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# Tutorial: Introduction of High Performance Cluster at CNIC



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Hands-on Tutorial @ CLUSTER25

中国科学院计算机网络信息中心
Computer Network Information Center,
Chinese Academy of Sciences

# Outline

- High Performance Cluster at CNIC
- Hardware & Software Environment
- Operation Commands
- Users Login

# Scientific Computing System of CAS

CNIC is the first organization to provide **public supercomputing service** for basic science in China.
Devoted to HPC environment building, software development and parallel optimization for years.

**1996, 6.4GFlops**
**SGI Power Challenge XL**

**Pilo**


**2014-, 2.36PFlops**
**Yuan Supercomputer**

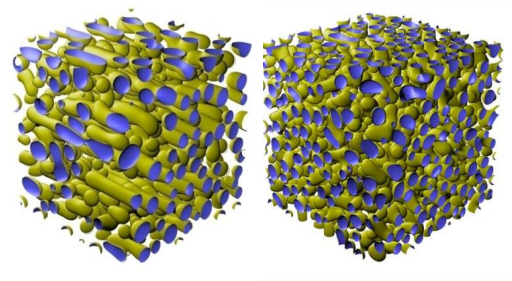
**ste**


**2019-, ORISE**

Since 1996, CNIC has deployed seven generations of supercomputing systems successively.

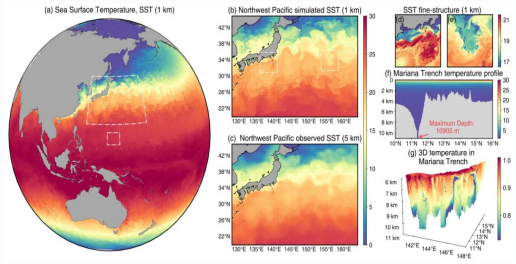
# Applications on CNIC Cluster

## Finalist for Gordon Bell Prize



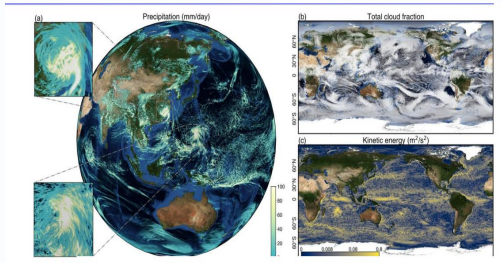
**2016 finalist for Gordon Bell Prize**

Extreme-Scale Phase Field Simulations of Coarsening Dynamics on the Sunway TaihuLight Supercomputer



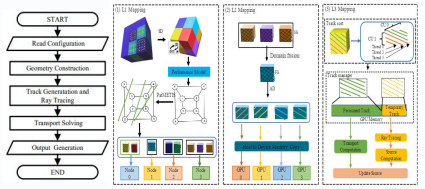

**2024 finalist for Gordon Bell Prize**

A Performance-Portable Kilometer-Scale Global Ocean Model on ORISE and New Sunway Heterogeneous Supercomputers



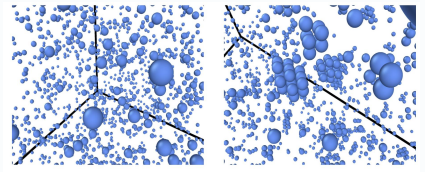

**2025 finalist for Gordon Bell Prize**

Kilometer-Scale AI-Powered and Performance-Portable Earth System Model (AP3ESM) to Achieve Year-Scale Simulation Speed on Heterogeneous Supercomputers



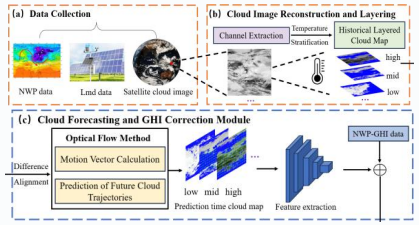

**Presented at SC'23**

ANT-MOC: Scalable Neutral Particle Transport Using 3D Method of Characteristics on Multi-GPU Systems



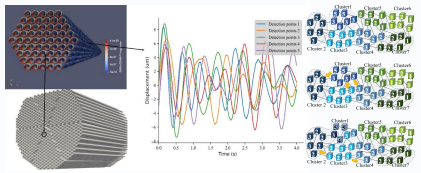
**Accepted by SC'25**

MISA-AKMC: Achieve Kinetic Monte Carlo Simulation of 20 Quadrillion Atoms on GPU Clusters



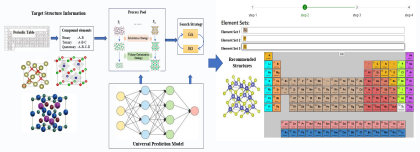

**Accepted by IJCAI' 25**

MCloudNet: An Ultra-Short-Term Photovoltaic Power Forecasting Framework With Multi-Layer Cloud Coverage



**Presented at SC'23**

Large-Scale Simulation of Structural Dynamics Computing on GPU Clusters

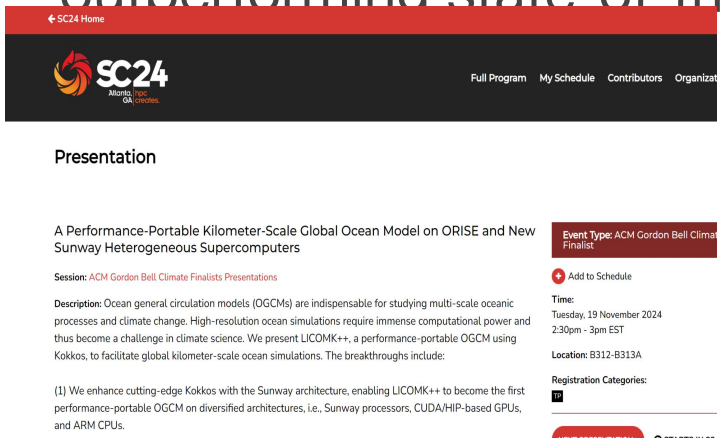


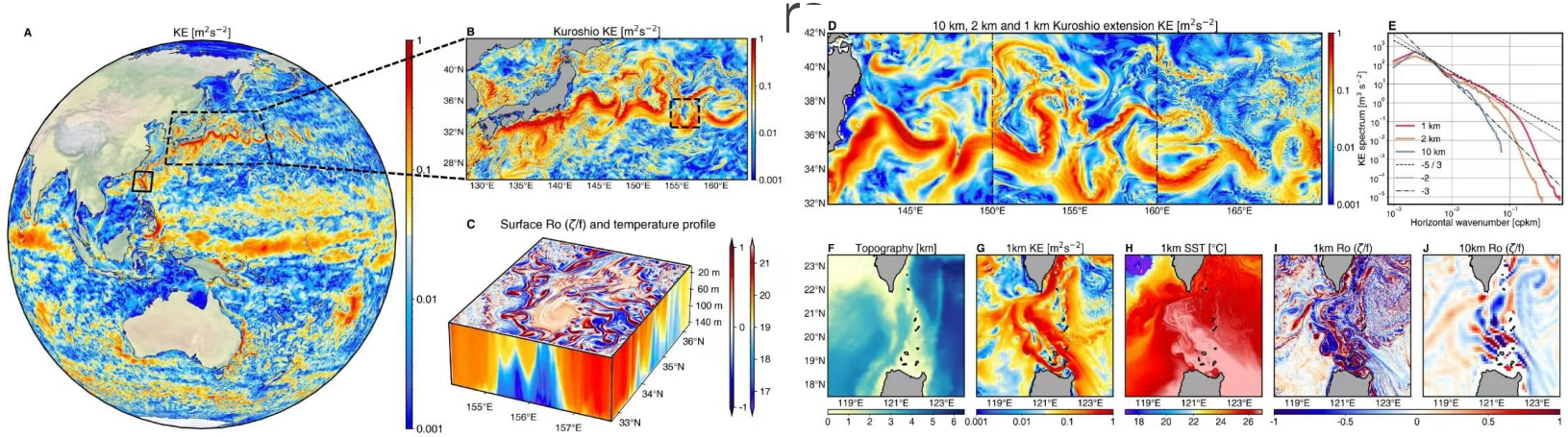
**Published in Inventions(MDPI)'25**

CrySPAI: A New Crystal Structure Prediction Software Based on AI

# LICOM++: Global Ocean Circulation Model

- **2024 finalist for Gordon Bell Prize**
- Establishing the world's first performance-portable ocean circulation model LICOMK++.
- The global 1km model can be scaled to the entire machine on **ORISE.**
- Exceeding 1 SYPD computational speed with parallel efficiency surpassing 50%, outperforming state-of-th

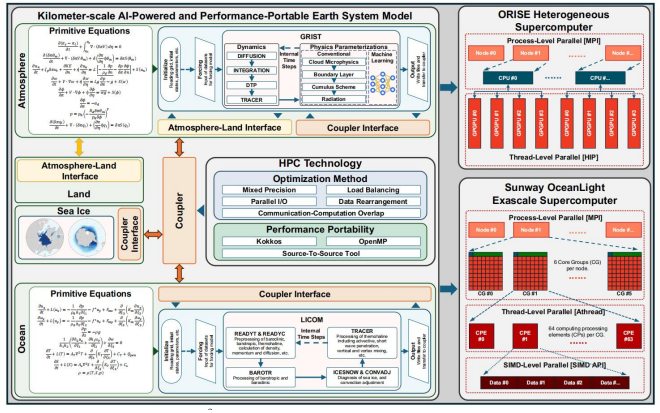


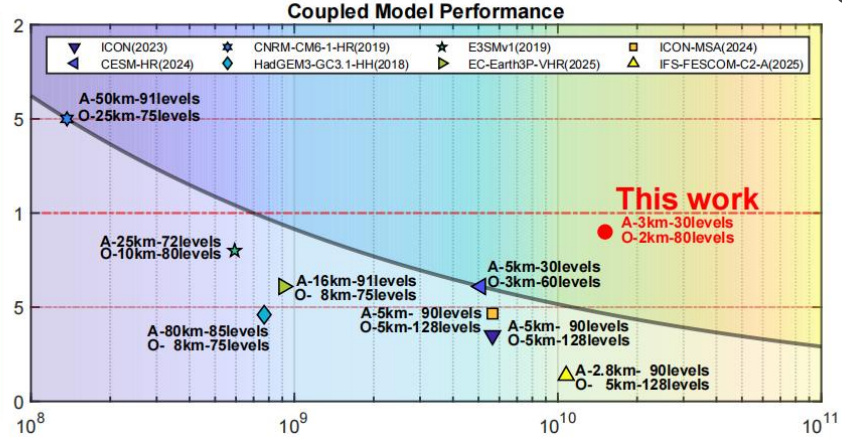



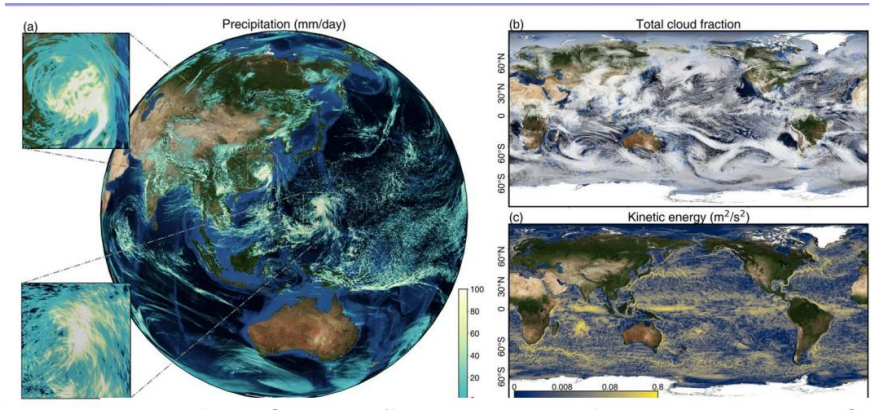

J. Wei et al., "A Performance-Portable Kilometer-Scale Global Ocean Model on ORISE and New Sunway Heterogeneous Supercomputers," SC24: International Conference for High Performance Computing, Networking, Storage and Analysis, Atlanta, GA, USA, 2024, pp. 1-12, doi: 10.1109/SC41406.2024.00009. keywords: {High performance computing;Ocean circulation;Climate change;Computational modeling;Supercomputers;Program processors;Computer architecture;Meteorology;Climatology;High-Performance Computing;Ocean General Circulation Model;Performance-Portable;Sunway Architecture}

# AP³ESM: Kilometer-Scale AI-Powered and Performance-Portable Earth System Model

- **2025 finalist for Gordon Bell Prize**
- Awarded the **'Best Supercomputing Application of the Year'** at the 21st National High Performance Computing Academic Conference hosted by the China Computer Federation (CCF).
- By employing Kokkos and OpenMP to achieve performance portability, this approach enables efficient operation on **ORISE** while minimizing development costs.



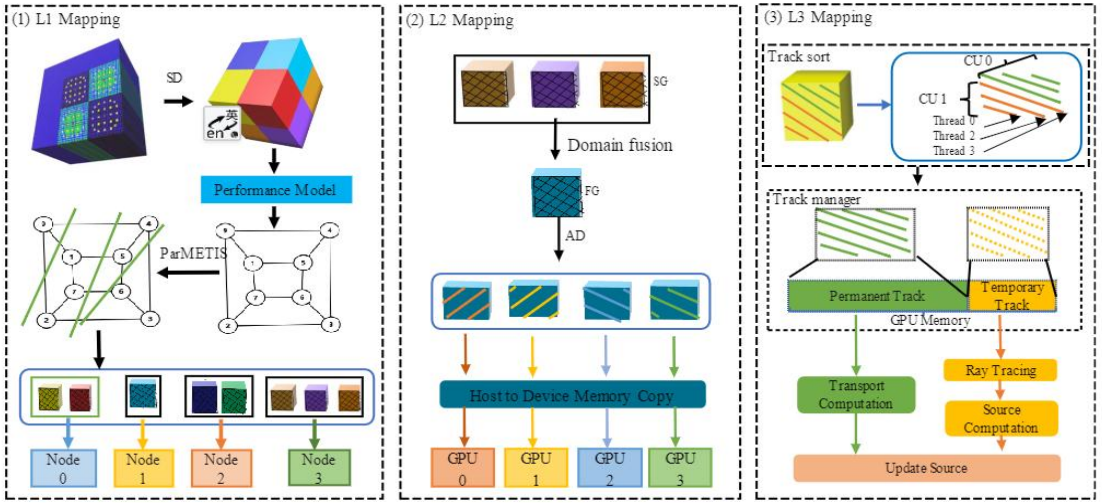



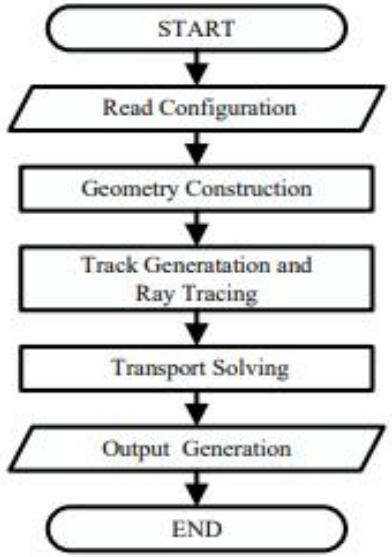



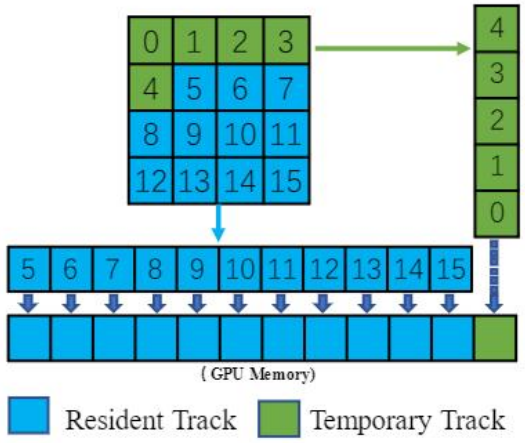

Kai Xu, Maoxue Yu, Yuhu Chen, Jie Gao, Shuang Wang, Jiaying Song, Xiaohui Duan, Junlin Wei, Jiangfeng Yu, Hailong Liu∗, Jinrong Jiang∗, Yi Zhang∗, Pengfei Lin∗, Tianyi Wang, Pengfei Wang, Weipeng Zheng, Jingwei Xie, Jiakang Zhang, Zilu Liu, Xiaoyu Jin, Jilin Wei, Qixin Chang, Qingxia Lin, Yanzhi Zhou, Yiwen Li, Weiguo Liu, Wei Xue, Haohuan Fu, Yue Yu, Xuebin Chi, Lixin Wu. 2025, Kilometer-Scale AI-Powered and Performance-Portable Earth System Model (AP3ESM) to Achieve Year-Scale Simulation Speed on Heterogeneous Supercomputers. *SC25: International Conference for High Performance Computing, Networking, Storage and Analysis* (CCF-A), Accepted.

# ANT-MOC: Scalable Neutral Particle Transport Using 3D Method of Characteristics on Multi-GPU Systems

- Awarded the **Only Double Nomination** for **Best Paper** and **Best Student Paper** at the 35th International Supercomputing Conference SC'23.
- Achieving high parallel efficiency within an ultra-large-scale parallel system comprising 16,000 GPUs, with strong scalability parallel efficiency reaching 70.69% and weak scalability parallel efficiency reaching 89.38%.



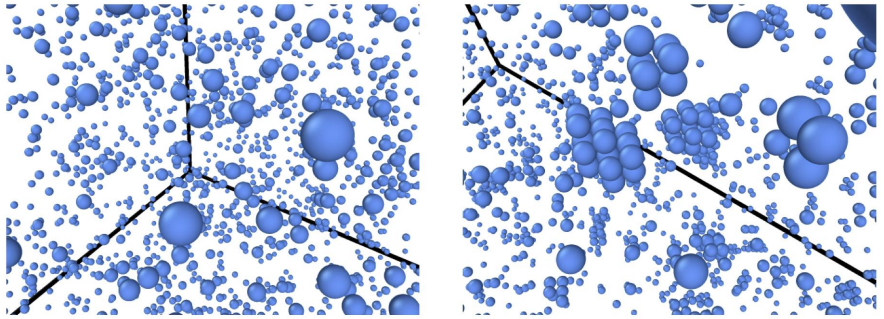




Shunde Li, Zongguo Wang, Lingkun Bu, Jue Wang, Zhikuang Xin, Shigang Li, Yangang Wang, Yangde Feng, Peng Shi, Yun Hu, and Xuebin Chi. 2023. ANT-MOC: Scalable Neutral Particle Transport Using 3D Method of Characteristics on Multi-GPU Systems. In The International Conference for High Performance Computing, Networking, Storage and Analysis (SC '23), November 12–17, 2023, Denver, CO, USA. ACM, New York, NY, USA, 12 pages

# MISA-AKMC: Achieve Kinetic Monte Carlo Simulation of 20 Quadrillion Atoms on GPU Clusters

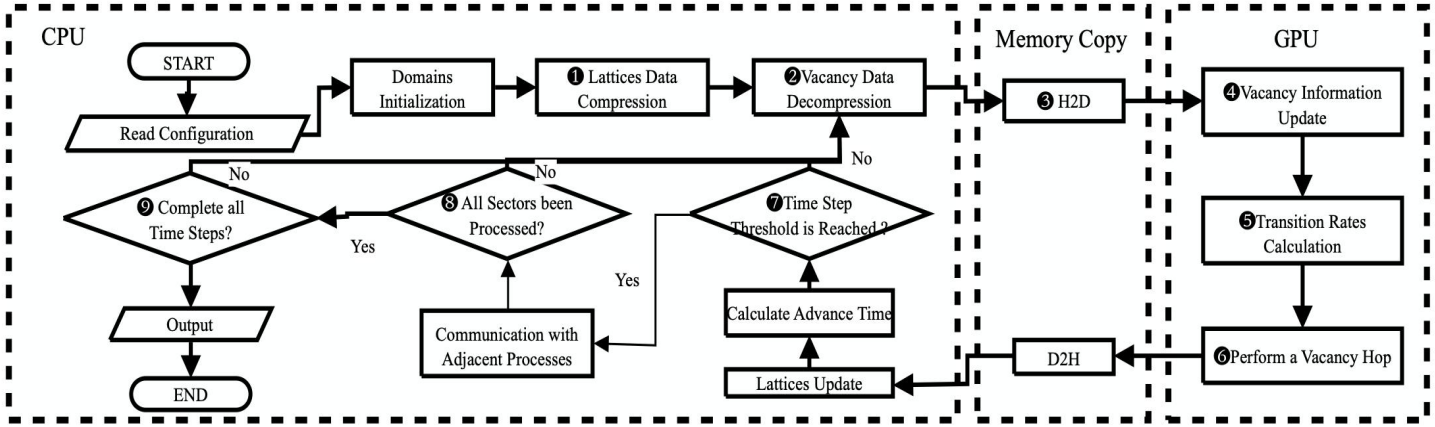
- Accepted by the International Supercomputing Conference **SC'25 (CCF A)**
- Self-developed new simulation software MISA-AKMC , for the first time achieving micrometer-scale atomic dynamics Monte Carlo simulations at a scale of $2*10^{16}$ atoms, setting a new benchmark in simulation scale within this field.
- Achieving high parallel efficiency within an ultra-large-scale parallel system comprising 16,000 GPUs, successfully overcoming the parallel computing bottleneck in atomic-level simulations.



(a) Initial state



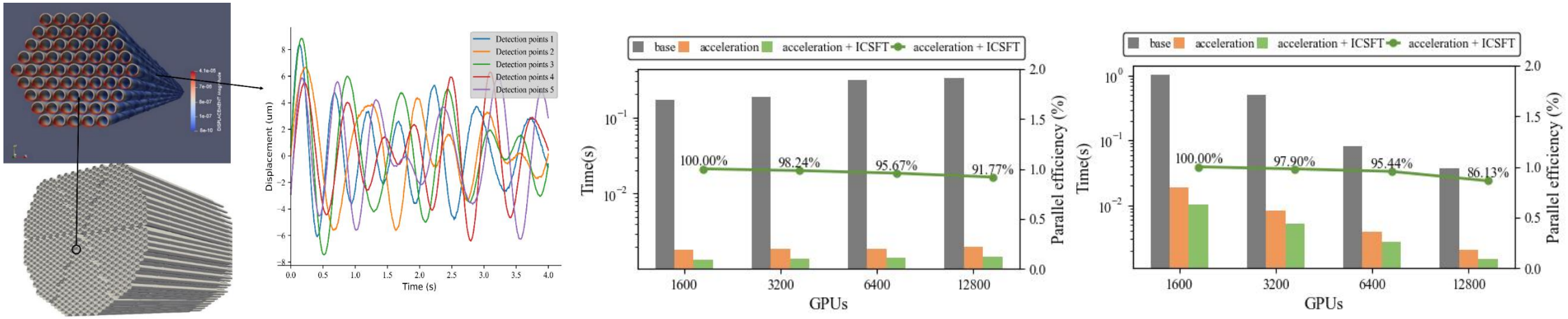
(b) Final state




Li Shunde, Pan Zhijie, Nie Ningming, Wang Jue*, Bai He, Chu Genshen, Zeng Yan, He Xinfu, Wang Yangang, Hu Changjun, Chi Xuebin. MISA-AKMC: Achieve Kinetic Monte Carlo Simulation of 20 Quadrillion Atoms on GPU Clusters. In Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis (SC '25).

# Large-Scale Simulation of Structural Dynamics Computing on GPU Clusters

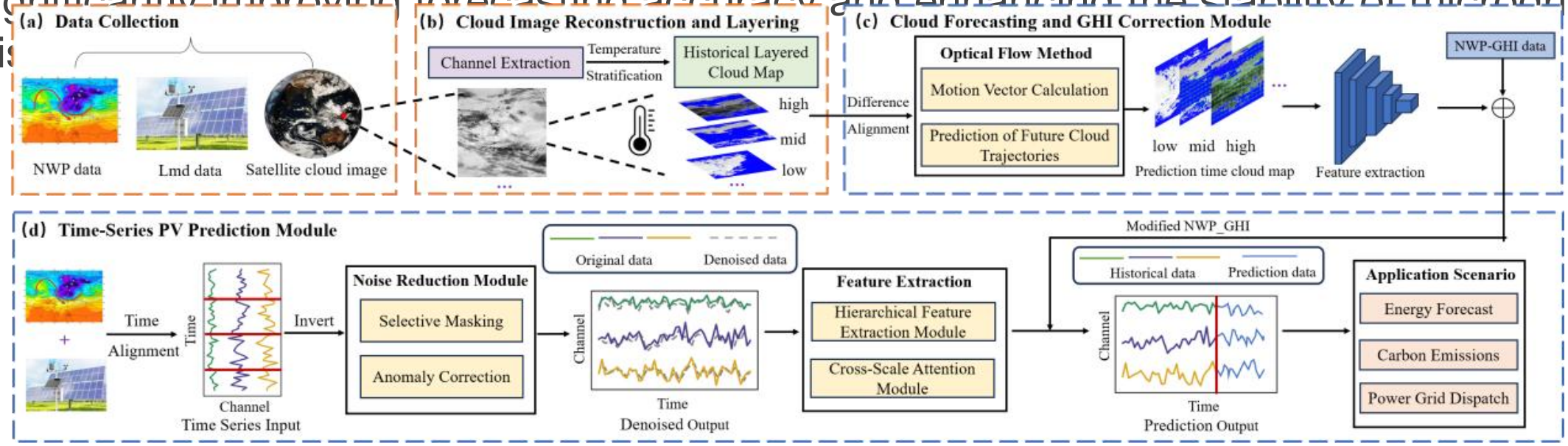
- Presented at SC'23
- Simulation of flow-induced vibration with a hundred-billion-mesh grid using 12,800 DCUs on **ORISE**.
- The maximum displacement at the top of the fuel assembly reached 9 micrometers, demonstrating accuracy comparable to test results from the US Westinghouse Test Centre, which illustrated the correctness of the simulation.




Y. Shi et al., "Large-Scale Simulation of Structural Dynamics Computing on GPU Clusters," SC23: International Conference for High Performance Computing, Networking, Storage and Analysis, Denver, CO, USA, 2023, pp. 1-14

# MCloudNet: An Ultra-Short-Term Photovoltaic Power Forecasting Framework With Multi-Layer Cloud Coverage

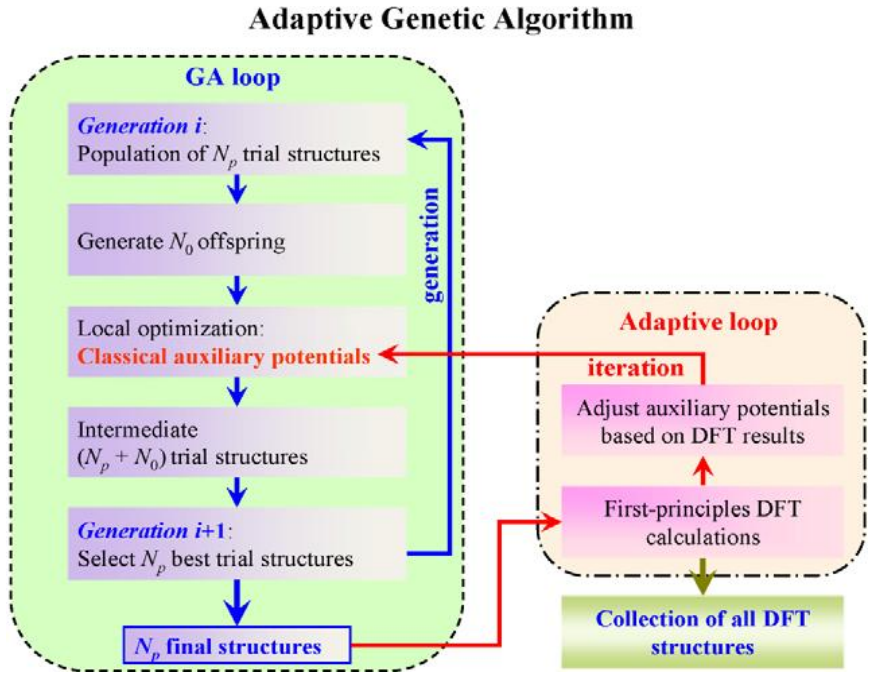
- Accepted by the International Joint Conference on Artificial Intelligence **IJCAI' 25 (CCF Class A)**
- MCloudNet enables ultra-short-term multi-cloud layer photovoltaic power forecasting.
- The model has been deployed across multiple photovoltaic power stations, significantly improving forecasting accuracy and enhancing the stability of microgrid dis

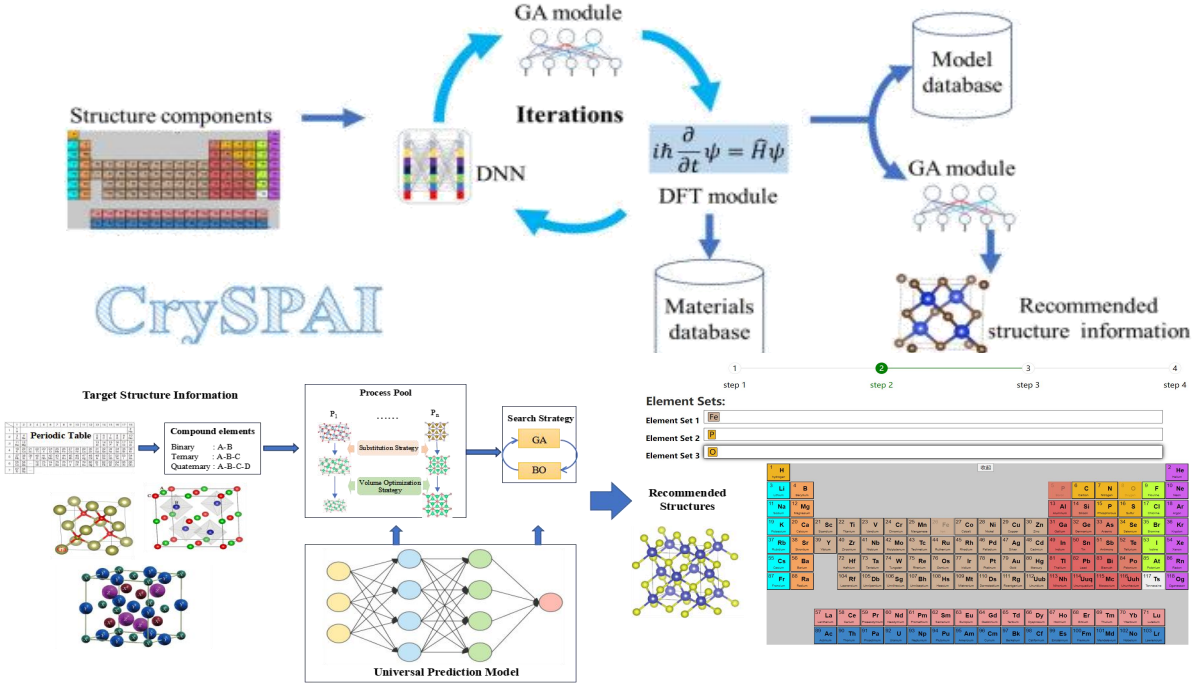



Meng Wan, Tiantian Liu, Yuxuan Bi, Jue Wang, Hui Cui, Rongqiang Cao, Jiaxiang Wang, Peng Shi, Ningming Nie, Yangang Wang. MCloudNet: An Ultra-Short-Term Photovoltaic Power Forecasting Framework With Multi-Layer Cloud Coverage. In Proceedings of the 34th International Joint Conference on Artificial Intelligence; IJCAI' 25.

# CrySPAI: A New Crystal Structure Prediction Software Based on AI

- Based on AGA framework,  AI method is introduced to form high performance material structure prediction software
- In 2010, we proposed an adaptive and iterative approach that combines the structural search speed of classical potentials with the accuracy of DFT calculations to improve the efficiency of DFT-based genetic algorithms by several orders of magnitude.




Wang, Z.; Chen, Z.; Yuan, Y.; Wang, Y. CrySPAI: A New Crystal Structure Prediction Software Based on Artificial Intelligence. Inventions 2025, 10, 26. https://doi.org/10.3390/inventions10020026

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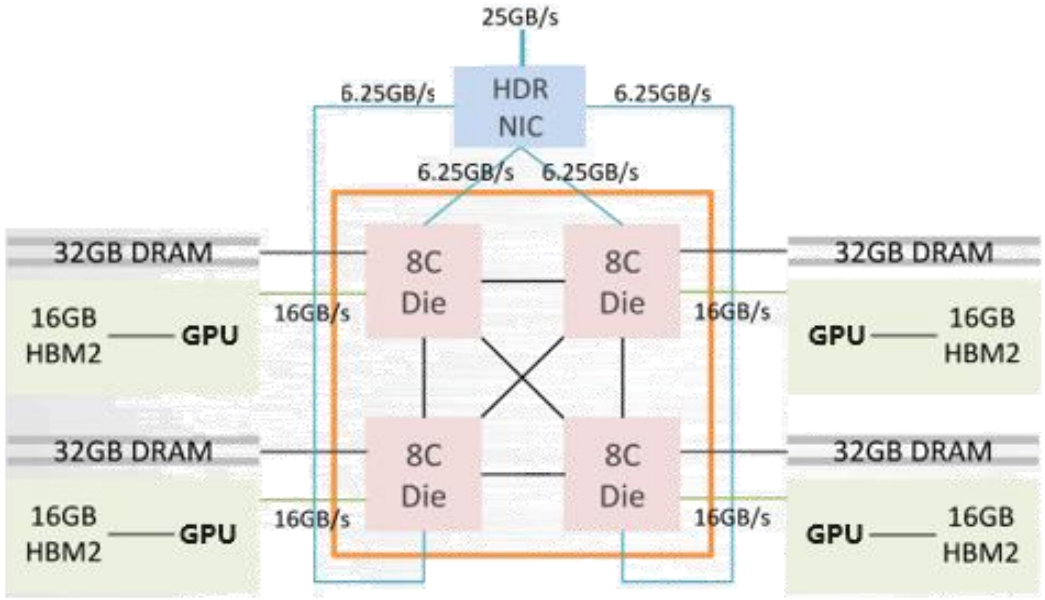
# High Performance Cluster at CNIC

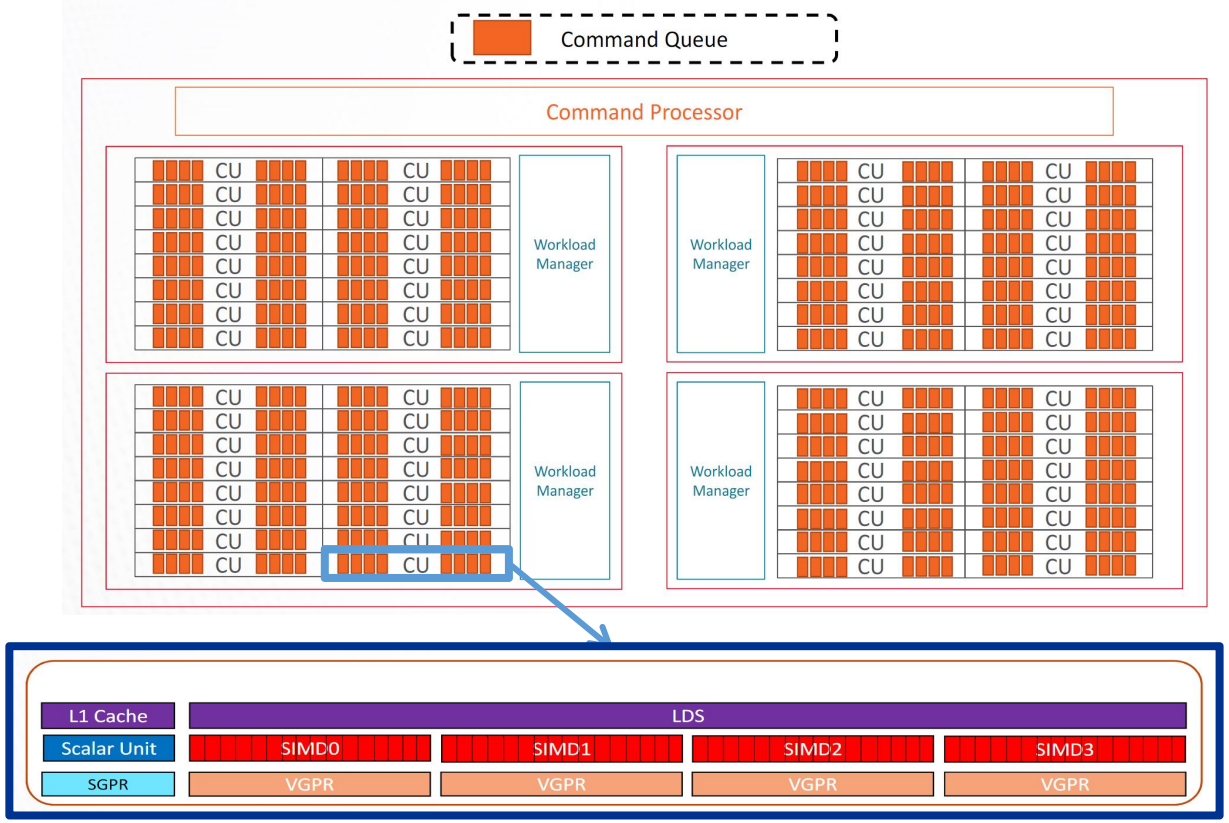



## NODES

- 32-core AMD Zen-based processor
- 128 GB host memory
- four AMD Instinct MI60 GPUs pre Node

## GPU

- 64 CUs
- 16 GB memory



# Software Environment

The system is equipped with complete, efficient and professional basic software, including operating system, compiler, mathematical library, parallel Computing environment software, etc. According to the user's needs, we will install and update the application software of various disciplines.

| ITEM | NAME | VERSION | PATH | MODULE NAME |
|---|---|---|---|---|
| CPU: C/Fortran Compiler | gcc/g++ | 7.3.1 | /opt/rh/devtoolse t-7 | compiler/devtoolset/7.3.1 |
| | gfortran | 7.3.1 | /opt/rh/devtoolse t-7 | compiler/devtoolset/7.3.1 |
| GPU Compiler | hipcc | 2.8.19361 | /opt/rocm/hip/ | compiler/rocm/2.9 |
| debugger | gdb | 8.0.1 36.el7 | /opt/rh/devtoolset-7/ | compiler/devtoolset/7.3.1 |
| MPI | hpcx-v2.7.4 | v2.7.4 | /opt/hpc/software/mpi/hpcx/v2.7.4 | mpi/hpcx/2.7.4/gcc-7.3.1 |
| miopen | miopen | 2.8.19361 | /opt/rocm/miopen/ | compiler/rocm/2.9 |
| rocblas | rocblas | 2.8.19361 | /opt/rocm/rocblas | compiler/rocm/2.9 |

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# Module Commands

| Module Commands | Usage |
|---|---|
| module av | View the available Modules |
| module list | View the currently loaded modules |
| module load modulefile | Load modules |
| module unload modulefile | Unload modules |
| module switch modulefile | Switch modules |
| module purge | Clear all loaded modules |
| module show modulefile | Show module content |

01 Check the available software in the system:
**$ module av**

02 To set the environment variables of a certain software, run the **module load** command. For example, to load the HDF5 library:
**$ module load mathlib/hdf5/1.9.20/intel**

03 View loaded environment usage:
**$ module list**

04 To uninstall software that is no longer needed using commands:
**$ module rm mathlib/hdf5/1.9.20/intel**

# Slurm Commands

| Commands | Usage | Example |
|---|---|---|
| sinfo | Displays the status of partitions and nodes | sinfo |
| squeue | Show job status | squene |
| srun | For interactive job submission | srun -n 2 -p p1-c1-2 hostname |
| sbatch | For batch job submission | sbatch -n 2 job.sh |
| salloc | For assignment mode job submission | salloc -p p1-c1-2 |
| scancel | Used to cancel a submitted job | scancel JOBID |
| scontrol | You can view and modify the slurm configuration and status, including querying node information or information about running jobs | scontrol show job JOBID |

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# Users Login

The login node of the GPU cluster is used to submit tasks.
You can log in to the assigned compute node only after the job scheduling system allocates resources.

The GPU cluster uses load balancing to allocate the login nodes. It is normal that the host name assigned to the login node may be different after each login.

| Login IP address: 60.245.128.10 | SSH Port : 65010 | ssh dfcs2025@60.245.128.10 –p 65010 |
|---|---|---|

**Login password Static password + dynamic password code**

Static password **is** dfcs20251234
**If the dynamic password is** 011594**, the password is** dfcs20251234011594

# Thanks!

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