SAND2010-1861P

Parallel Replica Dynamics

New LAMMPS features briefs

LAMMPS Users' Workshop @ CSRI

Thursday, Feb 25, 2010, 9:30 a.m.

Aidan Thompson

Sandia National Labs

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
```

E.g.

```
prd  1000000 100 10 10 100 comp1 54982
compute         comp1 all event/displace 0.5
```

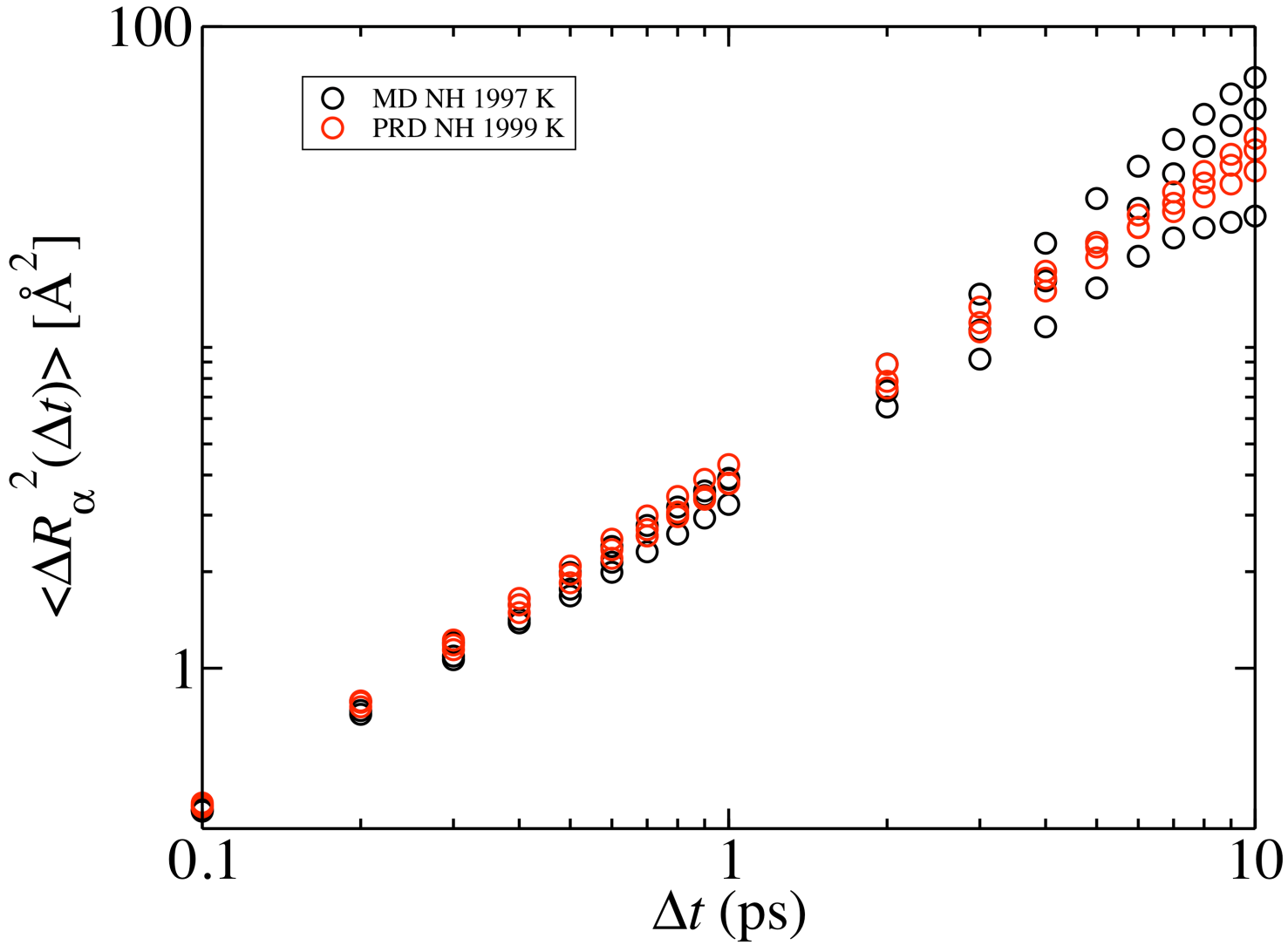
To run 128 replicas:

```
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



Test Problem: Vacancy Diffusion