VNIITF
ROSATOM

北京应用物理与计算数学研究所
Institute of Applied Physics and Computational Mathematics

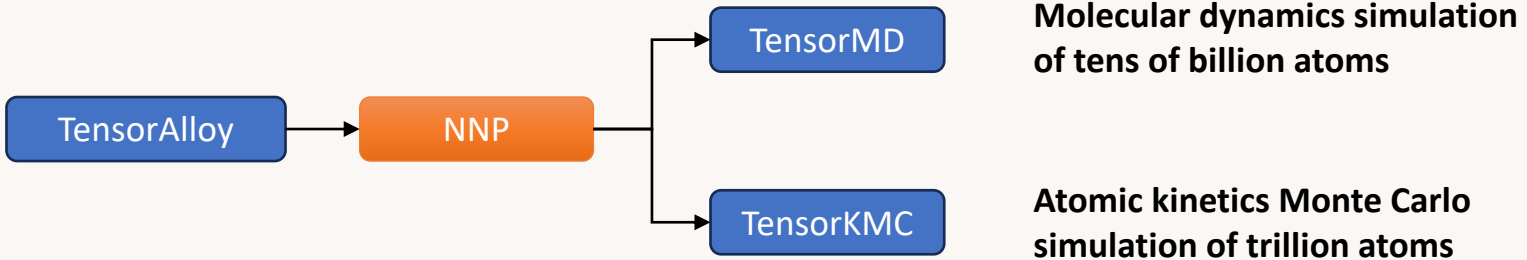
TensorKMC: Kinetic Monte Carlo Simulation of 50 Trillion Atoms Driven by Deep Learning on a New Generation of Sunway Supercomputer

Xin Chen
Institute of Applied Physics and Computational Mathematics
Beijing, China

铸国防基石 做民族脊梁

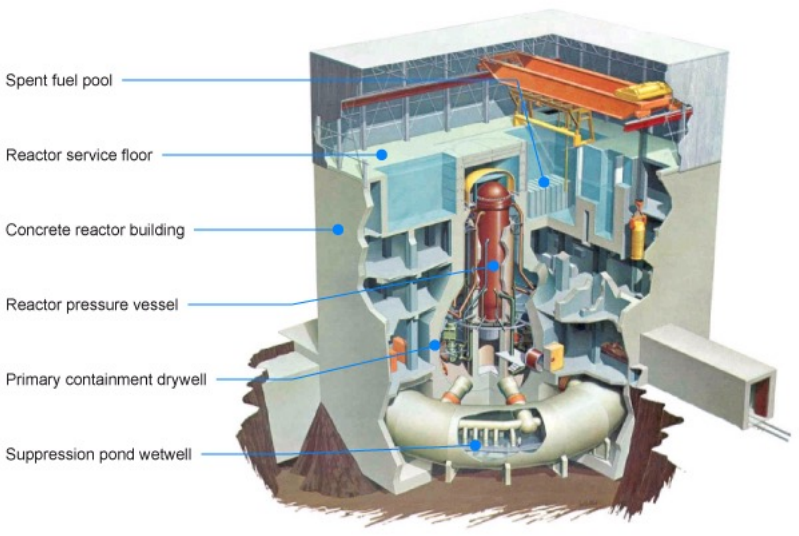
The presenter: Xin Chen

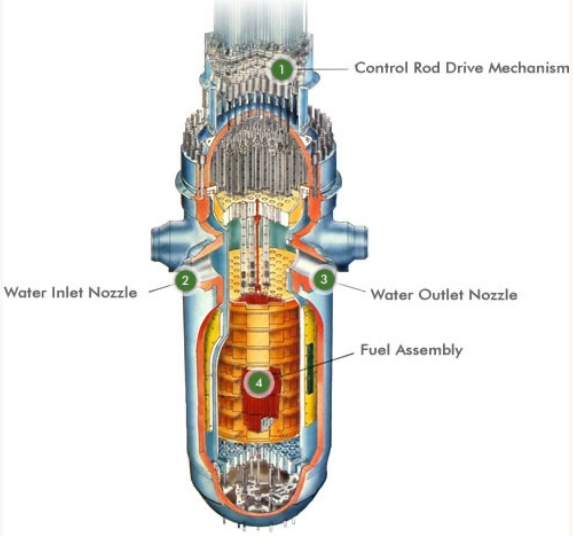
- Ph.D. degree in chemistry from Tsinghua University in 2018
- Assistant professor at the Institute of Applied Physics and Computational Mathematics, focusing on materials modeling and equation of state
- The core developer of TensorAlloy、TensorMD and TensorKMC



Reactor pressure vessel

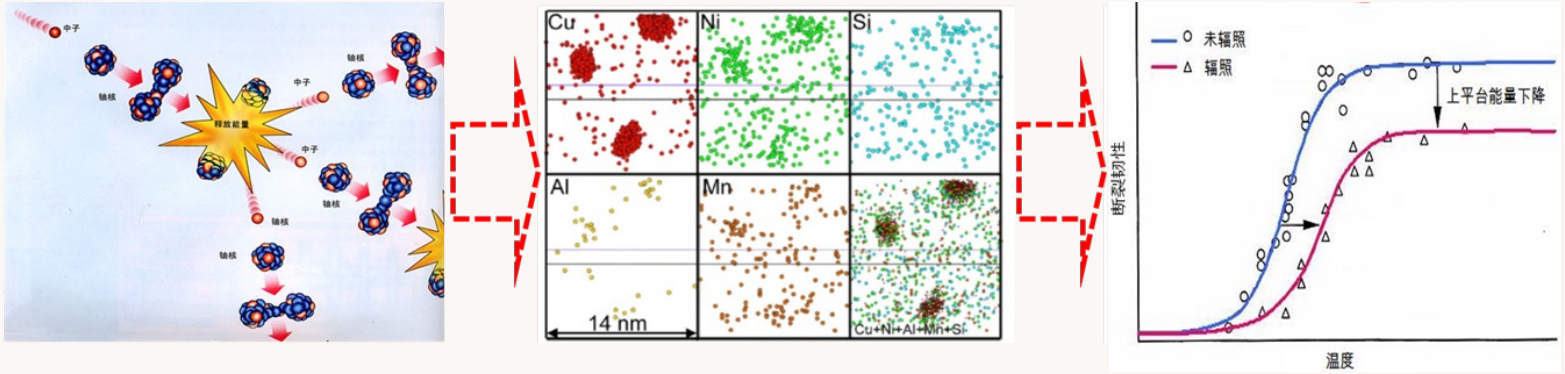
- Reactor pressure vessel (RPV) plays a critical role in safety of nuclear powerplant
- RPV is unsubstitutable
- RPV cylinder shell is the life-time limiting component for a nuclear reactor





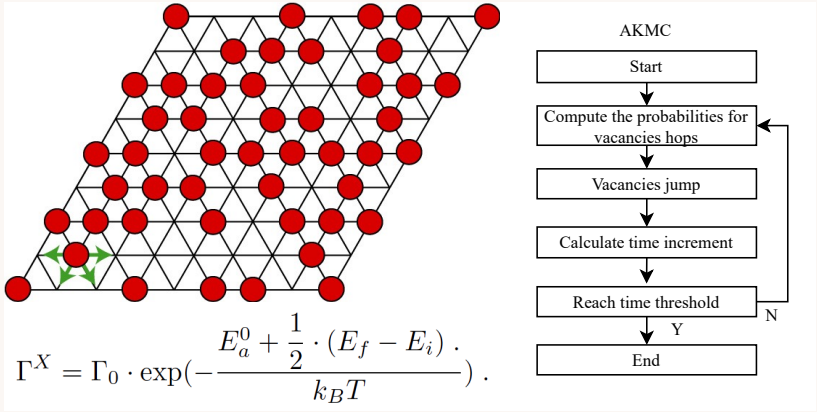
RPV aging

- The shell, primarily Fe-based alloy, is constantly bombarded by high-energy particles
- Defects accumulated over time, voids, bubbles, dislocation loops or lines, etc, formed
- Atoms segregate or aggregate
- Radiation hardens materials, but also lowers ductility
  - Losing ductility may lead to catastrophic failure without warning



Atomic Kinetic Monte Carlo

- Experimentally invetigating radiation-induced aging is difficult
- Theoretical study is also a challenge:
  - Phenomenons occured atomic level, accurate atomic modeling is required
  - Timescale is extremely large, molecular dynamics is not applicable
- **Atomic kinetic monte carlo (AKMC):** a combination of atomic modeling with meso-scale simulation

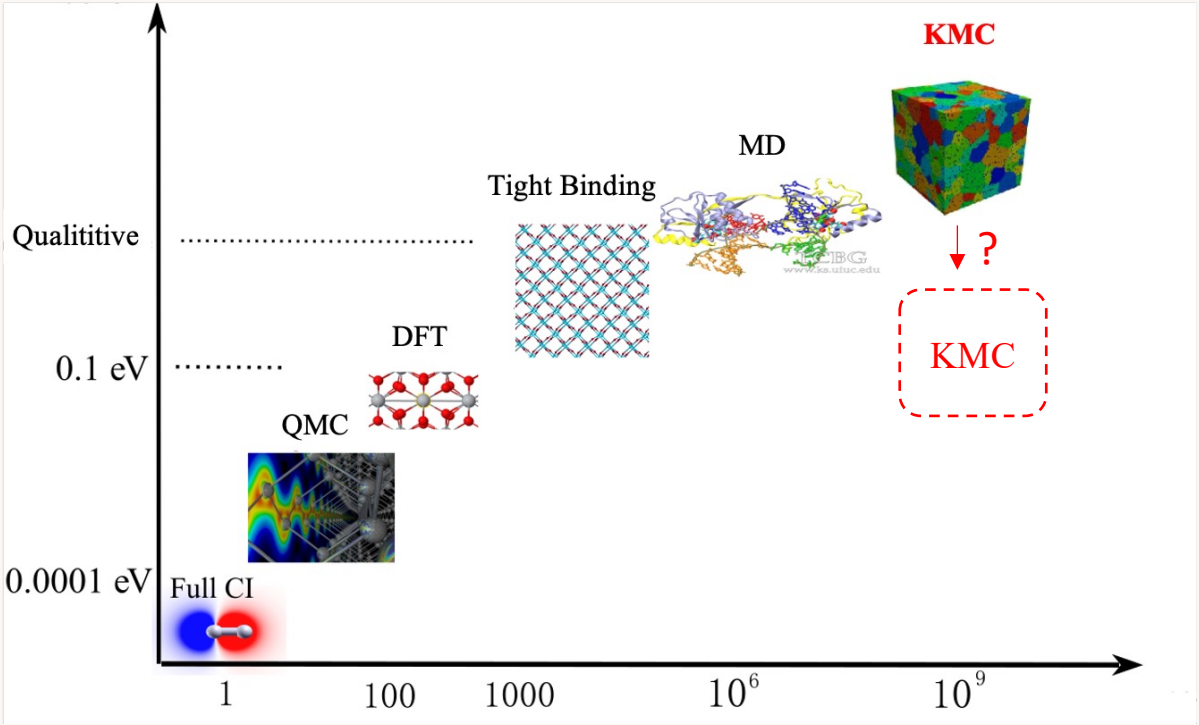


$$\Gamma^X = \Gamma_0 \cdot \exp(-\frac{E_a^0 + \frac{1}{2} \cdot (E_f - E_i)}{k_B T}) .$$

	AKMC
Spatial	nm - μm (10^4 – 10^7 atoms/proc)
Time	μs, s or longer
Driven by	Energy
Atoms	Always on lattice sites

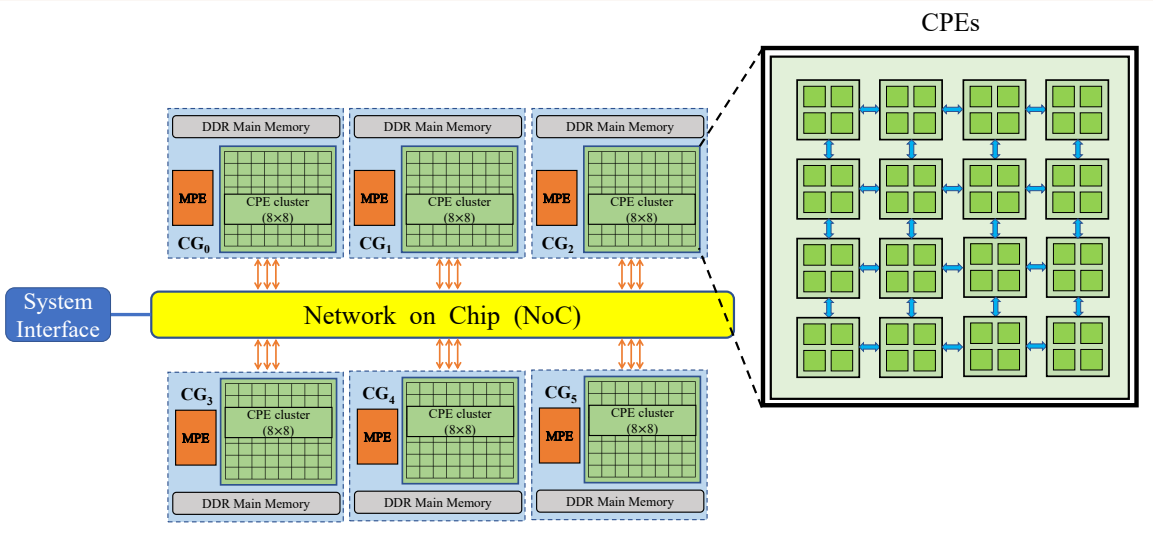
Atomic Kinetic Monte Carlo

- Traditionally AKMC is a qualititve simulation method as it often uses simplified interaction models
- Massively-paralleled AKMC with highly accurate energetic approach is needed for realistic modeling



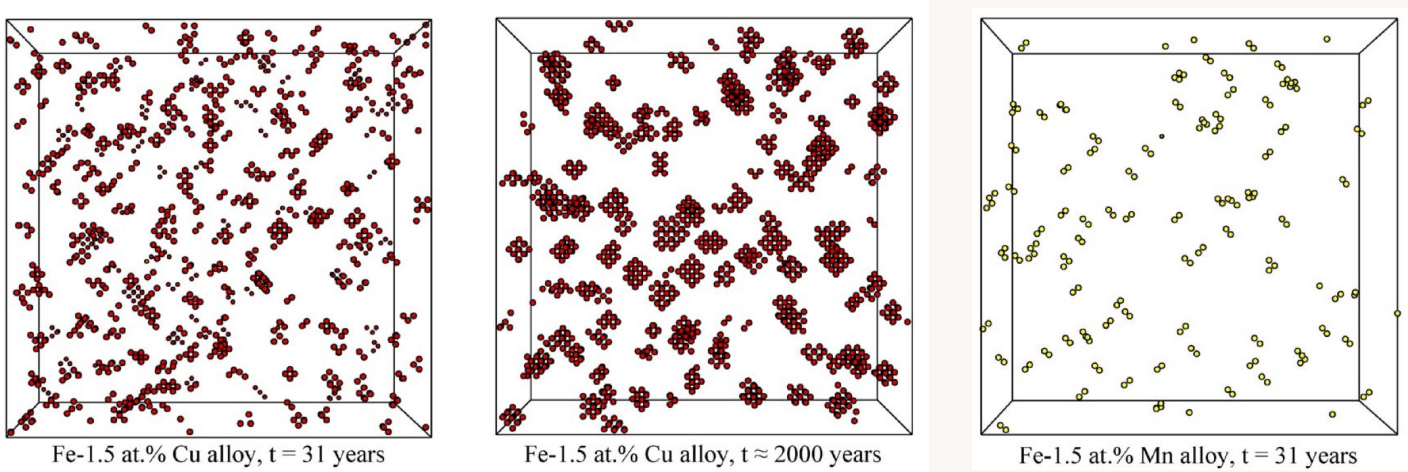
The new generation of Sunway

- Each SW26010pro many-core processor has 6 core groups (CGs)
- Each CG has 1 MPE, 8x8 CPEs, 16 GB main memory
- Each CPE has 256 kB high-speed manually controllable local device memory (LDM)



LAKIMOCA

- Developed by Électricité de France (EDF), owner of 58 power plants in France
- Capable of simulating long-term kinetics and atomic behaviors of dilute metal alloys
- Serial, empirical potentials, hundreds of thousands of atoms



Fe-1.5 at.% Cu alloy, t = 31 years

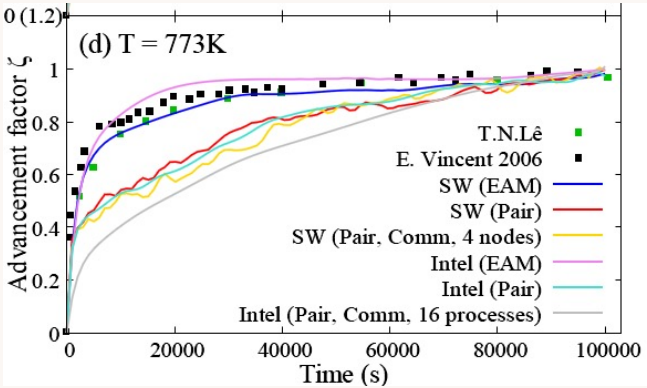
Fe-1.5 at.% Cu alloy, t ≈ 2000 years

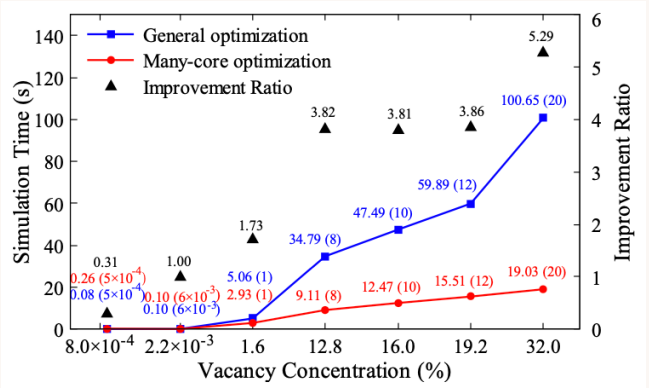
Fe-1.5 at.% Mn alloy, t = 31 years

Vincent et al., J. Nuc. Mater. 2006, 351, 88-99

OpenKMC

- Developed by Hong-Hui Shang and co-workers in 2019
- Can simulate up to hundreds of billions of atoms with empirical potentials
- Specially optimized for Sunway TaihuLight

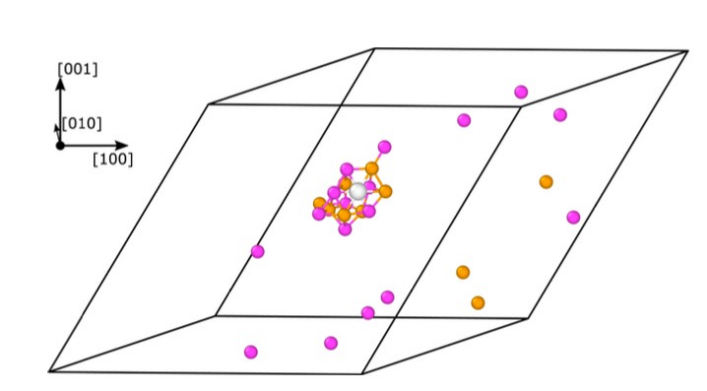


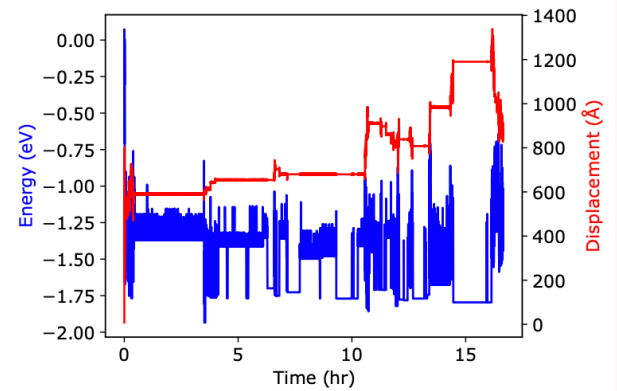


Kun Li and Hong-Hui Shang et al. SC' 19. doi: 10. 1145/3295500.3356165

i-PI

- i-Pi 2.0 is a universal force engine
- Neural network potential based AKMC simulates natural aging behavior of Al-6xxx alloys (~1500 atoms)





Jahn et al. Phys. Rev. M. 2021, 5, 053805
Kapil et al., Comp. Phys. Comm. 2018, 236, 214–223

1 Background

2 Related works

3 Key innovations

4 Performances

5 Application

TensorKMC

- **TensorKMC** is a massively parallel AKMC program integrated with highly accurate neural network potentials
  - **TensorAlloy**: an automatic atomistic neural network program for metals and alloys
    - Comput. Phys. Commun, 2020, 107057
    - Comput. Phys. Commun, 2021, 108132
  - **OpenKMC**: a KMC Design for Hundred-Billion-Atom Simulation Using Millions of Cores on Sunway TaihuLight
    - SC' 19. doi: 10. 1145/3295500.3356165

- **Major contributions:**
  - Triple-encodings and vacancy cache mechanism for largescale AKMC simulation
  - Extremely fast NNP implementation algorithms for many-core processor

Triple-Encodings

- Simulation domain of each process is large
- Vacancy concentration is extremely low: 0.0001%-0.01%
- Interatomic interaction has limited range, only atoms close to an active vacancy are "important"
- Hence, a large simulation domain can be decomposed to discrete vacancy systems

	AKMC
Spatial	nm - μm (10^4 – 10^7 atoms/proc)
Time	μs - s
Driven by	Energy
Atoms	Always on lattice sites

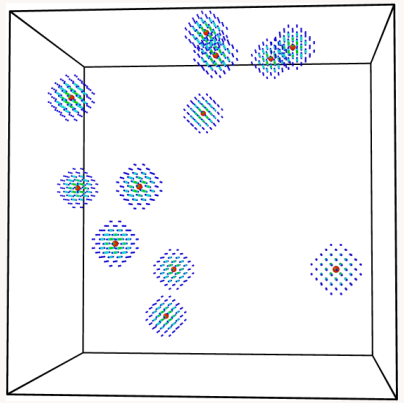
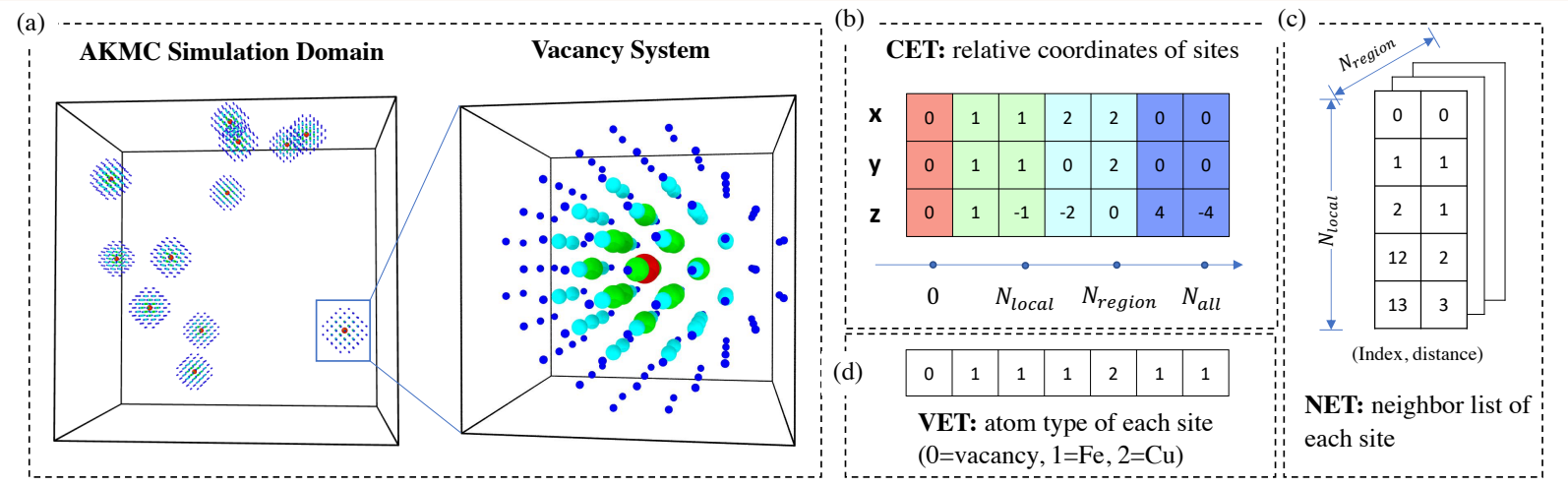


Illustration of domain decomposition

Triple-Encodings

- How to effectively represent these vacancies and atoms?
- **Triple-Encodings:** tabular arrays describing vacancy systems for BCC/FCC systems
  - 128 millions of atoms, 0.0008% vacancy concentration → 1024 vacancy systems
  - Large randomly accessed array → small continous dense block

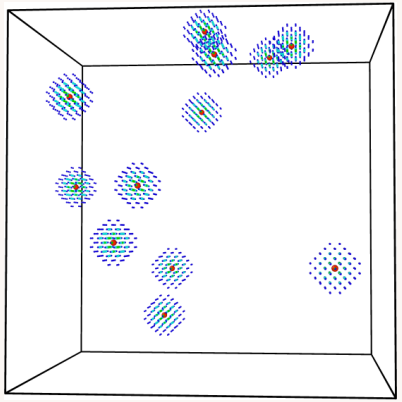


Vacancy cache and memory optimization

- **Cache mechanism:** only properties of atoms of vacancy systems need to be kept
  - Vacancy systems can be viewed as “big particles”
  - Update properties of a vacancy system only if it is close to a jump
  - OpenKMC stores properties of all atoms

- **Compute** the 1D index of a spatial position (i, j, k)
  - Applicable to BCC/FCC systems
  - OpenKMC uses a 3D array

- Overall memory cost reduces by ~66%

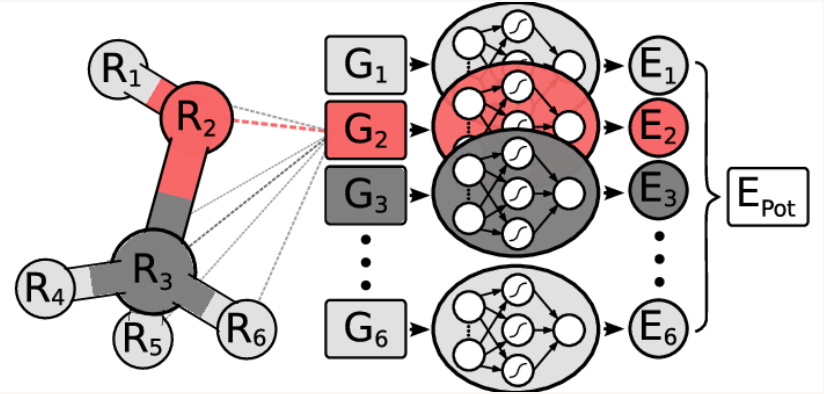


Atomic feature calculation

- The general NNP scheme: atomic positions → atomic features → atomic energy
- Atomic features are calculated with descriptor functions:
- In AKMC, interatomic distances are enumerable
- Tabular arrays can be used to compute features

$$f(r|p,q) = \sum_{j}^{N_{local}} \mathrm{TABLE(r,p,q)}$$

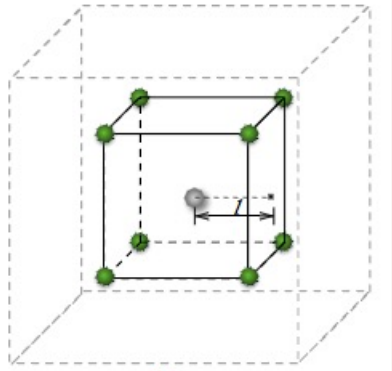
	AKMC
Spatial	nm - μm (10^4 – 10^7 atoms/proc)
Time	μs - s
Driven by	Energy
Atoms	Always on lattice sites



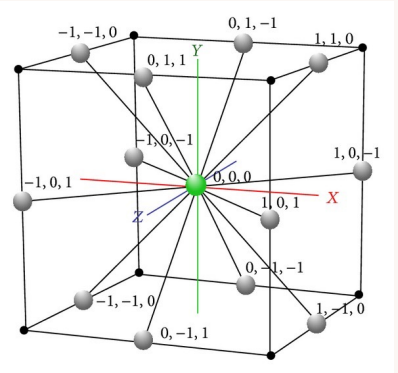
Atomic feature calculation

- A vacancy may jump to one of its N_f first nearest neighbors
  - BCC: $N_f = 8$
  - FCC: $N_f = 12$
- A total of $1 + N_f$ states should be computed each time

- Memory-bounded task:
  - #Ops = $\left(1 + N_f\right) \times N_{region} \times N_{local} \times N_{features}$
- Memory speed and bandwidth of SW26010pro is limited



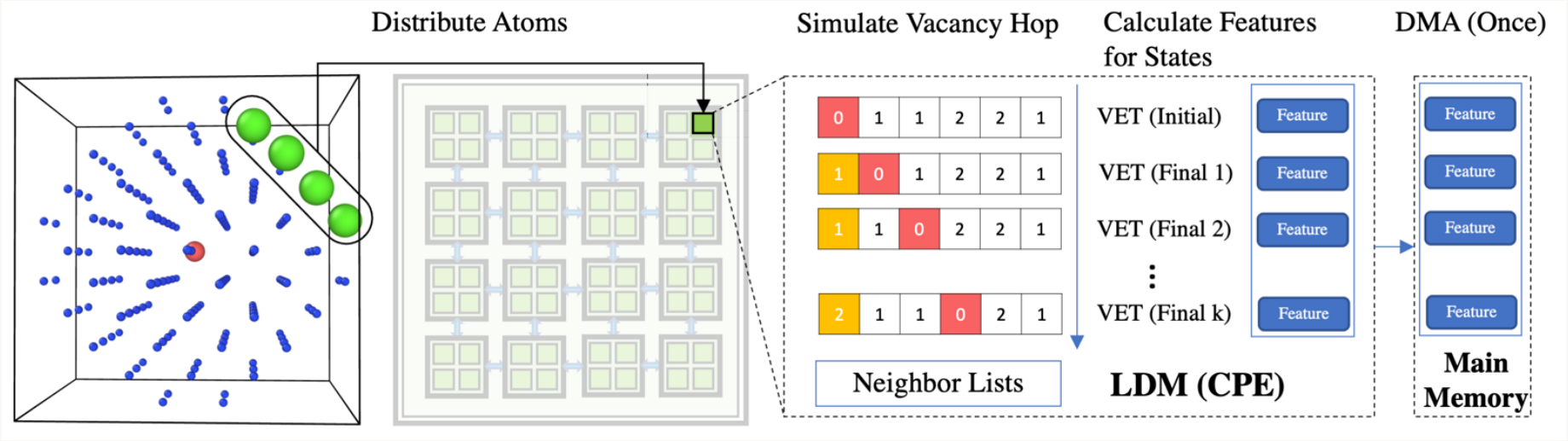
BCC



FCC

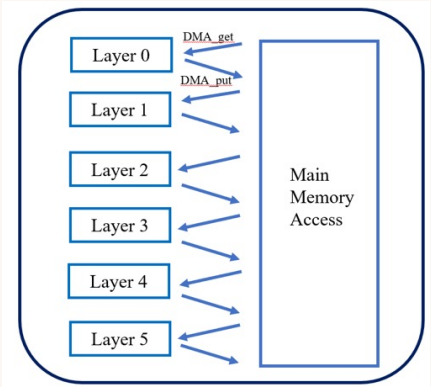
Atomic feature calculation

- A parallel CPEs-based feature operator
- Vacancy hopping simulation is moved to CPEs

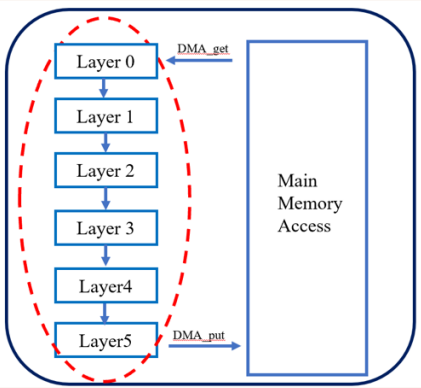


Energy calculation

- The energy calculation is achieved by a multi-layer convolutional neural network
  - Each batch corresponds to a state
- SW officially provides a highly-optimized DNN library (SWDNN)
  - Requires massive data exchange between CPEs and the main memory
- The big-fusion strategy
  - Minimize memory access
  - Hide data exchange behind computation



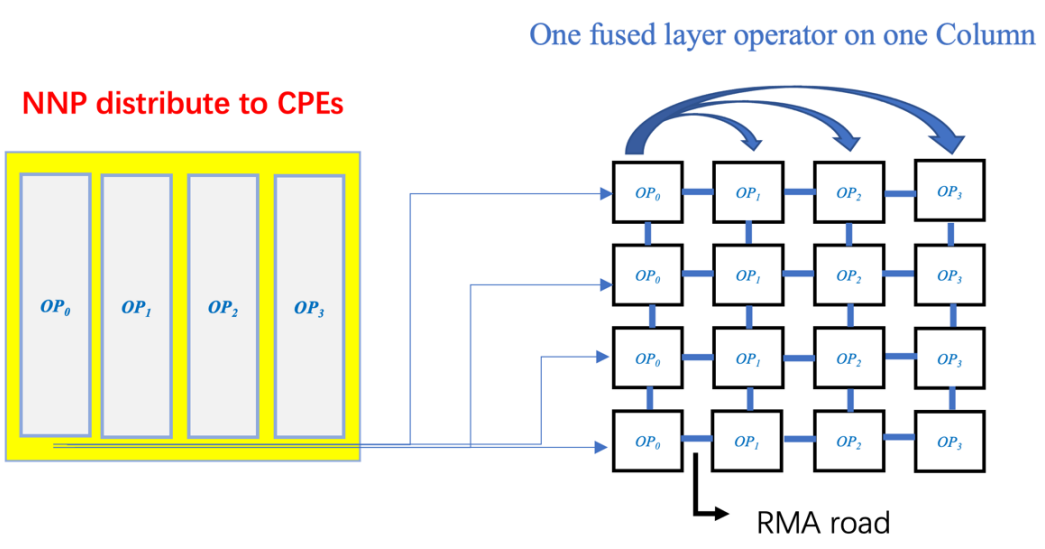
SWDNN



The big-fusion

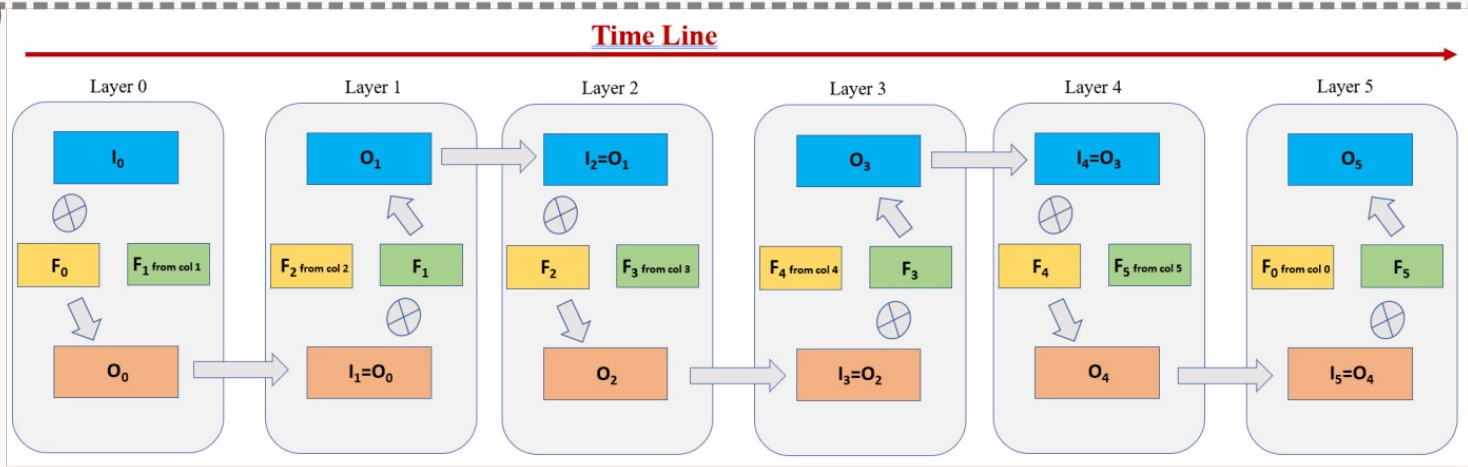
Energy calculation: the big-fusion strategy

- **CPEs act as "normal" cores**
- **LDM act as distributed storage**: NNP parameters are dispatched to CPEs
- Parameter sharing across CPEs is achieved by remote scratched memory access (RMA)



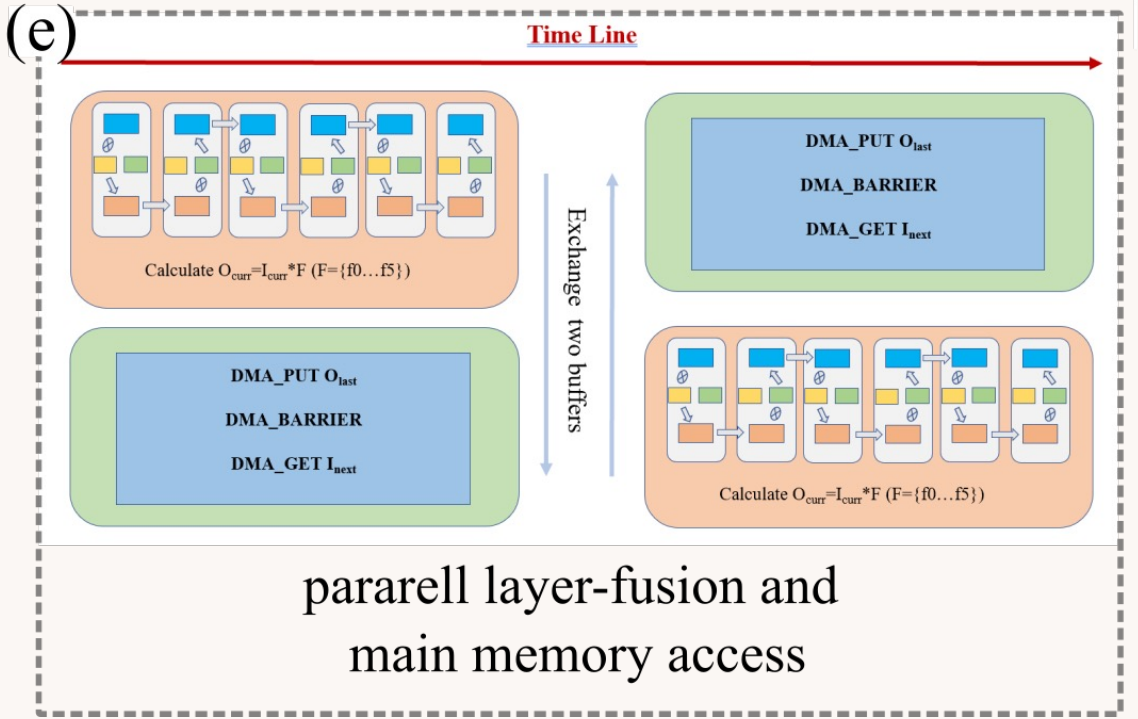
Energy calculation: the big-fusion strategy

(f)



the calculations flow on the Input to complete the kernel fusion , and at the same time hides RMA get the next layer filter in the current calculation

Energy calculation: the big-fusion strategy



1 Background

2 Related works

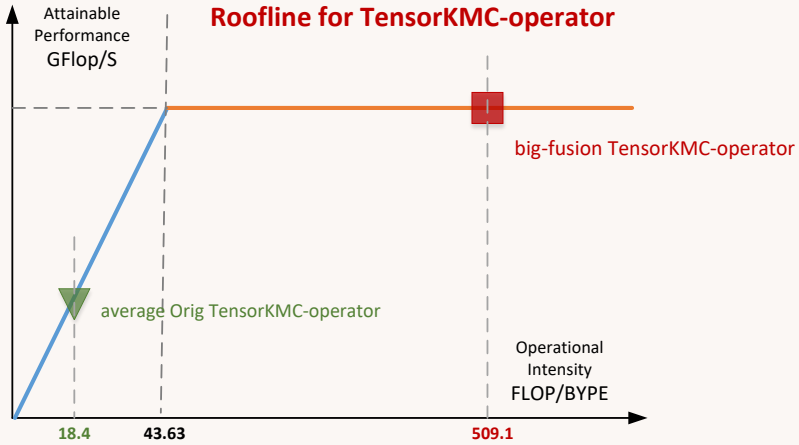
3 Key innovations

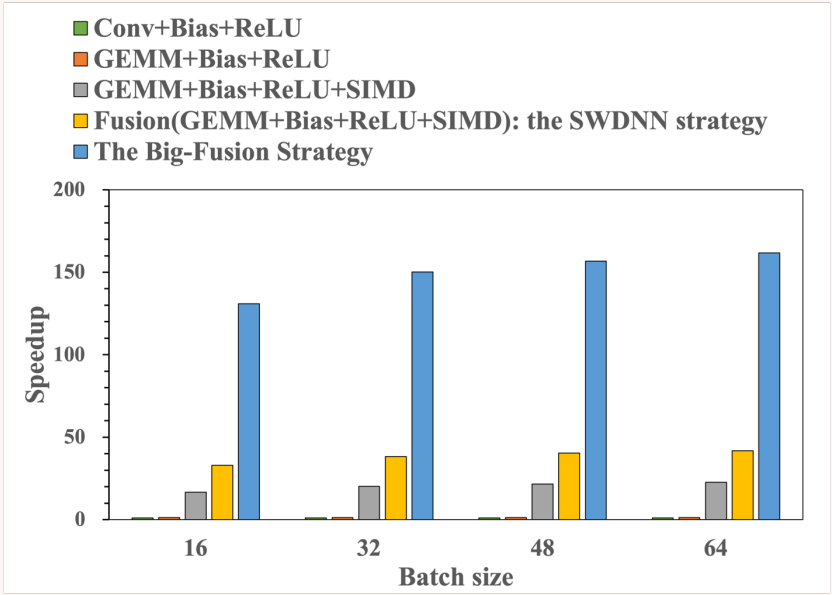
4 Performances

5 Application

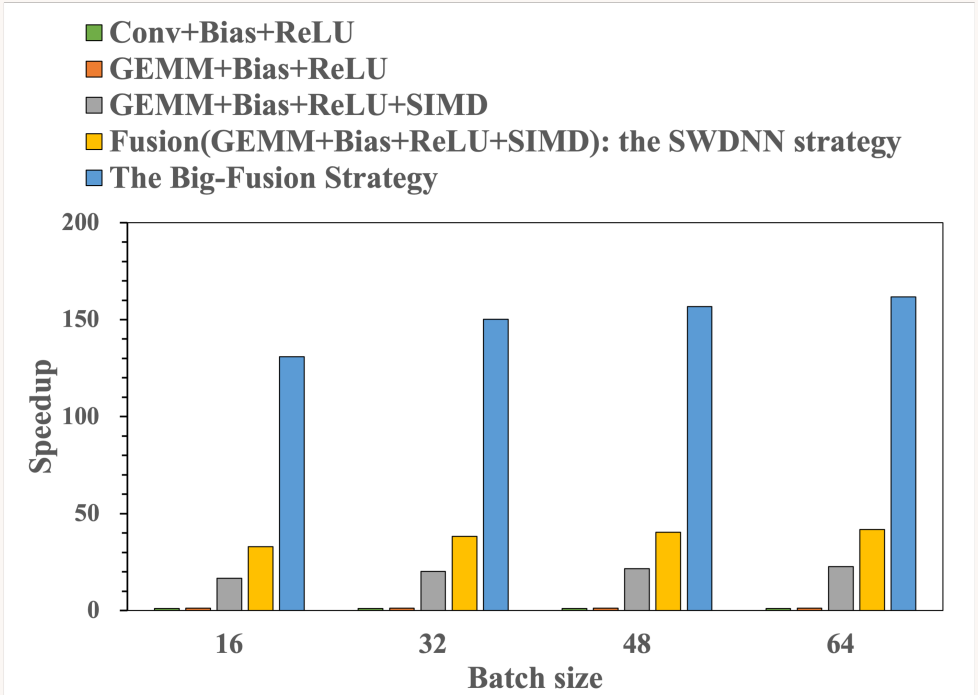
The Roofline analysis

Layer	In-c	Out-c	Memory (MB)	Volume (Gflop)	Intensity (flop/B)
1	64	128	10	0.125	12.8
2	128	128	12	0.25	21.3
3	128	128	12	0.25	21.3
4	128	128	12	0.25	21.3
5	128	64	8	0.25	21.3
6	64	1	2.06	0.001	0.48
Original			56.06	1.01	18.44
Big-fusion			2.03	1.01	509.05





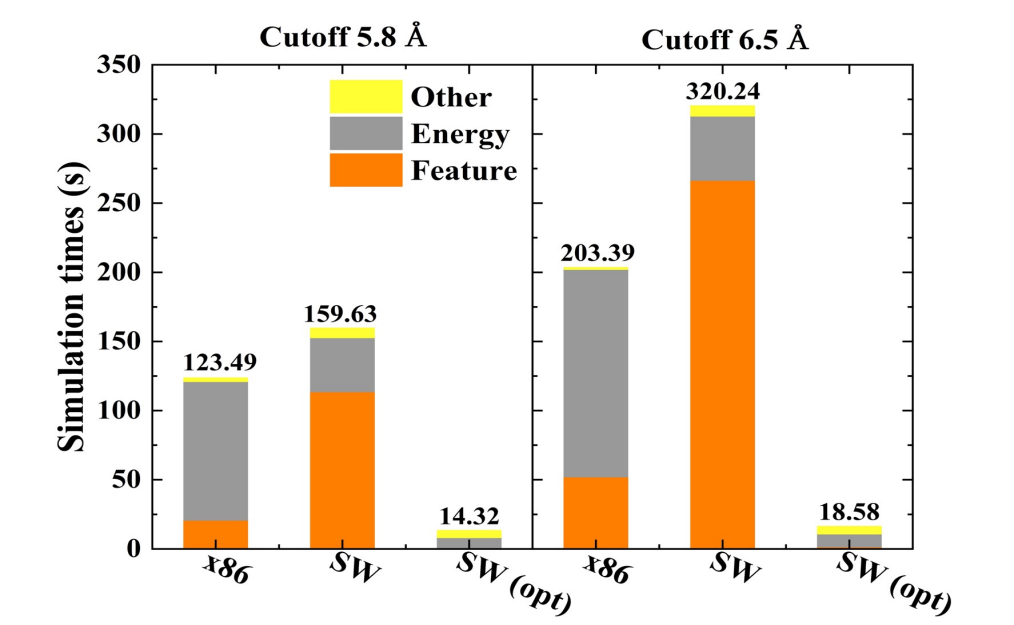
The big-fusion performances



Serial performances

- **Benchmark settings:**
  - 128 millions of atoms, 1.34% Cu concentration, 0.0008% vacancy concentration, 100 ns simulation time
- **X86:**
  - AMD EPYC, libtensorflow_cc, serial atomic feature calculation
- **SW:**
  - SW26010pro, libtensorflow_cc + SWDNN, serial atomic feature calculation
- **SW(opt):**
  - SW26010pro, customized operators

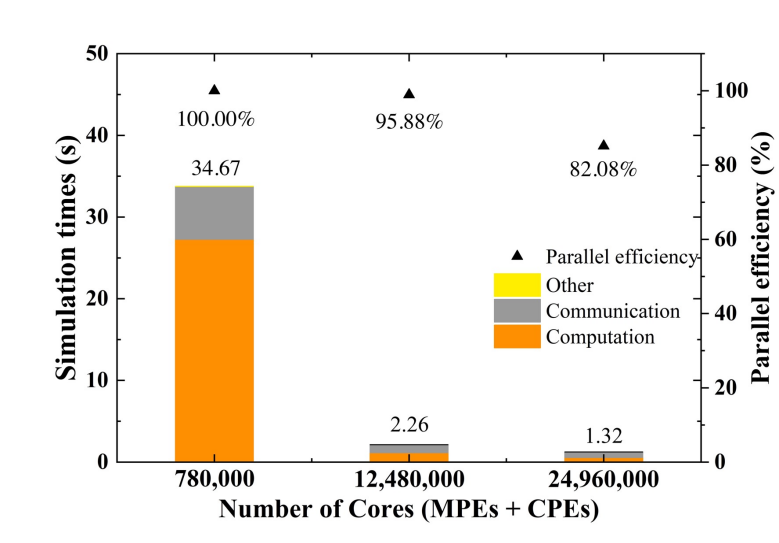
Serial performances

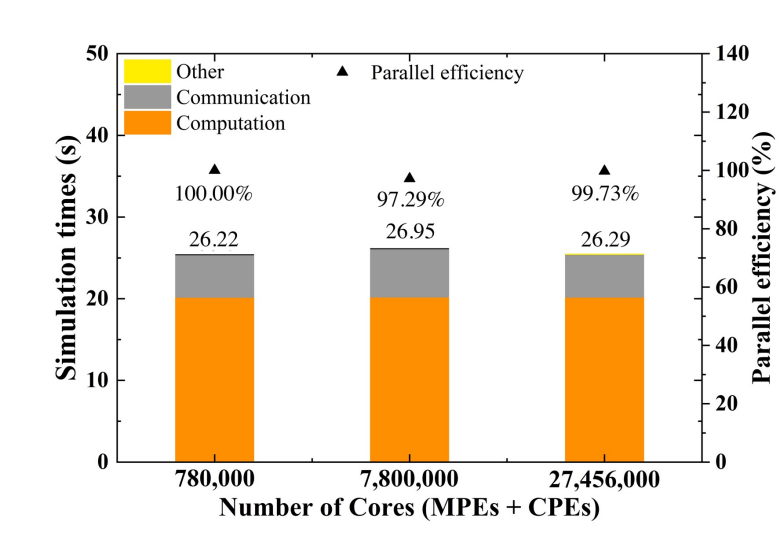


TensorKMC gains significant boost with customized operators

Parallel performances

- **Strong scaling:** 1.92 trillions of atoms
- **Weak scaling:** 128 millions of atoms / CG, maximum 54 trillions of atoms
- Synchronization interval: 20 ns





1 Background

2 Related works

3 Key innovations

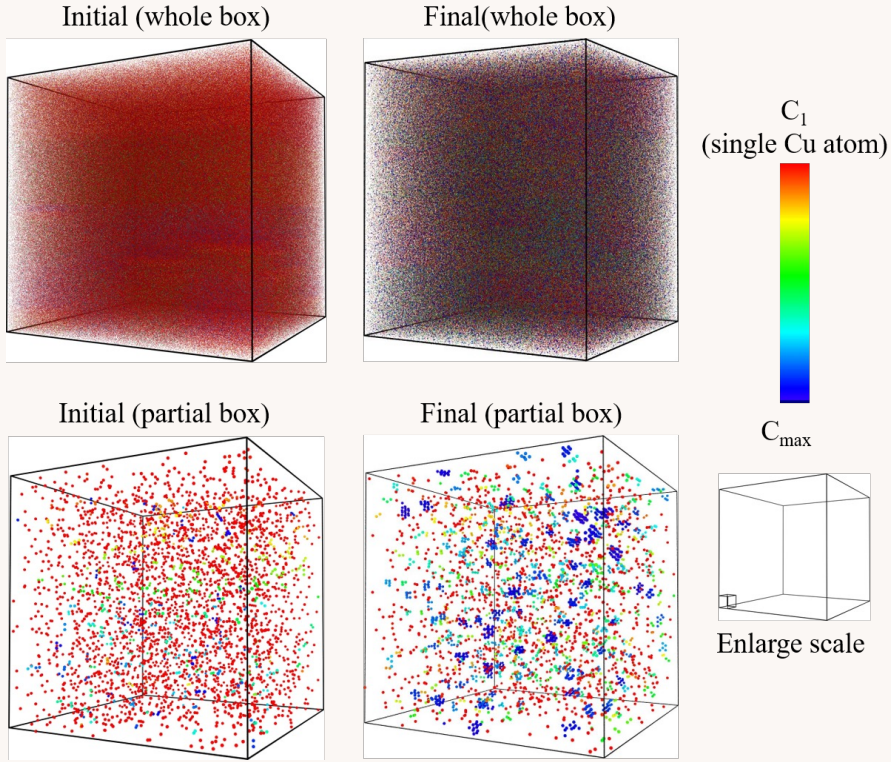
4 Performances

5 Application

Aging of Fe-Cu alloy

- 2.5 billions of atoms, 1.34% at. Cu, 0.0008% vacancy
- 1 second, 573K

- After a long-term evolution, considerable Cu cluster precipitations are observed while isolated Cu atoms are significantly reduced



Conclusion

- **TensorKMC: deep learning driven massively parallel AKMC code**
  - A successful integration of TensorAlloy and OpenKMC
  - Mesoscaling simulation on exscale machine

- The first reported micron-long kinetic simulation of 50 trillion atoms with ab initio accuracy

Papers

- **Machine learning interaction potential**
  1. TensorAlloy: an automatic atomistic neural network program for alloys. *Comput. Phys. Commun. 2020, 250, 107057*
  2. Machine learning enhanced empirical potentials for metals and alloys. *Comput. Phys. Commun. 2021, 269, 108132*

- **Atomic Kinetics Monte Carlo**
  1. **NNP-based:** TensorKMC: kinetic Monte Carlo simulation of 50 trillions of atoms driven by deep learning on a new-generation of Sunway supercomputer. *In The International Conference for High Performance Computing, Networking, Storage, And Analysis (SC'21). November 14-19, 2021*. ACM St. Louis, MO, USA.
  2. **Empirical potential based:** Redesigning OpenKMC for Multi-Component Trillion-Atom Simulations on the New Sunway Supercomputer. *IEEE Transactions on Parallel and Distributed Systems.* 2023, Just accepted.

Thanks for your attention