Parallel Replica Dynamics
New LAMMPS features briefs
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The PRD Method

Invented by Art Voter:

A. F. Voter, "Parallel replica method for dynamics of infrequent events", *Phys Rev B* **57** **1**3985 (1998) (146 citations up to Feb 2010)

Core Idea:

- Many atomistic simulations are characterized by long periods of localized virbration within a basin, punctuated by brief transitions between basins

- We assume the transitions between basins occur randomly (Markovian, Poisson process, first-order kinetics.) Then t_{ij}, the time spent in state i until a transtion to state j, obeys the follow probability law:

$$P(t_{ij} > t) = \exp(-k_{ij}t)$$

- If we run R independent simulations, the probability law becomes:

$$P(t_{ij}^1, \ldots, t_{ij}^R > t) = \prod_{r=1}^{R} P(t_{ij}^r > t) = \exp(-k_{ij}Rt)$$

- Hence, by running *R* independent replicas, the transition kinetics are conserved, but time is rescaled by a factor of *R*.

- This only works for first-order kinetics

The PRD Algorithm
(as implemented in LAMMPS by Mike Brown)

while (time remains):

   1. dephase for $N_{dephase}$ * $T_{dephase}$ steps

   2. until (event occurs on some replica):

      run dynamics for T_{event} steps

      quench and check for event on any replica

   3. until (no correlated event occurs):

      run dynamics for $T_{correlate}$ steps

      quench and check for event on this replica

   4. event replica shares state with all replicas

PRD in LAMMPS

Command Syntax

```
prd N t_event n_dephase t_dephase t_corr compute-ID seed
```

Example

```
prd   1000000 100 10 10 100 comp1 54982
compute         comp1 all event/displace 0.5
```
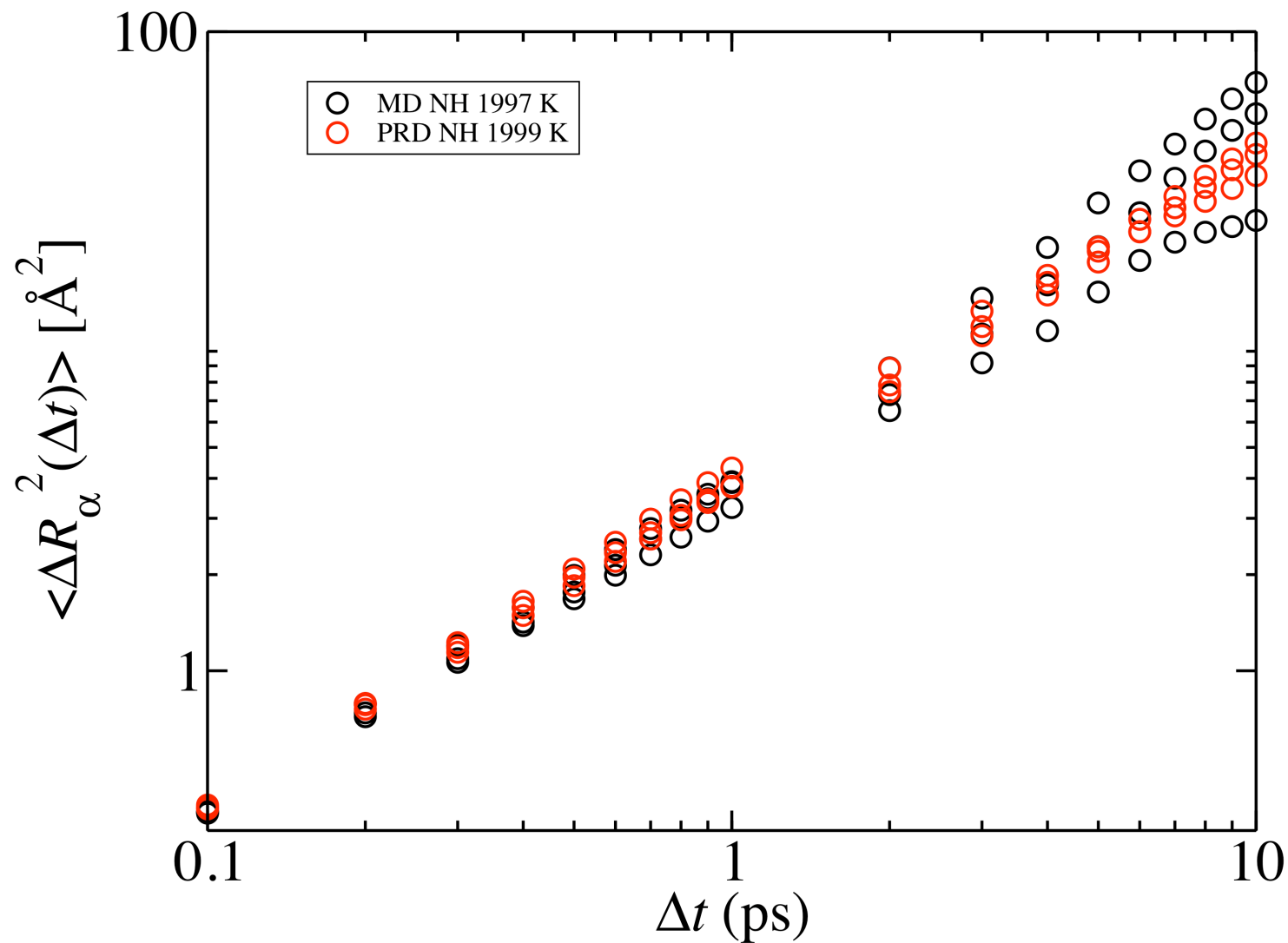
To run 128 replicas:

```
mpiexec -np 128 lmp_tbird -partition 128x1 -in in.si_prd
```

Test Problem: Vacancy Diffusion

- Created a single vacancy in a 4x4x4x8 Silicon crystal
- Ran 100 ps NVT MD at 2000 K using Stillinger-Weber potential
- Quenched every 0.1 ps and dumped atoms with coordination != 4
- From dump file, obtained $\mathbf{R}_{vac}(t)$, the vacancy "center-of-mass" as a function of time
- Ran PRD run style for 1 ns with 1 replica
- Important note: For PRD, the time given in the dump file is the timestep count for 1 replica, which is not a good measure of physical time. This is more accurately represented by the "clock time", reported for each event in the master log file.

Test Problem: Vacancy Diffusion

$\langle \Delta R_\alpha^{\,2}(\Delta t) \rangle$ [$\mathring{A}^2$]

Δt (ps)

- ○ MD NH 1997 K
- ○ PRD NH 1999 K

Test Problem: Vacancy Diffusion