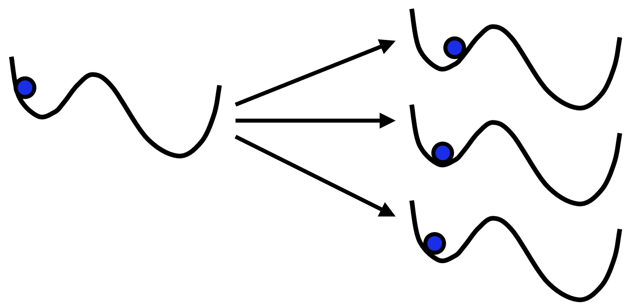
Parallel Replica Dynamics



A very brief introduction

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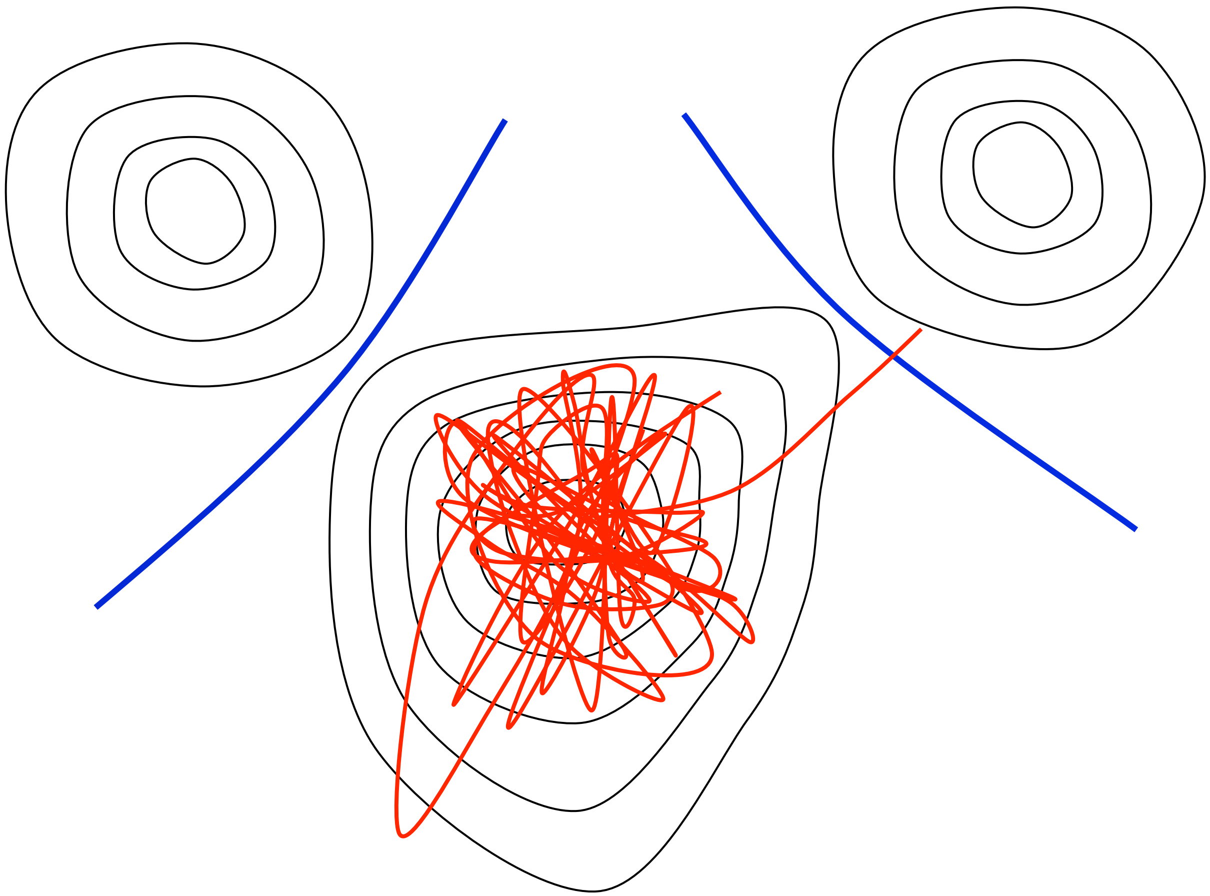
DOE/BES, LANL LDRD, DOE/ASCR, DOE/SciDAC

Parallel Replica Dynamics



The system vibrates in 3-N dimensional basin many times before finding an escape path. Using many trajectories in parallel, we can find a correct escape event more quickly. (I.e., the probability for escaping along a certain path should be proportional to the rate constant for that path.)

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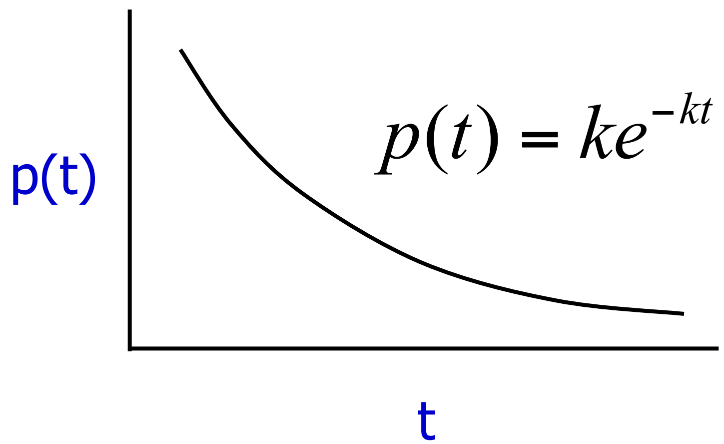
Parallel Replica Dynamics

Parallelizes time evolution

Assumptions:

- infrequent events
- exponential distribution of first-escape times



AFV, Phys. Rev. B, 57, R13985 (1998)

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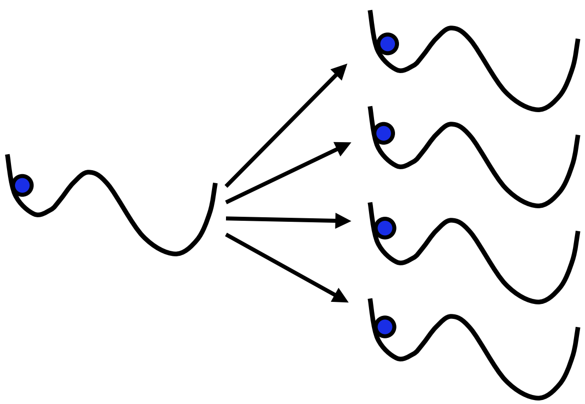
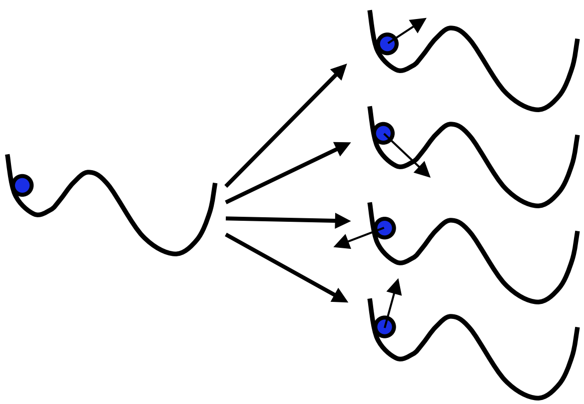
Parallel Replica Dynamics Procedure

Replicate entire system on each of M processors.



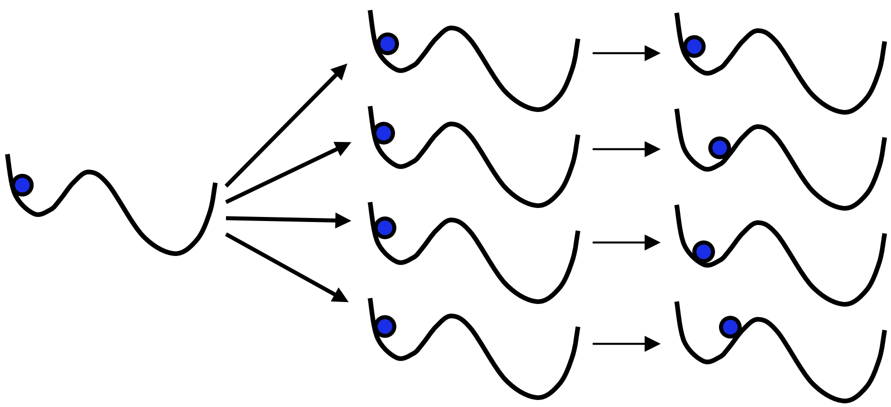
Parallel Replica Dynamics Procedure

Randomize momenta independently on each processor.



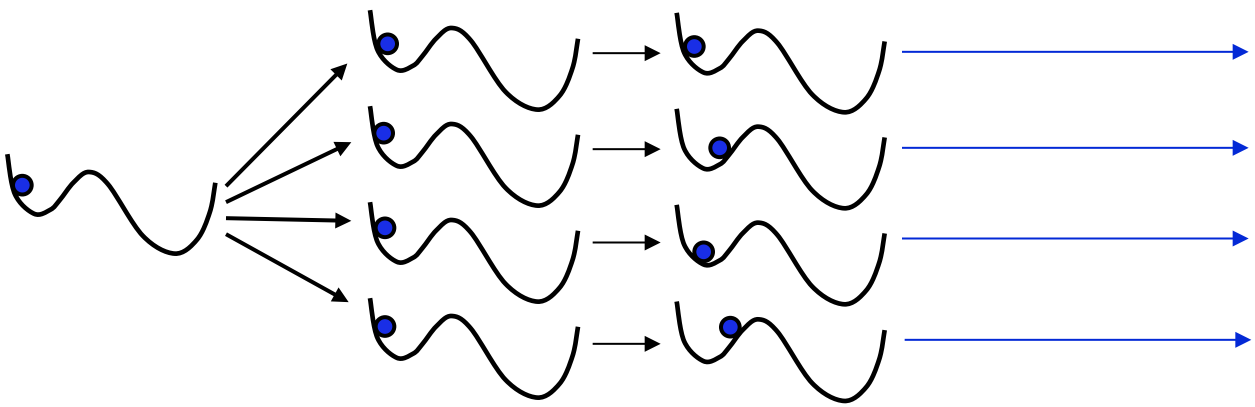
Parallel Replica Dynamics Procedure

Run MD for short time ($\tau_{dephase}$) to dephase the replicas.



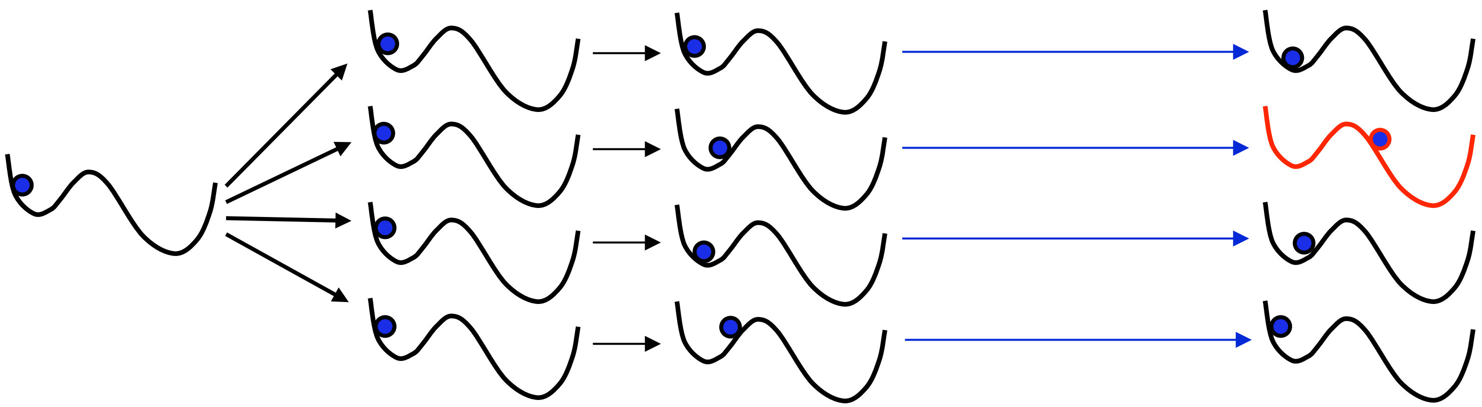
Parallel Replica Dynamics Procedure

Start clock and run thermostatted MD on each processor.
Watch for transition…



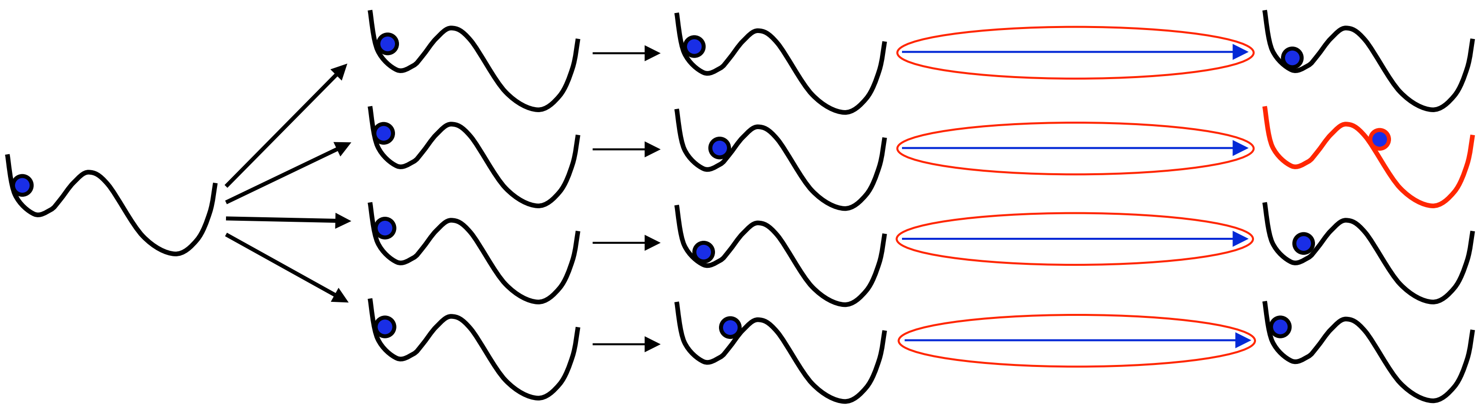
Parallel Replica Dynamics Procedure

Stop all trajectories when first transition occurs on *any* processor.



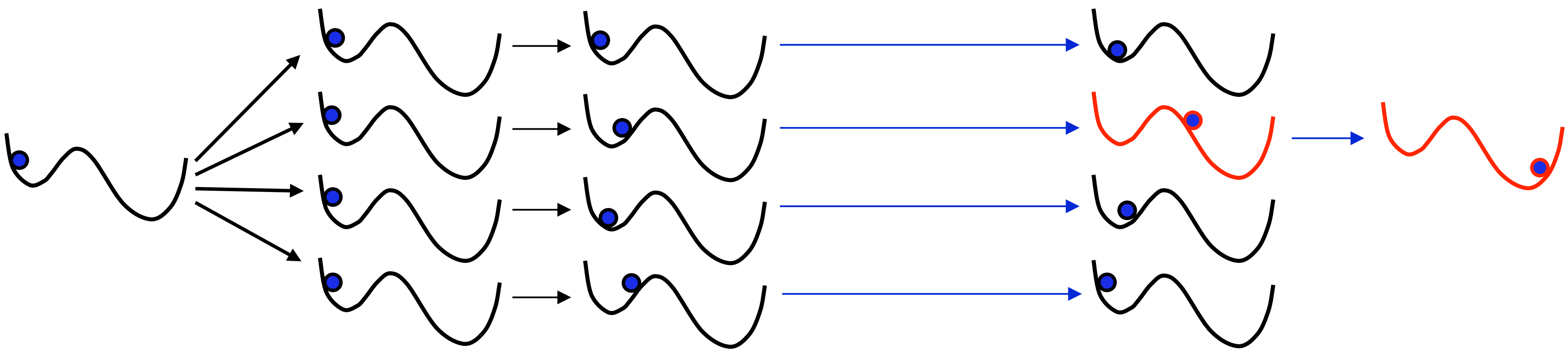
Parallel Replica Dynamics Procedure

Sum the trajectory times over all M processors. Advance simulation clock by this t_{sum}



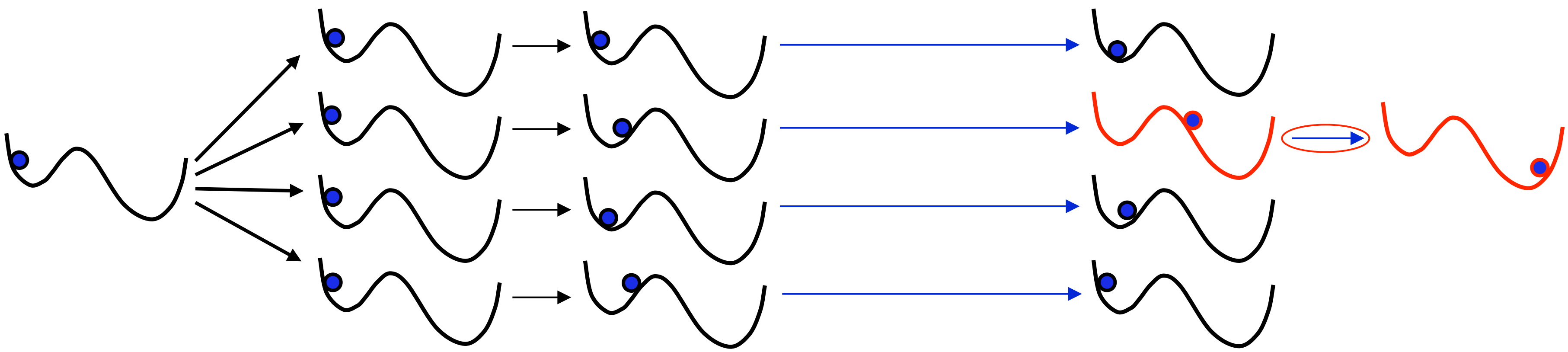
Parallel Replica Dynamics Procedure

On the processor where a transition occurred, continue trajectory for a time τ_{corr} to allow correlated dynamical events.



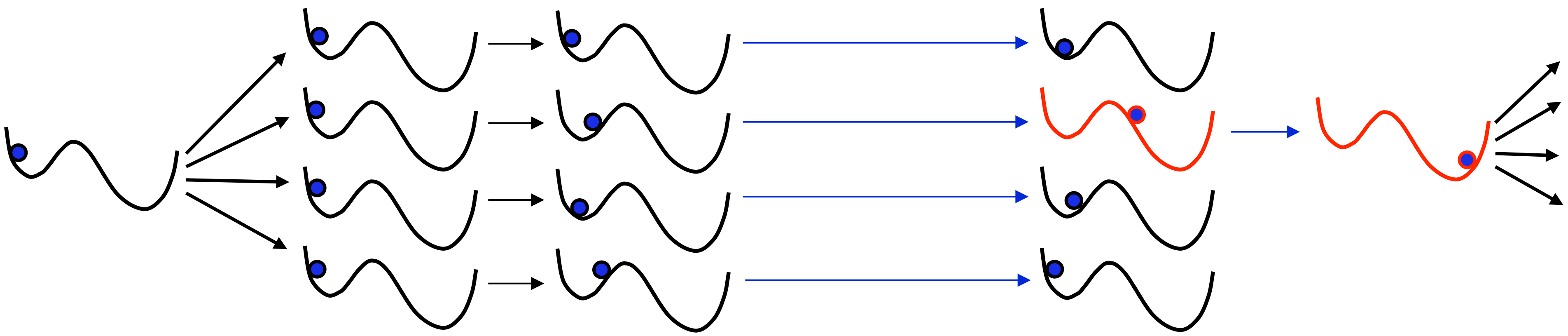
Parallel Replica Dynamics Procedure

Advance simulation clock by τ_{corr}.

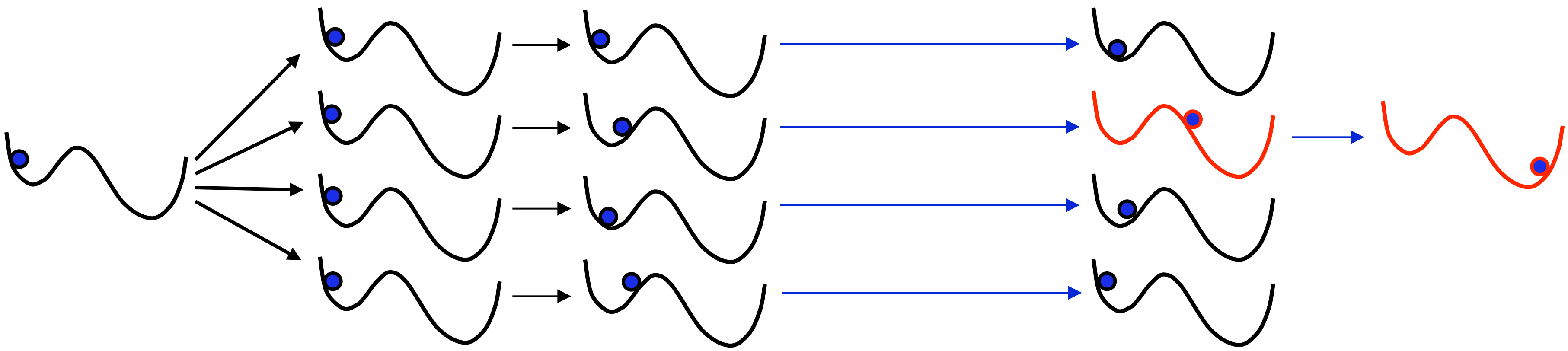


Parallel Replica Dynamics Procedure

Replicate the new state and begin procedure again.



Parallel Replica Dynamics



The summed time (t_{sum}) obeys the correct exponential distribution, and the system escapes to an appropriate state.

State-to-state dynamics are thus correct; τ_{corr} stage even releases the TST assumption [AFV, Phys. Rev. B, 57, R13985 (1998)].

Good parallel efficiency if τ_{rxn} / M >> $\tau_{dephase}$+τ_{corr}

Applicable to any system with exponential first-event statistics

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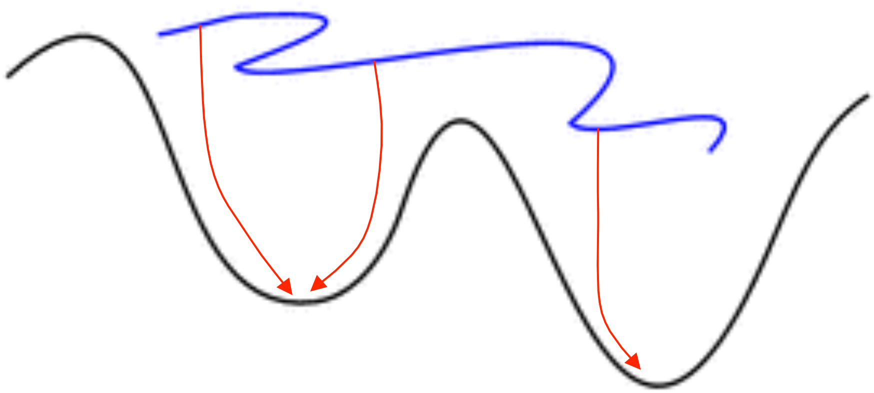
Detecting a transition

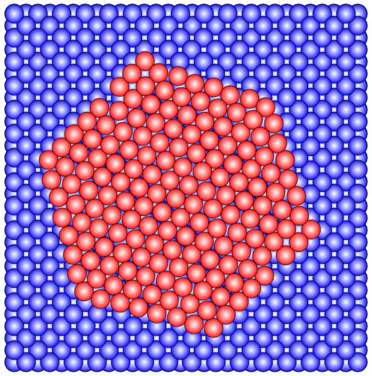
- best method depends on the system

- simple method for EAM metal systems:
  periodically perform steepest-descent quench;
  see if geometry at basin minimum has changed

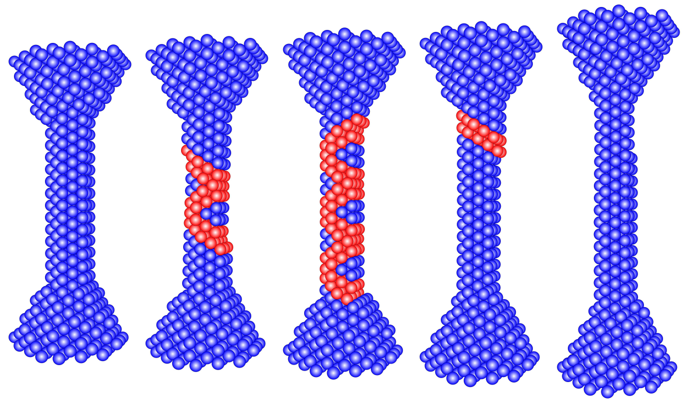


- can also use:
  - change in bond connectivity (Kum, Uberuaga)
  - change in local order parameter

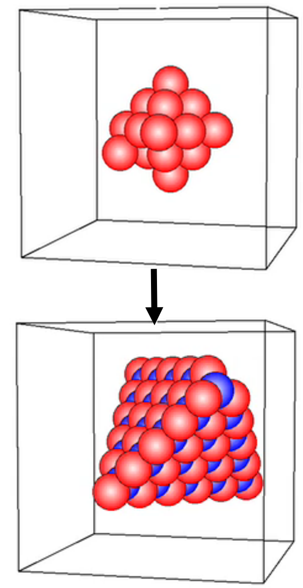
Examples of ParRep studies



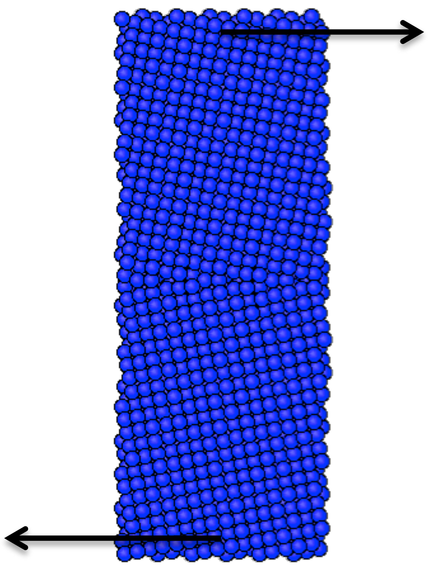
Ag_{169}/Cu(100), magic cluster, Uche et al, 2009.



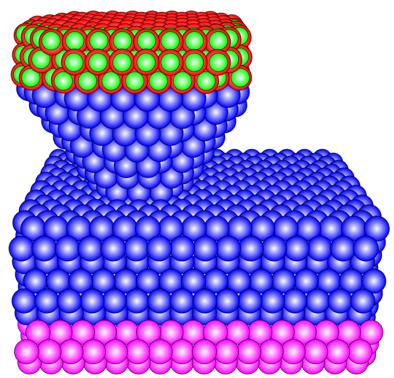
Ag nanowire stretch, μs - ms, Perez et al.



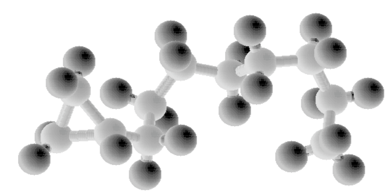
Cu void collapse to SFT, μs, Uberuaga et al, 2007.



Driven Cu GB sliding, 500 μm/s Mishin et al, 2007.



Friction force microscopy, Dong et al, 2009, 2010, 2011.



Hexadecane pyrolysis, μs, Kum et al, 2004.

Recent brief AMD review: Perez et al, Ann. Rep. Comp. Chem. **5**, 79 (2009)

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