CHAOFENG HOU

Dr. Chaofeng Hou is an associate professor at the Institute of Process Engineering of the Chinese Academy of Sciences. Currently, his research fields are focused on prediction of thermodynamic properties of low-dimensional nanomaterials and construction of a corresponding virtual simulation platform, high performance computing of solid functional materials, and mesoscale mechanism of chemical vapor deposition process. Dr. Hou is the originator of a Chinese patent of invention. In 2012, he obtained the best paper nomination award in the annual conference of high performance computing in China. He was also the recipient of the best application award for high performance computing granted by the Chinese Academy of Sciences.

Large-scale Molecular Dynamics Simulation of Thermal Conductivity of Silicon Nanowires on the Sunway TaihuLight Supercomputer

Large-scale Molecular Dynamics Simulation of Thermal Conductivity of Silicon Nanowires on the Taihulight Supercomputer

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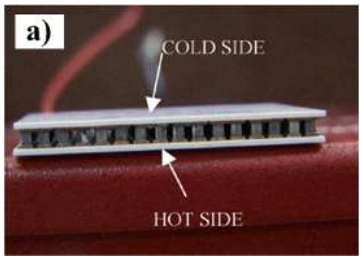
Background

Importance of silicon

unit cell
for crystalline silicon

heat dissipation

microelectronics
MEMS



thermoelectric devices

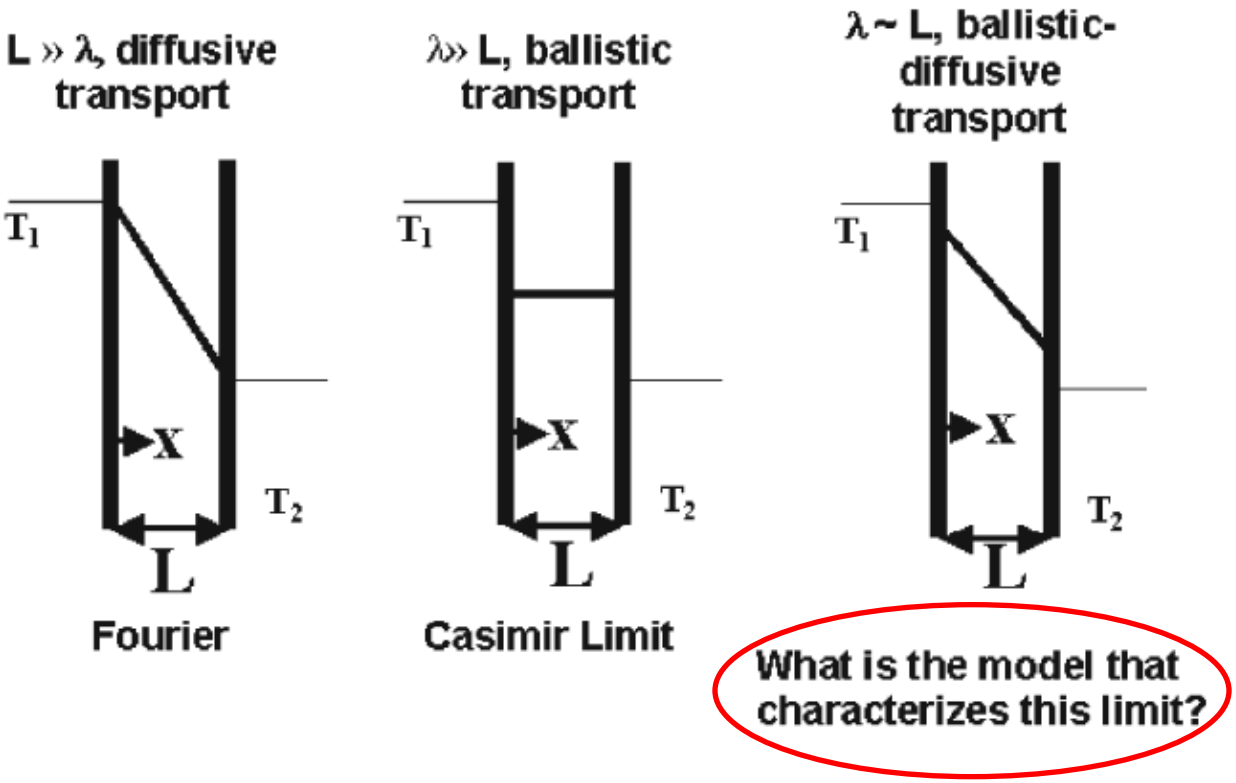
Photovoltaic

MD Simulation of Crystalline Silicon

- **EMD: fluctuation-dissipation theory, Green-Kubo formula, homogeneous, long time**

- **NEMD: Fourier's law, nanostructure, direct, rapid**

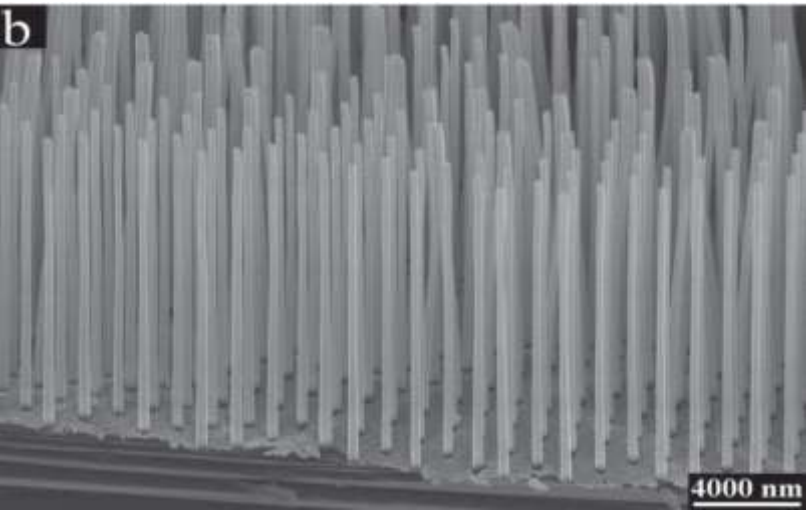
Importance of Size/Scale in Simulation



simulation size >> MFP of phonons (Mean Free Path)

One Dimensional Silicon Structure

(Si Nanowires)



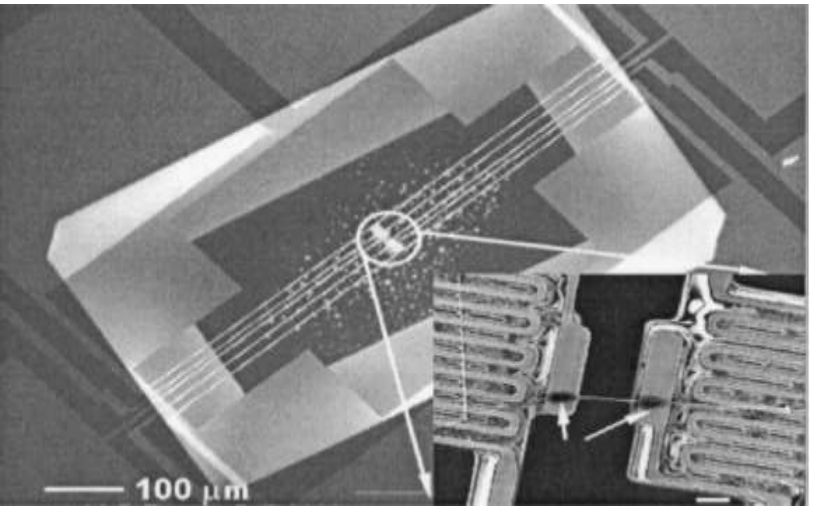
Applications:

Transistor: FET, MOS

Sensor, LCD

Thermoelectric devices

(Advanced Materials 2011, 23, p285)



Typical dimensions:

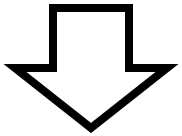
D > 10 nm, L – μm~mm

(Applied Physics Letters 2003, 83, p2934)

Atomistic Simulation of Crystalline Silicon

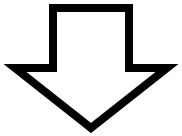
Large simulation size/scale

L> 1 micrometer, D>10 nm

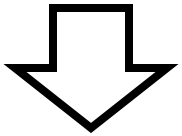


Enormous amount of atoms

> 100 millions atoms



Huge data and computational workload



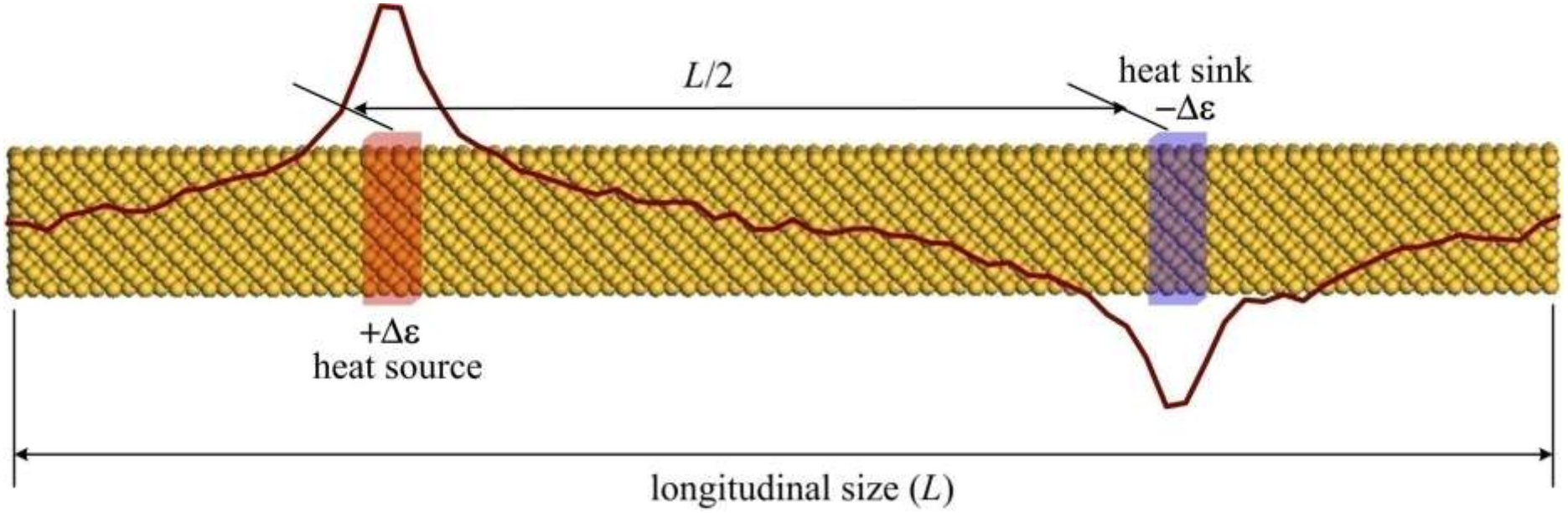
Acceleration hardware

large-scale parallelization

Numerical Models

Simulation Framework

- **NVE ensembles**
- **Heat current density: 1.3E-4 eV/nm^2**
- **PBC conditions + fixed layer**



Potential model

Bond order potential such as Tersoff model (many-body interaction)

$$E_{total} = \frac{1}{2}\sum_{i \neq j} V_{ij}(r_{ij}) = \frac{1}{2}\sum_{i \neq j} f_C(r_{ij})[V_R(r_{ij}) + B_{ij}V_A(r_{ij})]$$

$$f_C(r) = \begin{cases} 1, & r < R - D \\ \frac{1}{2} - \frac{1}{2}\sin[\frac{\pi}{2}(r - R)/D], & R - D < r < R + D \\ 0, & r > R + D \end{cases}$$

$$B_{ij} = (1 + \beta^n \zeta_{ij}{}^n)^{-1/2n}$$

(J. Tersoff, *Physical Review B*, 37(12), 6991-7000, 1988)

Three features:

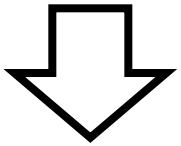
1) Complex operations

2) Heterogeneous data

3) Many-body asymmetry

Complex operations

- **Different from pairwise potential: LJ, Morse etc.**
- **Different from angle and dihedral interaction in biomolecules:**
- **Depend on all other neighbors:**
- **Nonlinear math functions: pow, exp, division**



tricky treating!

complex data structure and data interaction

Heterogeneous data

Position: vector

Velocity: vector

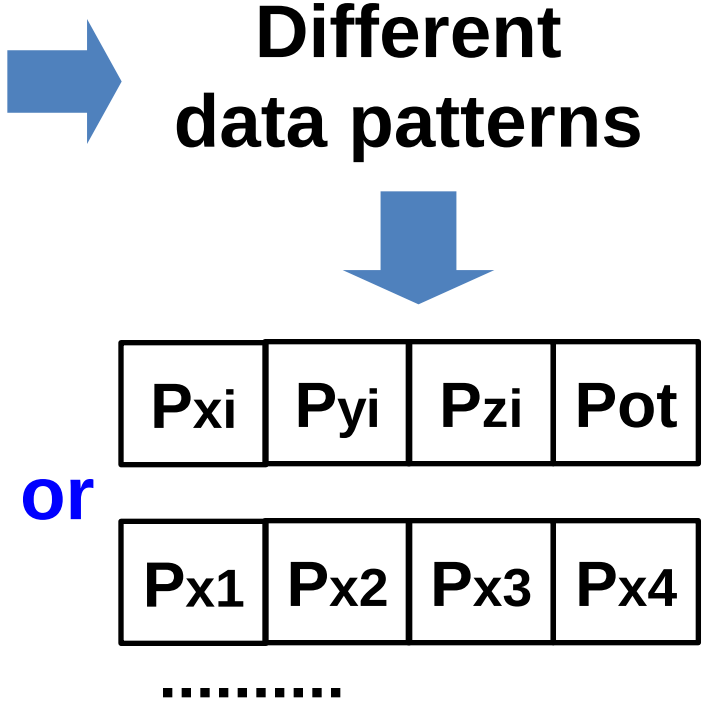
Potential energy: scalar

Kinetic energy: scalar

Temperature: scalar

Neighbor index: scalar

Model parameters:



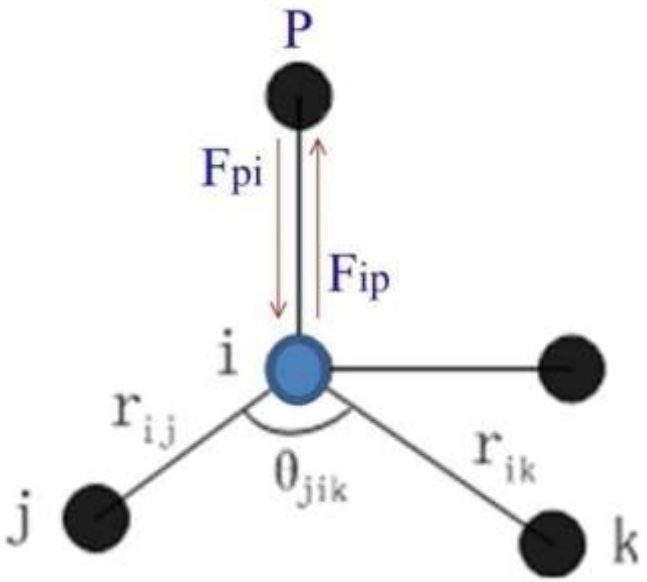
Many-body asymmetry

Dependence on all other neighbors

$F_{ip} \neq F_{pi}$

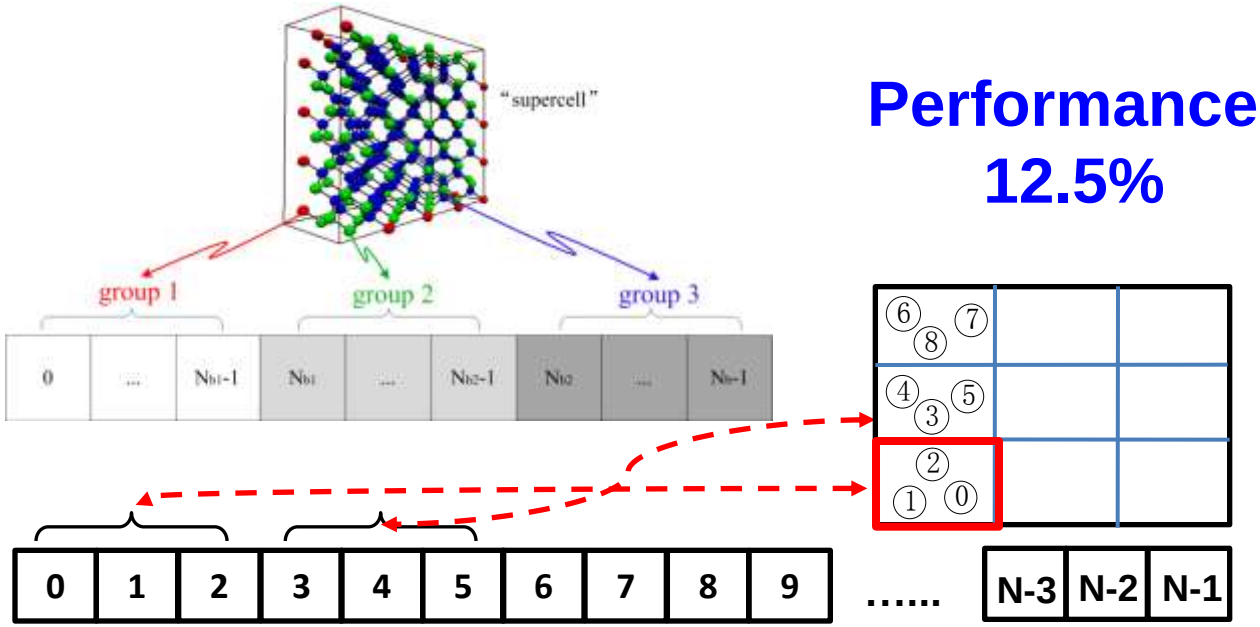
Interactive force between atom i and p:
$0.5*(F_{ip}+F_{pi})$

Resultant force on atom i :
F_i
8 times of computation




Optimizations

Data ordering



Performance: 12.5%

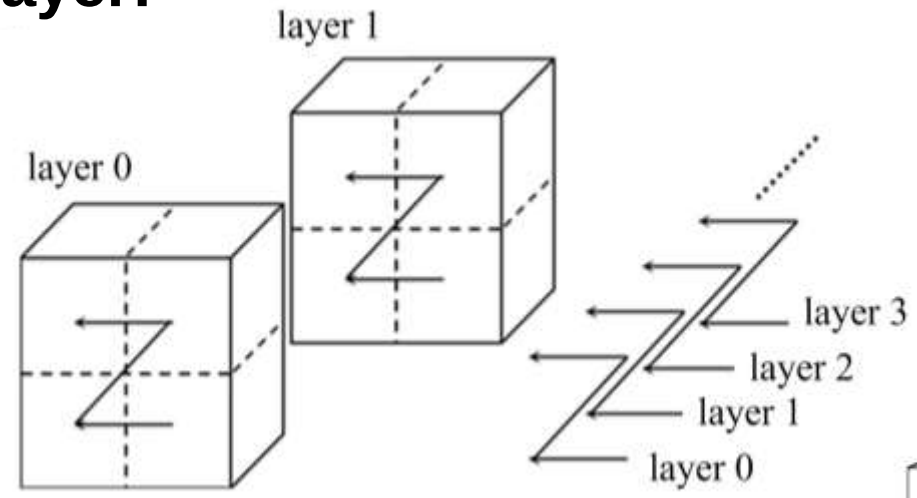
- **Fixed neighbors**
- **Reordering atoms: SLP, "supercell"**
- **Atom sorting: three types**
- $N_{atom} = m * N_b$
- **Correspondence between cells and threads**

Selection of cells (size & shape)

Atom number in different "supercells"	Dimensions in three directions	Atom number in the first group	Atom number in the second group	Atom number in the third group	Fraction of the third group (%)
64	2 × 2 × 2	10	27	27	42.19
128	2 × 2 × 4	14	51	63	49.22
192	2 × 3 × 4	16	71	105	54.69
216	3 × 3 × 3	16	75	125	57.87
256	2 × 4 × 4	18	91	147	57.42
288	3 × 3 × 4	18	95	175	60.76
384	3 × 4 × 4	20	119	245	63.80
512	4 × 4 × 4	22	147	343	66.99

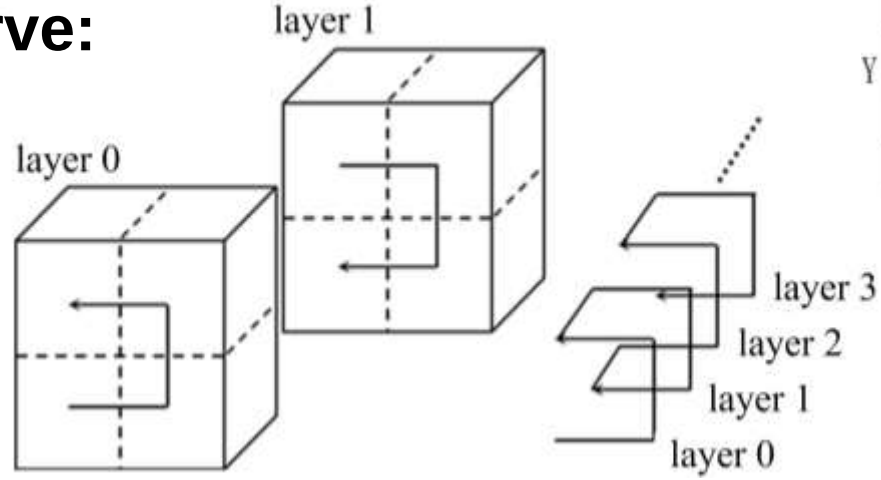
The optimal cell corresponds to 3x4x4 units cells (8 atoms per unit cell), so the total atom number in one cell is 384.

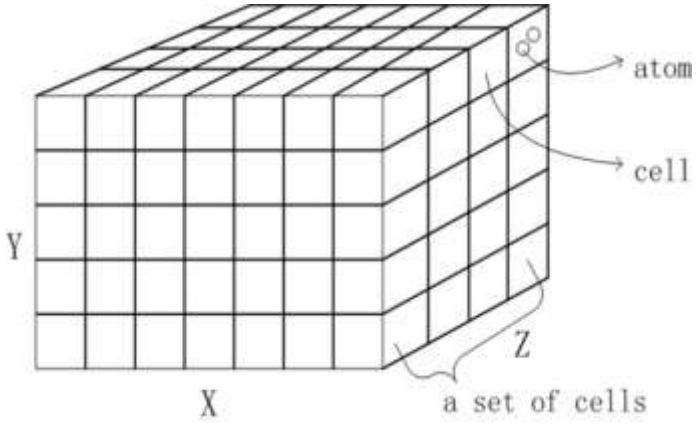
Layer by layer:



Performance: 15.1%

Hilbert curve:





Division of simulation domain into cells

Other specific optimizations

Aiming at the three forementioned complex model features

1) Efficient use of hierarchical memory

local memory **global memory**

2) SIMD vectorization

3) Nonlinear mathematical functions

4) Overlap between computation and memory access

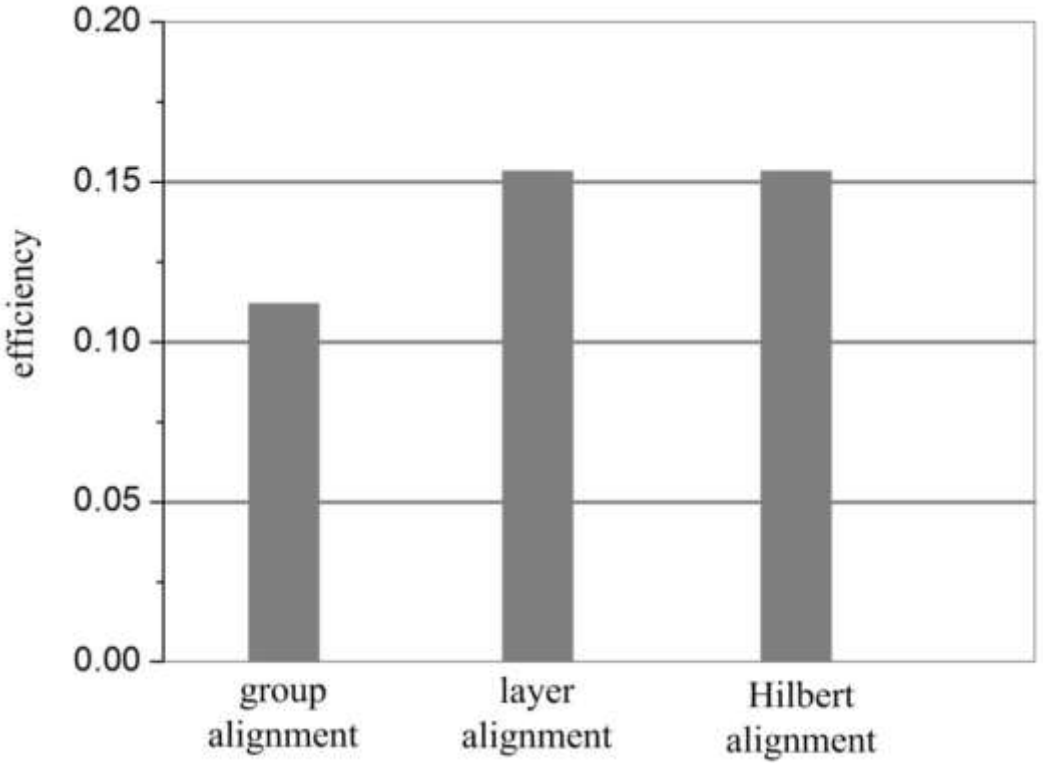
Performance comparison with reports

- **Updating rate of simulated atoms (/step/atom/GHz):**

  Lammps: 1.0778E-6 (s)

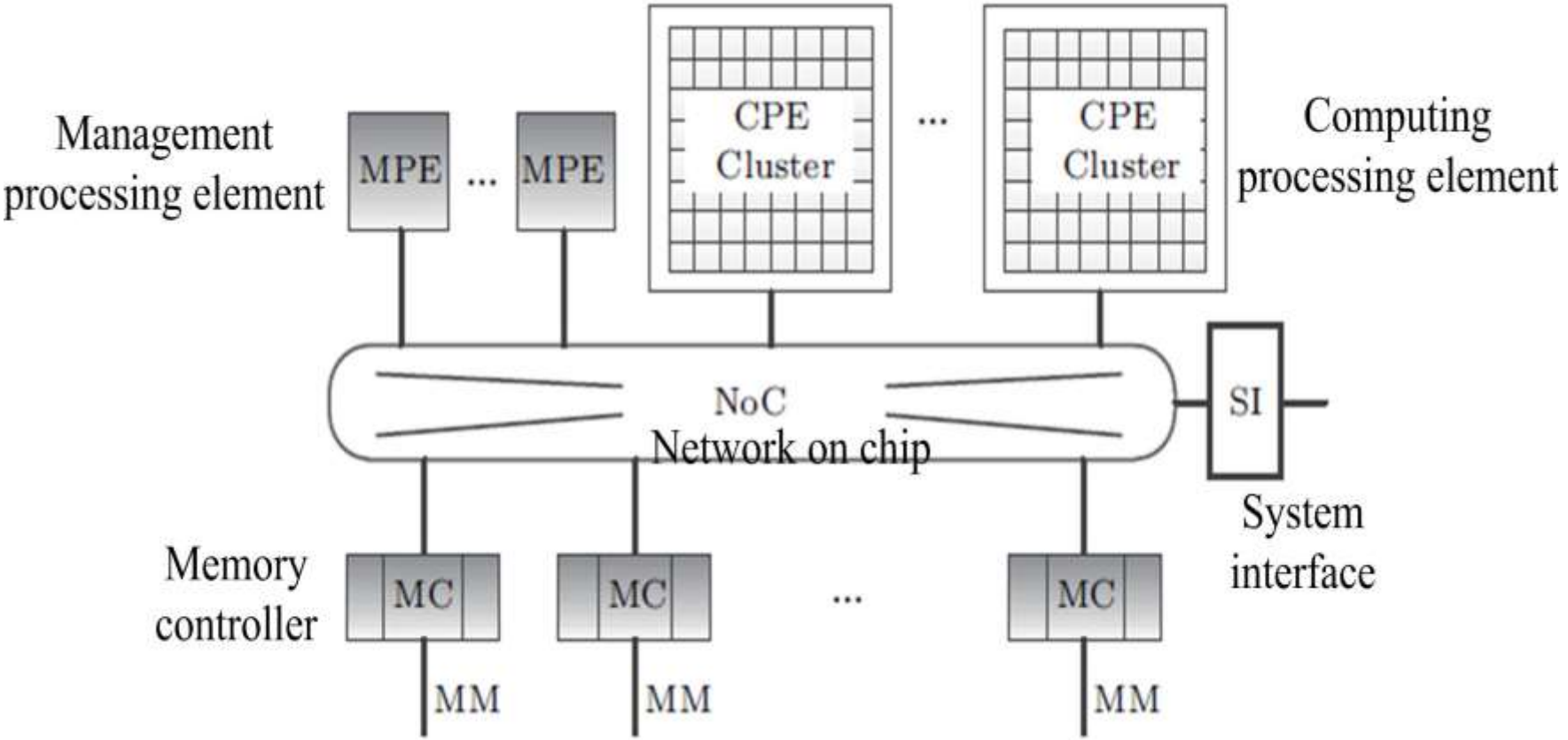
  Our work: 0.74653E-6 (s)

1.44 times



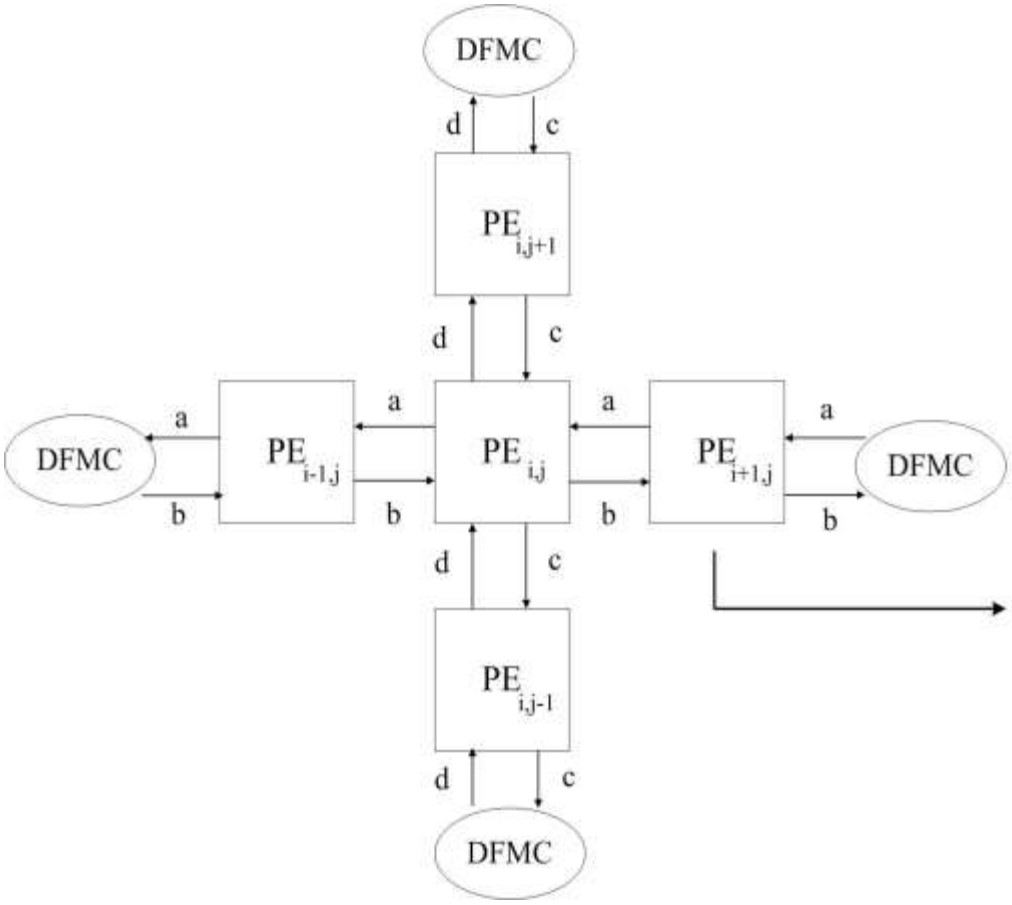

Performance

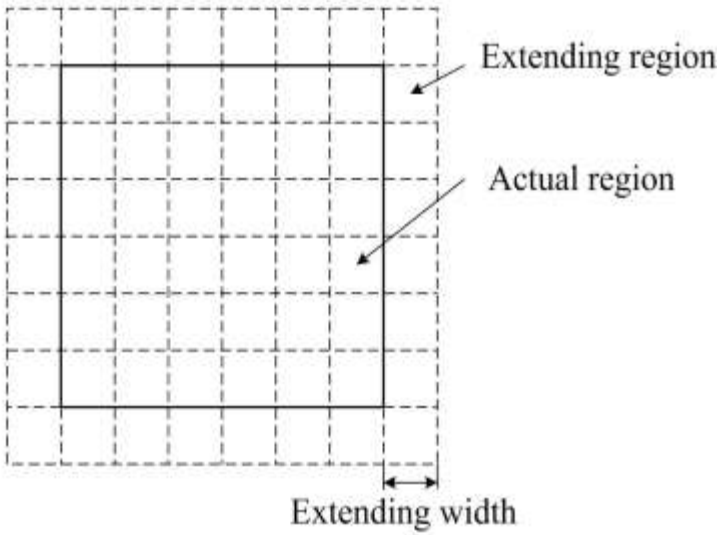
Architecture of one node on The Sunway Taihulight Supercomputer



- **Inter-node Parallelization**

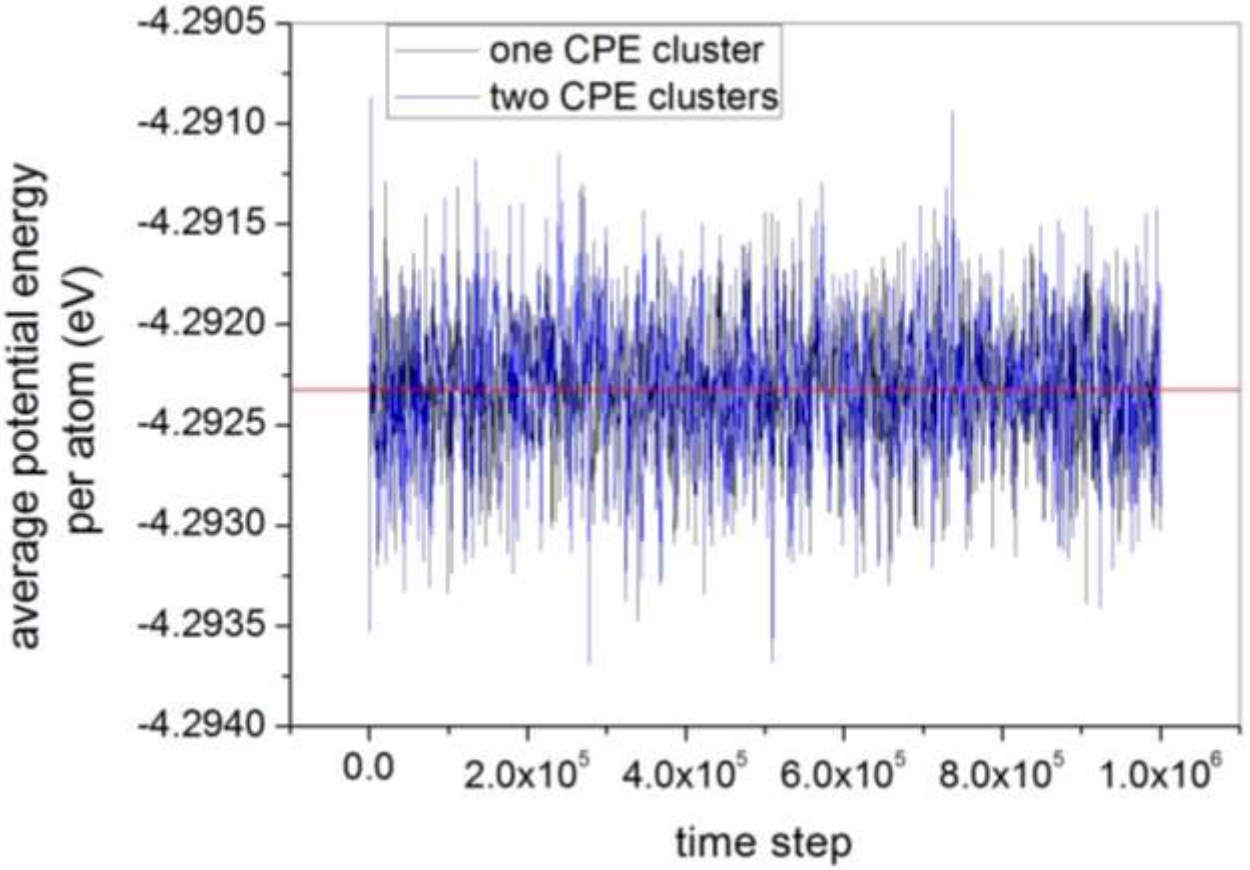
  shift-style **multi-level: CPU, threads**



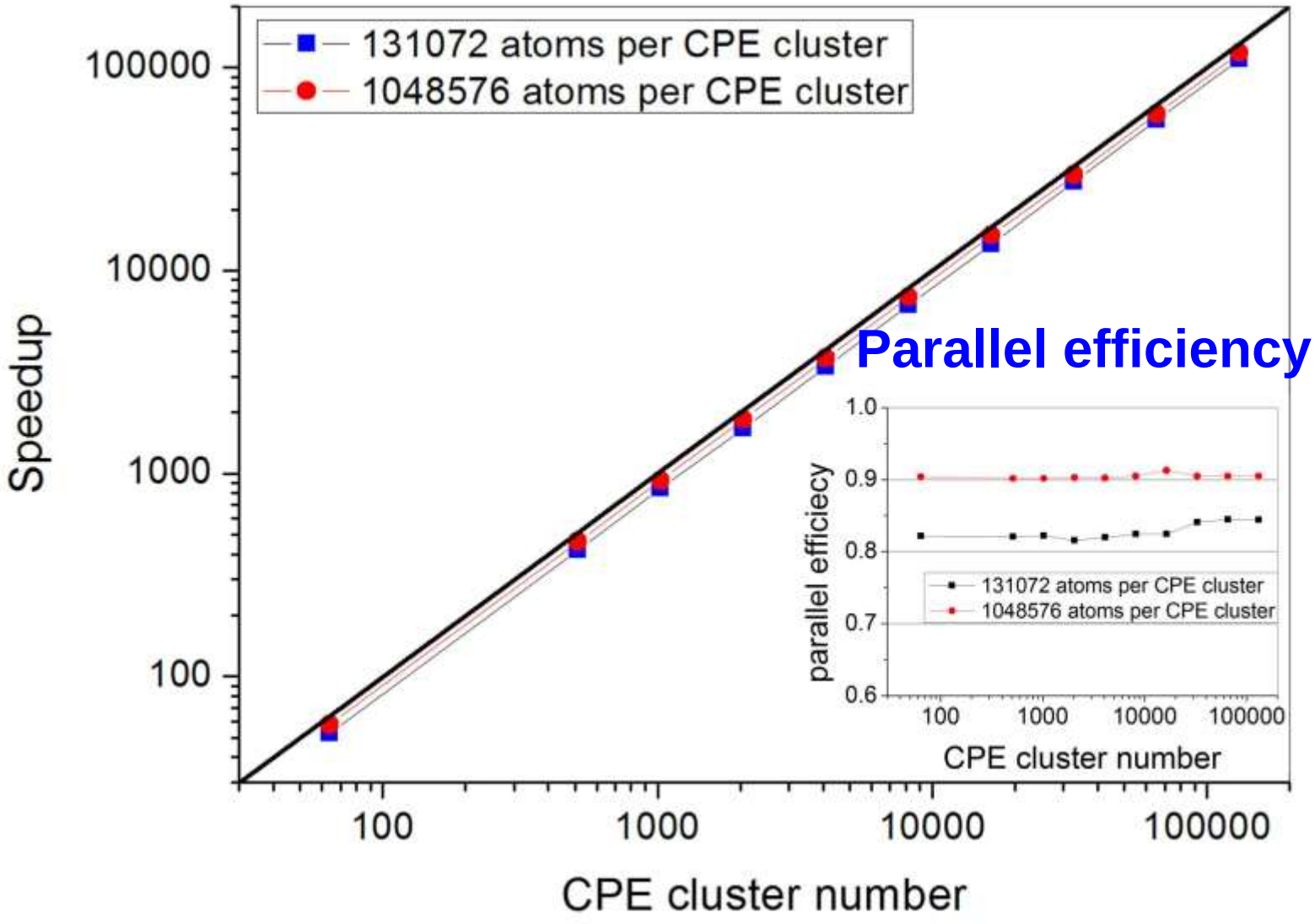


Algorithm Validation

- **NVE**
- **Initial temperature: 500K**
- **16384 atoms per CPE cluster**

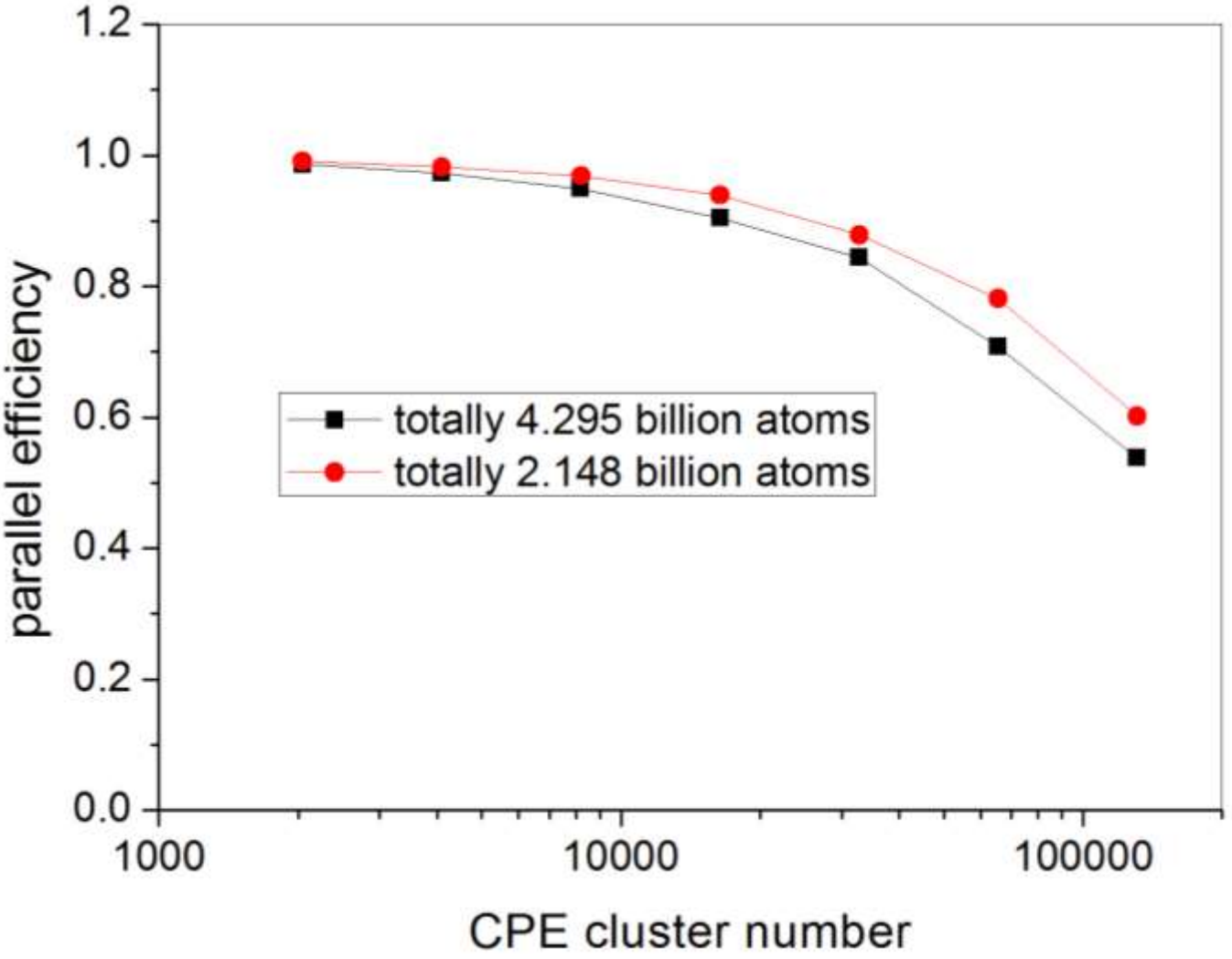


Measurement of Weak Scaling

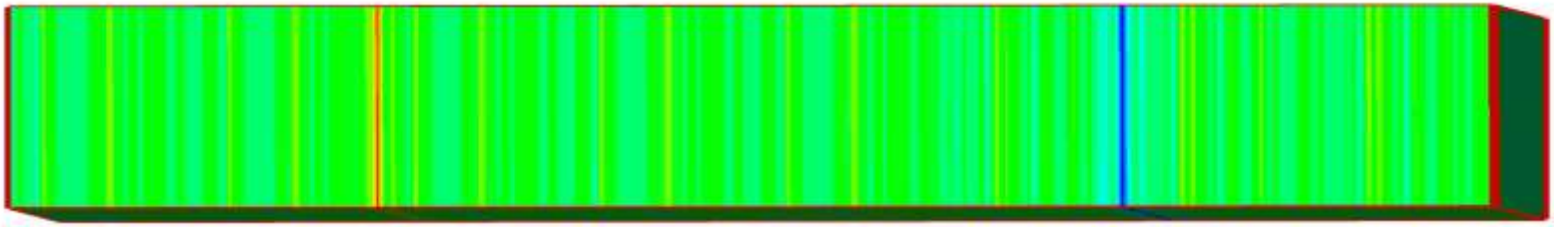


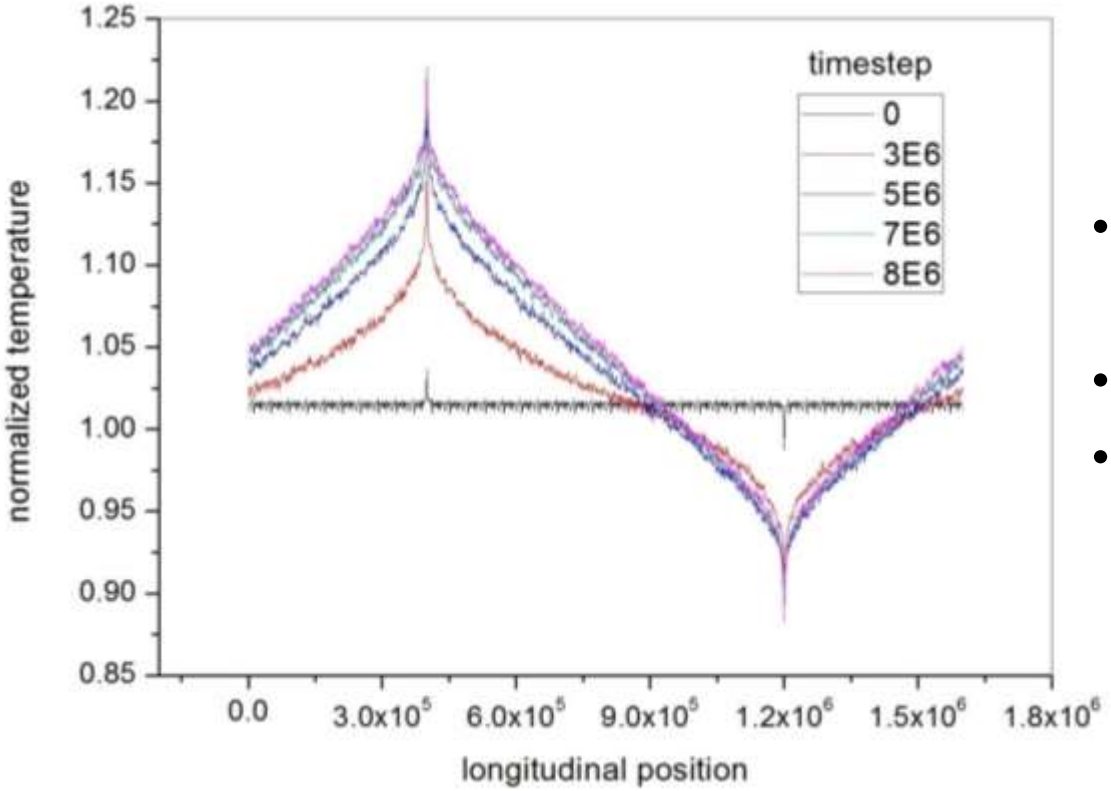
Parallel efficiency: >80%

Measurement of Strong Scaling



Longitudinal temperature distribution





- **cross-section area: 6.75nm*6.75nm**
- **length: 8.9μm**
- **temperature: 500K**

Conclusions & Prospects

Conclusions

- **MD simulation of 8.51 Pflops with 10.27 million cores from 160512 CPE clusters. projected performance of 17.55 Pflops**
- **Excellent strong and weak scalability.**
- **15.1% of peak performance of a single CPE cluster.**
- **Overcoming the longitudinal size effects, and lateral sizes compared with the experiment.**

Prospects

1) **New algorithm and optimization for higher performance.**

   Expected performance of about 22 Pflops.

2) **Simulation of nanostructures with defects.**

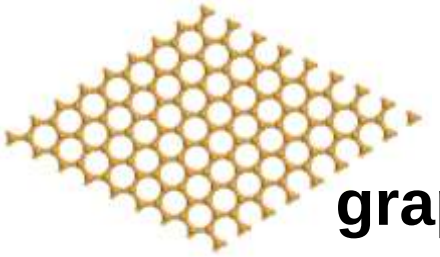
   Coupled computation of MPE and CPE cluster.

3) **Designing hardware structure:**

   Register number, local memory size.

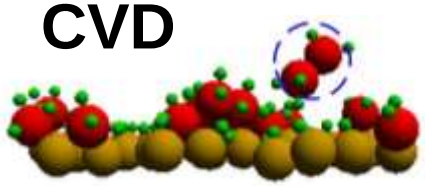
4) Other solid covalent materials such as carbon et al and their low dimensional structures

CNT



graphene

CVD



5) Directly achieve trans-scale simulation bridging microscopic and macroscopic scale.

Thank you
for your attention!