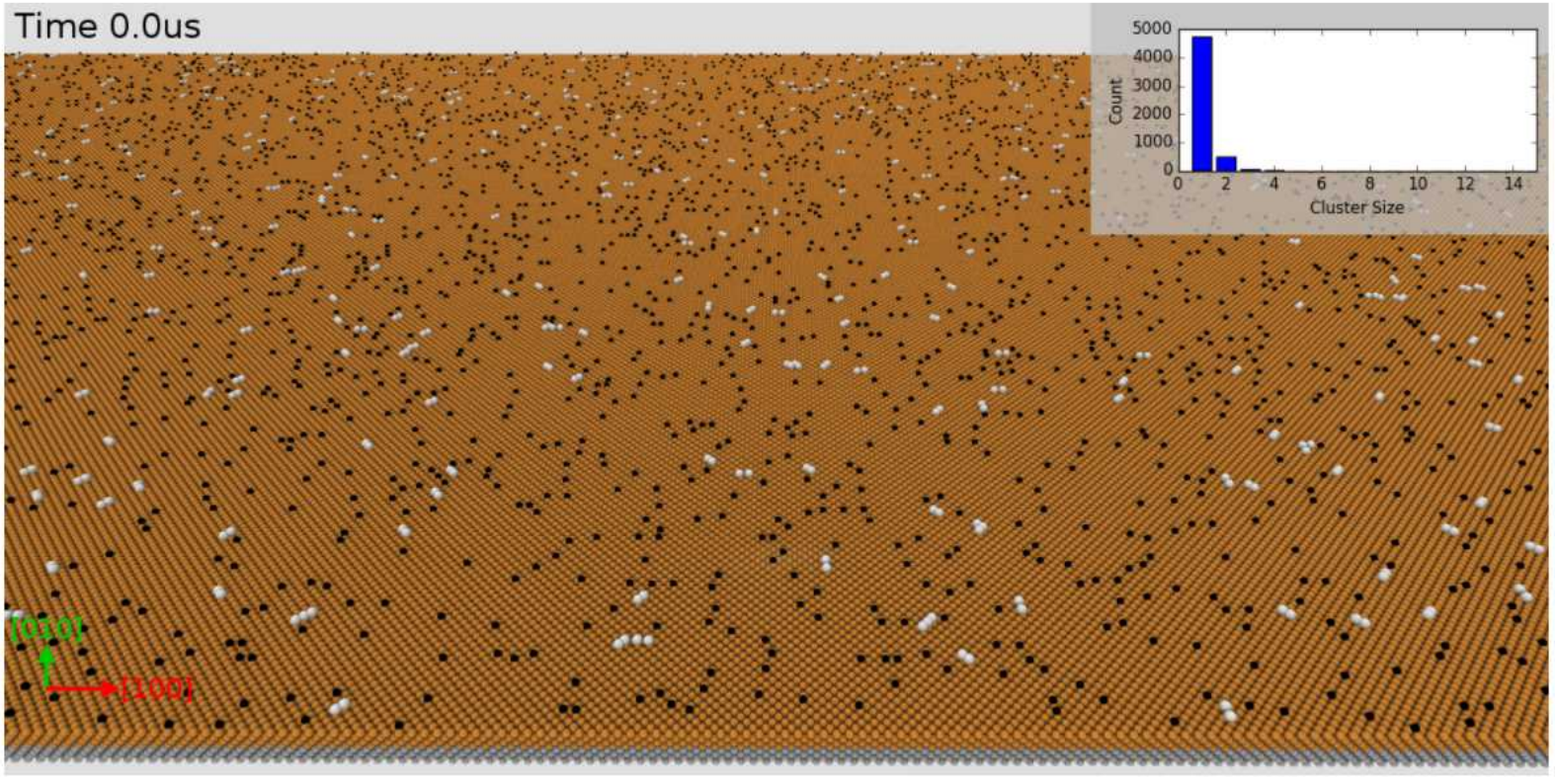


Movie

- Not just adatom motion, **substrate atoms** part of every event
- Mobile monomers, dimers, trimers
- Two stages of movie, two speeds
- Larger clusters are immobile, except around perimeter



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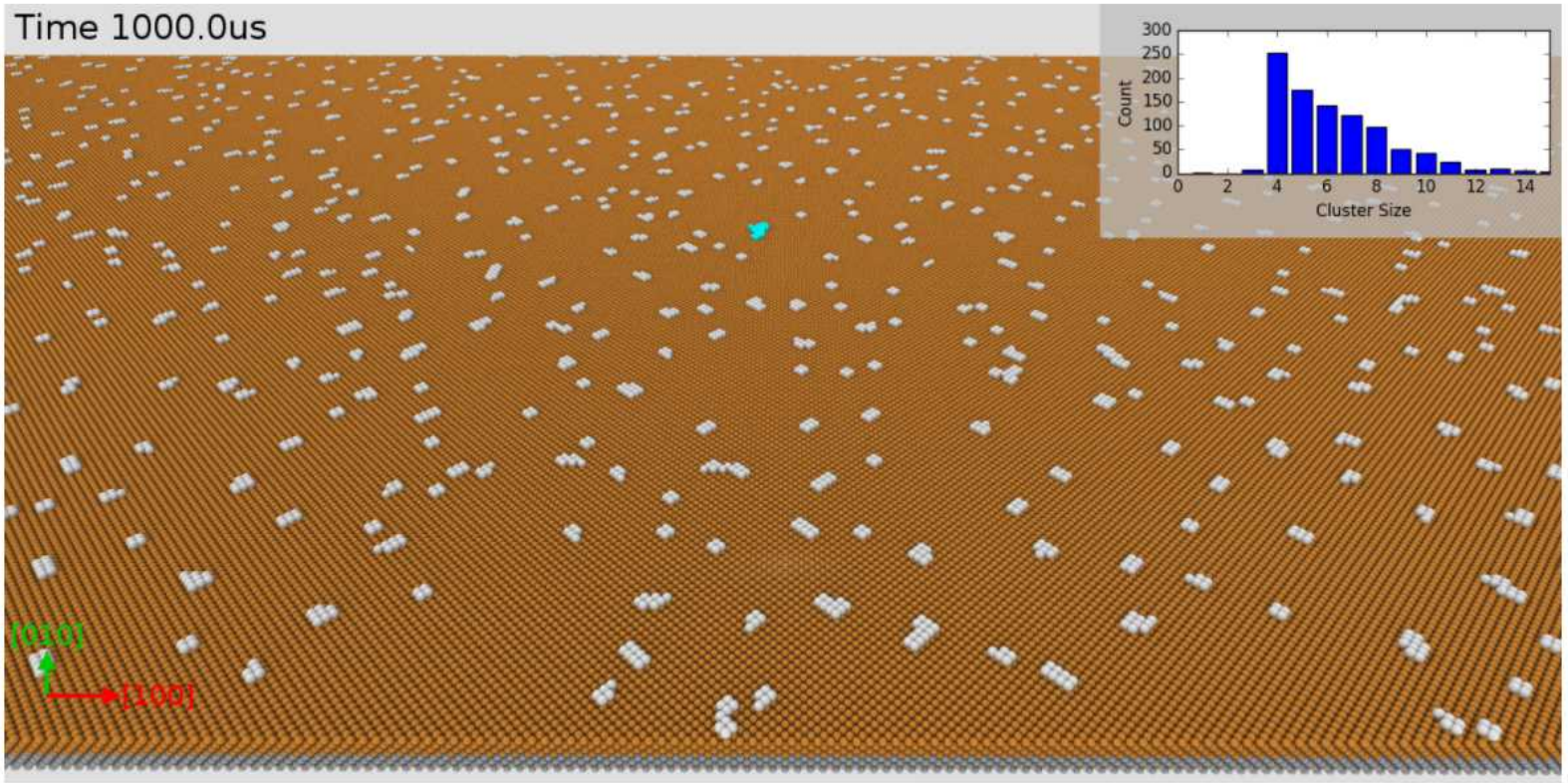

- **OVITO** help: thanks to Mitch Wood (Sandia)

Running a HD simulation in an MD code

Via new **hyper** command in LAMMPS

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Via new **hyper** command in LAMMPS

- Choose V_{max}, q, **T**, and B_{target}
- Save initial quench state of system
- Loop:
  - run 100 steps of **MD** with Langevin thermostat
    add **HD bias** at every step to select atom pair(s)
  - save dynamic state
  - perform **quench**
  - check if any **events** occurred (relative to previous quench)
  - if yes:
    archive event info
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    recreate bond list = I,J pairs, equilibrium R_0
  - restore dynamic state

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Usual **parallel** MD and quench (spatial partitioning of atoms)

Extra operations and data for computing HD bias

- Bias **every bond** that is local max-strain bond within R_{cut}
- R_{cut} = distance at which one event influences another
- $\sim$2x cutoff for EAM = 10 Å $\Rightarrow$ **700** neighbor bonds/bond

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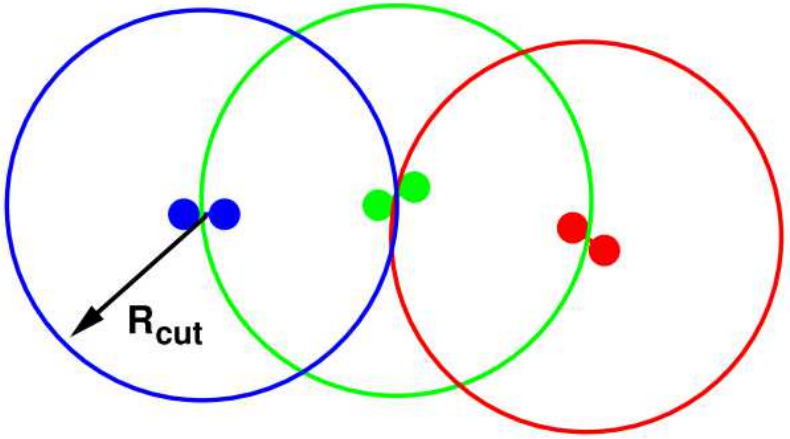

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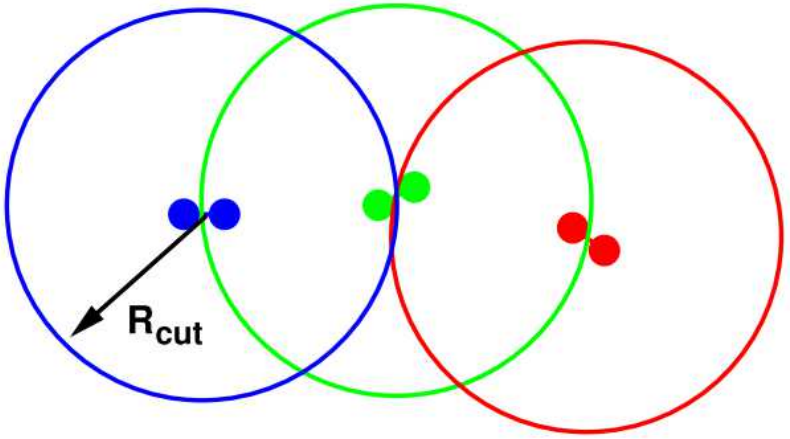
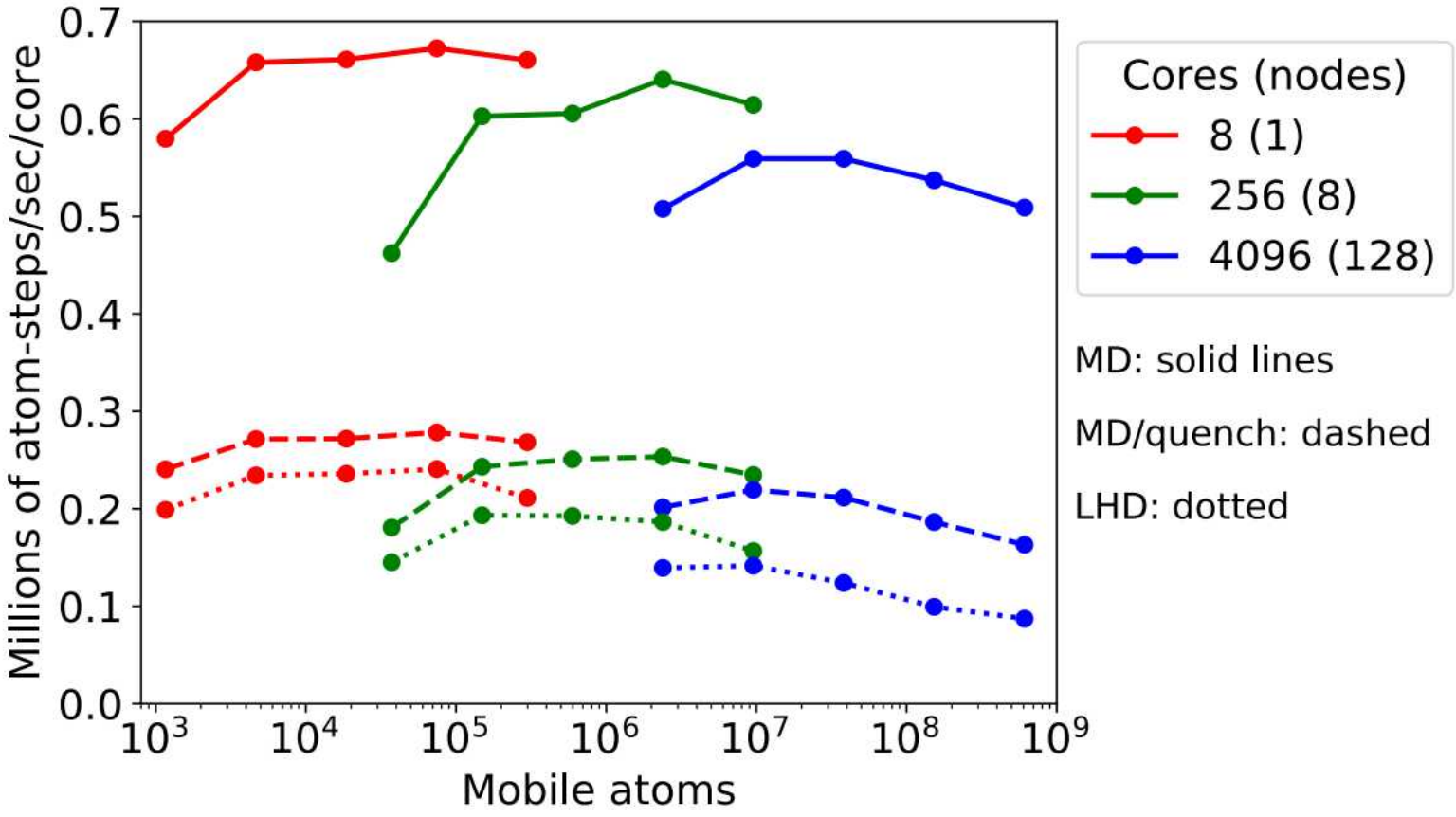


- Create and loop over **2nd neighbor list** out to R_{cut}
- **Communication** to acquire strain info for ghost atoms

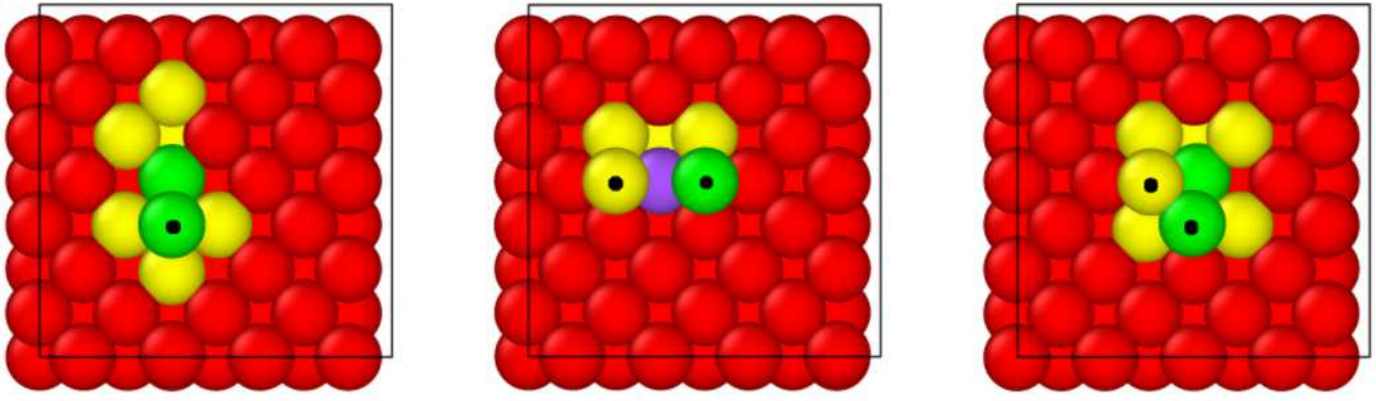
Parallel scaling for local HD is similar to MD



- For cheap EAM, HD is ~**3-5x** more expensive than MD
- Majority is careful **quench**, rest is comp/comm out to **Rcut**

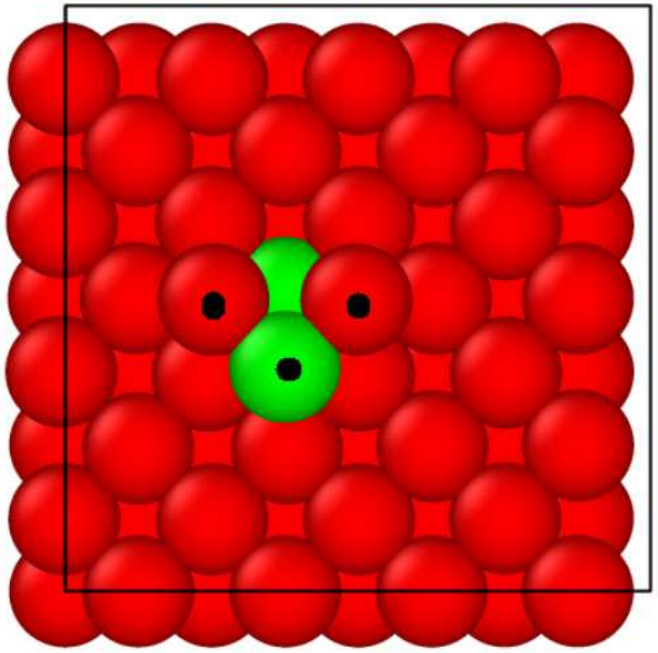
Exchange event and dimer diffusion

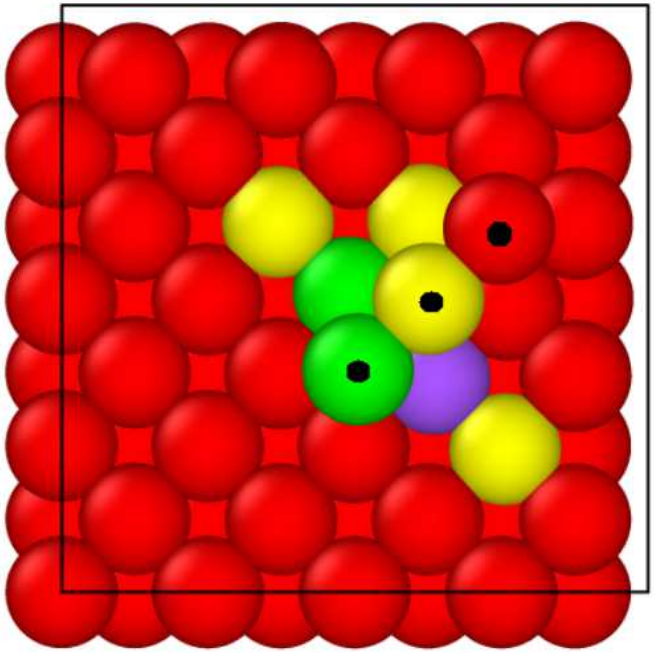
Green: atom moves > 1.0 Å during event
Purple: > 0.2 Å, **Yellow**: > 0.1 Å, **Red**: < 0.1 Å



Exchange barrier = **0.656 eV**, hop barrier = 1.25 eV (too high)
Hop barrier when next to another adatom = **0.635 eV**
Successive exchanges enable **dimer diffusion**

Trimer duck-under and bend





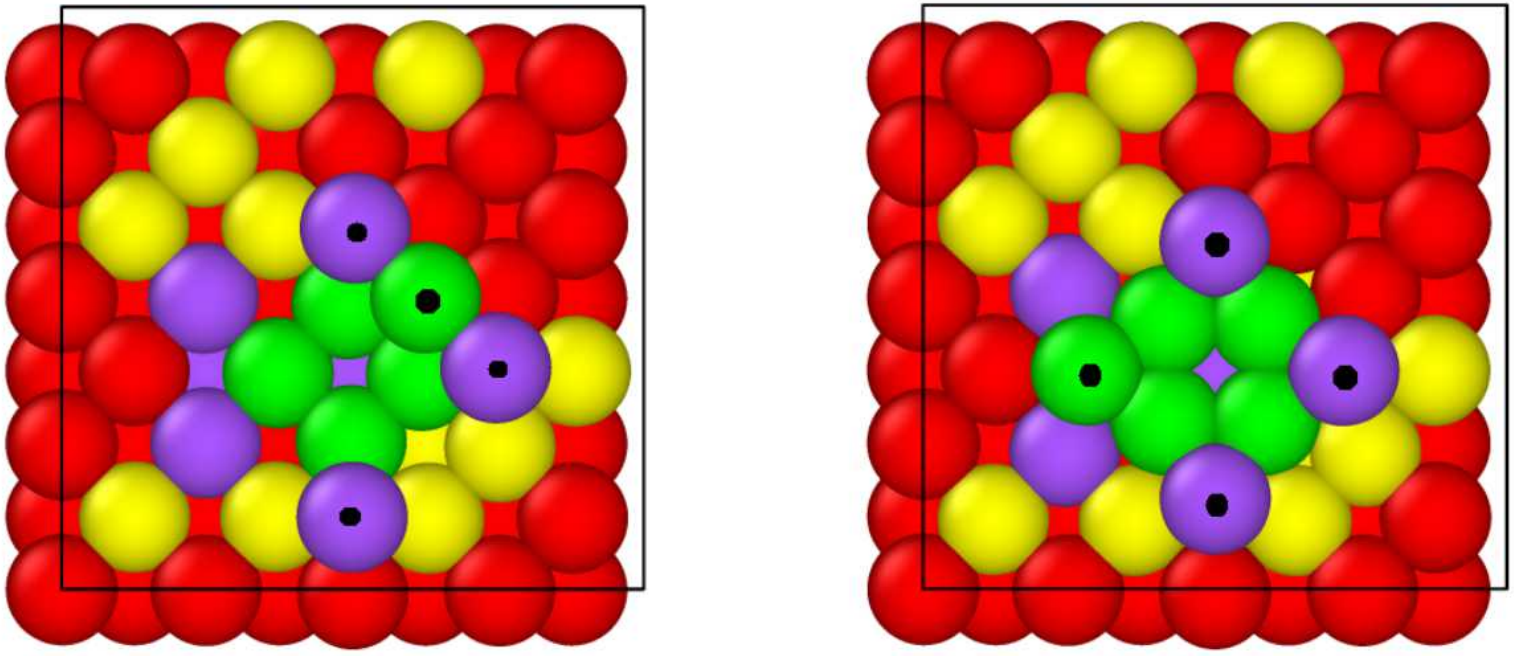
Duck-under barrier = 0.41 eV, bend = 0.67 eV

Lowest barrier event, recall we chose $V_{max} = 0.4$ eV

Successive bends & un-bends enable **trimer diffusion**

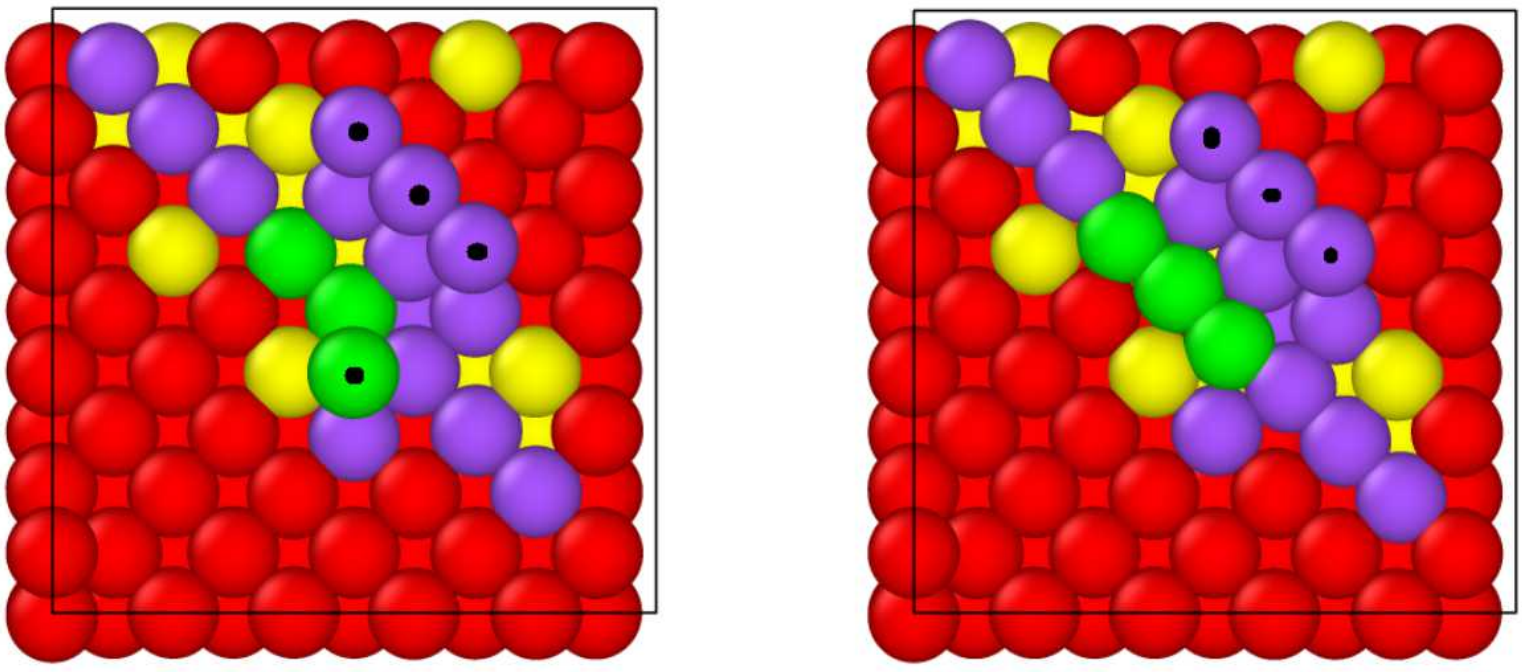
Flower formation event

Highly technical name!



Barrier = 0.772 eV, when adatom is near a linear trimer
Reverse event can result in **long-distance trimer move**

Crowdion event



Barrier = 0.771 eV (induced by nearby trimer)

Reverse event can displace adatom by 2 lattice sites in (110)

Hyperdynamics summary

Key points:

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Lower temperatures for $V_{max} = 0.4$ eV:

- 400K $\Rightarrow$ 4000x boost $\Rightarrow$ 50M steps $\Rightarrow$ 1 ms
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Challenges:

- Can we perform cheaper quenches
- Often do not know all barrier heights *a priori*
  - allowed time boost is function of current lowest barrier height
  - **ideal**: on-the-fly adaptation of T_{boost}, V_{max}, q

Thanks and links

- Funding from DOE **exascale computing program** (ECP)
- EXA**ALT** = exascale atomistics for accuracy, length, time

- LAMMPS MD package: **http://lammps.sandia.gov**
  - hyper command in REPLICA package, examples/hyper