INFORMATION TECHNOLOGY CENTER
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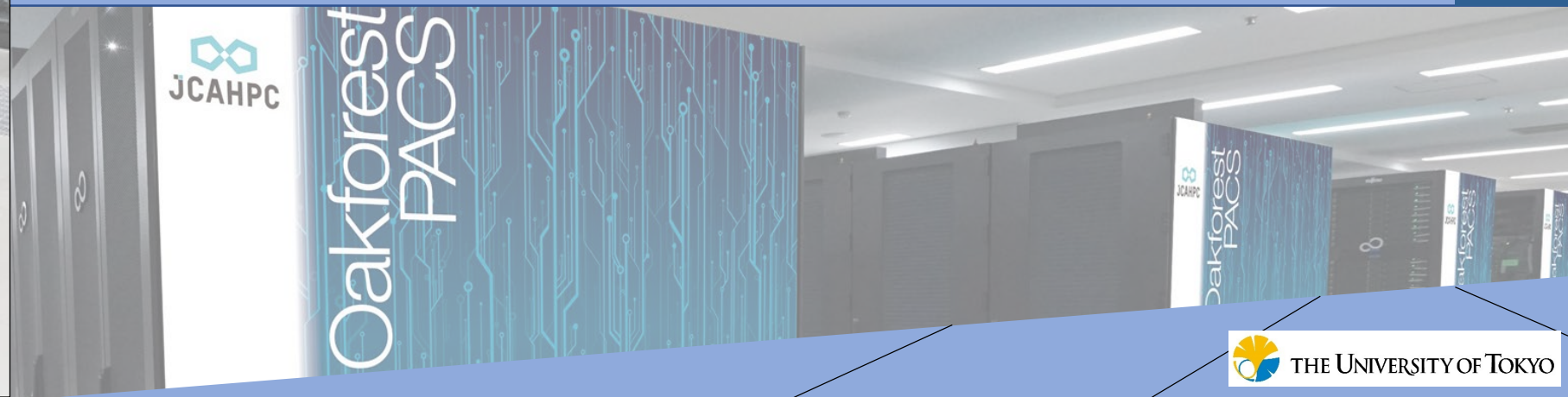
JCAHPC

Research Activities of SCD/U-Tokyo



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Contents

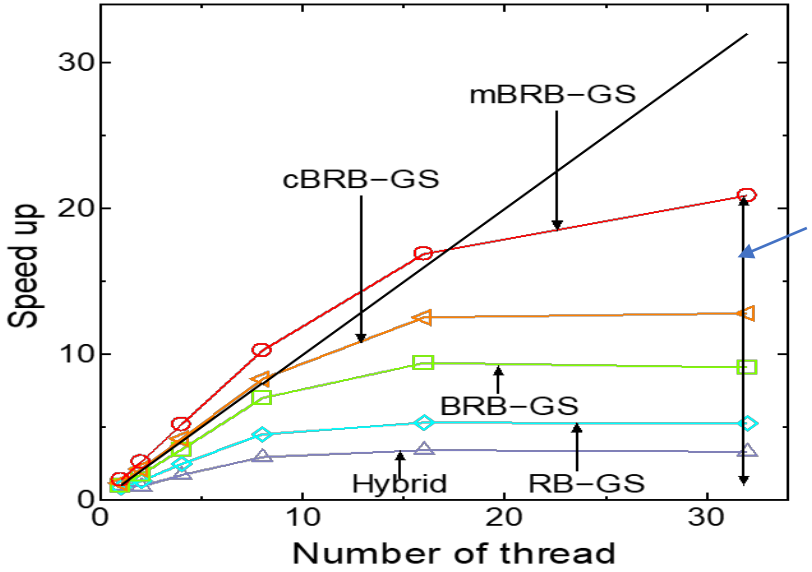
- Location of movies:
  https://www.cc.u-tokyo.ac.jp/en/public/isc21.php
- Research activities to improve HPC
  - Development of high-performance iterative solvers for SLEs
  - High Performance Framework for Many-core Clusters
- Research activities utilizing HPC
  - Accelerating Simulations of Computational Fluid Dynamics (CFD)
  - Toward Acceleration of Molecular Dynamics
  - Exploration of dark matter sub-halos by using *N*-body simulations

Development of High-performance Iterative Solvers for SLEs

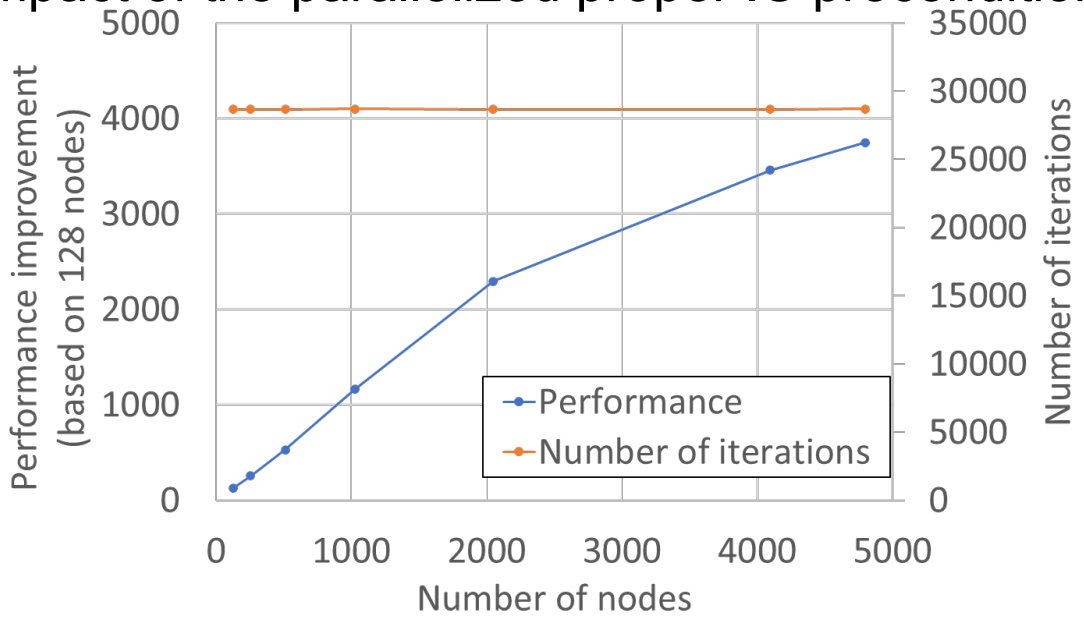
- PI: Masatoshi Kawai
- Research of iterative methods for
  - ✓Static and dynamic analysis
  - ✓Eigenvalue problems

  with high-performance
  - ✓Multigrid method, preconditioner
  - ✓IC preconditioner
- Outcomes
  - ✓Multiplicative-Schwartz type Block multi-color GS smoother
  - ✓SIMDization of the GS method
  - ✓Massively parallelization of a proper IC preconditioner

Effect of MS-BMC-GS smoother



Impact of the parallelized proper IC preconditioner



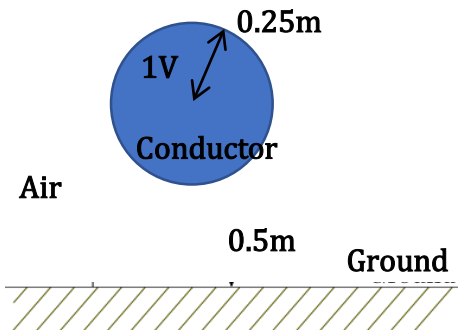
High Performance Framework for Many-core Clusters

Tetsuya Hoshino

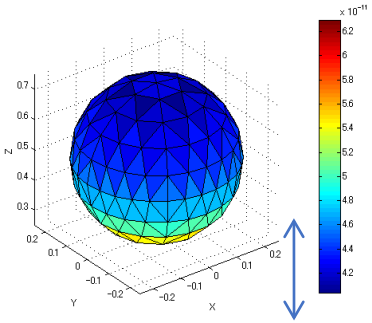
Research topics

- ✓ **Performance optimizations and modeling for many-core processors**
  - ✓ **A64FX, GPUs, Intel Knights Landing**
- ✓ **Auto-tuning, parallel algorighms**
  - ✓ **Semi-auto-vectorization for HACApK library**
    - ✓ **$\mathcal{H}$ACApK library :https://github.com/Post-Peta-Crest/ppOpenHPC/tree/MATH/HACApK**
  - ✓ **Load-balancing-aware algorithm of H-matrices for GPUs**

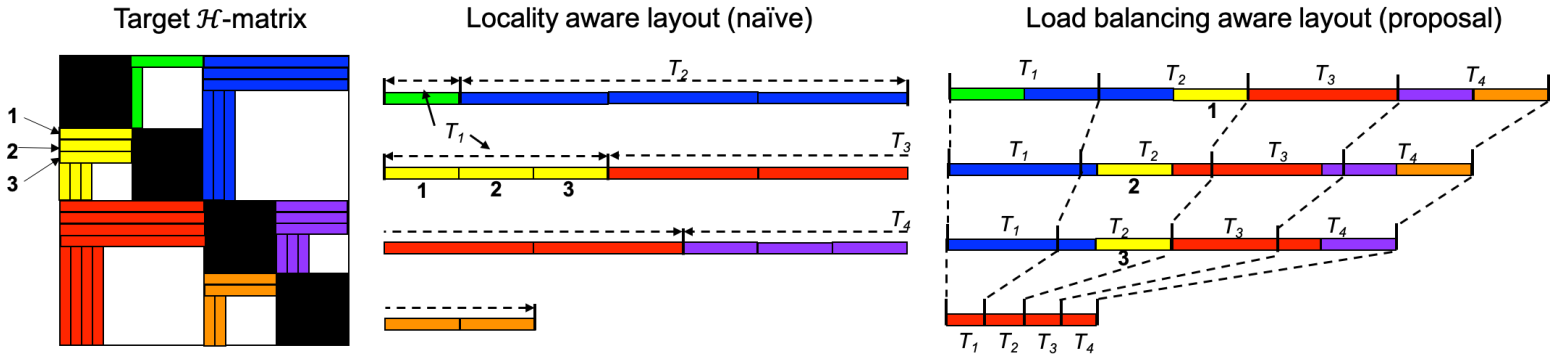
Analysis condition



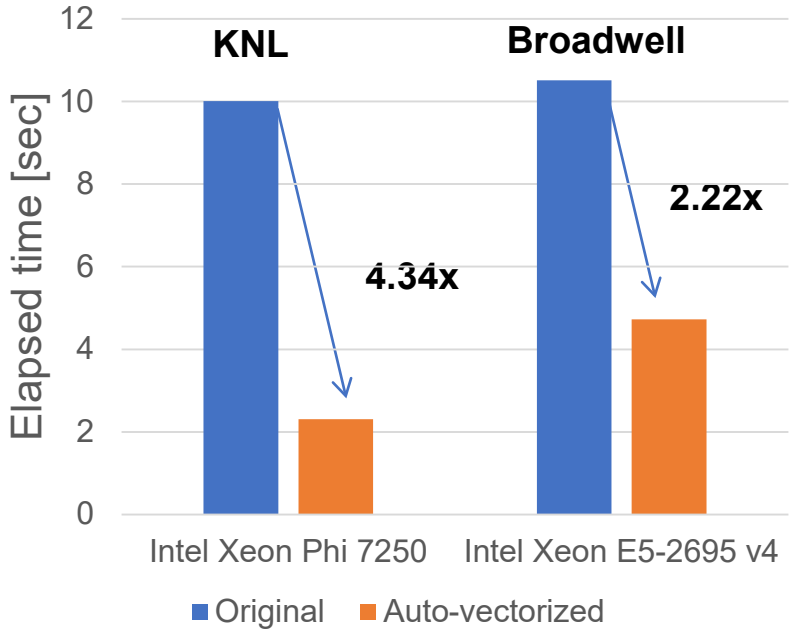
Analysis result



New data storage method of H-matrix for GPUs



Semi-auto-vectorization of H-matrix generation



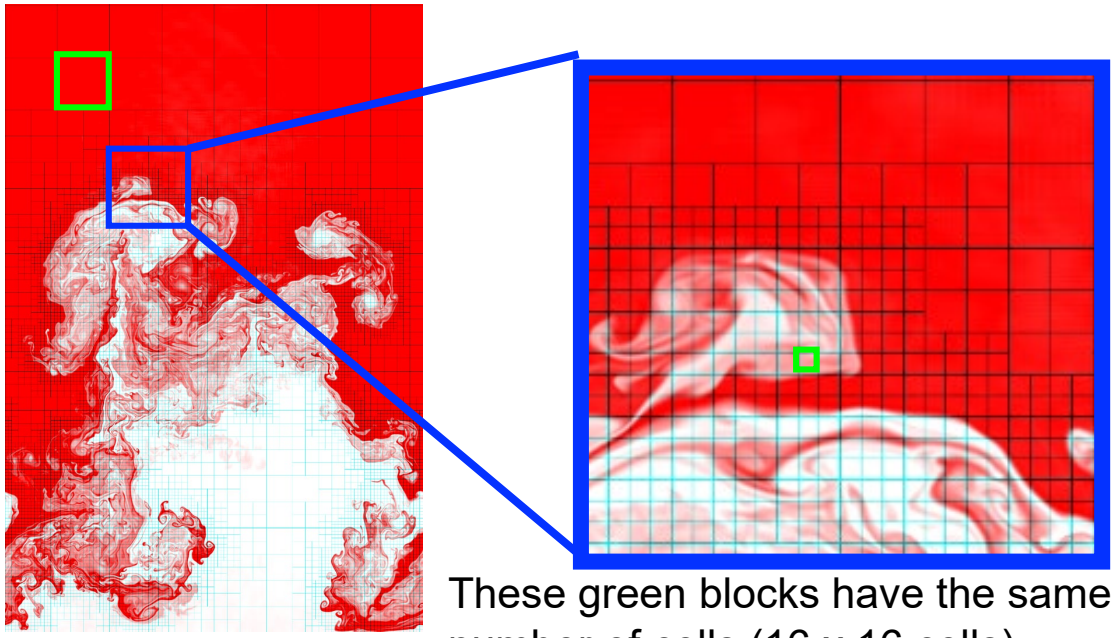
Accelerating Simulations of Computational Fluid Dynamics (CFD)

Takashi Shimokawabe

Research topics

- Large-scale CFD simulations on GPU supercomputers
- Adaptive mesh refinement (AMR) framework for GPU supercomputers
- Machine-learning-based fast surrogate model for CFD simulations

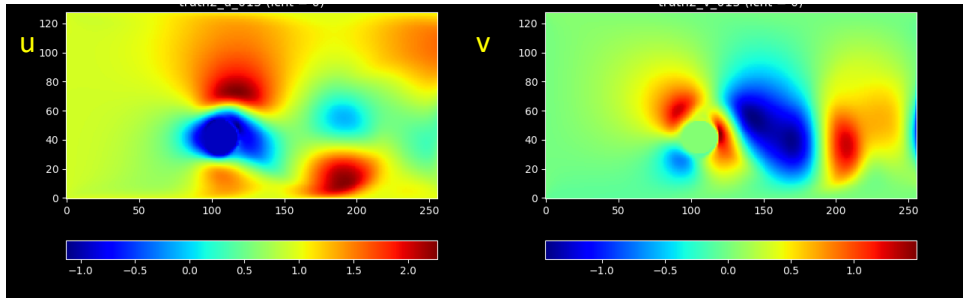
Rayleigh-Taylor Instability Simulation



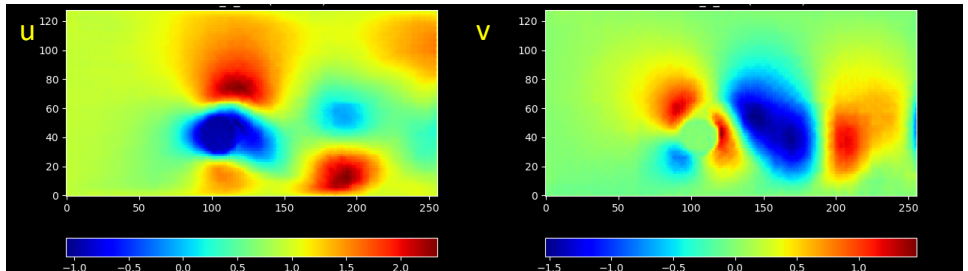
These green blocks have the same number of cells (16 x 16 cells)

CFD results predicted by deep learning

Ground truth (LBM simulation)



Prediction (DNN)



Toward Acceleration of Molecular Dynamics

Hayato Shiba

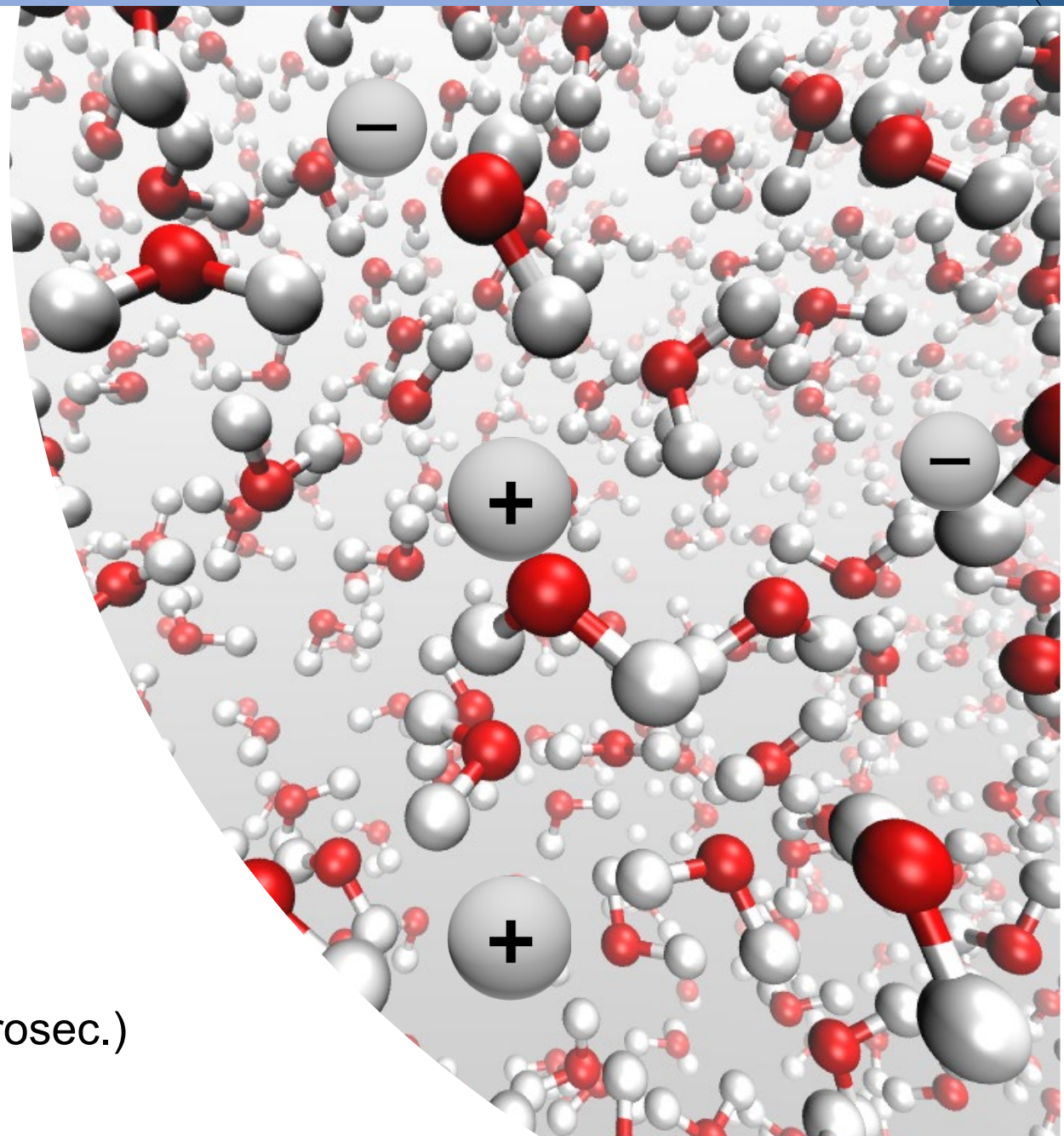
Molecular Dynamics for Liquid / Soft Matter

Current research topics

superparallel molecular simulations
& enhanced sampling methods
for electrolyte solutions

- Machine-learning-assisted path sampling of reaction coordinate
  beyond limitation of communication wall

- Long-wave phenomena on interfaces with solvated ions
  toward the mesoscale (billion-atom + microsec.)



Exploration of Dark Matter Sub-halos by Using *N*-body Simulations

- PI: Yohei MIKI
- Missing satellite problem: cosmological simulations overproduce dark matter (DM) sub-halos [$\mathcal{O}(100)$] compared to observed satellites around Milky Way-size galaxies [$\mathcal{O}(10)$]
  - Hypothesis: ~10% DM sub-halos succeeded to form stars
- Challenge: observational estimation of DM sub-halo counts
  - Gap detection in stellar streams
  - Feasibility studies using gravitational *N*-body simulations are on-going (➔)