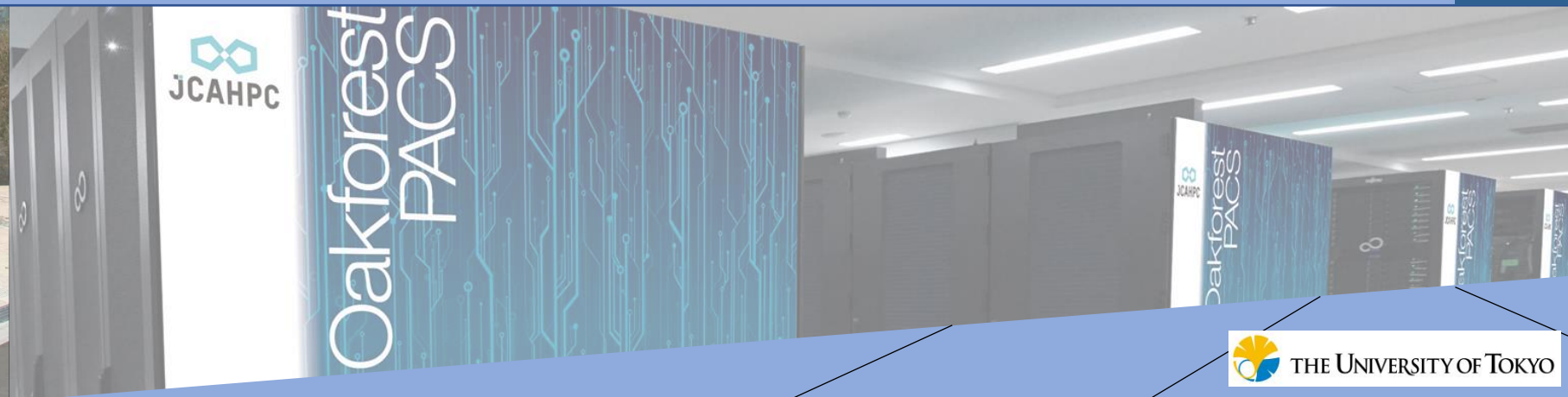
INFORMATION TECHNOLOGY CENTER
THE UNIVERSITY OF TOKYO

JCAHPC

Research activities



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Contents

- Location of movies:
  https://www.cc.u-tokyo.ac.jp/public/sc20.php
- Research activities to improve HPC
  - SH/HW Optimizations for Next-Generation Supercomputing
  - Development of high-performance iterative solvers for SLEs
  - $\mathcal{H}$**ACApK** : $\mathcal{H}$-matrices Library for distributed memory systems
  - 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

SW/HW Optimizations for Next-Generation Supercomputing

Eishi Arima, Ph.D

✉ arima@cc.u-tokyo.ac.jp

My broader research interests are principally in computer architecture, system software, and high performance computing, while the major focus is on software/hardware cooperative optimizations for emerging architectures including such as novel memory subsystems and wide SIMD machines in order to improve performance, energy efficiency, and other perspectives.

Topics:

- **Footprint-Aware Power Capping:** An in-node power management scheme explicitly aware of problem scale [ISC'20paper][Youtube]
- **Large-Scale Power Evaluation:** A case for power control features of A64FX processor using over 20K Fugaku nodes [Youtube]
- **Pattern-Aware Staging:** A compiler-based data optimization technique for hybrid main memories [ISC'20paper][Youtube]
- **Classification-Based Caching:** A sophisticated cache replacement mechanism useful for modern microprocessors [DSD'20paper]
- **Footprint-Aware Co-Scheduling:** A scheduler-based approach to improve resource utilizations (ongoing work) [ICPP'19abst][Poster]
- **Older Contents:** NVRAM-based hardware cache architectures/implementation [DATE'13paper][ICCD'15paper][ISSCC'16paper]

Grants:

- **PI**, "Coscheduling Methods for Next-Generation Large-Scaled Systems with Heterogeneous Memories", *JSPS Grant-in-Aid for Early-Career Scientist*, 4.29M JPY, FY2020-FY2021
- **PI**, "Exploiting High-Bandwidth and Large-Capacity on Hybrid Main Memories through Pattern-Aware Optimization", *JSPS Grant-in-Aid for Early-Career Scientist*, 4.16M JPY, FY2018-FY2019
- **PI**, "Memory System Optimization for Energy Efficient Big Data Processing", *JSPS Grant-in-Aid for Research Activity Start-up*, 2.99M JPY, FY2016-FY2017

Professional Activities:

- **ACM CF'21 Special Session Chair**, **ACM CF'20 Program Chair**, **IEEE Cluster'19 Publications Chair**, IEEE NVMSA'18 Web Chair
- **Program Committee: IPDPS'21**, HPC ASIA'21, **HiPC'20**, IA^3@SC'20, CANDAR'20, Cluster'20 (Posters), ISC'20 PhD Forum, CANDAR'19, ISC'19 PhD Forum, CANDAR'18, NVMSA'18, **ICPP'18**, SCAsia'18, HPC ASIA'18, CANDAR'17, NVMSA'17, (xSIG'19,'20)

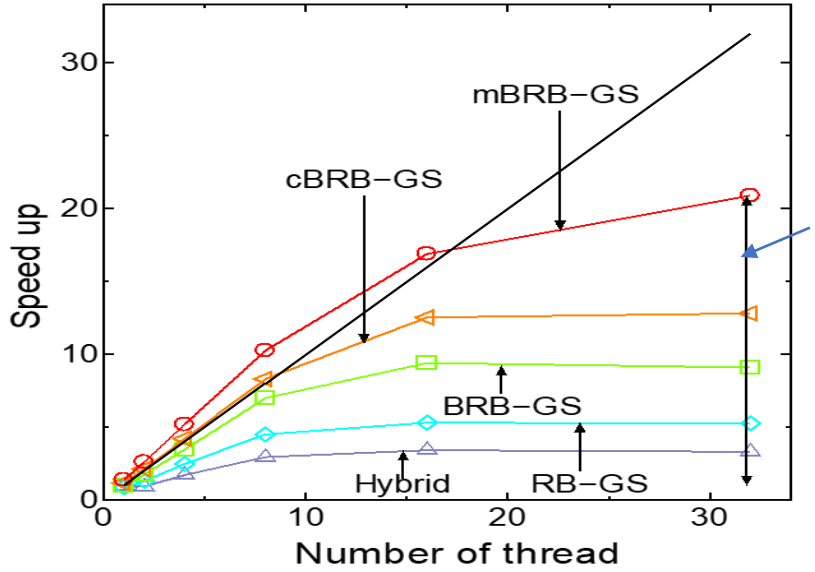
🌐 https://www.cspp.cc.u-tokyo.ac.jp/arima/index-e.html

Development of high-performance iterative solvers for SLEs

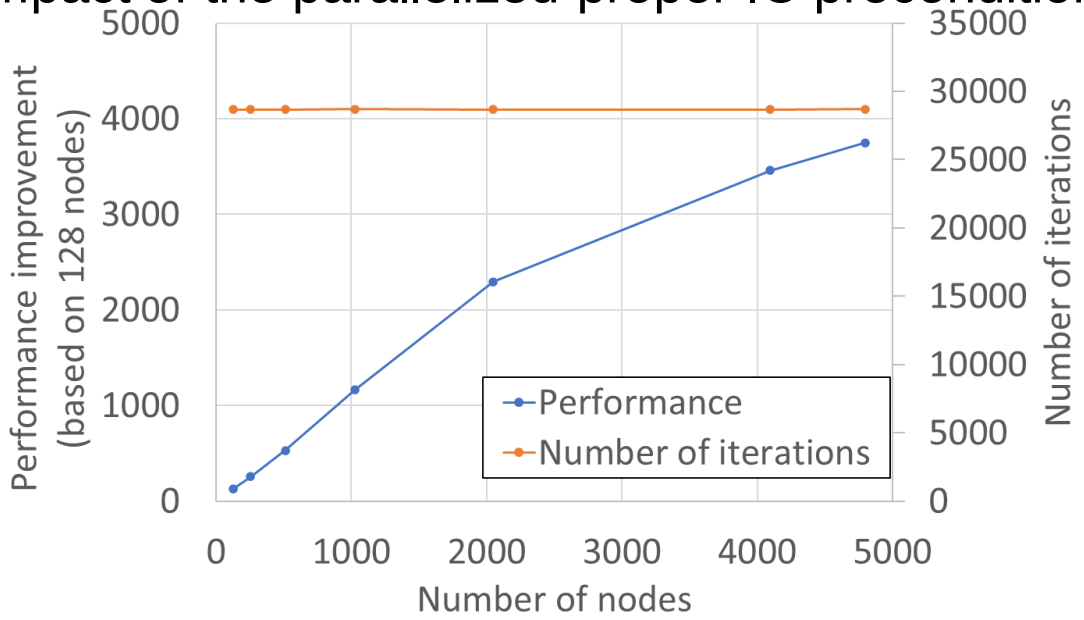
- PI: Masatoshi Kawai
- Research of iterative methods for
  - ✓Static and dynamic analysis
  - ✓Eigenvalue problems

  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

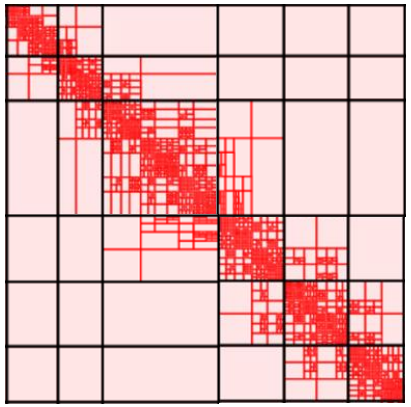


$\mathcal{H}$ACApK : $\mathcal{H}$-matrices Library for distributed memory systems

Ida, Akihiro (✉ ida@cc.u-Tokyo.ac.jp)

► **$\mathcal{H}$ACApK library :**

- **enables us to conduct large-scale simulations based on the boudary integral equation method.**
- **is developed for CPU-based clusters, and partialy ported to multi-GPU platforms.**
- **is an open-source software (MIT license).**



► **Available formats**

- (Lattice) $\mathcal{H}$-matrices
- Block low rank

► **Available operations**

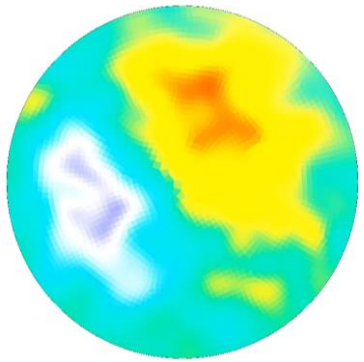
- Matrix-vector product
- LU factorization
- QR factortrization

► **Downloaded from web-site :**

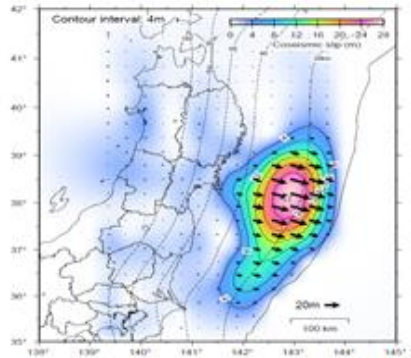
https://github.com/Post-Peta-Crest/ppOpenHPC/tree/MATH/HACApK

► **Example analyses**

- Spin torque oscillator

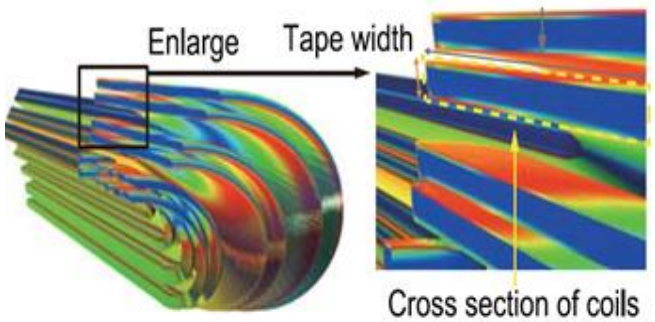


- Earthquake cycle



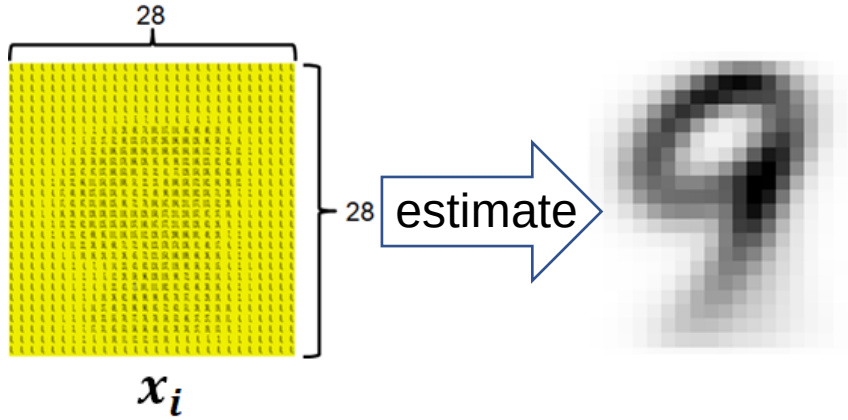
・Transcribed from **Ohtani at al (2011)**

- Superconductor



・Transcribed from **Tominaga *et al* (2018)**

- Machine lerning

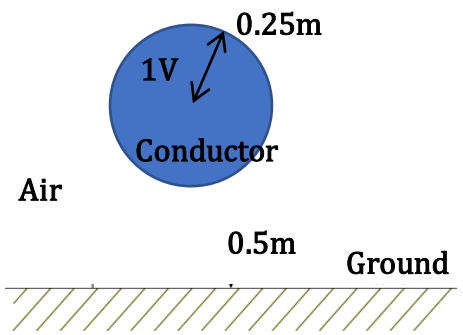


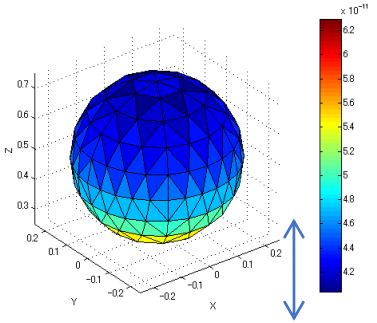
Tetsuya Hoshino

Research topics

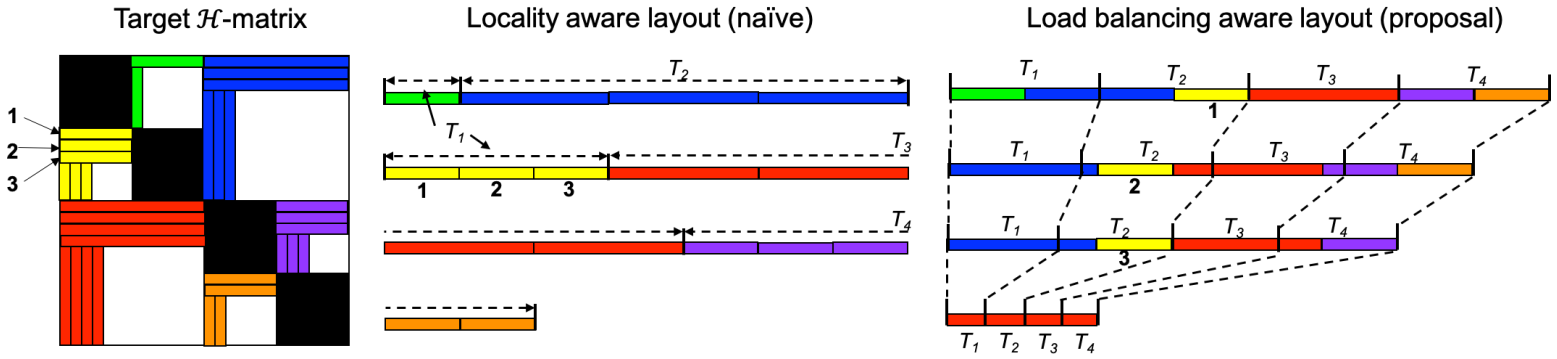
- ✓ Extended OpenACC compiler framework for data layout optimization
- ✓ Semi-auto-vectorization for HACApK library
- ✓ Load-balancing-aware algorithm of H-matrices for GPUs

Analysis condition **Analysis result**

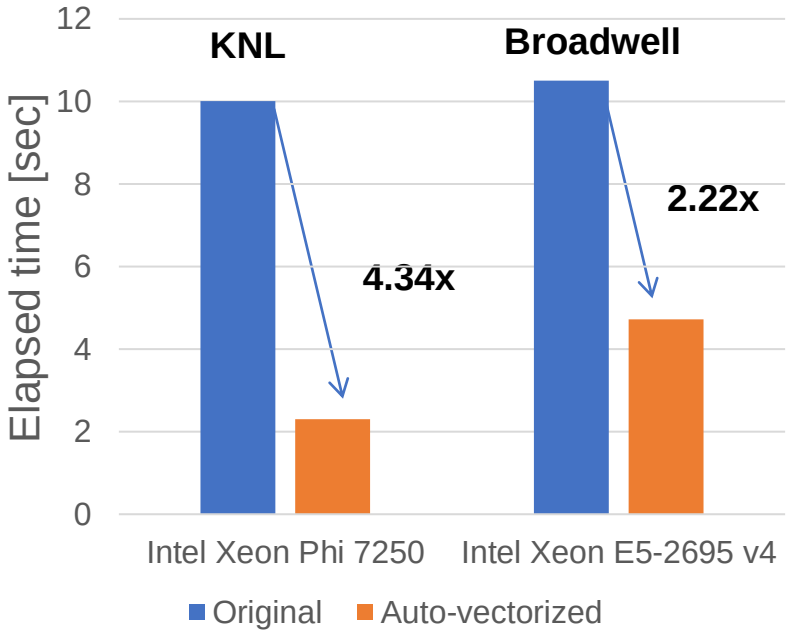




New data storage method of H-matrix for GPUs



Semi-auto-vectorization of H-matrix generation



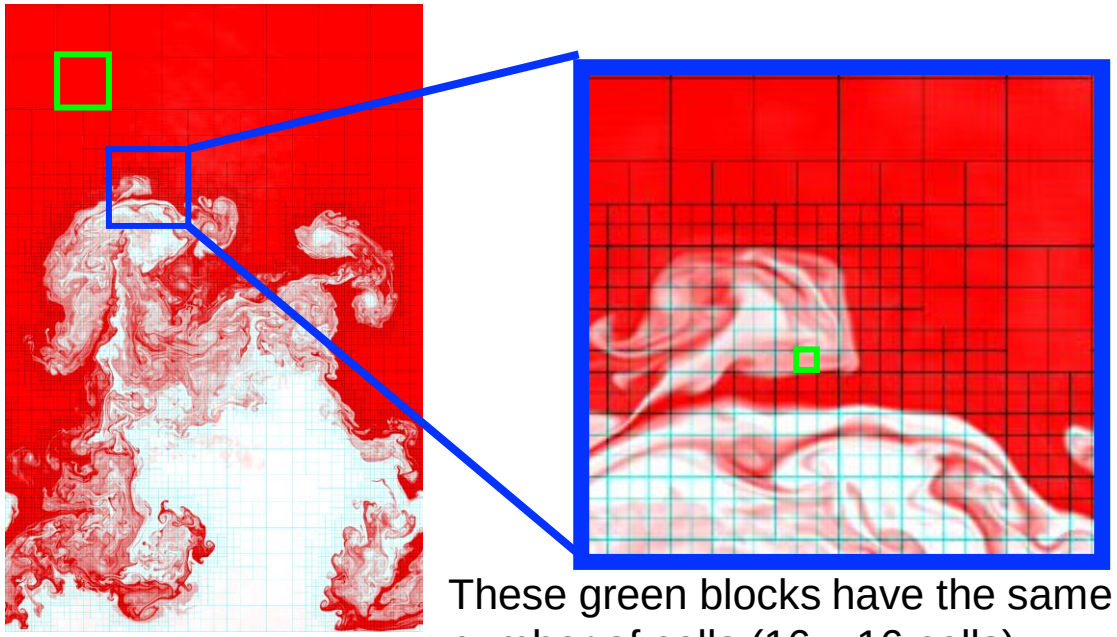
Accelerating Simulations of Computational Fluid Dynamics (CFD)

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

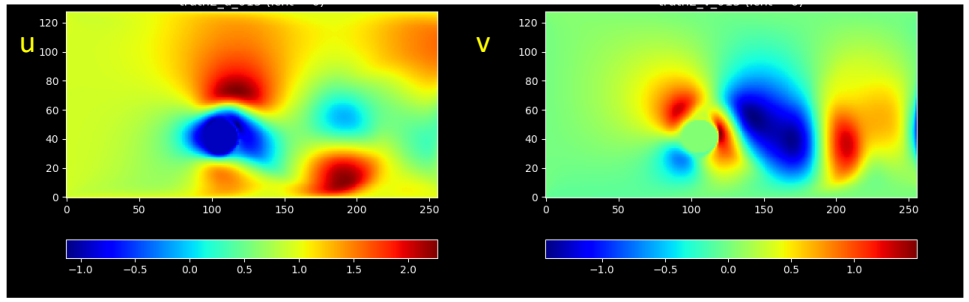
Rayleigh-Taylor Instability Simulation



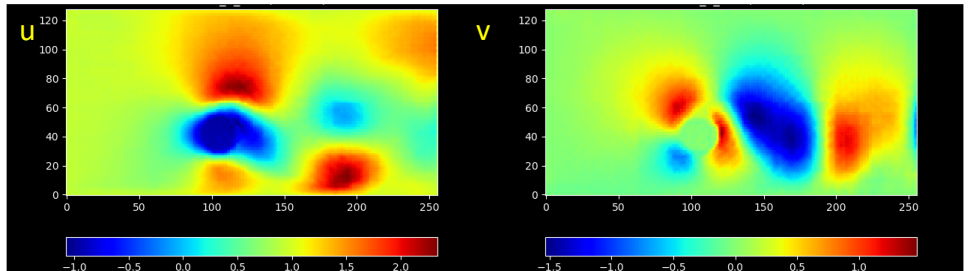
These green blocks have the same number of cells (16 x 16 cells)

CFD results predicted by deep learning

Ground truth (LBM simulation)



Prediction (DNN)



Toward Acceleration of Molecular Dynamics

Hayato Shiba

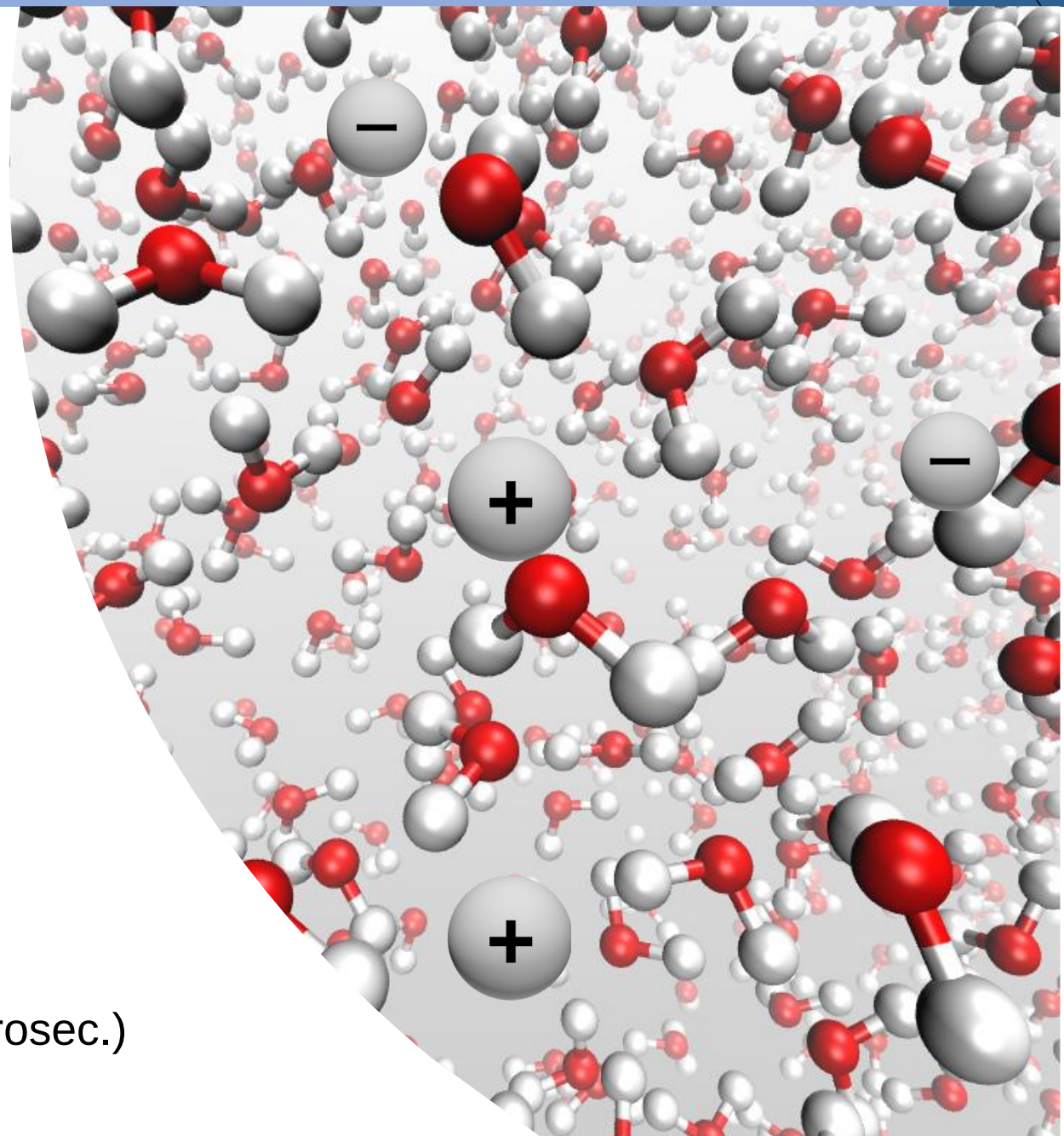
Molecular Dynamics for Liquid / Soft Matter

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 (➔)