ppOpen-HPC

Open Source Infrastructure for Development and Execution of Large-Scale Scientific Applications on Post-Peta Scale Supercomputers with Automatic Tuning (AT)

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Summary

- ppOpen-HPC is an open source infrastructure for development and execution of optimized and reliable simulation code on post-peta-scale (pp) parallel computers based on many-core architectures with automatic tuning (AT), and it consists of various types of libraries, which cover general procedures for scientific computation.

ppOpen-HPC: Overview

- Application framework with automatic tuning (AT)
  - “pp” : post-peta-scale
- Five-year project (FY.2011-2015) (since April 2011)
  - Lead P.I.: Kengo Nakajima (ITC, The University of Tokyo)
  - Part of “Development of System Software Technologies for Post-Peta Scale High Performance Computing” funded by JST/CREST (Supervisor: Prof. Mitsuhisa Sato, Co-Director, RIKEN AICS)

- Team with 7 institutes, >50 people (5 PDs) from various fields: Co-Design
  - ITC/U.Tokyo, AORI/U.Tokyo, ERI/U.Tokyo, FS/U.Tokyo
  - Hokkaido U., Kyoto U., JAMSTEC

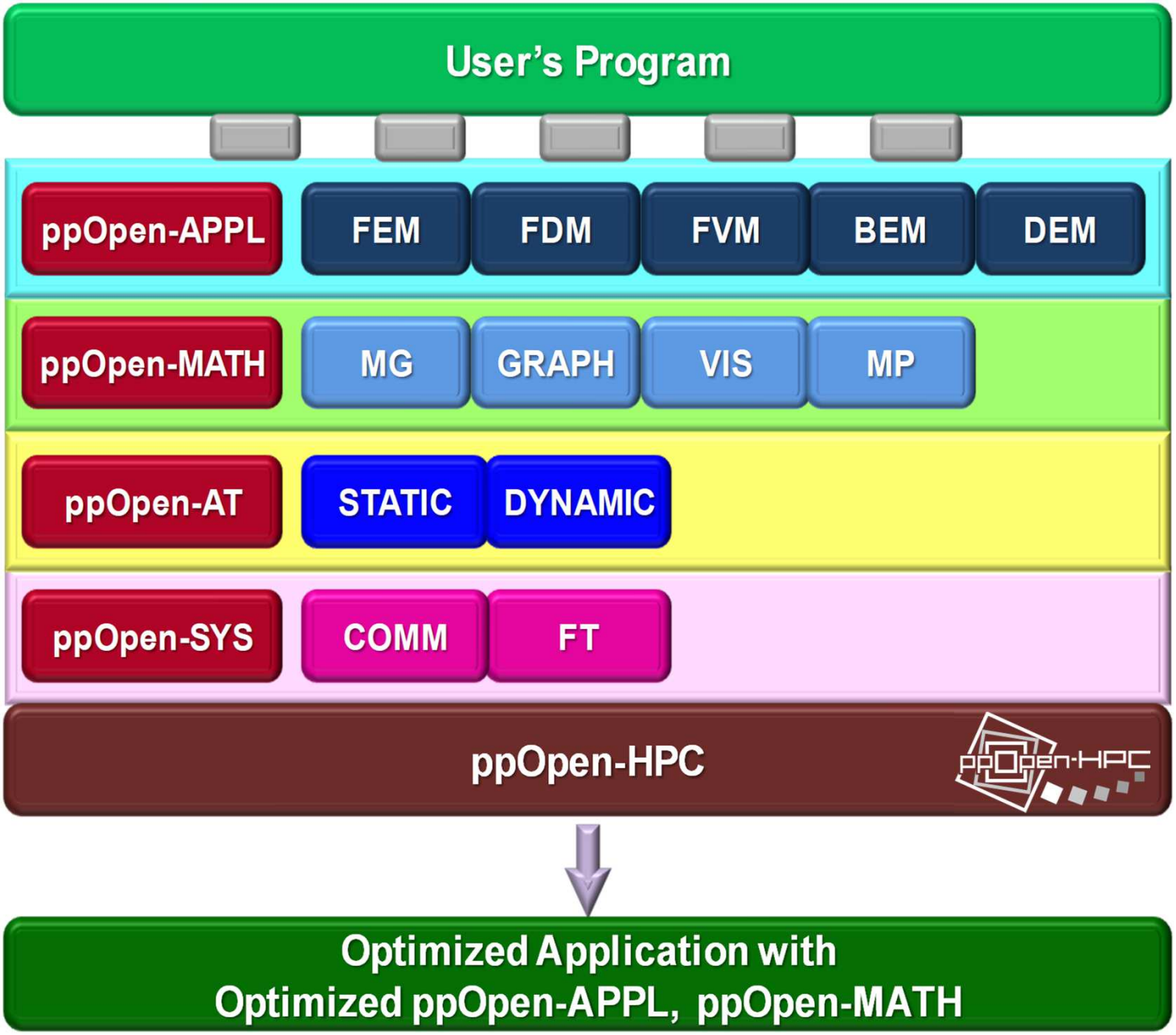
独立行政法人
科学技術振興機構
Japan Science and Technology Agency
CREST
戦略的創造研究推進事業
Core Research for Evolutionary Science and Technology

Framework Appl. Dev.

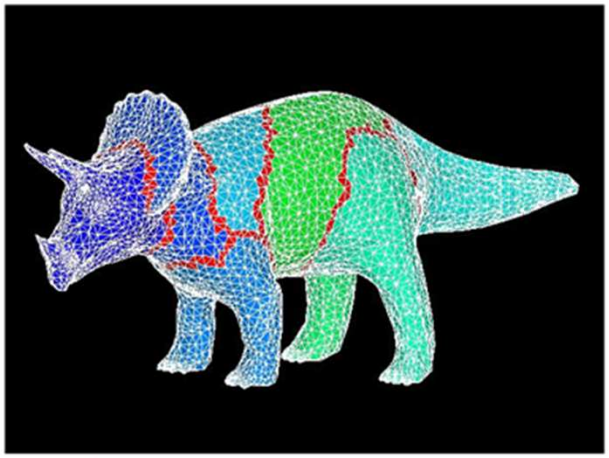
Math Libraries

Automatic Tuning (AT)

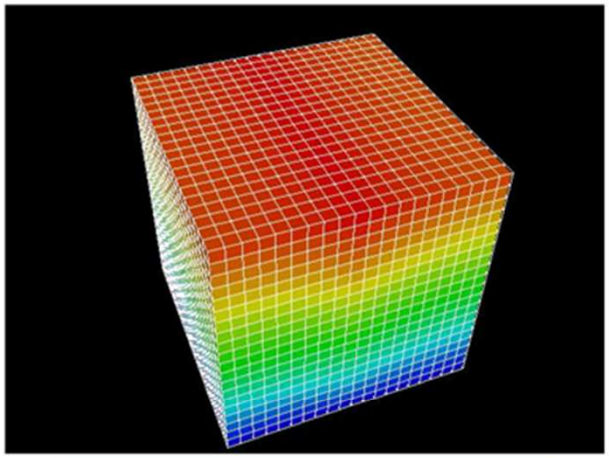
System Software



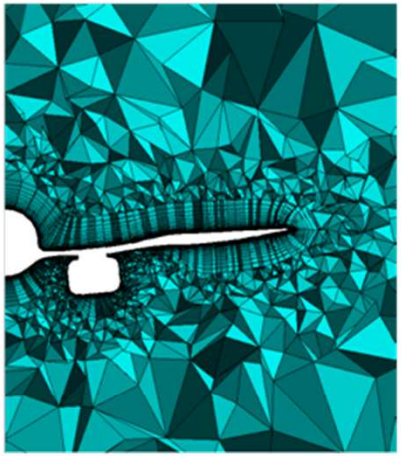
ppOpen-HPC covers …



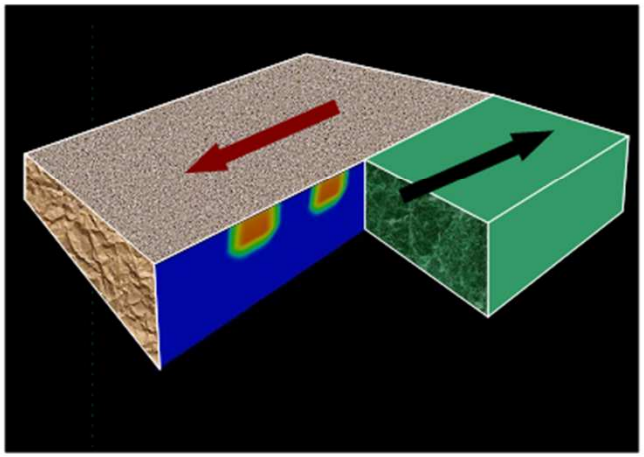
FEM
Finite Element Method



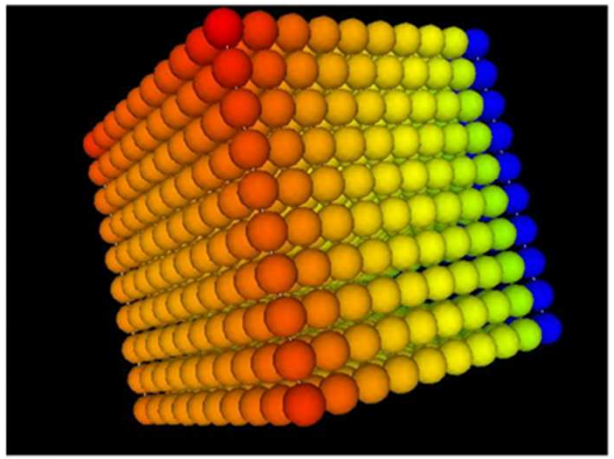
FDM
Finite Difference Method



FVM
Finite Volume Method



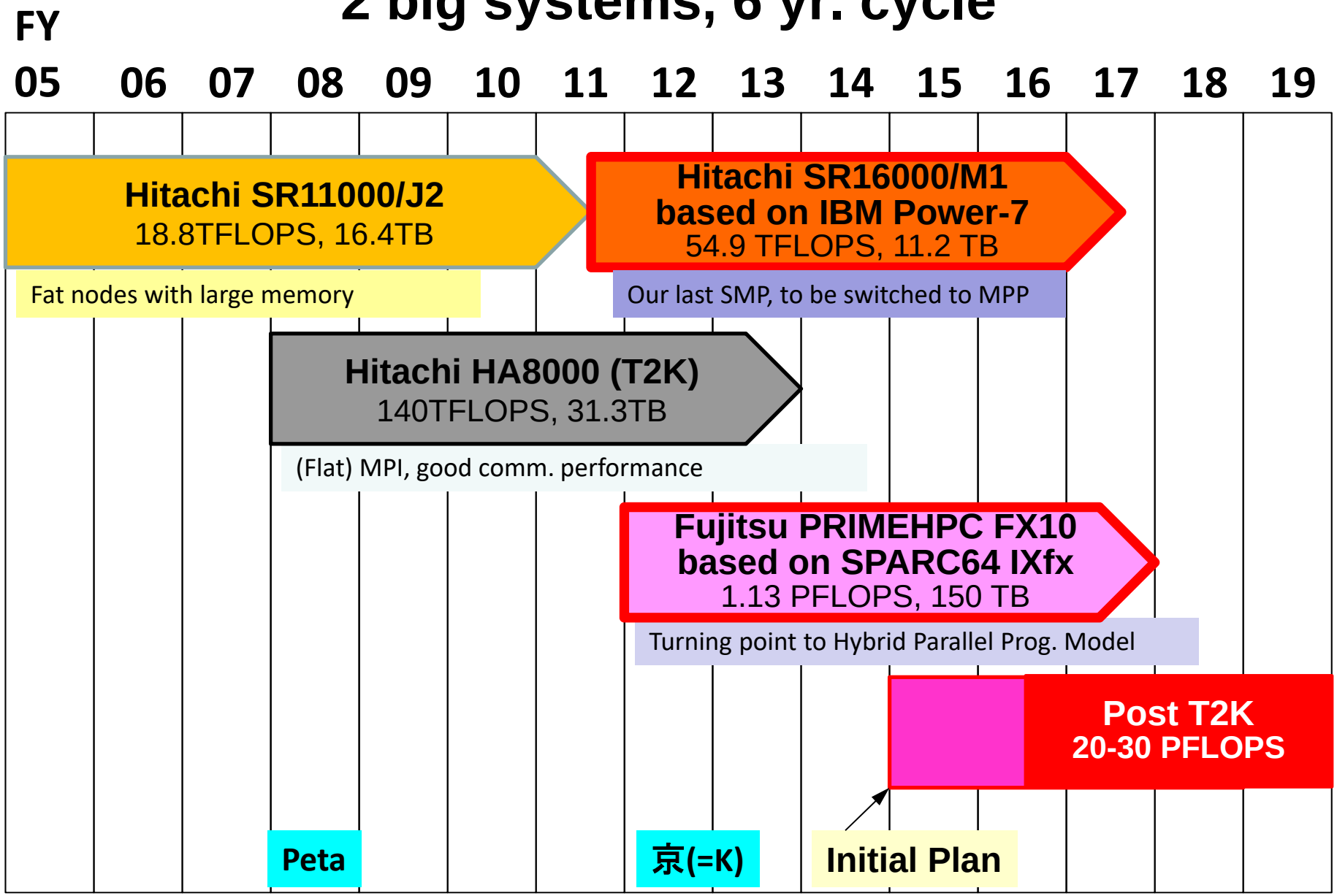
BEM
Boundary Element Method



DEM
Discrete Element Method

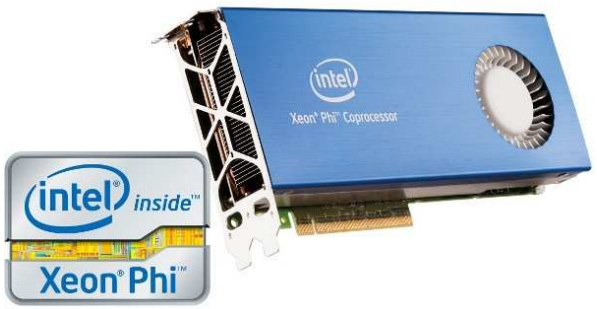
Supercomputers in U.Tokyo

2 big systems, 6 yr. cycle



Target of ppOpen-HPC: Post T2K System

- Target system is Post T2K system
  - 25+ PFLOPS, FY.2016
    - ✓ JCAHPC (Joint Center for Advanced High Performance Computing): U. Tsukuba & U. Tokyo
    - ✓ http://jcahpc.jp/
  - Many-core based (e.g. Intel MIC/Xeon Phi)
    - ✓ MPI + OpenMP + X
  - ppOpen-HPC helps smooth transition of users (> 2,000) to new system
- K/FX10, Cray, Xeon clusters are also in scope



JCAHPC

Oakforest-PACS

- Full Operation started on December 1, 2016
- 8,208 Intel Xeon/Phi (KNL), 25 PF Peak Performance
  - Fujitsu
- **TOP 500 #7 (#1 in Japan), HPCG #5 (#2) (June 2017)**
- **JCAHPC: Joint Center for Advanced High Performance Computing)**
  - University of Tsukuba
  - University of Tokyo
    - New system will installed in Kashiwa-no-Ha (Leaf of Oak) Campus/U.Tokyo, which is between Tokyo and Tsukuba
  - http://jcahpc.jp

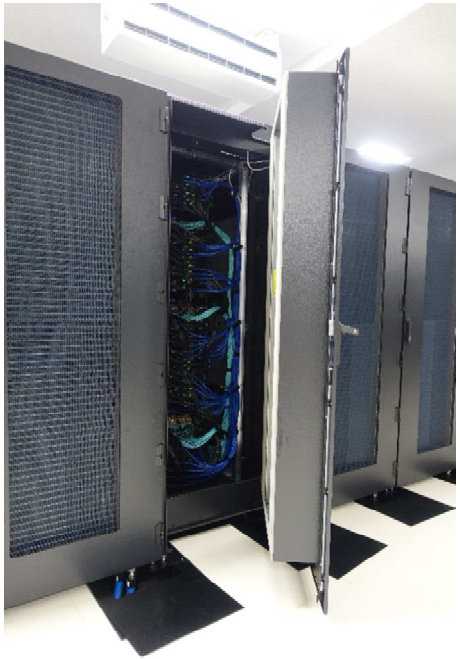
JCAHPC

東京大学 THE UNIVERSITY OF TOKYO

筑波大学 University of Tsukuba

Computation node (Fujitsu next generation PRIMERGY) with single chip Intel Xeon Phi (Knights Landing, 3+TFLOPS) and Intel Omni-Path Architecture card (100Gbps)

Chassis with 8 nodes, 2U size



15 Chassis with 120 nodes per Rack

東京大学情報基盤センター
INFORMATION TECHNOLOGY CENTER, THE UNIVERSITY OF TOKYO

計算科学研究センター
Center for Computational Sciences

Schedule of Public Release

(with English Documents, MIT License)

http://ppopenhpc.cc.u-tokyo.ac.jp/

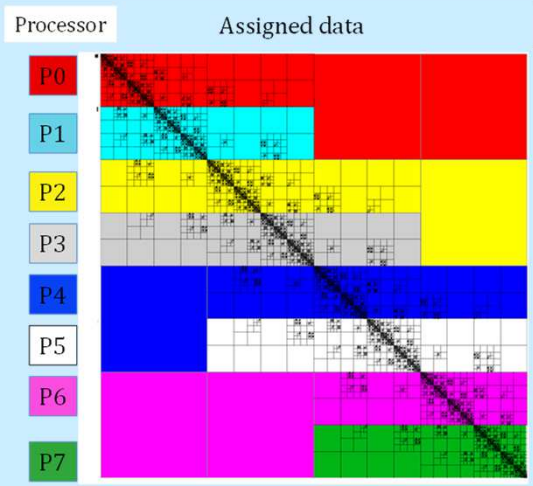
- Released at SC-XY (or can be downloaded)
- Multicore/manycore cluster version (Flat MPI, OpenMP/MPI Hybrid) with documents in English
- We are now focusing on MIC/Xeon Phi
- Collaborations are welcome

- History
  - SC12, Nov 2012 (Ver.0.1.0)
  - SC13, Nov 2013 (Ver.0.2.0)
  - SC14, Nov 2014 (Ver.0.3.0)
  - SC15, Nov 2015 (Ver.1.0.0)

New Features in Ver.1.0.0

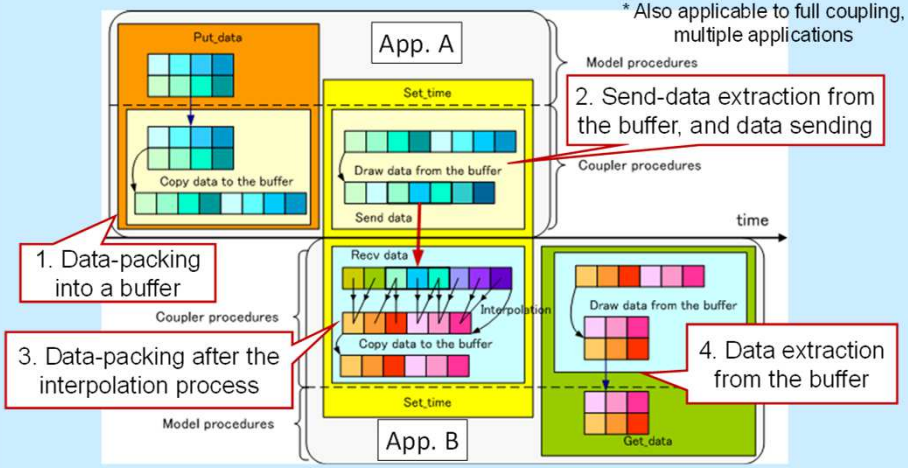
http://ppopenhpc.cc.u-tokyo.ac.jp/

- **HACApK library for H-matrix comp. in ppOpen-APPL/BEM (OpenMP/MPI Hybrid Version)**
  - **First Open Source Library by OpenMP/MPI Hybrid**
- ppOpen-MATH/MP (Coupler for Multiphysics Simulations, Loose Coupling of FEM & FDM)
- Matrix Assembly and Linear Solvers for ppOpen-APPL/FVM



Assign a^c to P_k if $S(a^c{}_{ij})$ in $R(P_k)$

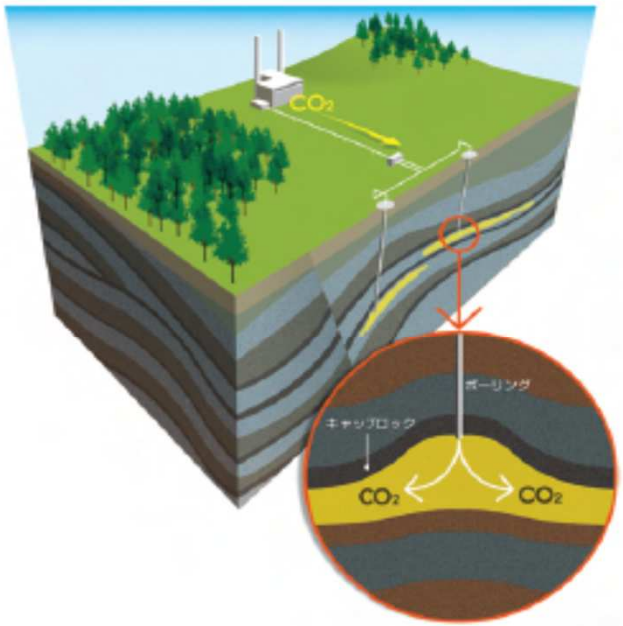
A : Whole matrix
A_{IJ} : The entry in the I-th row and the J-th column of A
a^c: A small submatrix of A
$a^c{}_{ij}$: The entry in the i-th row and the j-th column of a^c
N : Number of rows of A
n : Number of processors
P_k : The k-th processor
l_k : $1 = l_0 < \cdots < l_k < \cdots < l_{n+1} = N + 1$
R : $R(P_k) = \{i \mid l_k \le i < l_{k+1}\}$
S : $S(a^c{}_{ij}) = I$ when $a^c{}_{ij} = A_{IJ}$



Collaborations, Outreaching

- Collaborations
  - International Collaborations
    - Lawrence Berkeley National Lab.
    - National Taiwan University, National Central University
    - ESSEX-II/SPPEXA/DFG, Germany
    - IPCC（Intel Parallel Computing Center）
- Outreaching, Applications
  - Large-Scale Simulations
    - Geologic CO_2 Storage
    - Astrophysics
    - Earthquake Simulations etc.
    - ppOpen-AT, ppOpen-MATH/VIS, ppOpen-MATH/MP, Linear Solvers
  - Intl. Workshops (2012,13,15)
  - Tutorials, Classes

Simulation of Geologic CO_2 Storage



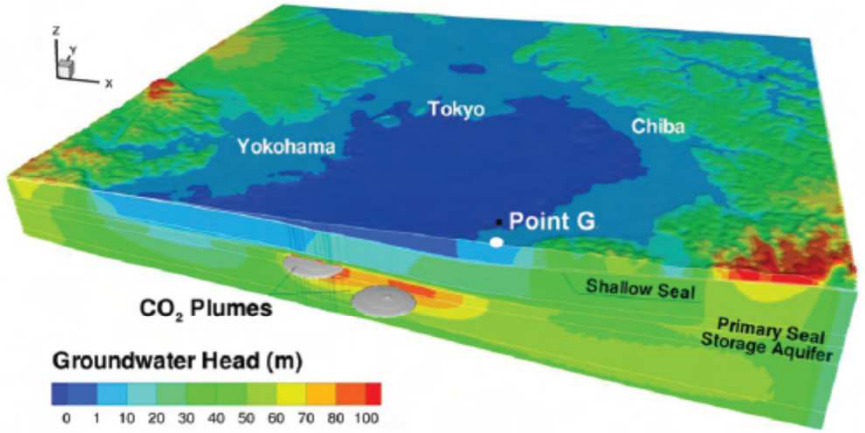
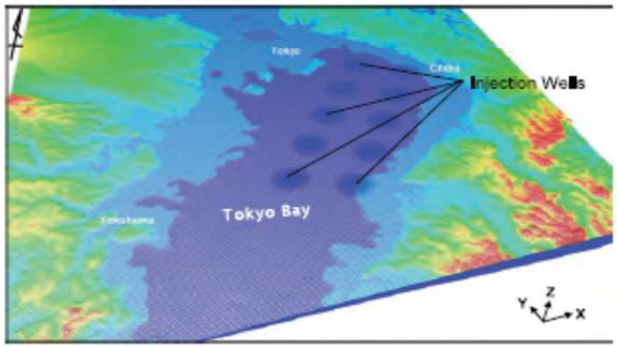
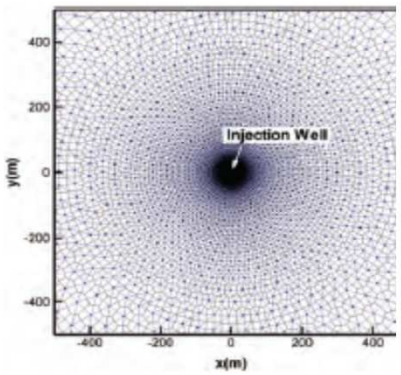
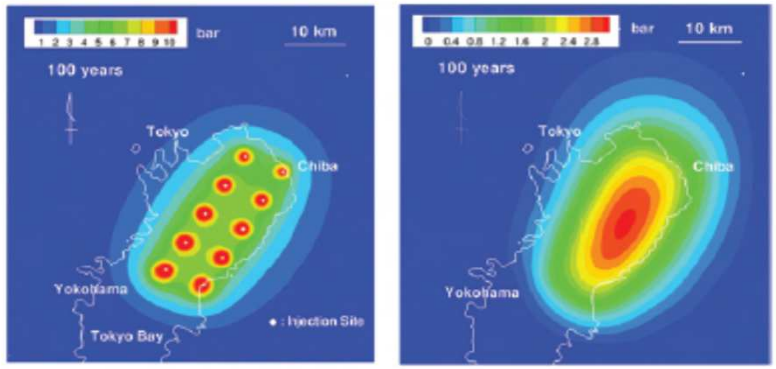


図 -4　CO_2 圧入後の地下水圧（全水頭換算）の分布（100 年後）







(a) 深部遮蔽層下面　　(b) 浅部遮蔽層下面

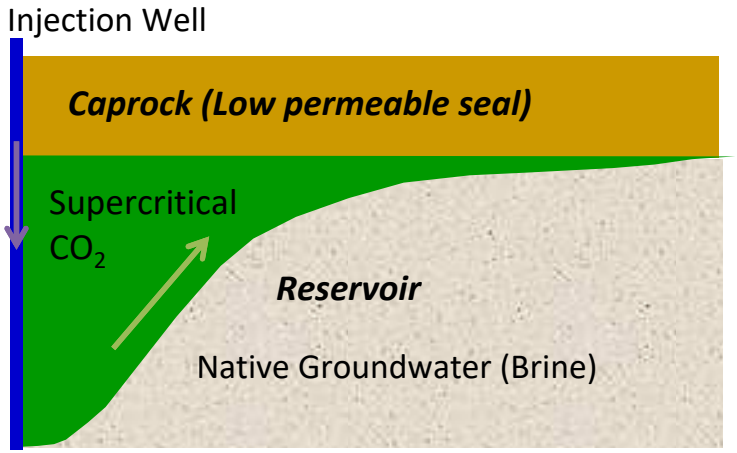
図 -5　圧力上昇量の平面分布（初期状態からの増分、圧入開始から 100 年後）

[Dr. Hajime Yamamoto, Taisei]

Simulation of Geologic CO_2 Storage

- Science
  - Behavior of CO_2 in supercritical state at deep reservoir
- PDE's
  - 3D Multiphase Flow (Liquid/Gas) + 3D Mass Transfer
- Method for Computation
  - TOUGH2 code based on FVM, and developed by Lawrence Berkeley National Laboratory, USA
    - More than 90% of computation time is spent for solving large-scale linear equations with more than 10^7 unknowns
- Numerical Algorithm
  - Fast algorithm for large-scale linear equations developed by Information Technology Center, the University of Tokyo
- Supercomputer
  - Earth Simulator II (NEX SX9, JAMSTEC, 130 TFLOPS)
  - Oakleaf-FX (Fujitsu PRIMEHP FX10, U.Tokyo, 1.13 PFLOPS

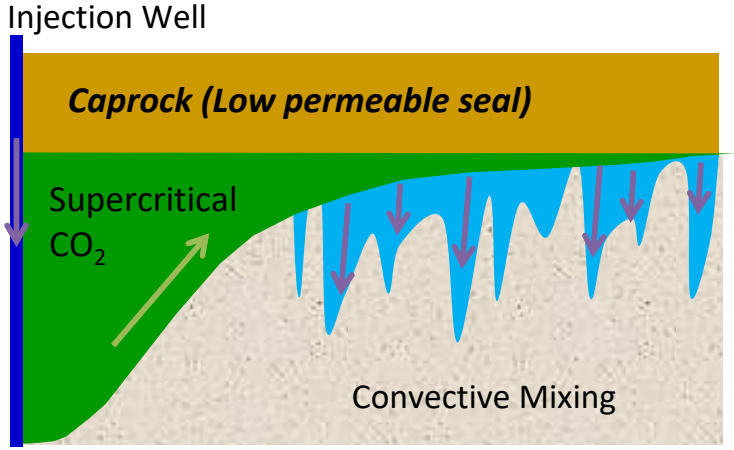
Diffusion-Dissolution-Convection Process



- **Buoyant $scCO_2$ overrides onto groundwater**
- **Dissolution of CO_2 increases water density**
- **Denser fluid laid on lighter fluid**
- **Rayleigh-Taylor instability invokes convective mixing of groundwater**

[Dr. Hajime Yamamoto, Taisei]

Diffusion-Dissolution-Convection Process



- **Buoyant scCO$_2$ overrides onto groundwater**
- **Dissolution of CO$_2$ increases water density**
- **Denser fluid laid on lighter fluid**
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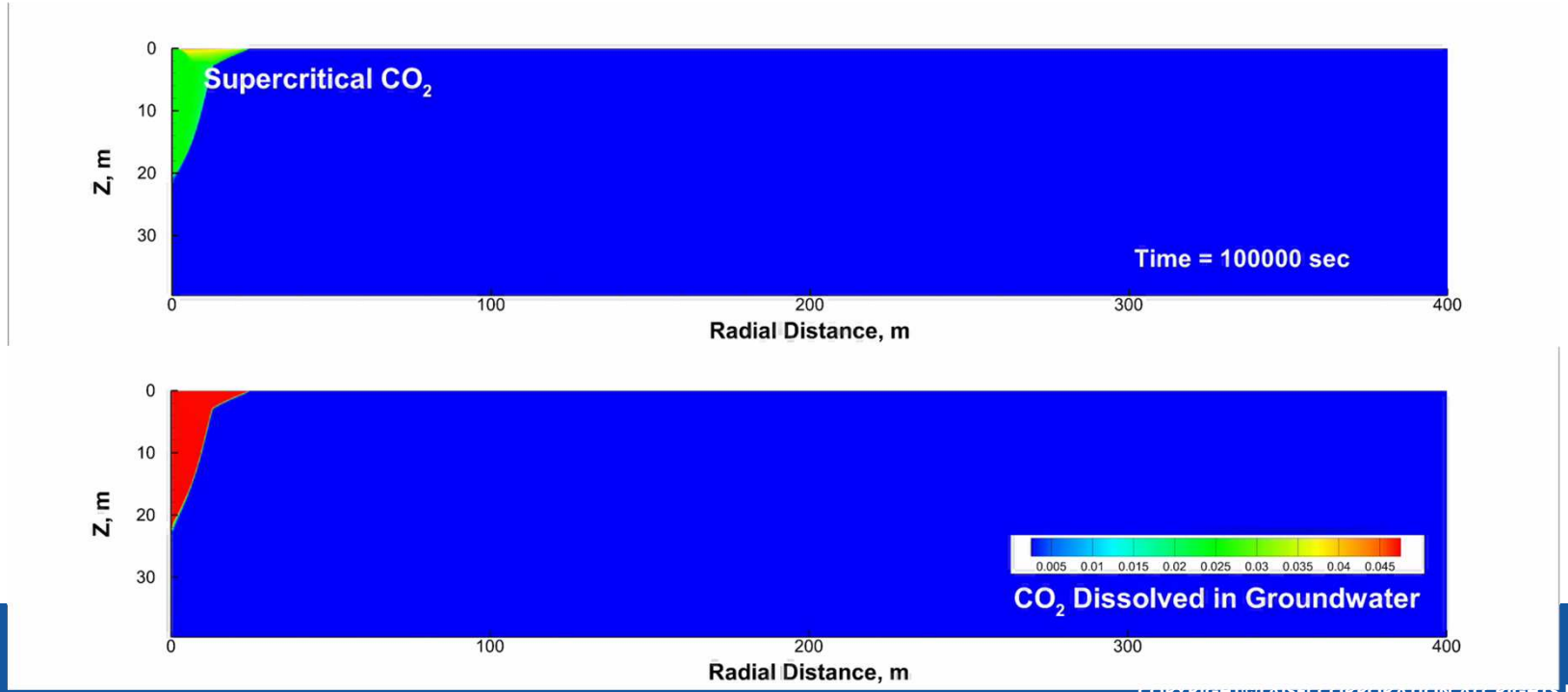
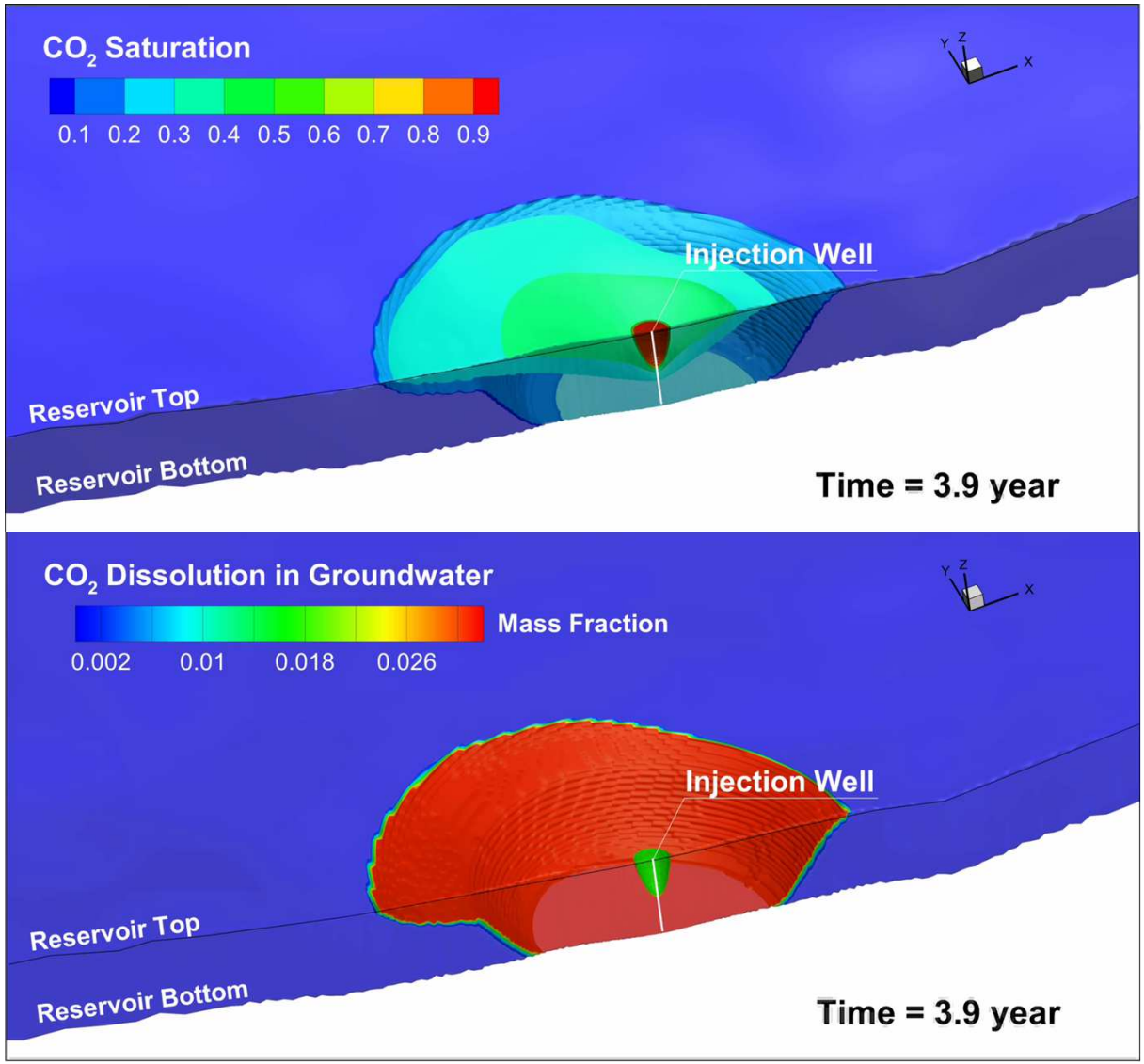
The mixing significantly enhances the CO$_2$ dissolution into groundwater, resulting in more stable storage

Preliminary 2D simulation (Yamamoto et al., GHGT11) [Dr. Hajime Yamamoto, Taisei]





Density convections for 1,000 years:

Flow Model

Only the far side of the vertical cross section passing through the injection well is depicted.

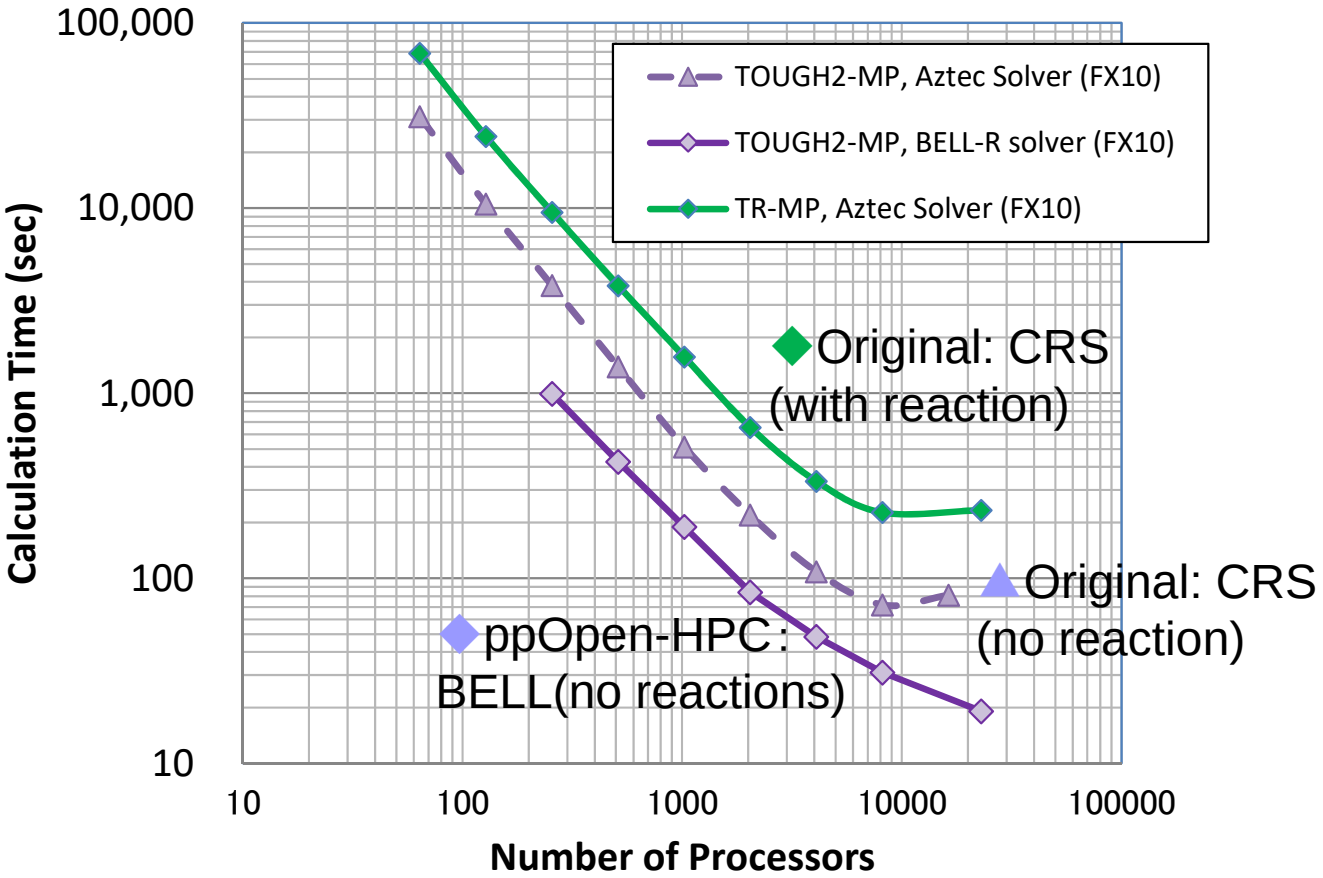
[Dr. Hajime Yamamoto, Taisei]

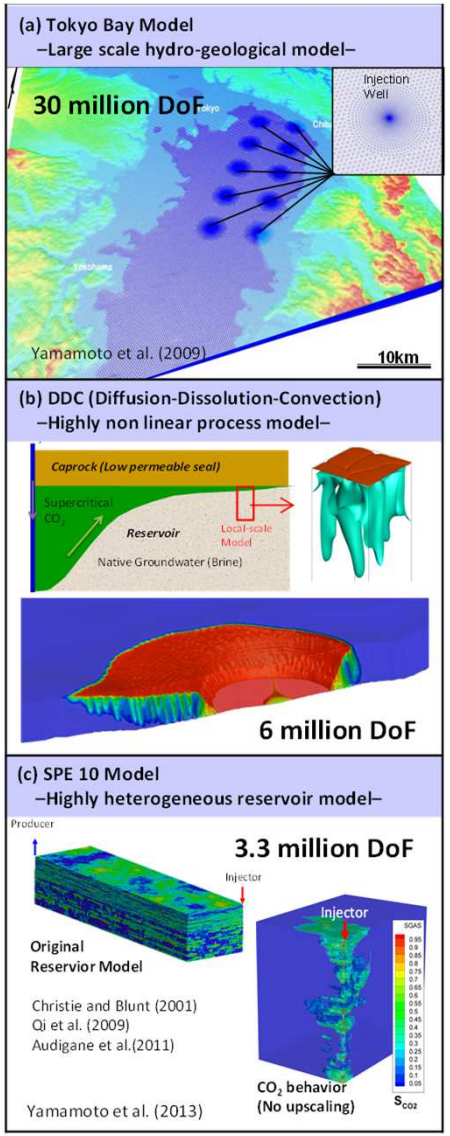
- The meter-scale fingers gradually developed to larger ones in the field-scale model
- Huge number of time steps (> 10^5) were required to complete the 1,000-yrs simulation
- Onset time (10-20 yrs) is comparable to theoretical (linear stability analysis, 15.5yrs)

Performance: Heterogeneous, Non-linear models

The scalability may be suppressed depending on the problem size as well as the severity of heterogeneity and non-linearity of models

[Dr. Hajime Yamamoto, Taisei]





※DOF: degrees of freedom

Fujitsu FX10（Oakleaf-FX），30M DOF: 2x-3x improvement