Sciences on K computer

Large scale numerical simulations for strongly correlated quantum systems

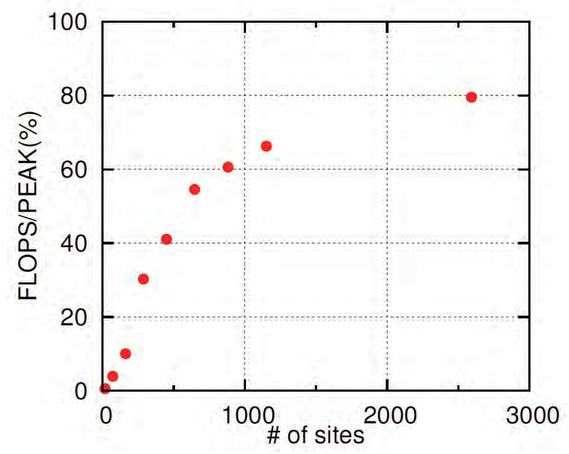
What is a strongly correlated quantum systemsin condensed matters?

- We have investigated "strongly correlated electron systems" , in which
  - electrons are governed by the quantum mechanics; wave-particle duality, Pauli exclusion principle, spin degree of freedom
  - Coulomb interactions between electrons can not be ignored; go beyond the band theory
- Combination of the quantum nature of electrons and many-body effects gives rise to <u>remarkable properties</u> of matters and <u>difficulties</u> in the problems
  - High-Tc superconductivity in Cu oxides
  - Colossal magnetoresistance in Mn oxides
  - exponentially large Hilbert space
  - analytical method very often fails

⇒ We need efficient and reliable computational methods.

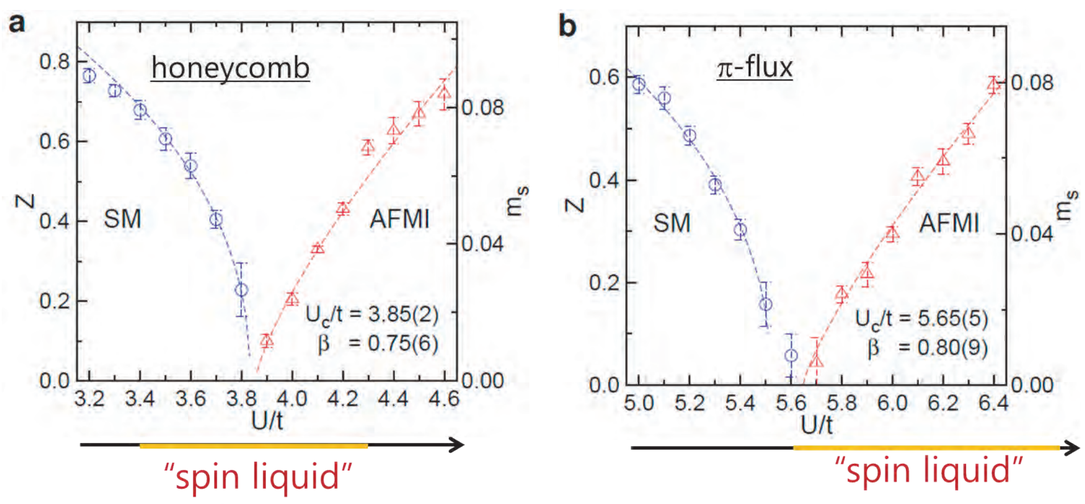
Computational methods for quantum many-body problems

- We have developed approximation-free and highly-efficient simulation codes on K computer.
  - Quantum Monte Carlo (QMC)
    - system size: ∼ 1,000 sites
    - applicable to 2 and 3 dim.
    - "negative sign problem" is exponentially serious.
  - Density Matrix Renormalization Group (DMRG)
    - system size: ∼ 100 sites
    - affordable up to 2 dim.
    - less restricted to symmetry or parameter



Result #1 : Ground-state phase diagram of interacting Dirac Fermions

"spin liquid" phases were predicted in interacting Dirac fermions on lattices as intermediate phases between semimetal and antiferromagnetic Mott insulator



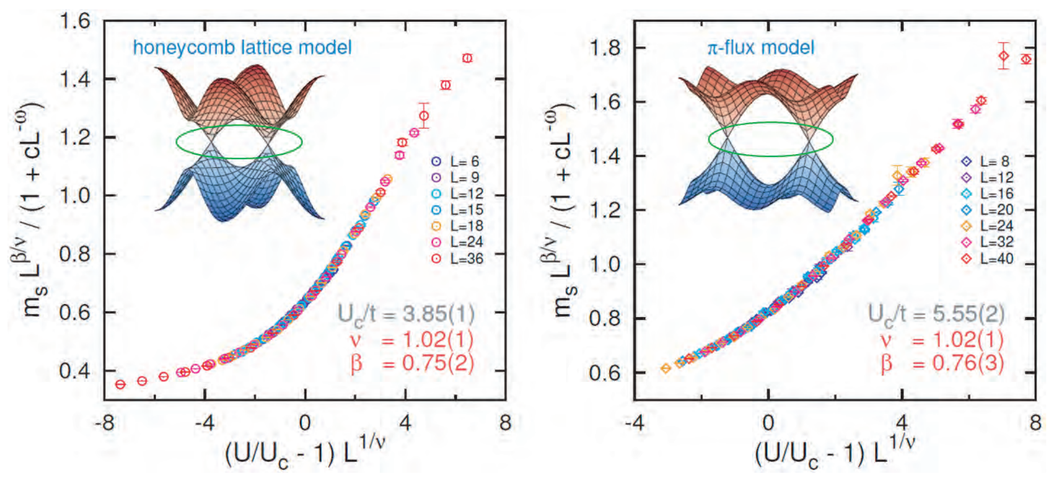
Meng et al., Nature (2010) Chang, Scalettar, Phys. Rev. Lett. (2012)

✓ Direct and continuous transition between SM and AFMI
→ spin liquid phase is unlikely.

Sorella, Otsuka, Yunoki, Scientific Reports 2, 992 (2012)

Result #2 : Fermionic quantum criticality in interacting Dirac electrons

Dirac electrons: electronic systems with a linear dispersion near the Fermi level e.g. graphene, topological insulators, d-wave High-Tc



✓ Highly accurate calculations of order parameters by large-scale QMC simulations
✓ Critical exponents for two different models are the same within statistical errors;
→ Numerical validation of universality class

cf. Gross-Neveu model in particle physics

Sorella, Otsuka, Yunoki, Scientific Reports 2, 992 (2012)

NTChem: Quantum Chemistry Calculations on Massively Parallel Computers

Quantum chemistry calculations based on Hartree-Fock and DFT have O(N3 ~ N4) computational scaling, where N is proportional to the system size. Therefore it is very time consuming to compute large systems. To solve this problem, we have developed the following effective methods that take advantage of massively parallel computing and have integrated them into our group's NTChem quantum chemistry program.

Pseudospectral (PS) Method

<u>Acceleration of two-electron integral</u>

$$(\mu\nu|\lambda\sigma) = \iint \phi_\mu(\mathbf{r}_1)\phi_\nu(\mathbf{r}_1)\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}\phi_\lambda(\mathbf{r}_2)\phi_\sigma(\mathbf{r}_2)\,d\mathbf{r}_1\,d\mathbf{r}_2$$

Computational cost $O(N^4)$

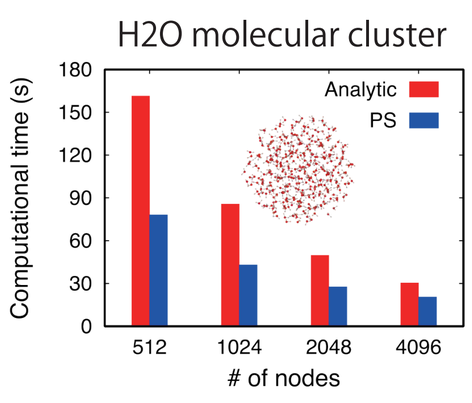
Replacement of an analytic integral with a numerical integral

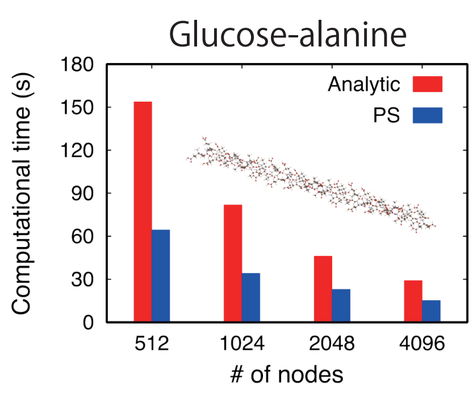
$$(\mu\nu|\lambda\sigma)_{\mathrm{PS}} = \sum_{g=1}^{M} w_g \phi_\mu(\mathbf{r}_g)\phi_\nu(\mathbf{r}_g)\int \frac{\phi_\lambda(\mathbf{r}_2)\phi_\sigma(\mathbf{r}_2)}{|\mathbf{r}_g-\mathbf{r}_2|}\,d\mathbf{r}_2$$

Computational cost $O(MN^2)$ (M: # grid points)

<u>Performance Tests</u>

Pure DFT (BP86), Def2-SVP basis set





Diagonalization Free Methods

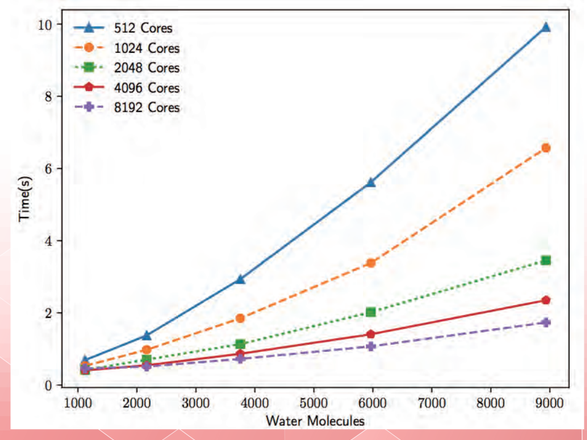
Diagonalization free methods are based on computing the functions of sparse, symmetric matrices.
We have developed a library of matrix function solvers that can compute a variety of functions in linear time.
Core routine: Sparse Matrix-Matrix Multiplication.
Large scale hybrid MPI-OpenMP parallelization.

<u>Feature Set</u>

Standard Polynomials
Chebyshev Polynomials
Trigonometric Functions
Exponential and Logarithm
pth Root
Inverse pth Root
Inverse
Matrix Sign Function
Density Matrix Minimization
Density Matrix Purification
Distributed File I/O

<u>Performance Tests</u>

STO Basis Set, Compute the Inverse Square Root.
Demonstrated strong scaling for even small matrices.



Sciences on K computer

Computational Structural Biology Research Unit

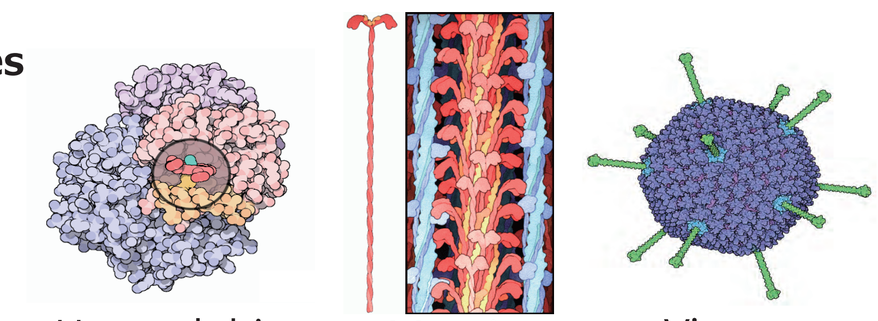
Structural biology and big data: high performance computing needed

・Biomolecules accomplish core biological functions and dysfunction may result in severe diseases.

・A critical step to understand function of biological molecules is determining their 3-dimensional structure.

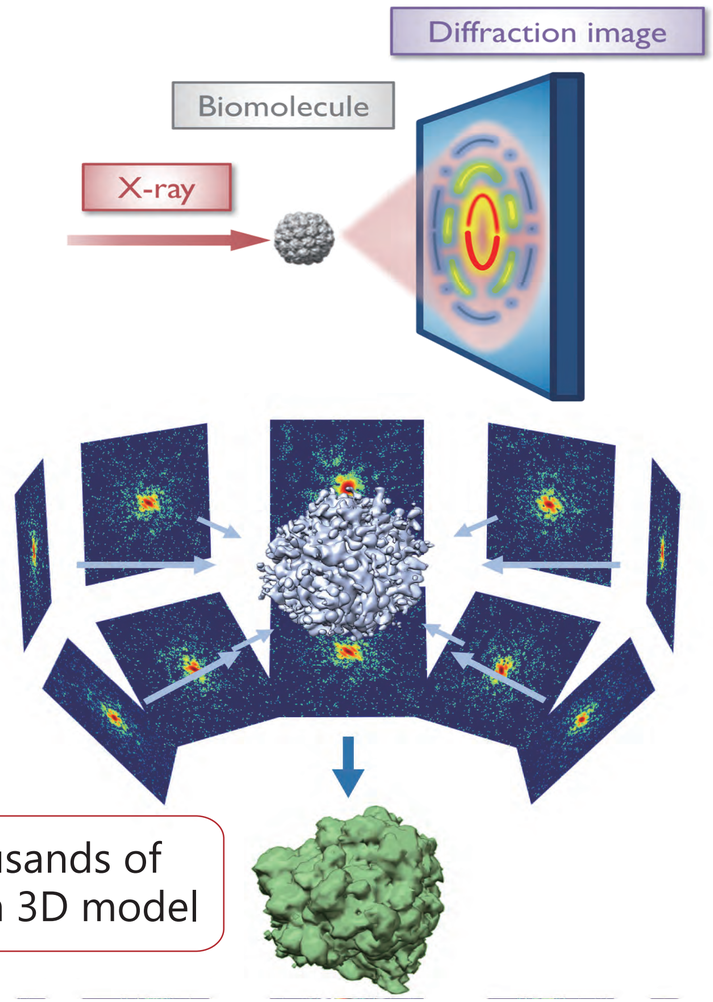
X-ray free electron laser (XFEL):
new experimental approach to image directly single molecules

Example of biological molecules



Hemoglobin　Myosin　Virus

Development of computational tools to solve 3D structures of biological molecules from 2D images from XFEL experiments



Computational time (16 cores, 1,000,000 images)

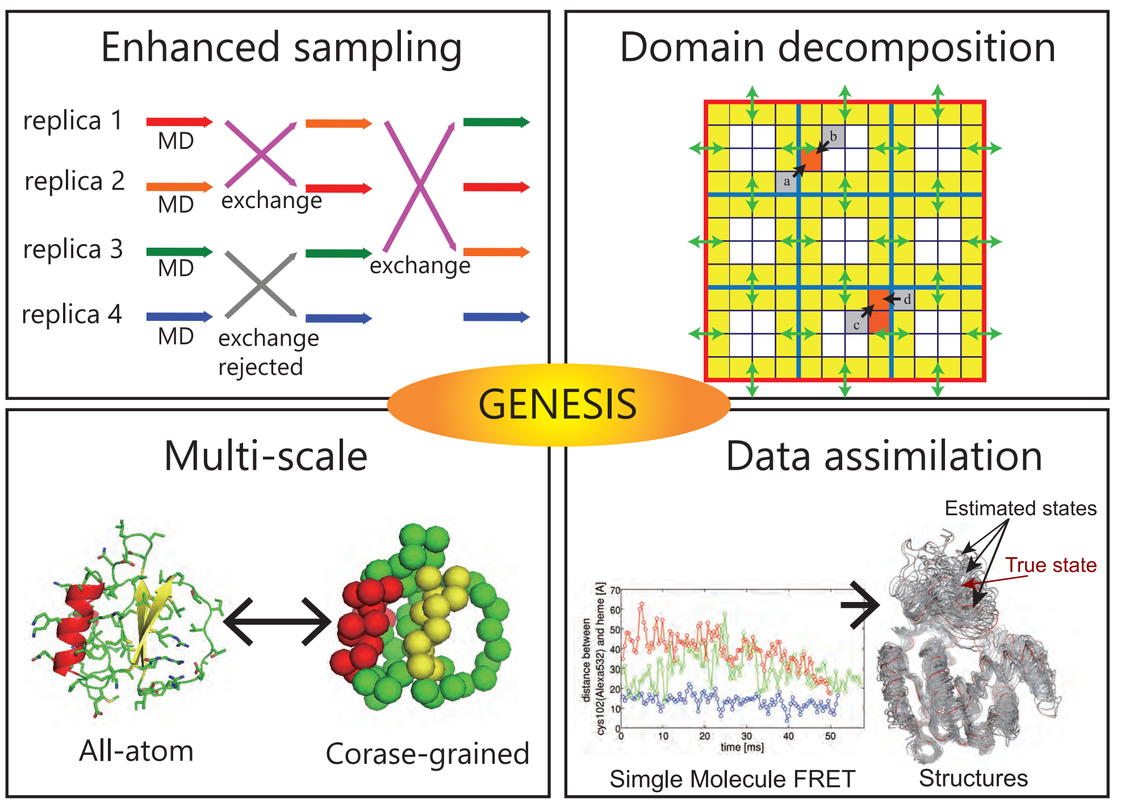
Image size (pixel)	128^2	640^2
2D matching (30 iterations)	7 days	~100 days
Phase retrieval (100 trials)	1 day	125 days

Assembling thousands of 2D images into a 3D model

Computational Biophysics Research Team

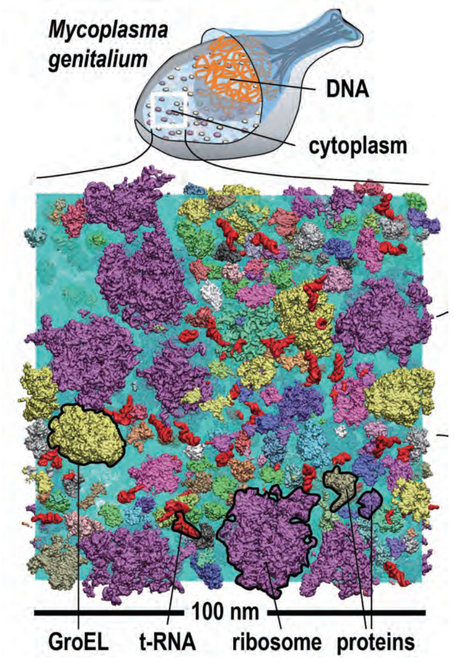
GENESIS
Generalized-ensemble simulation system

1. Domain decomposition with hybrid parallelization
2. Enhanced sampling algorithm for free energy calculation
3. Multi-scale MD (All atom, Coarse-Grained, QM/MM)
4. Data assimilation



Target application

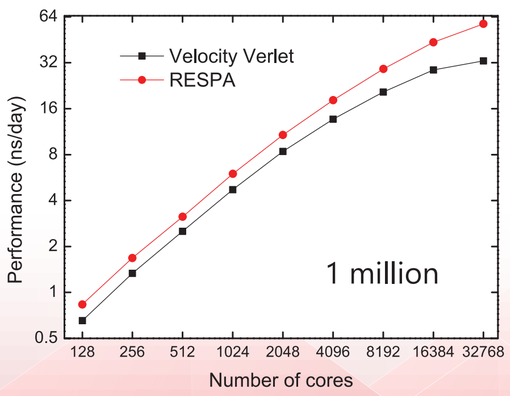
1. Molecular crowding
2. Structure/Dynamics of biomolecules
3. Reaction pathway
4. Data driven simulations

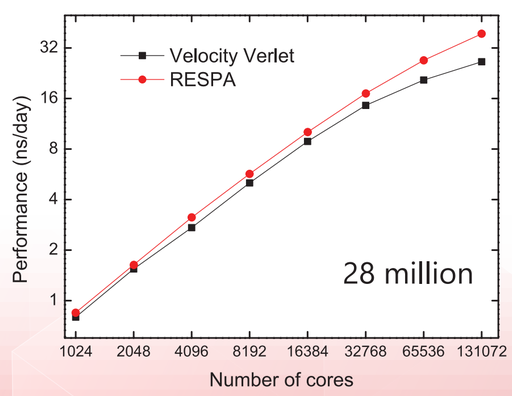


Cytoplasm system performed by GENESIS (*eLife* **5**, e19274 (2016))

URL: http://www.aics.riken.jp/labs/cbrt/

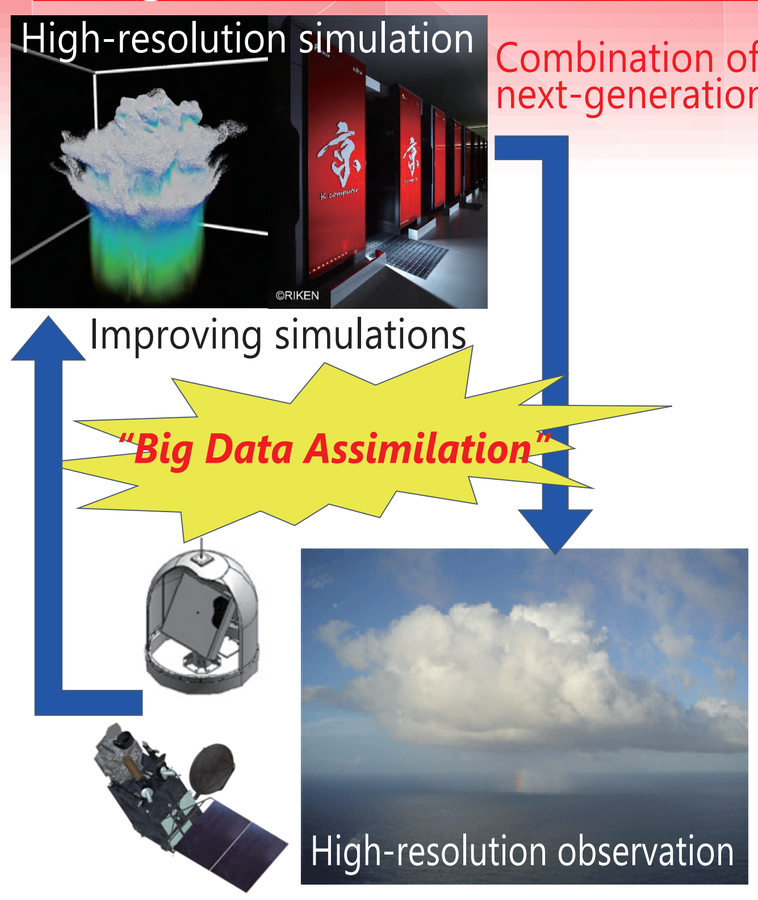
Performance of GENESIS



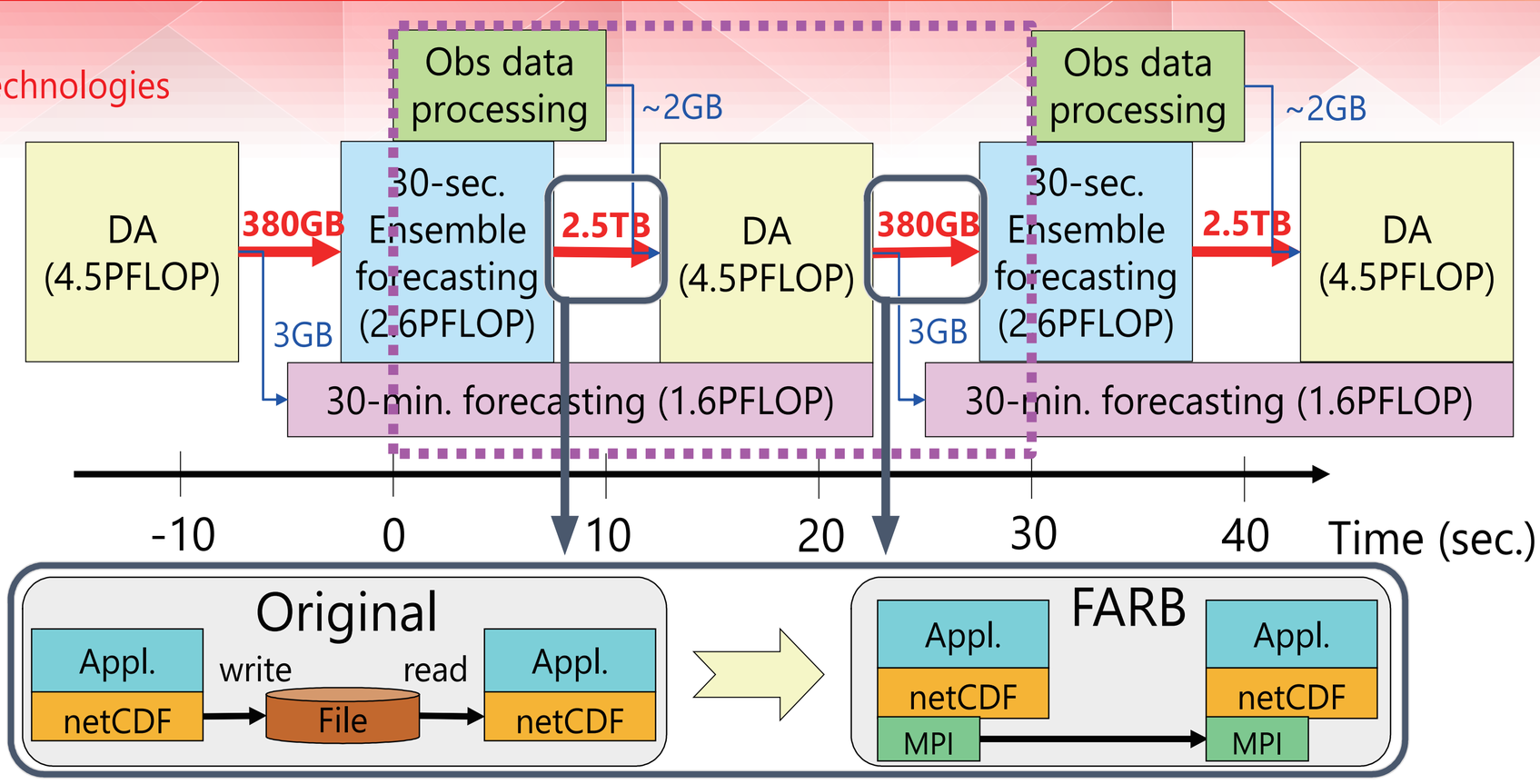


Innovating "big data assimilation" technology for revolutionizing very-short-range severe weather prediction

Big Data Assimilation *(Miyoshi et al. 2016, Proc. of IEEE, doi:10.1109/JPROC.2016.2602560)*



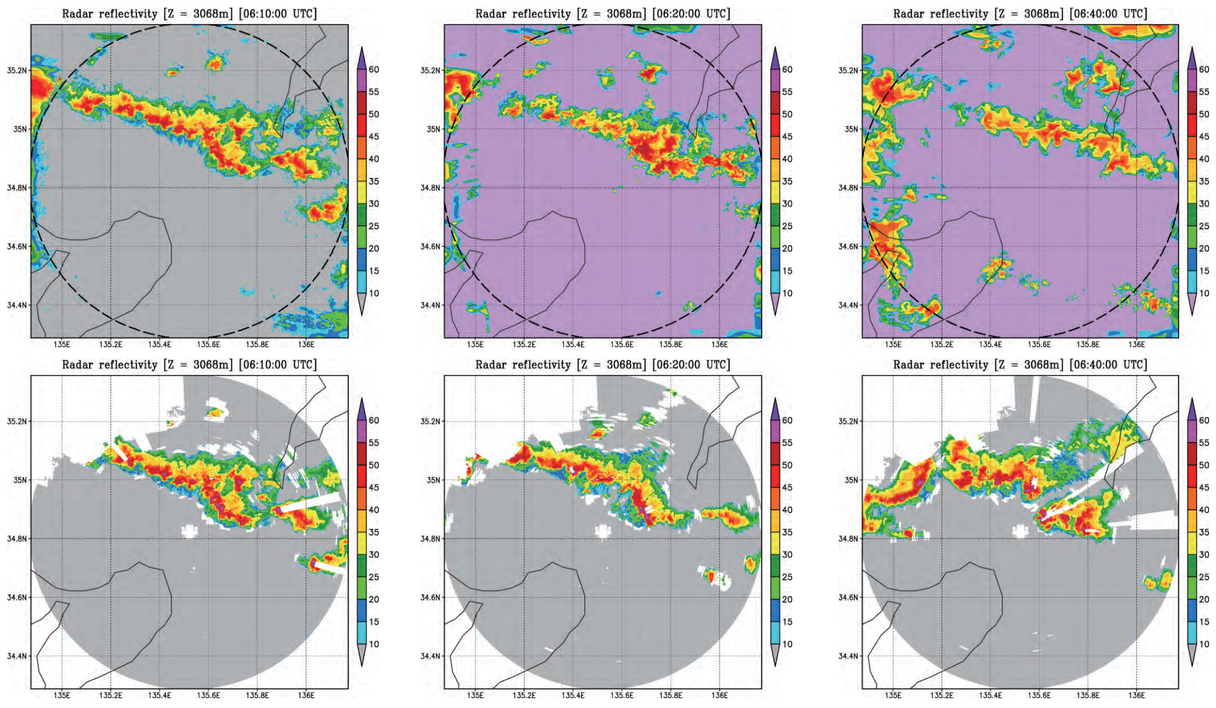
Combination of next-generation technologies

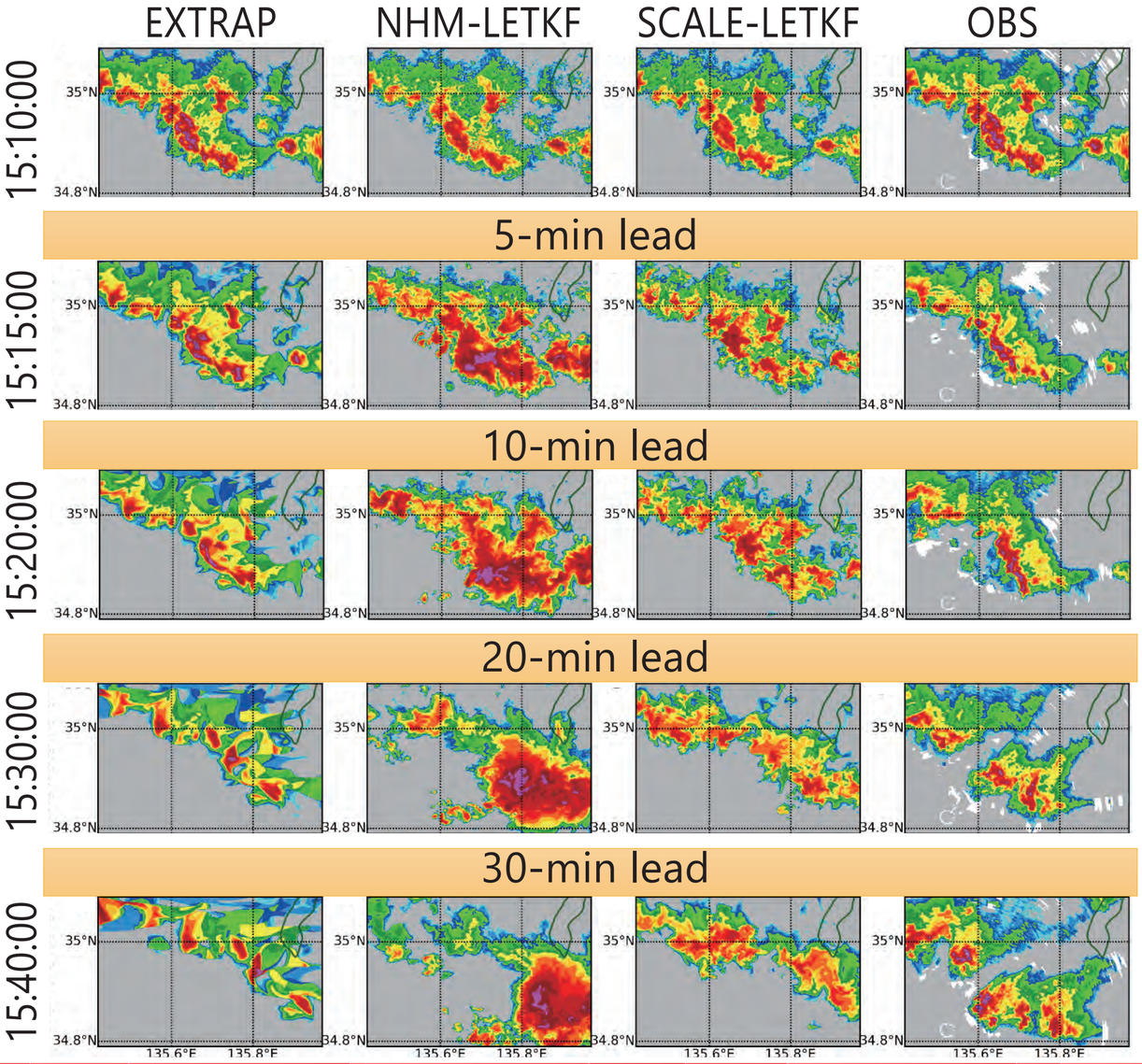


Case1 (7/13/13 Kyoto)

with 1km/100m resolution & 100-member NHM-LETKF

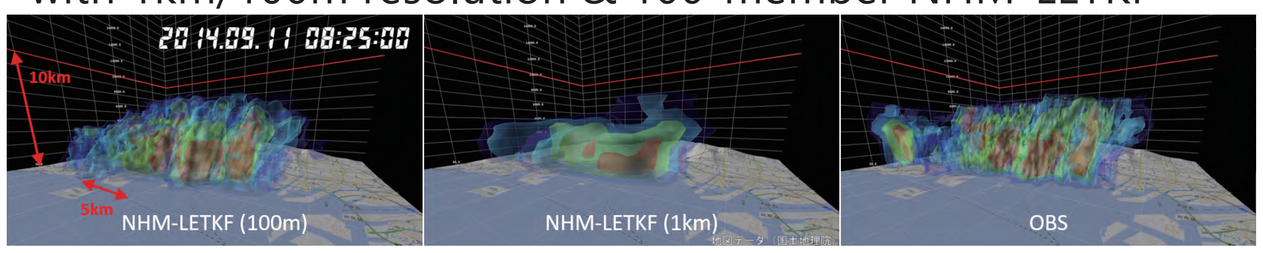
15:15:00 JST





Case2 (9/11/14 Kobe)

with 1km/100m resolution & 100-member NHM-LETKF



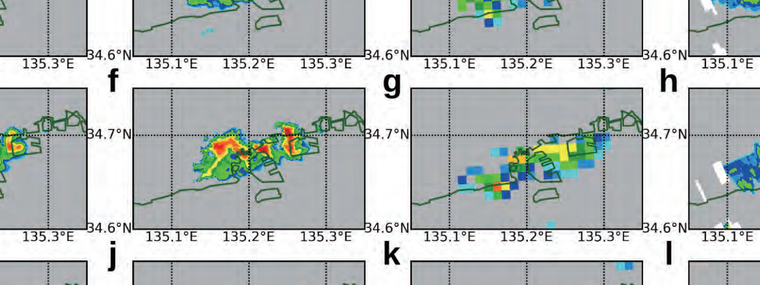
LETKF: Local Ensemble Transform Kalman Filter
NHM: Nonhydrostatic Model
SCALE: Scalable Computing for Advanced Library and Environment
EXTRAP: Extrapolation

Computation time

ensemble forecasts + data assimilation

Original proposal: 100-m mesh, 100 ensemble members, every 30 seconds

Measured



Alternative strategies: degrade resolution, ensemble size, and/or frequency

Estimated