

Introduction to Parallel Programming for Multicore/Manycore Clusters

General Introduction

Invitation to Supercomputing

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Motivation for Parallel Computing (and this class)

- Large-scale parallel computer enables fast computing in large-scale scientific simulations with detailed models. Computational science develops new frontiers of science and engineering.
- Why parallel computing ?
 - faster & larger
 - “larger” is more important from the view point of “new frontiers of science & engineering”, but “faster” is also important.
 - + more complicated
 - Ideal: Scalable
 - Solving N^x scale problem using N^x computational resources during same computation time (weak scaling)
 - Solving a fix-sized problem using N^x computational resources in $1/N$ computation time (strong scaling)

Scientific Computing = SMASH

Science

Modeling

Algorithm

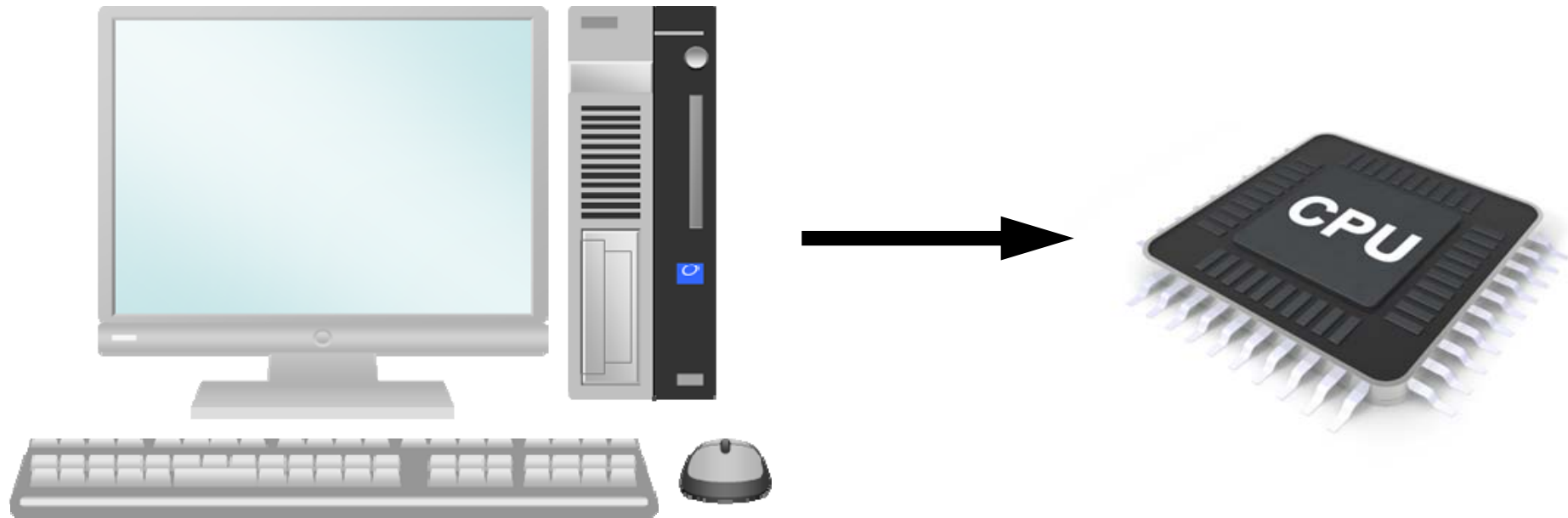
Software

Hardware

- You have to learn many things.
- Collaboration (or Co-Design) will be important for future career of each of you, as a scientist and/or an engineer.
 - You have to communicate with people with different backgrounds.
 - It is more difficult than communicating with foreign scientists from same area.
- (Q): Computer Science, Computational Science, or Numerical Algorithms ?

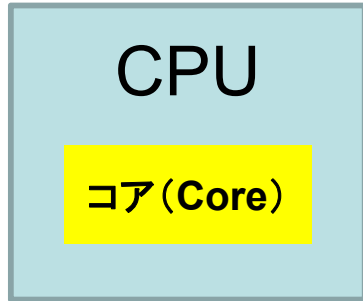
- **Supercomputers and Computational Science**
- Overview of the Class

Computer & CPU

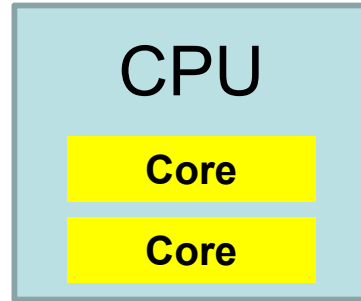


- Central Processing Unit (中央处理装置): CPU
- CPU's used in PC and Supercomputers are based on same architecture
- GHz: Clock Rate
 - Frequency: Number of operations by CPU per second
 - GHz -> 10^9 operations/sec
 - Simultaneous 4-8 instructions per clock

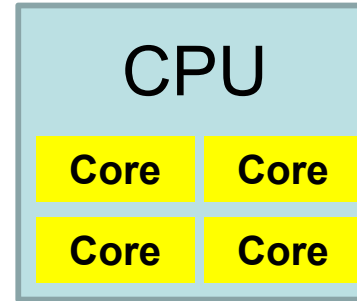
Multicore CPU



Single Core
1 cores/CPU

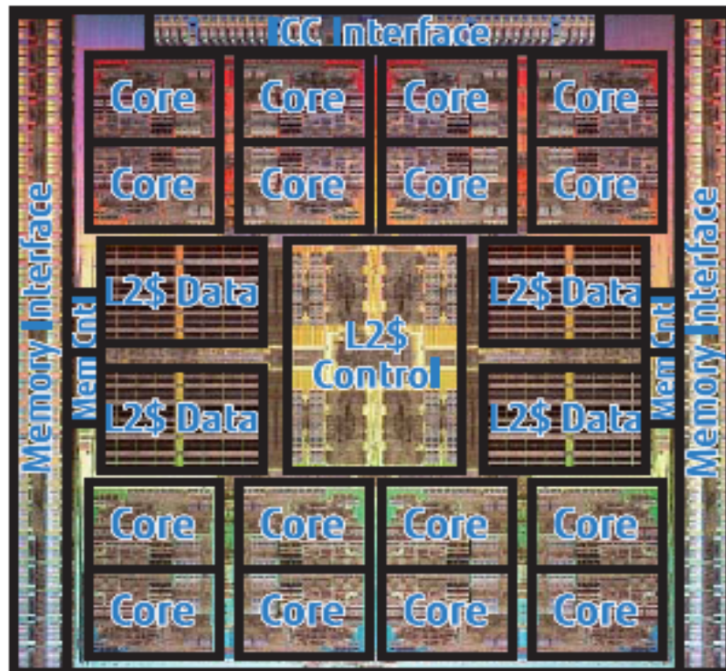


Dual Core
2 cores/CPU



Quad Core
4 cores/CPU

- Core= Central part of CPU
- Multicore CPU's with 4-8 cores are popular
 - Low Power

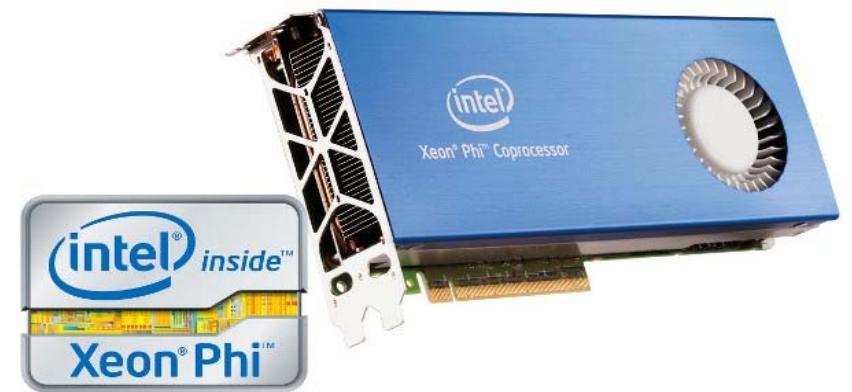


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- GPU: Manycore
 - $O(10^1)$ - $O(10^2)$ cores
- More and more cores
 - Parallel computing
- Oakleaf-FX at University of Tokyo: 16 cores
 - SPARC64™ IXfx

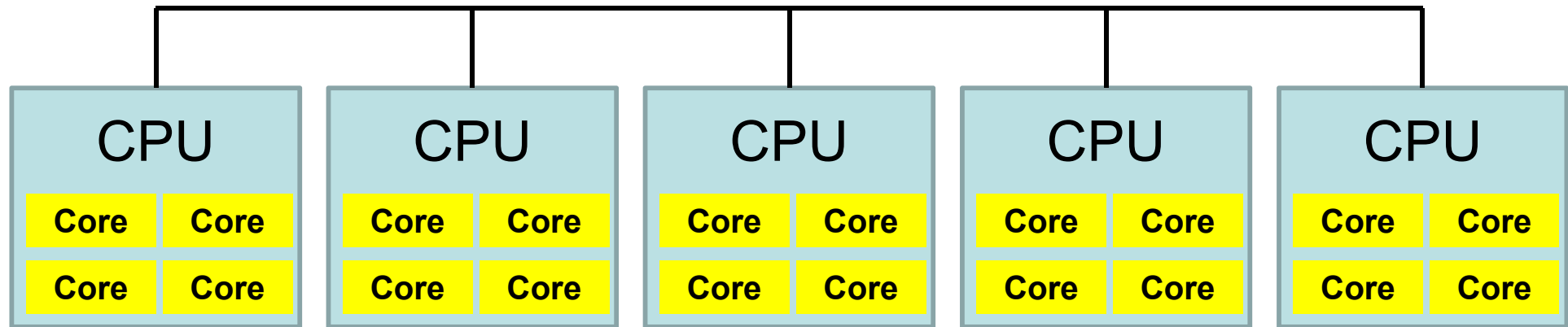
GPU/Manycores

- GPU : Graphic Processing Unit
 - GPGPU: General Purpose GPU
 - $O(10^2)$ cores
 - High Memory Bandwidth
 - Cheap
 - NO stand-alone operations
 - Host CPU needed
 - Programming: CUDA, OpenACC
- Intel Xeon/Phi: Manycore CPU
 - >60 cores
 - High Memory Bandwidth
 - Unix, Fortran, C compiler
 - Currently, host CPU needed
 - Stand-alone: Knights Landing

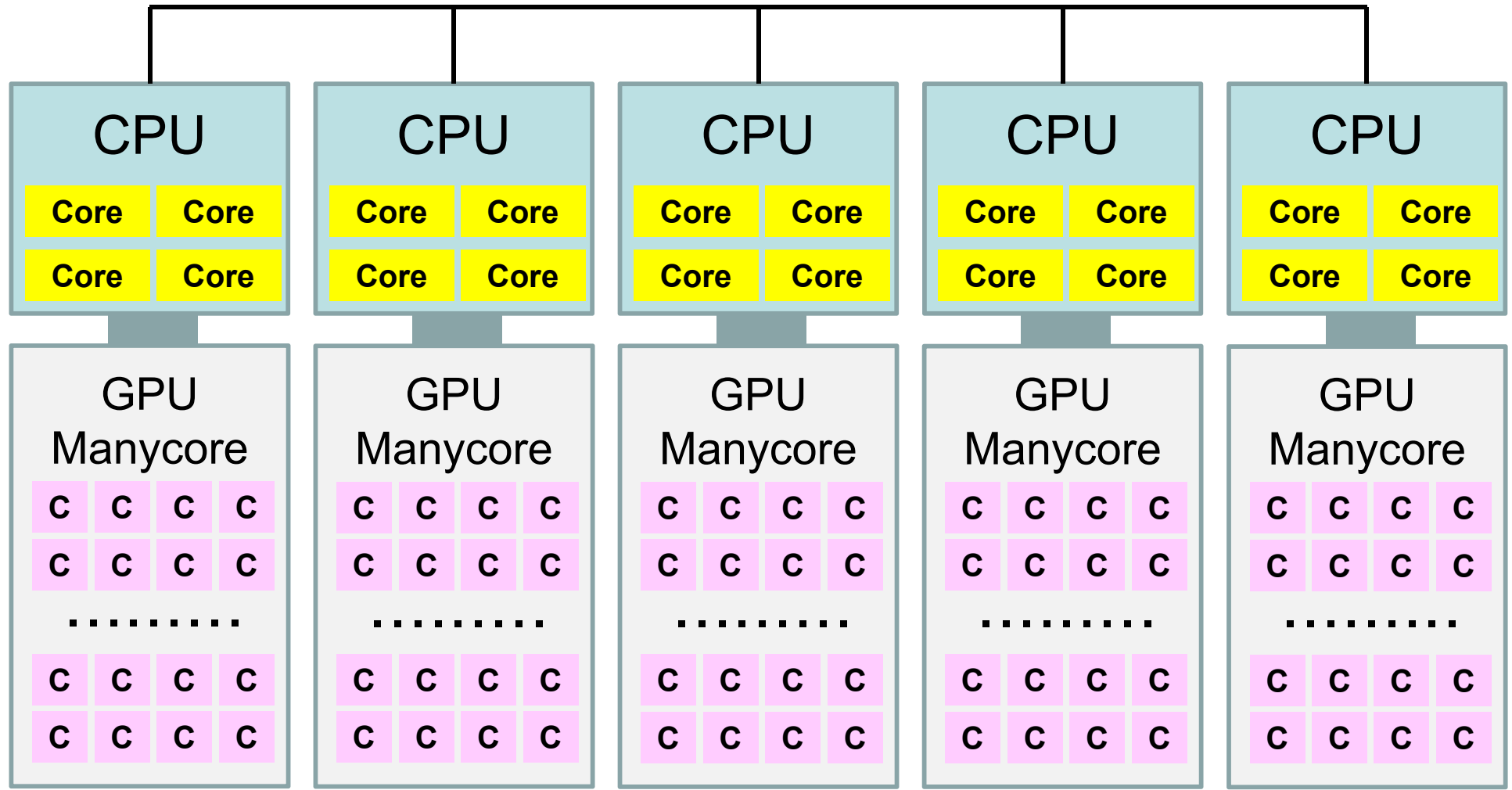


Parallel Supercomputers

Multicore CPU's are connected through network



Supercomputers with Heterogeneous/Hybrid Nodes

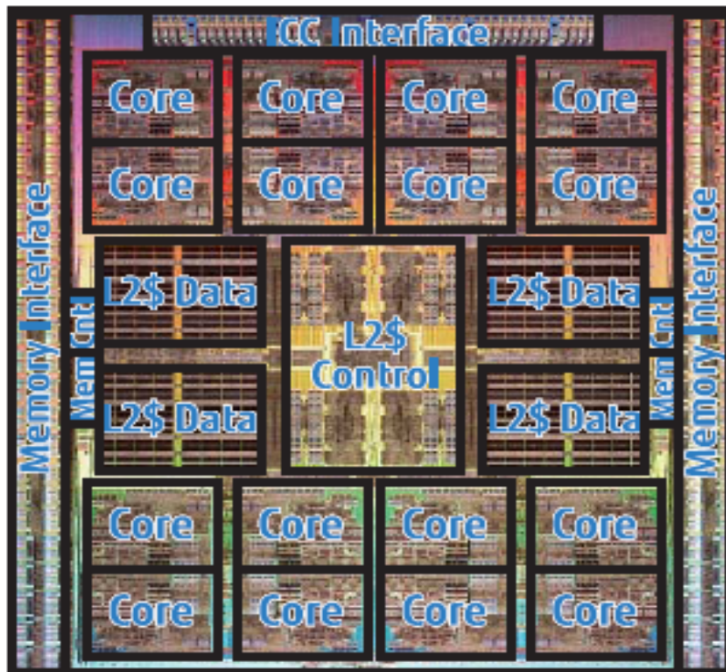


Performance of Supercomputers

- Performance of CPU: Clock Rate
- FLOPS (Floating Point Operations per Second)
 - Real Number
- Recent Multicore CPU
 - 4-8 FLOPS per Clock
 - (e.g.) Peak performance of a core with 3GHz
 - $3 \times 10^9 \times 4(\text{or } 8) = 12(\text{or } 24) \times 10^9 \text{ FLOPS} = 12(\text{or } 24) \text{ GFLOPS}$
 - $10^6 \text{ FLOPS} = 1 \text{ Mega FLOPS} = 1 \text{ MFLOPS}$
 - $10^9 \text{ FLOPS} = 1 \text{ Giga FLOPS} = 1 \text{ GFLOPS}$
 - $10^{12} \text{ FLOPS} = 1 \text{ Tera FLOPS} = 1 \text{ TFLOPS}$
 - $10^{15} \text{ FLOPS} = 1 \text{ Peta FLOPS} = 1 \text{ PFLOPS}$
 - $10^{18} \text{ FLOPS} = 1 \text{ Exa FLOPS} = 1 \text{ EFLOPS}$

Peak Performance of Oakleaf-FX

Fujitsu PRIMEHPC FX10 at U.Tokyo



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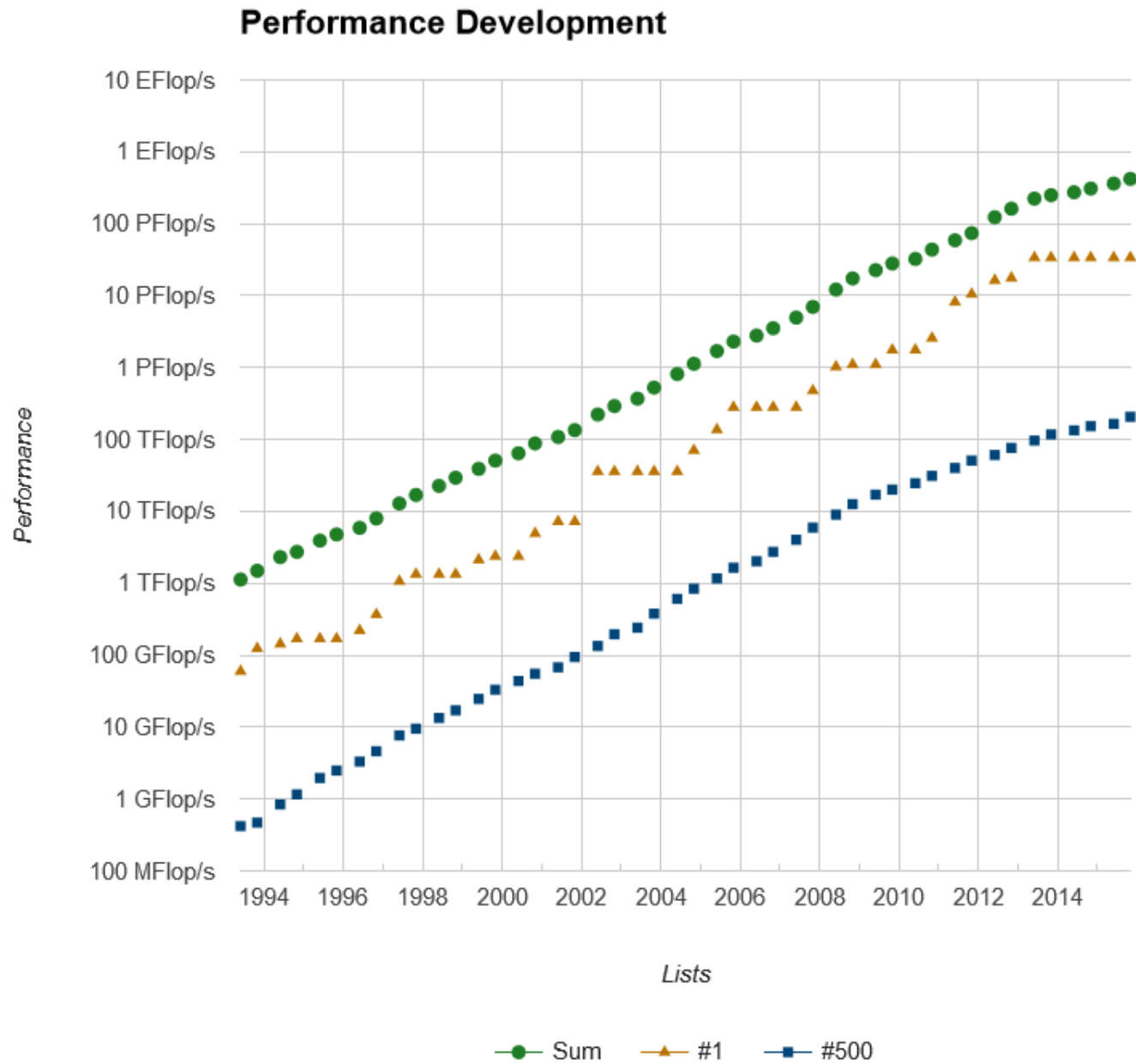


- 1.848 GHz
- 8 FLOP operations per Clock
- Peak Performance (1 core)
 - $1.848 \times 8 = 14.78$ GFLOPS
- Peak Performance (1 node/16 cores)
 - 236.5 GFLOPS
- **Peak Performance of Entire Performance**
 - 4,800 nodes, 76,800 cores
 - **1.13 PFLOPS**

TOP 500 List

<http://www.top500.org/>

- Ranking list of supercomputers in the world
- Performance (FLOPS rate) is measured by “Linpack” which solves large-scale linear equations.
 - Since 1993
 - Updated twice a year (International Conferences in June and November)
- Linpack
 - iPhone version is available



- PFLOPS: Peta ($=10^{15}$) Floating OPerations per Sec.
- Exa-FLOPS ($=10^{18}$) will be attained after 2020

48th TOP500 List (November, 2016)

	Site	Computer/Year Vendor	Cores	R _{max} (TFLOPS)	R _{peak} (TFLOPS)	Power (kW)
1	National Supercomputing Center in Wuxi, China	Sunway TaihuLight , Sunway MPP, Sunway SW26010 260C 1.45GHz, 2016 NRCP	10,649,600	93,015 (= 93.0 PF)	125,436	15,371
2	National Supercomputing Center in Tianjin, China	Tianhe-2 , Intel Xeon E5-2692, TH Express-2, Xeon Phi, 2013 NUDT	3,120,000	33,863 (= 33.9 PF)	54,902	17,808
3	Oak Ridge National Laboratory, USA	Titan Cray XK7/NVIDIA K20x, 2012 Cray	560,640	17,590	27,113	8,209
4	Lawrence Livermore National Laboratory, USA	Sequoia BlueGene/Q, 2011 IBM	1,572,864	17,173	20,133	7,890
5	DOE/SC/LBNL/NERSC USA	Cori , Cray XC40, Intel Xeon Phi 7250 68C 1.4GHz, Cray Aries, 2016 Cray	632,400	14,015	27,881	3,939
6	Joint Center for Advanced High Performance Computing, Japan	Oakforest-PACS , PRIMERGY CX600 M1, Intel Xeon Phi Processor 7250 68C 1.4GHz, Intel Omni-Path, 2016 Fujitsu	557,056	13,555	24,914	2,719
7	RIKEN AICS, Japan	K computer , SPARC64 VIIIfx , 2011 Fujitsu	705,024	10,510	11,280	12,660
8	Swiss Natl. Supercomputer Center, Switzerland	Piz Daint Cray XC30/NVIDIA P100, 2013 Cray	206,720	9,779	15,988	1,312
9	Argonne National Laboratory, USA	Mira BlueGene/Q, 2012 IBM	786,432	8,587	10,066	3,945
10	DOE/NNSA/LANL/SNL, USA	Trinity , Cray XC40, Xeon E5-2698v3 16C 2.3GHz, 2016 Cray	301,056	8,101	11,079	4,233

R_{max}: Performance of Linpack (TFLOPS)

R_{peak}: Peak Performance (TFLOPS), Power: kW

<http://www.top500.org/>

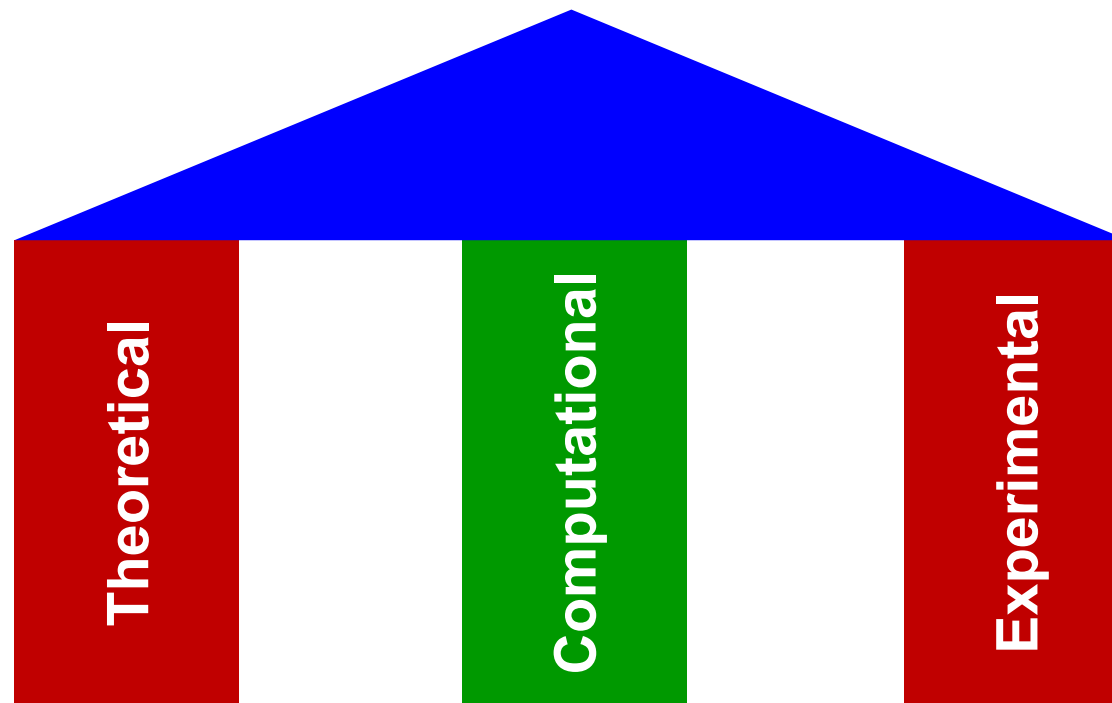
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104	ITC/U. Tokyo Japan	Oakleaf-FX SPARC64 IXfx, 2012 Fujitsu	76800	1043	1135	1177

Computational Science

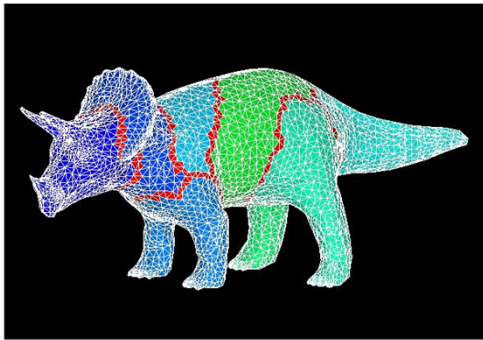
The 3rd Pillar of Science

- Theoretical & Experimental Science
- Computational Science
 - The 3rd Pillar of Science
 - Simulations using Supercomputers

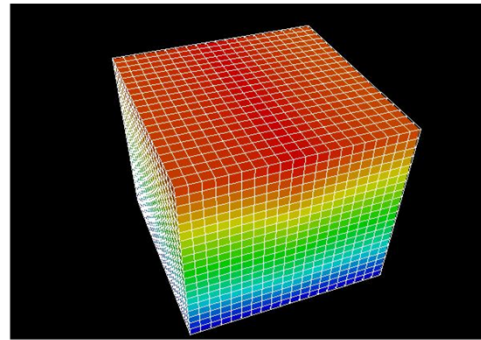


Methods for Scientific Computing

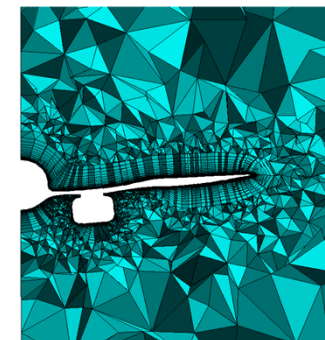
- Numerical solutions of PDE (Partial Diff. Equations)
- Grids, Meshes, Particles
 - Large-Scale Linear Equations
 - Finer meshes provide more accurate solutions



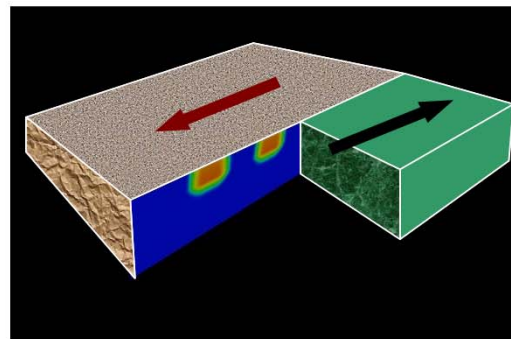
有限要素法
Finite Element Method
FEM



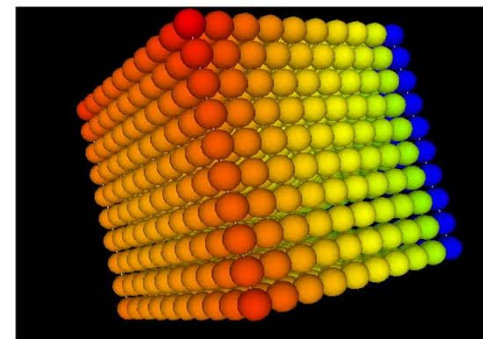
差分法
Finite Difference Method
FDM



有限体積法
Finite Volume Method
FVM



境界要素法
Boundary Element Method
BEM

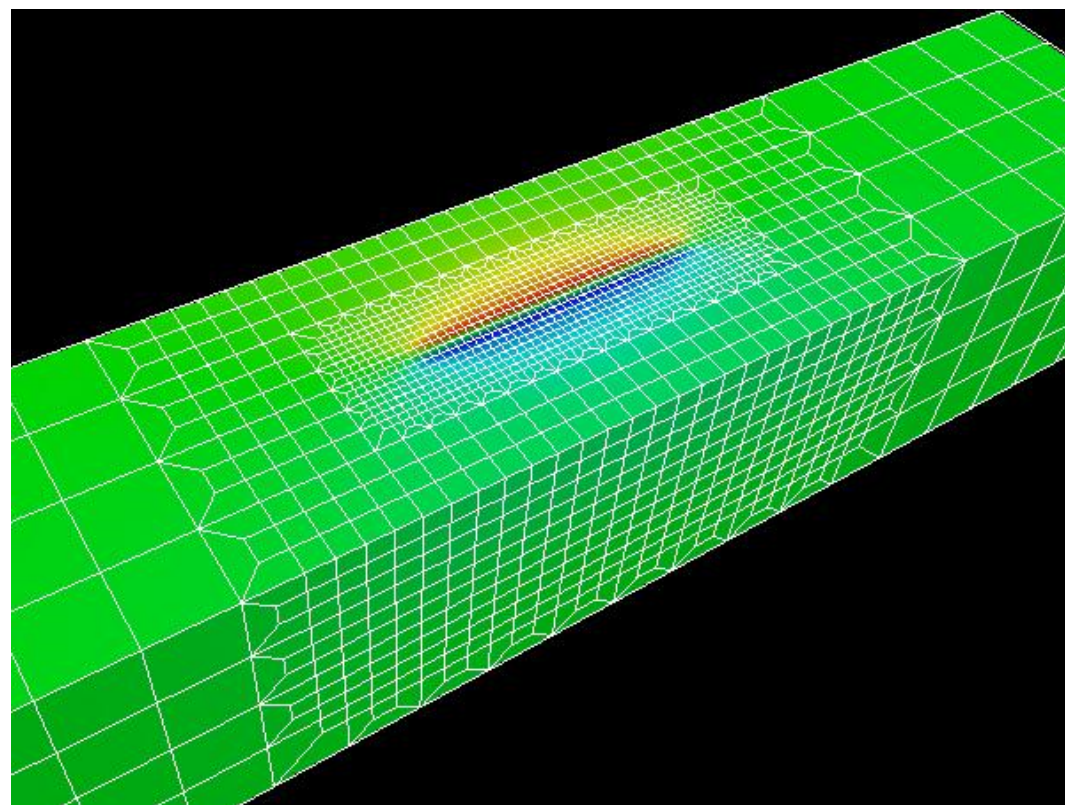
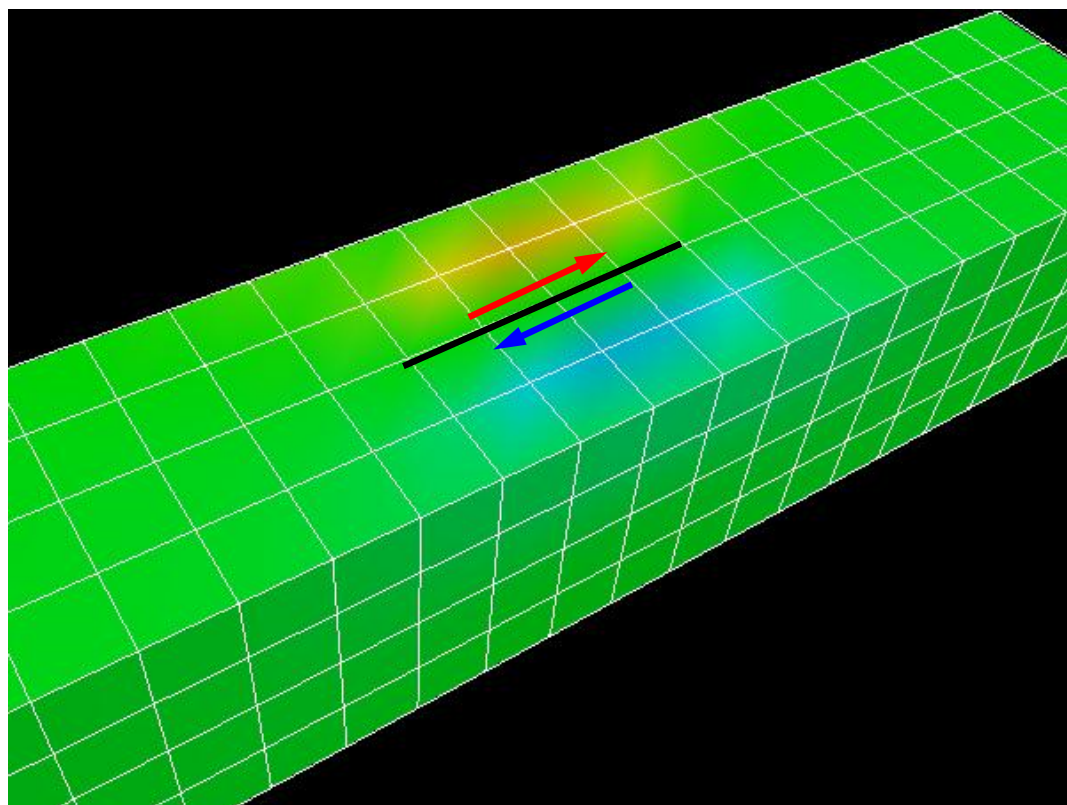


個別要素法
Discrete Element Method
DEM

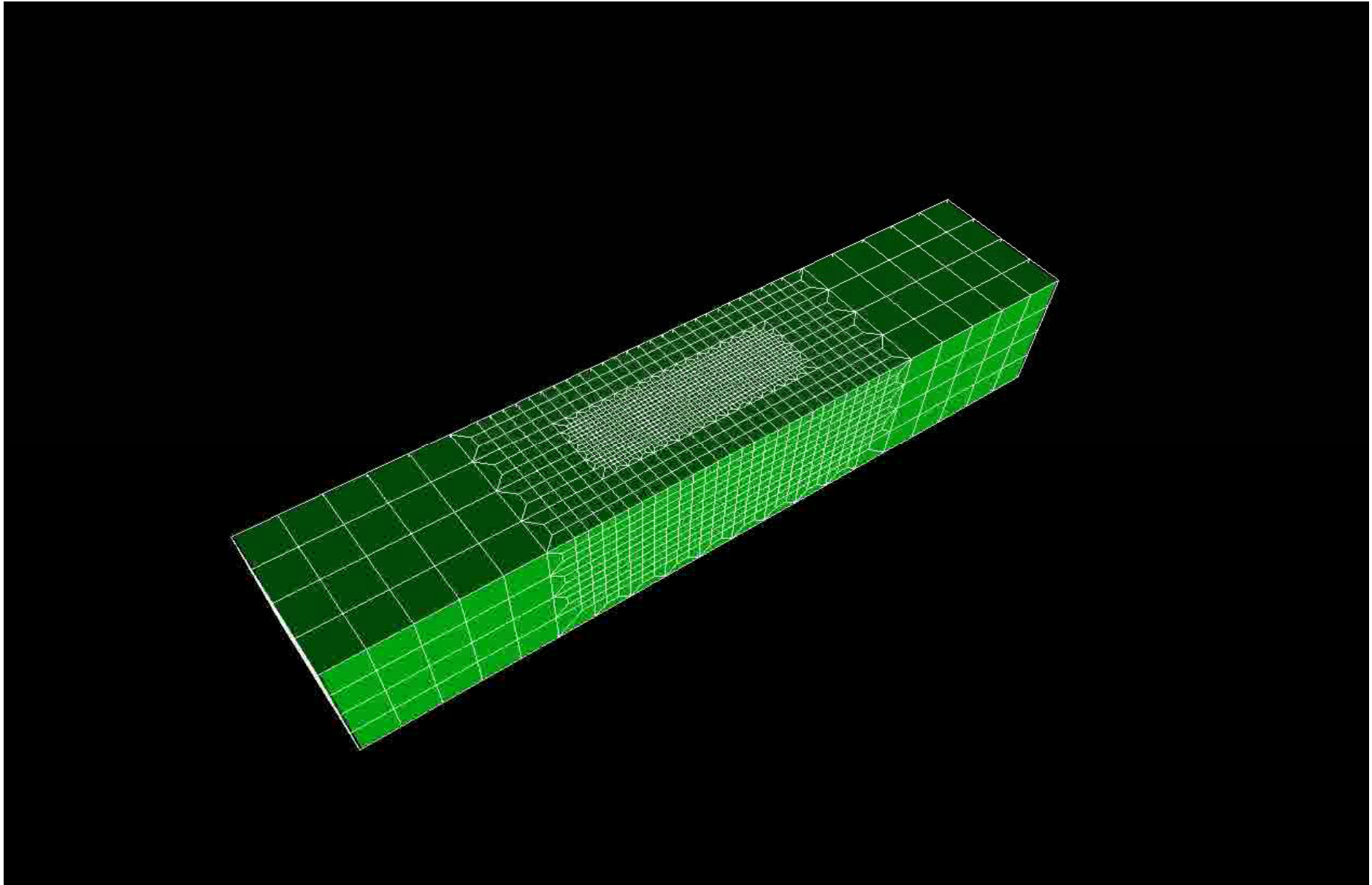
3D Simulations for Earthquake Generation Cycle

San Andreas Faults, CA, USA

Stress Accumulation at Transcurrent Plate Boundaries

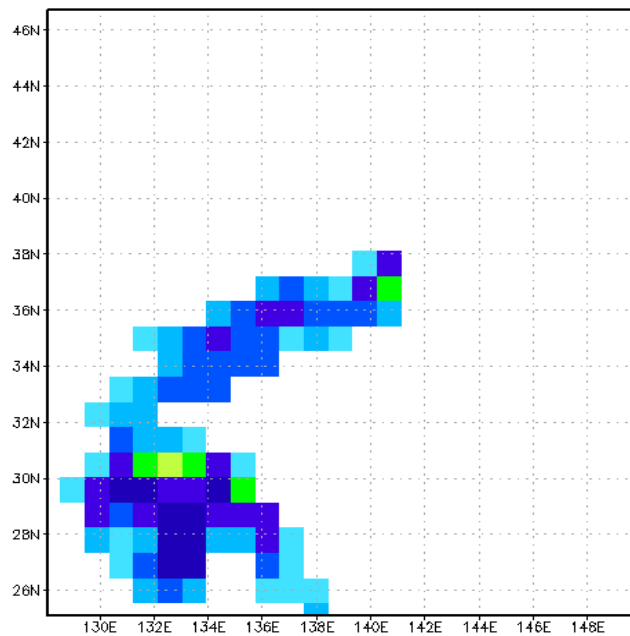


Adaptive FEM: High-resolution needed at meshes with large deformation (large accumulation)

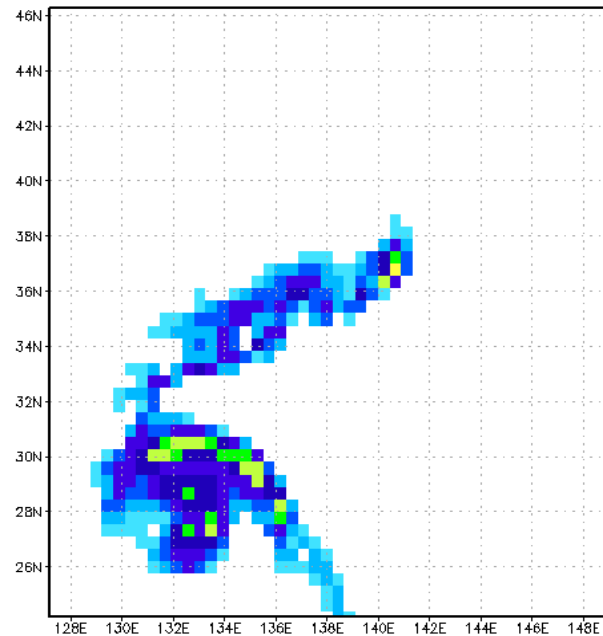


Typhoon Simulations by FDM

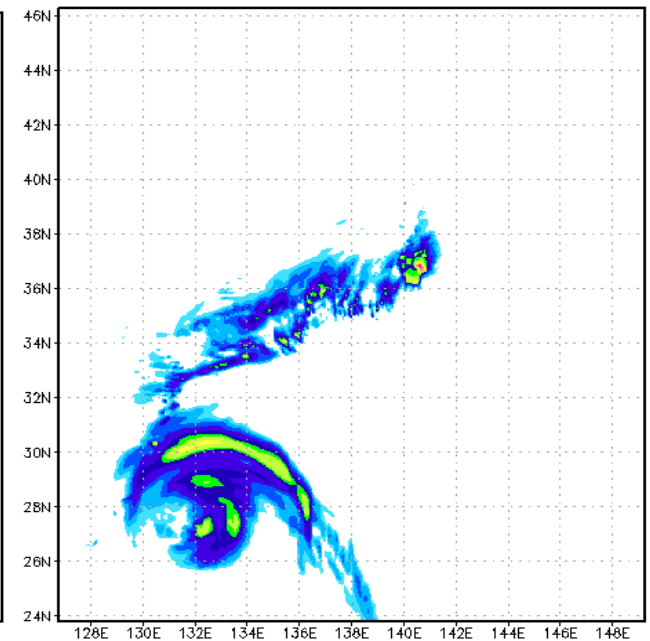
Effect of Resolution



$\Delta h = 100\text{km}$

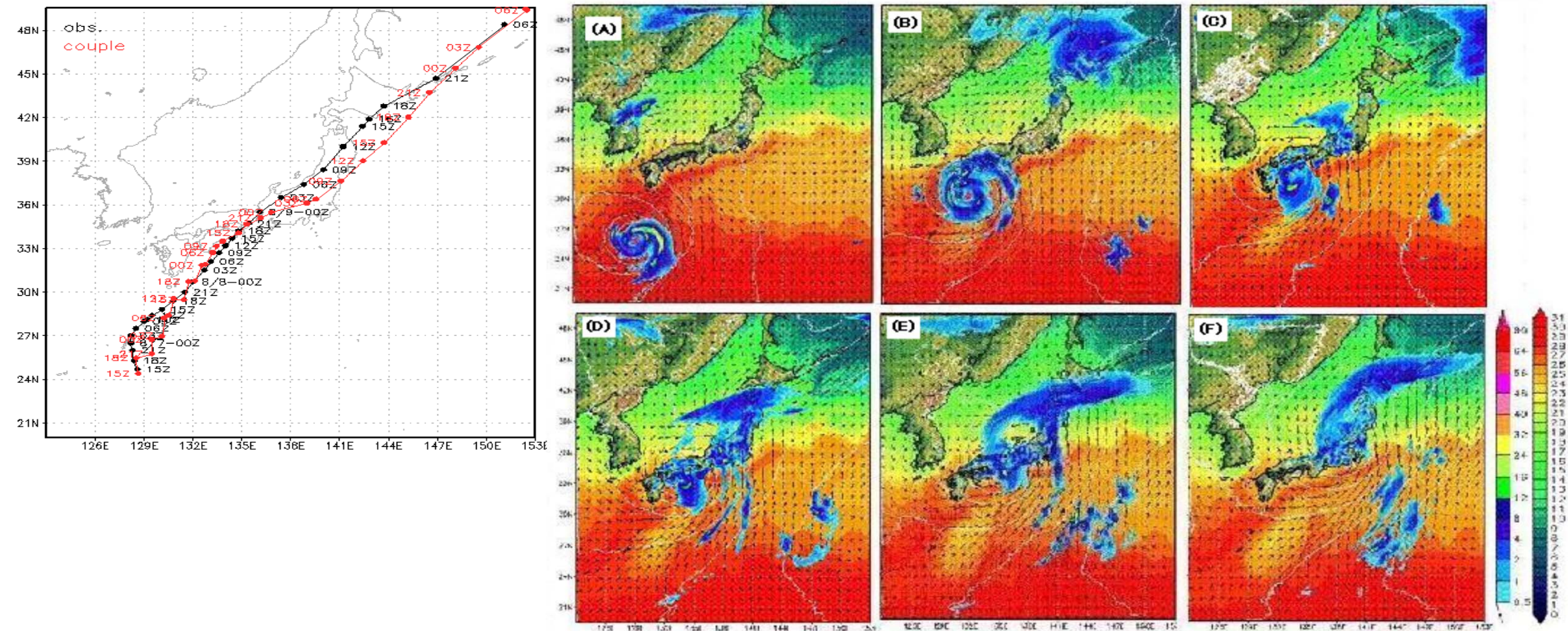


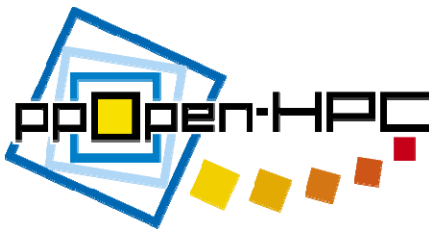
$\Delta h = 50\text{km}$



$\Delta h = 5\text{km}$

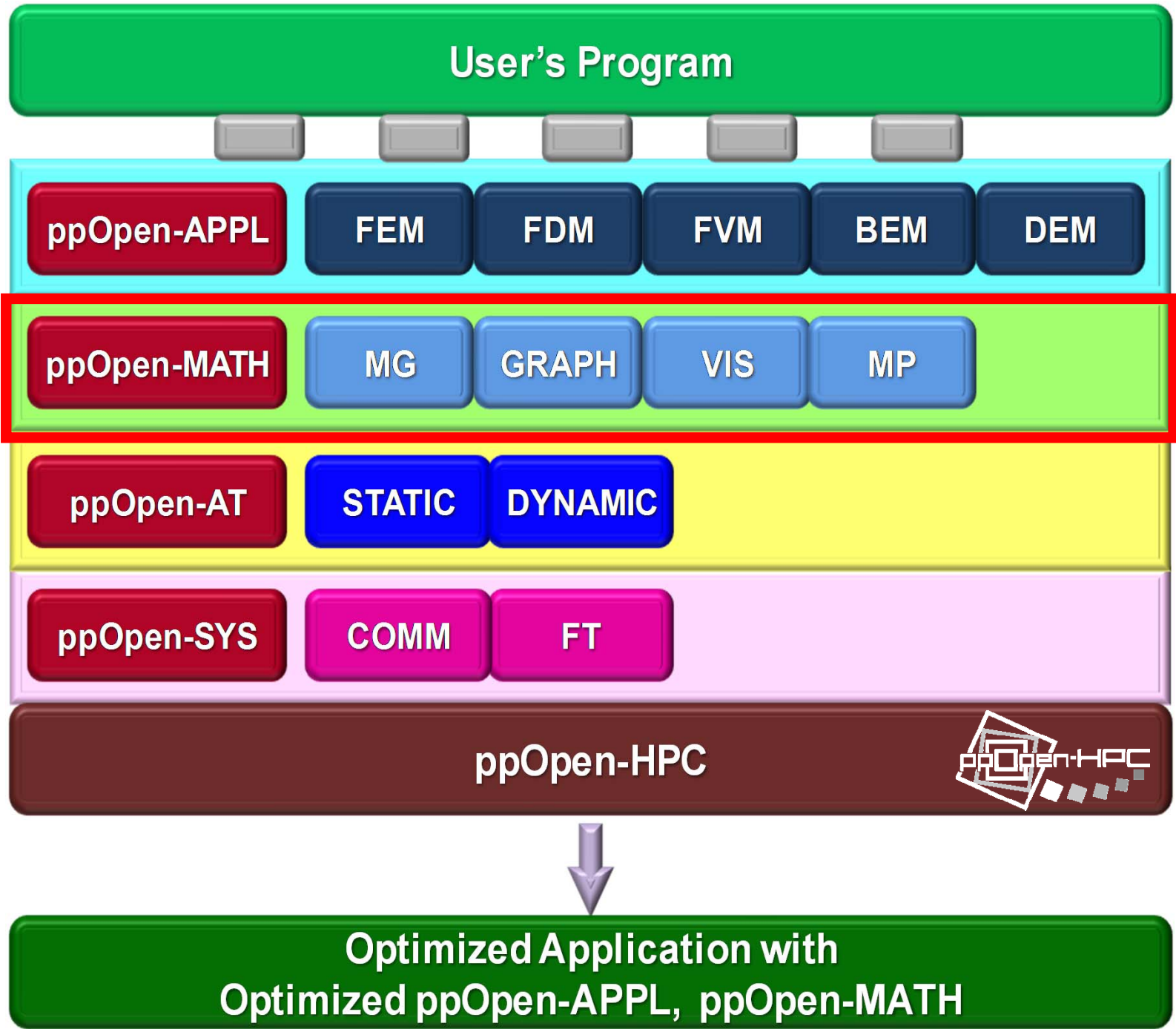
Simulation of Typhoon MANGKHUT in 2003 using the Earth Simulator

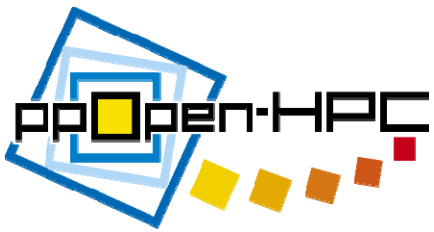




ppOpen-HPC

- 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.
- Software
 - Source Files, English Documents
 - MIT License
 - <http://ppopenhpc.cc.u-tokyo.ac.jp/>





ppOpen-MATH

- A set of common numerical libraries
 - Multigrid solvers (ppOpen-MATH/MG)
 - Parallel graph libraries (ppOpen-MATH/GRAPH)
 - Multithreaded RCM for reordering (under development)
 - Parallel visualization (ppOpen-MATH/VIS)
 - Library for coupled multi-physics simulations (loose-coupling) (ppOpen-MATH/MP)
 - Originally developed as a coupler for NICAM (atmosphere, unstructured), and COCO (ocean, structured) in global climate simulations using K computer
 - Both codes are major codes on the K computer.
 - » Prof. Masaki Satoh (AORI/U.Tokyo): NICAM
 - » Prof. Hiroyasu Hasumi (AORI/U.Tokyo): COCO
 - Developed coupler is extended to more general use.
 - Coupled seismic simulations

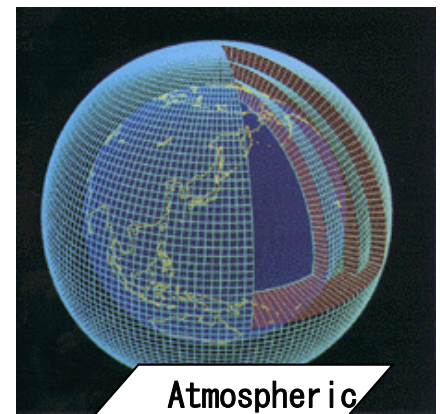
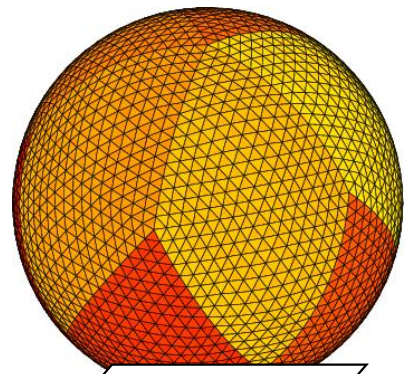
Motivation for Parallel Computing (again)

- Large-scale parallel computer enables fast computing in large-scale scientific simulations with detailed models. Computational science develops new frontiers of science and engineering.
- Why parallel computing ?
 - faster & larger
 - “larger” is more important from the view point of “new frontiers of science & engineering”, but “faster” is also important.
 - **+ more complicated**
 - Coupled Problems (Fluid + Structure)
 - Multiple PDE (Partial Differential Equations)
 - Actually, most of the real world problems are “coupled” ones

NICAM:
Semi-Structured Grid

MIROC-A:
FDM/Structured Grid

NICAM-
Agrid
NICAM-
ZMgrid



MIROC-A

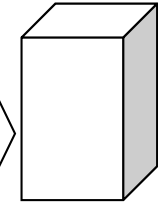
Atmospheric
Model-1

Atmospheric
Model-2

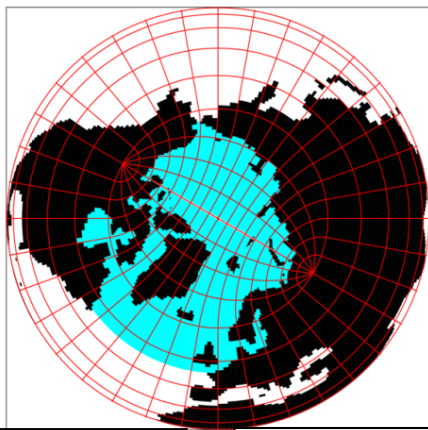
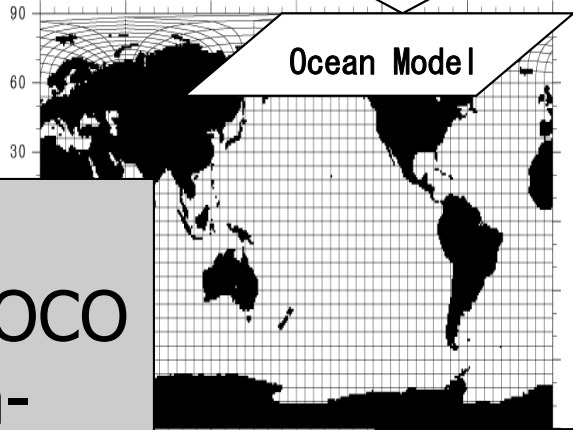
ppOpen-MATH/MP Coupler

- Grid Transformation
- Multi-Ensemble
- IO
- Pre- and post-process
- Fault tolerance
- M × N

J-cup



Post-Peta-Scale
System
-System S/W
-Architecture



COCO
Regional COCO
Matsumura-
model

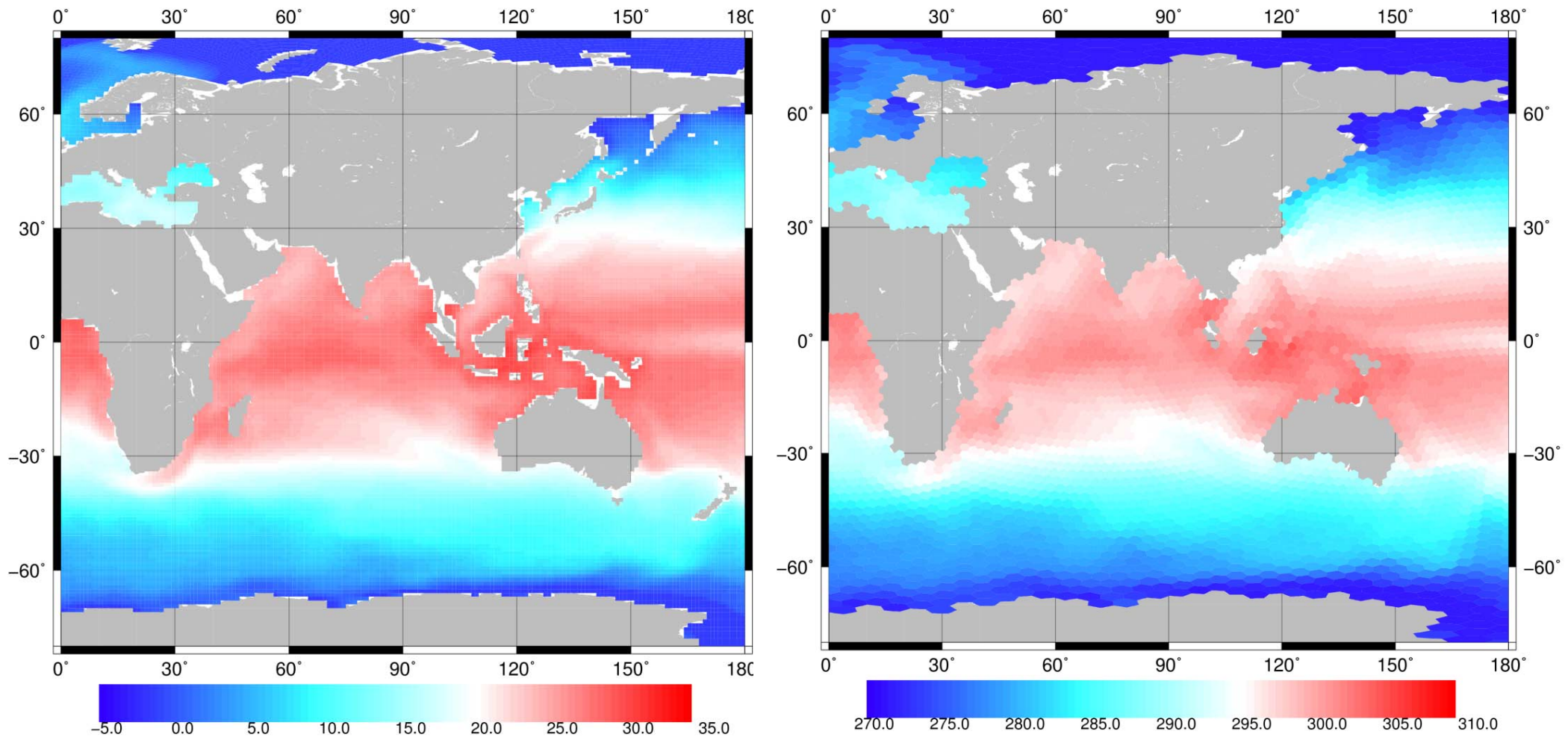
COCO: Tri-Polar FDM

Regional Ocean Model
Non Hydrostatic Model

c/o T.Arakawa,
M.Satoh

c/o T.Arakawa, M.Satoh

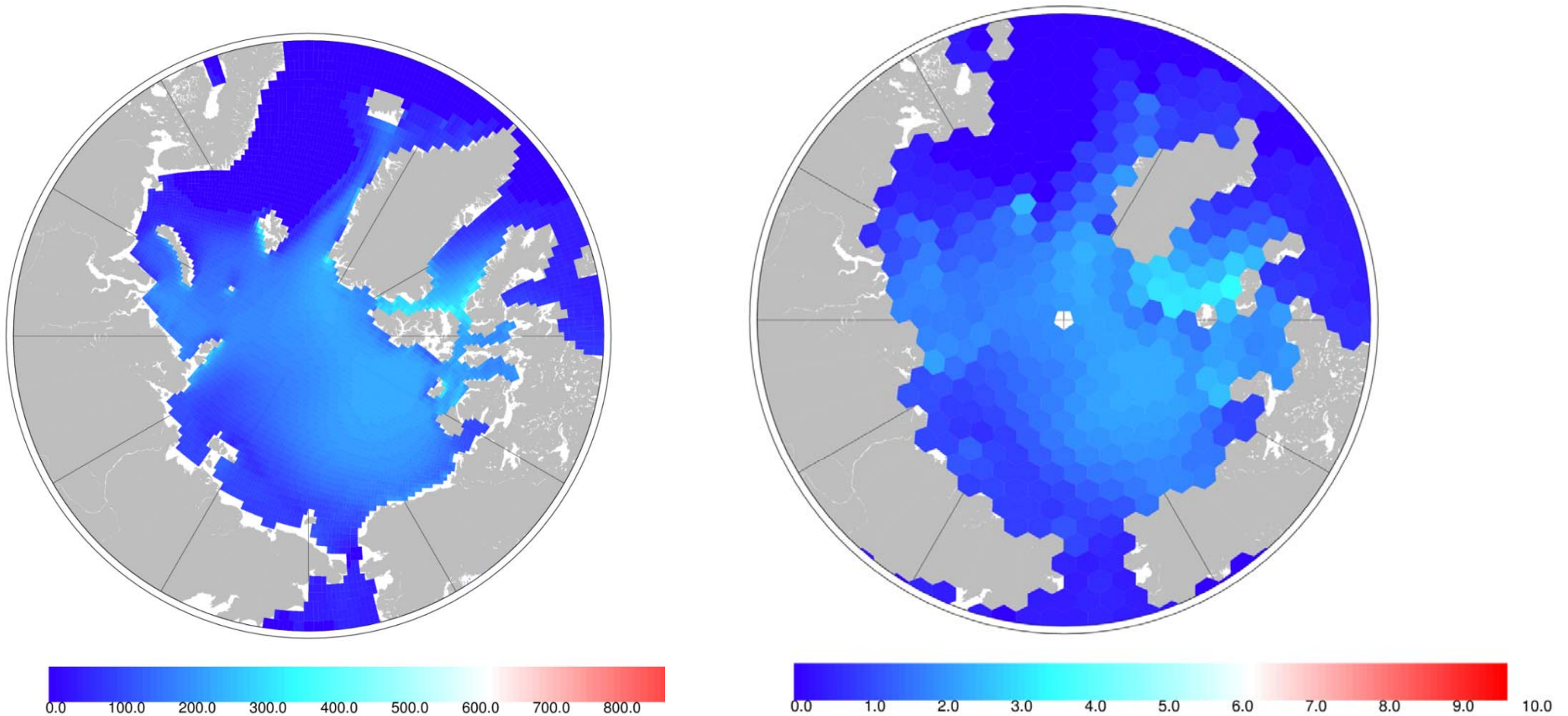
Sea surface temperature (OSST)



left: COCO (Ocean: Structured), right: NICAM (Atmospheric: Semi-Unst.)

c/o T.Arakawa, M.Satoh

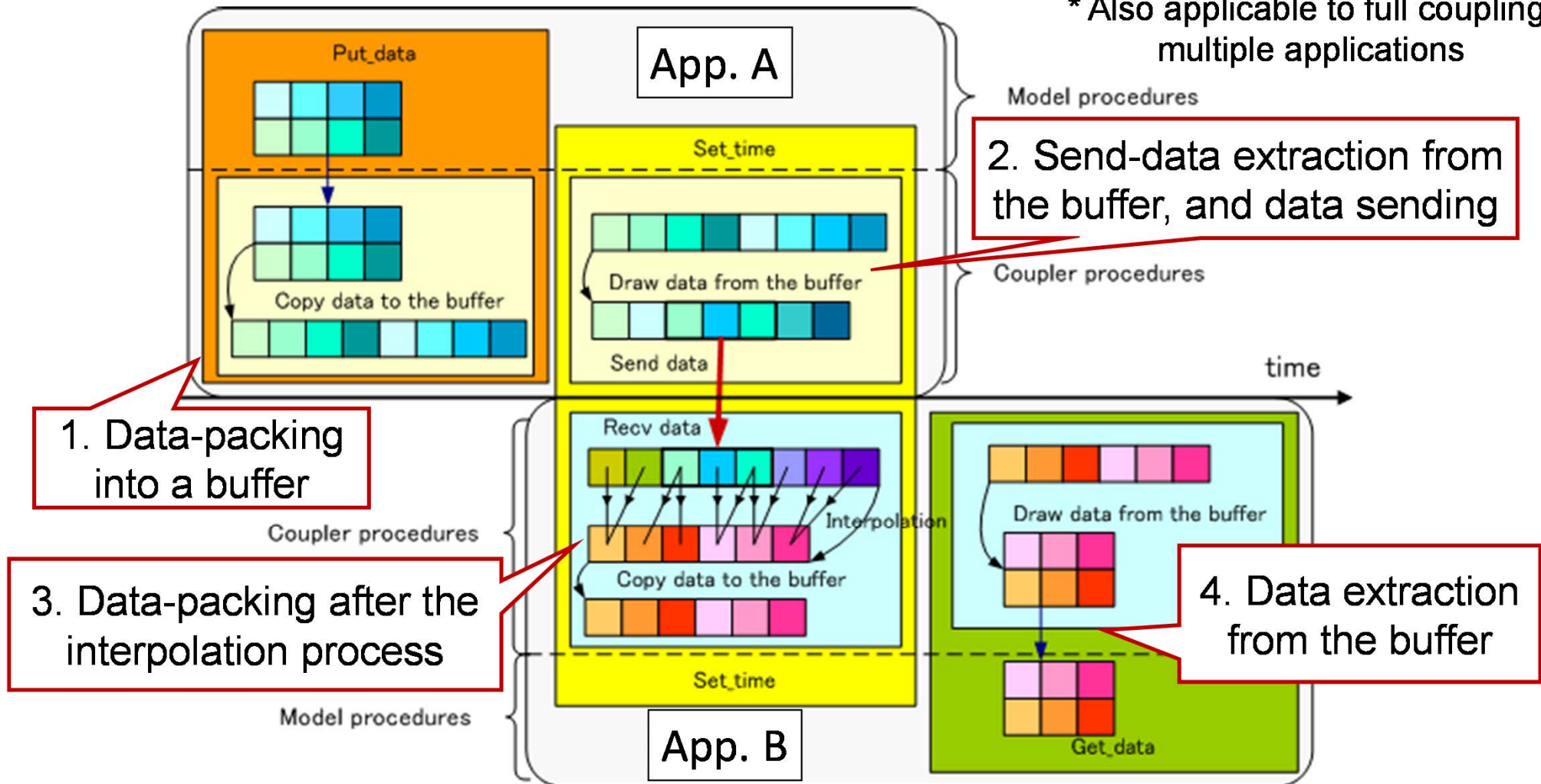
Thickness of Sea Ice (OHI)



left: COCO (Ocean: Structured), right: NICAM (Atmospheric: Semi-Unst.)

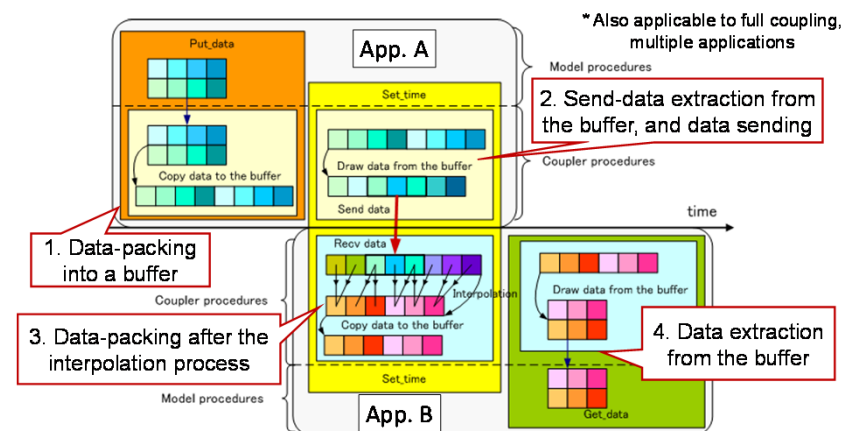
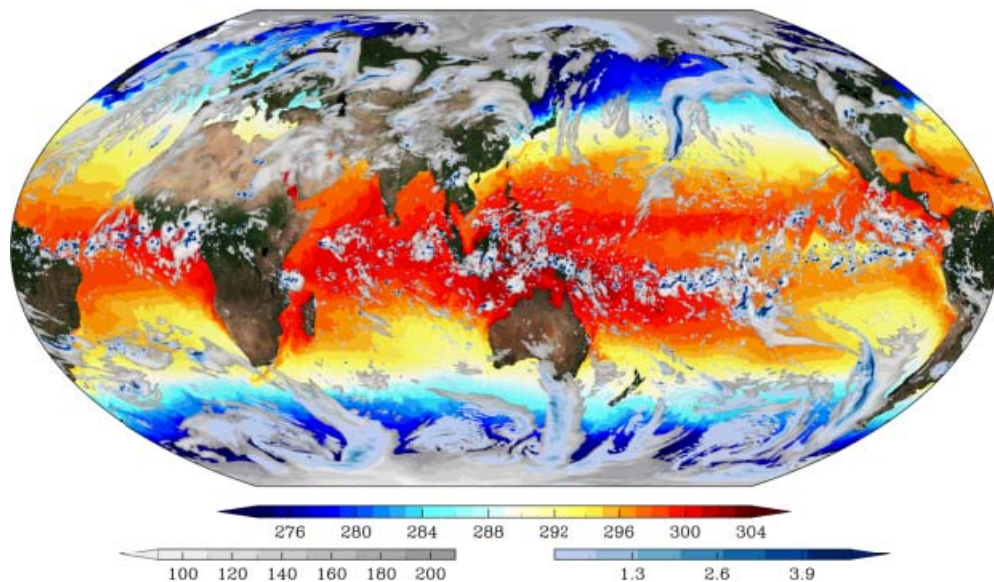
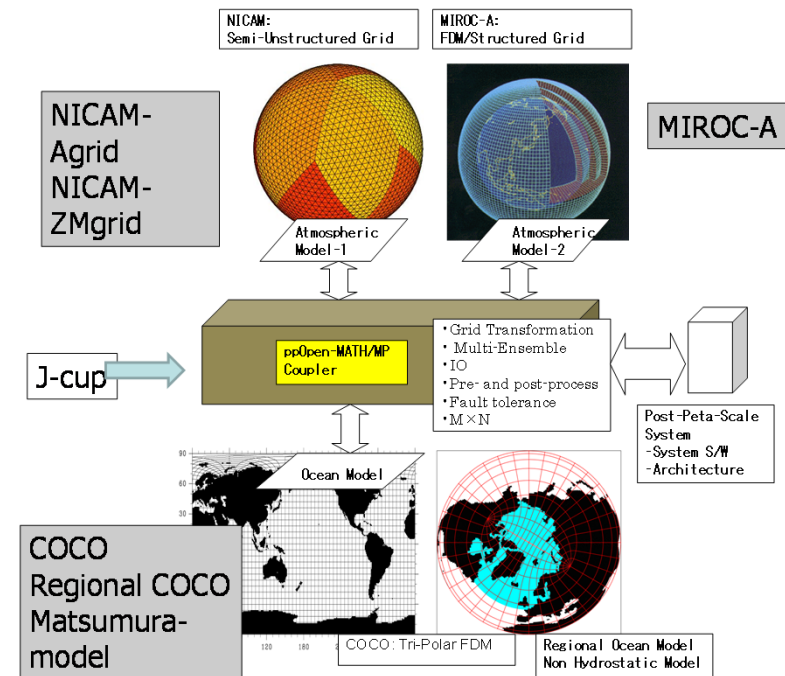
Dataflow of ppOpen-MATH/MP*

* Also applicable to full coupling, multiple applications



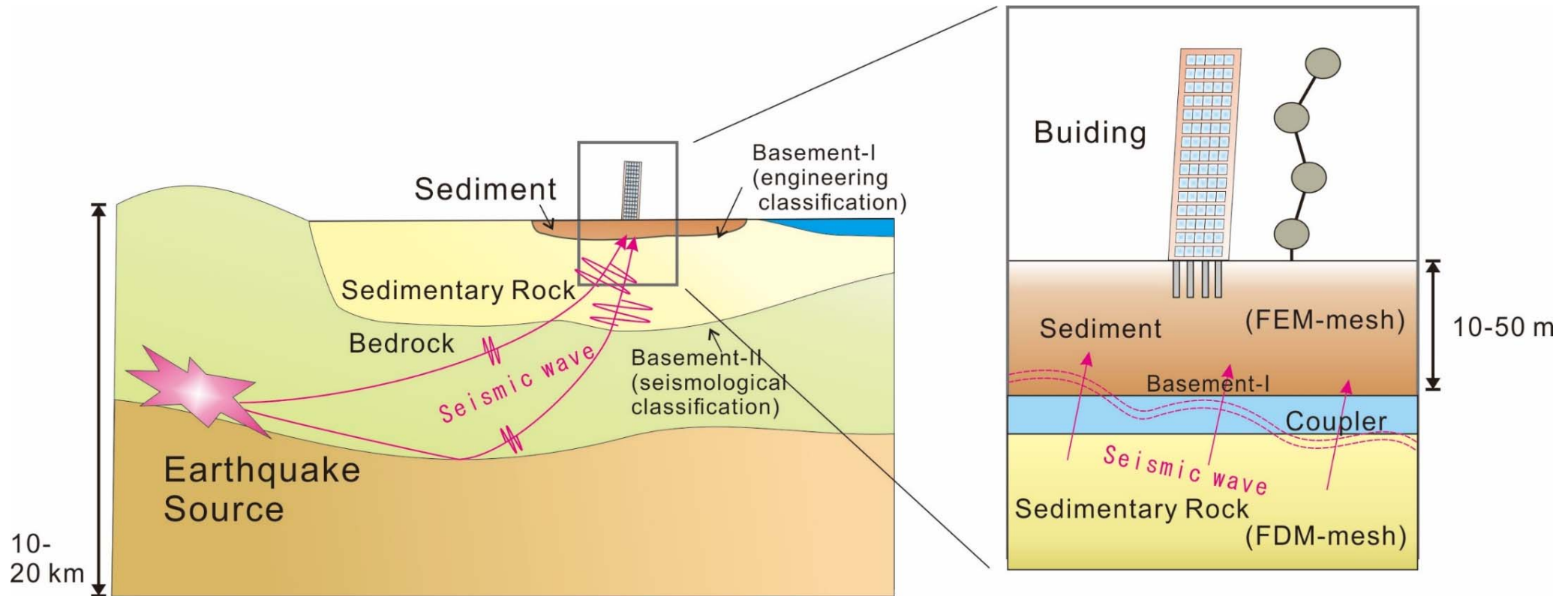
Atmosphere-Ocean Coupling on OFP by NICAM/COCO/ppOpen-MATH/MP

- High-resolution global atmosphere-ocean coupled simulation by NICAM and COCO (Ocean Simulation) through ppOpen-MATH/MP on the K computer is achieved.
 - ppOpen-MATH/MP is a coupling software for the models employing various discretization method.
- An O(km)-mesh NICAM-COCO coupled simulation is planned on the Oakforest-PACS system.
 - A big challenge for optimization of the codes on new Intel Xeon Phi processor
 - New insights for understanding of global climate dynamics



Coupling Simulation of Seismic Waves and Building Vibrations

1



The coupling simulation refers to one-way data communication from **FDM** (seismic wave propagation) to **FEM** (dynamic structure).

Numerical Model Description

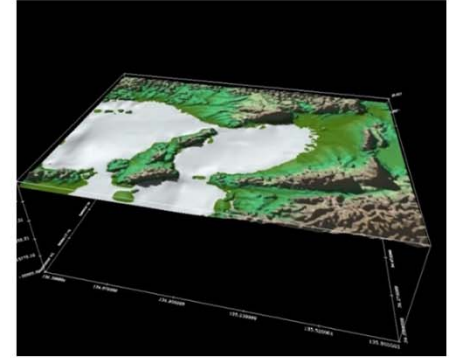
Seism3D+ (composed of ppOpen-APPL/FDM)

Explicit FDM Application for Seismic Wave Analysis

$$\rho \frac{\partial v_p}{\partial t} = \left(\frac{\partial \sigma_{xp}}{\partial x} + \frac{\partial \sigma_{yp}}{\partial y} + \frac{\partial \sigma_{zp}}{\partial z} + f_p \right), \quad (p = x, y, z)$$

v : velocity
 σ : stress
 f : external force
 λ, μ : Lamé's constant

$$\frac{\partial \sigma_{pq}}{\partial t} = \lambda \left(\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} \right) \delta_{pq} + \mu \left(\frac{\partial v_p}{\partial q} + \frac{\partial v_q}{\partial p} \right), \quad (p, q = x, y, z)$$

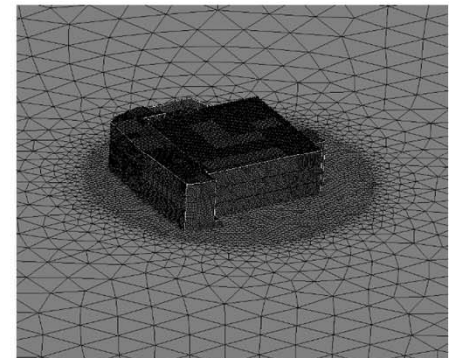


FrontISTR++ (composed of ppOpen-APPL/FEM)

Implicit FEM Application for Structural Analysis

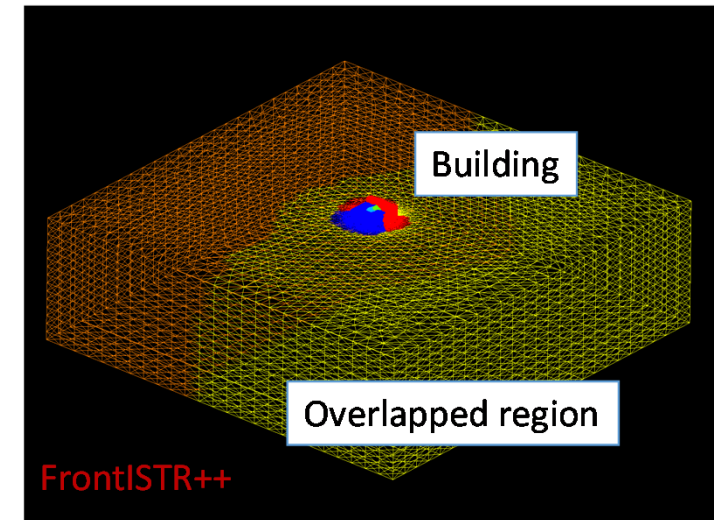
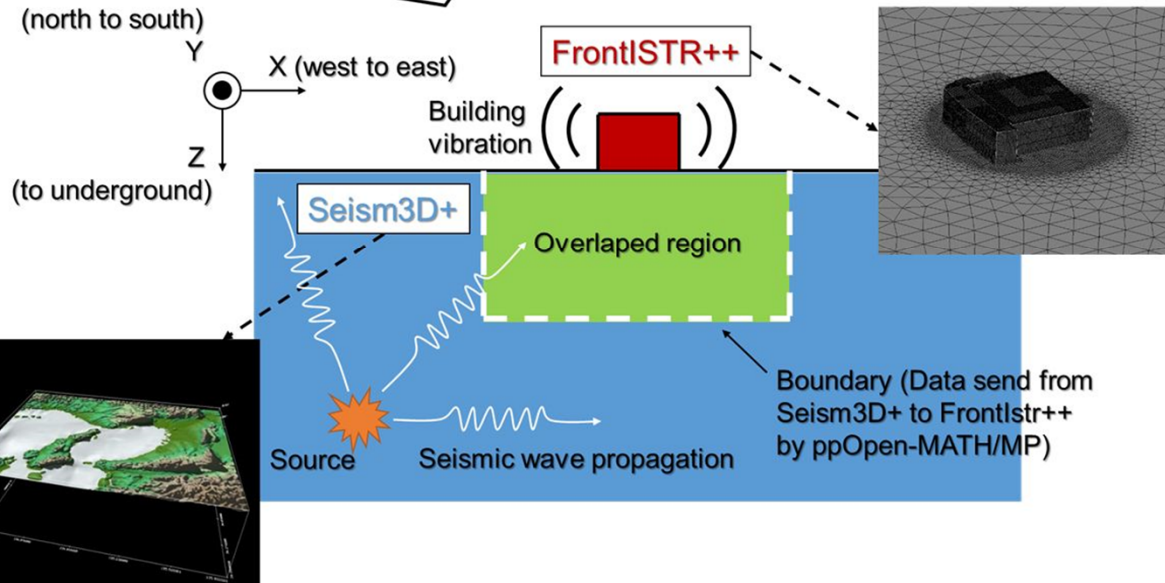
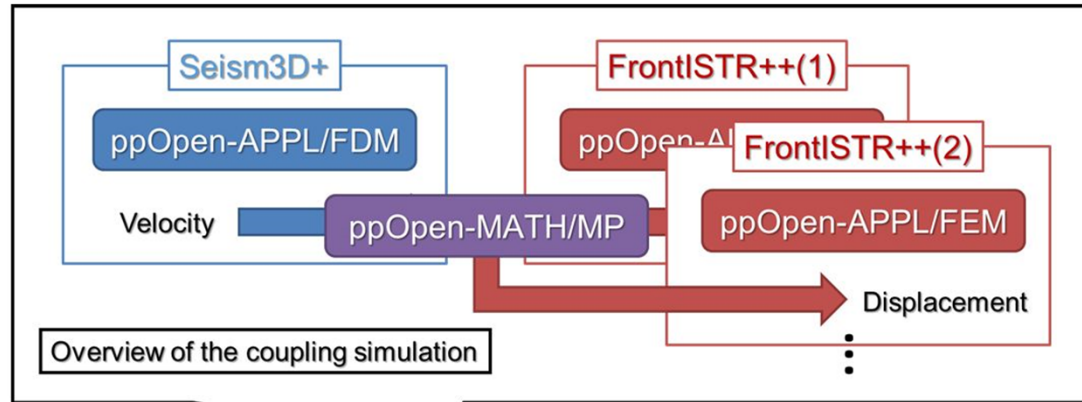
$$\mathbf{M}\ddot{\mathbf{d}} + \mathbf{C}\dot{\mathbf{d}} + \mathbf{K}\mathbf{d} = \mathbf{F}$$

M: mass matrix
C: damping matrix
K: stiffness matrix
F: nodal load vector
d: nodal displacement vector



Computational load: **Seism3D+** < **FrontISTR++**

Implementation of the Coupling Simulation



Unstructured mesh used in **FrontISTR++**
 Colors: MPI process (64 processes)
 (Partitioning by METIS)

Practical Simulation on Oakleaf-FX

The simulation target is the earthquake that occurred at Awaji Island on 13 April, 2013. The computational domain of Seism3D+ is 60 km² from Awaji Island and that of FrontISTR++ is the actual building of RIKEN Advanced Institute for Computational Science (AICS), Port Island, Kobe, modeled by an unstructured mesh.

Seism3D+ Grid Points $(x, y, z) = (1536, 1536, 1600)$
 Parallelization 2560 processes/16 threads

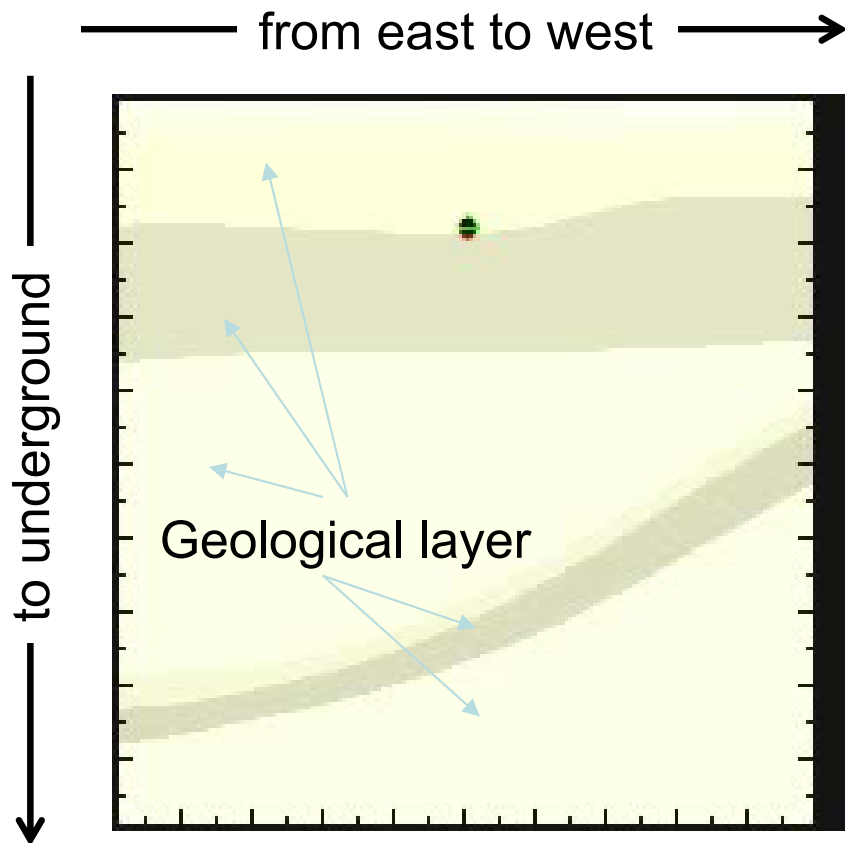
FrontISTR++ Grid Points 600 million (AICS building)
 Parallelization 1000 processes/16 threads
 (@Port Island)
 1000 processes/16 threads
 (@Kobe Stadium)

Total 4560 nodes on Oakleaf-FX
 (Seism3D+: 2560 nodes, FrontISTR++: 2000 nodes)

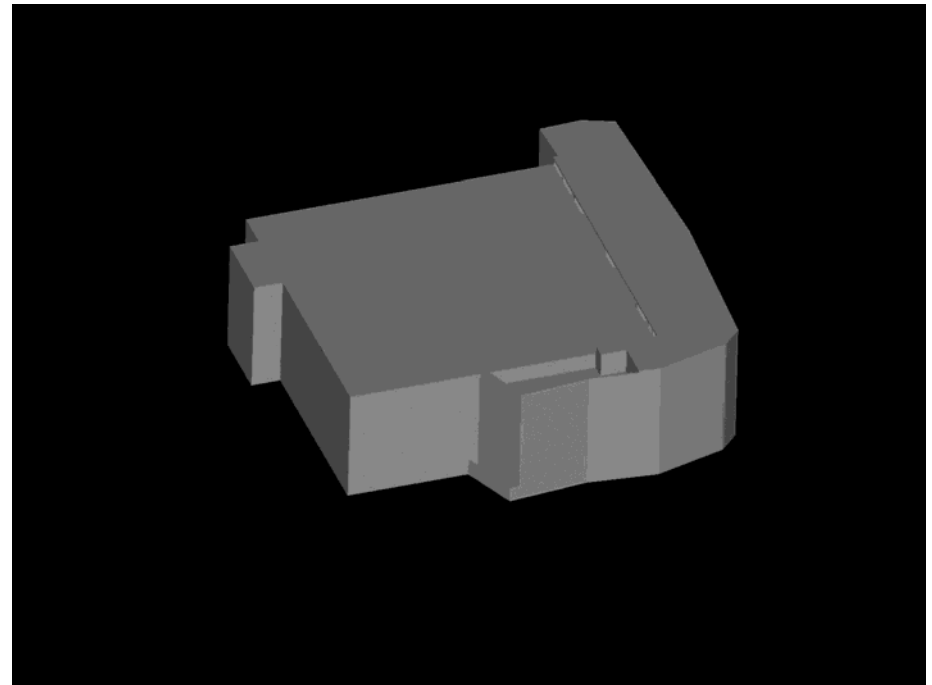


Computational domain
 of Seism3D+

2,560 nodes for FDM, 2,000 nodes for FEM = 4,560 nodes of FX10



Seismic wave propagation by [Seism3D+](#)
(Red: P-wave, Green: S-wave)



Building vibration by [FrontISTR++](#)

2,560 nodes for FDM, 2,000 nodes for FEM = 4,560 nodes of FX10

- ✓ Coupling simulation was executed on large-scale computational resources of Oakleaf-FX supercomputer system.
- ✓ Seismic wave propagations (**Seism3D+**) for the simulation time of 90 sec., and building vibrations (**FrontISTR++**) for the simulation time of 20 sec. were calculated.

Comparison between sim. time and exe. time

	Sim. Time	Exe. Time
Seism3D+	90 sec.	6 hours
FrontISTR++	20 sec.	16 hours

- ✓ It was revealed that the manner in which memory allocation occurs in the coupler has some problem when such a large-scale simulation is performed.

Simulation of Geologic CO₂ Storage

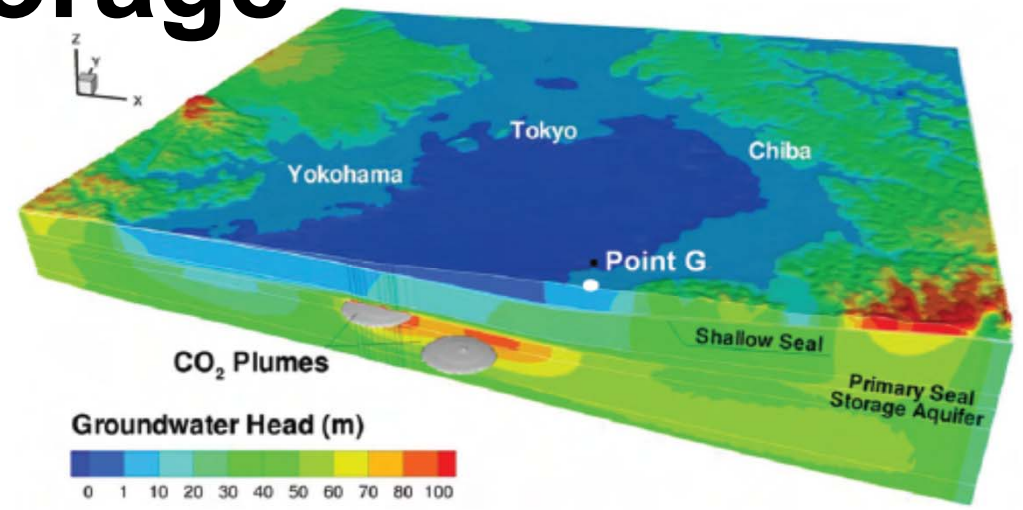
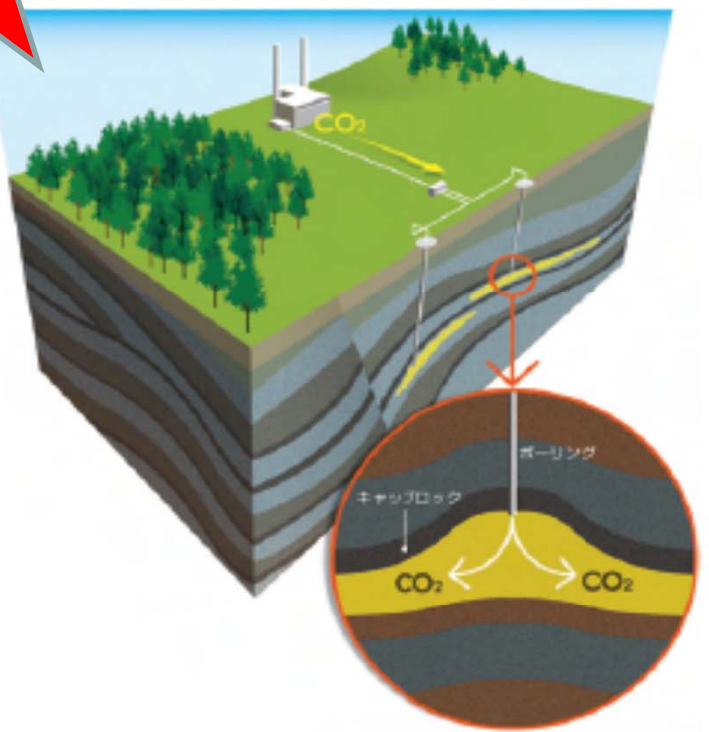
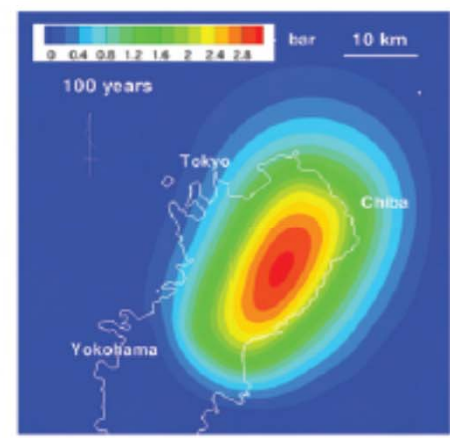
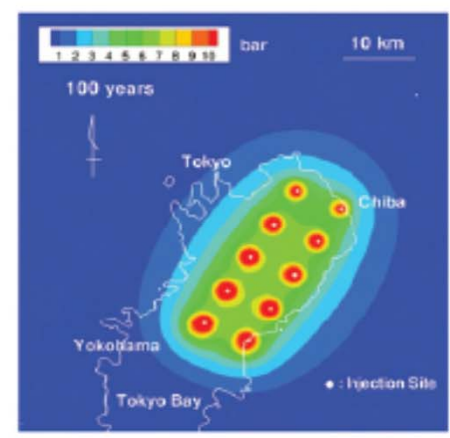
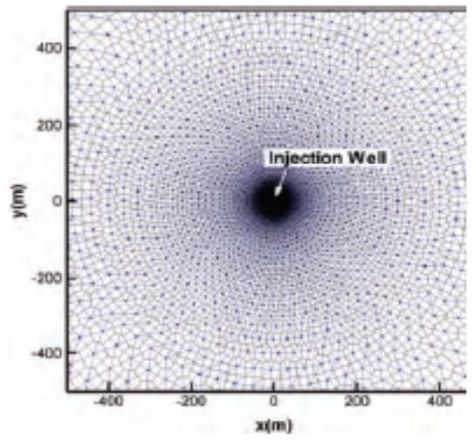
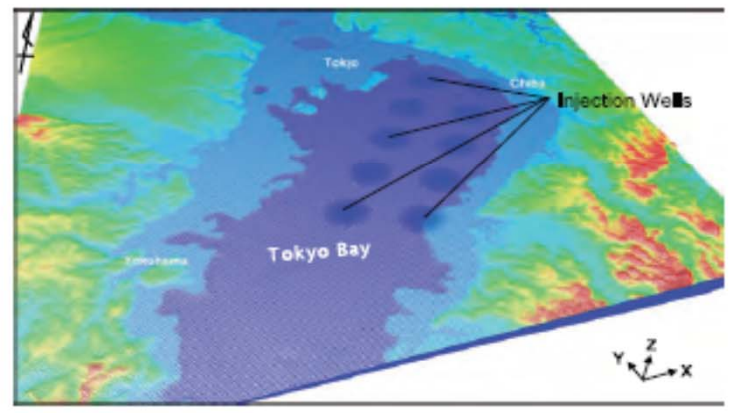


図-4 CO₂ 圧入後の地下水圧 (全水頭換算) の分布 (100 年後)



(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 CO₂ Storage

- International/Interdisciplinary Collaborations
 - Taisei (Science, Modeling)
 - Lawrence Berkeley National Laboratory, USA (Modeling)
 - Information Technology Center, the University of Tokyo (Algorithm, Software)
 - JAMSTEC (Earth Simulator Center) (Software, Hardware)
 - NEC (Software, Hardware)
- 2010 Japan Geotechnical Society (JGS) Award

Science

Modeling

Algorithm

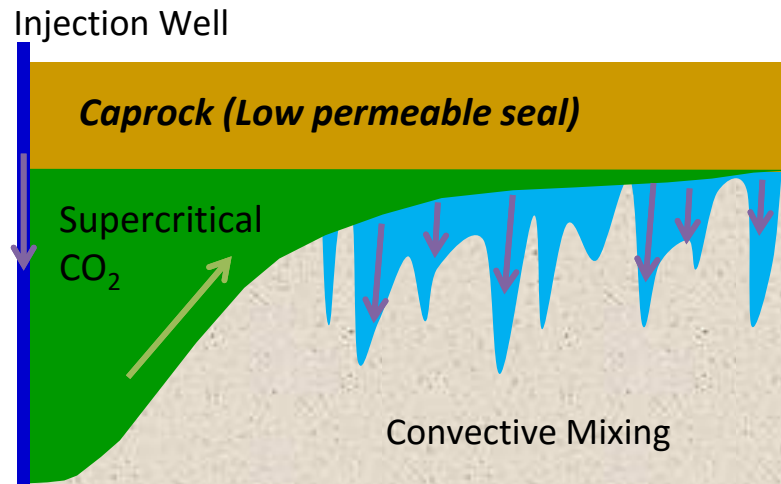
Software

Hardware

Simulation of Geologic CO₂ Storage

- Science
 - Behavior of CO₂ 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)

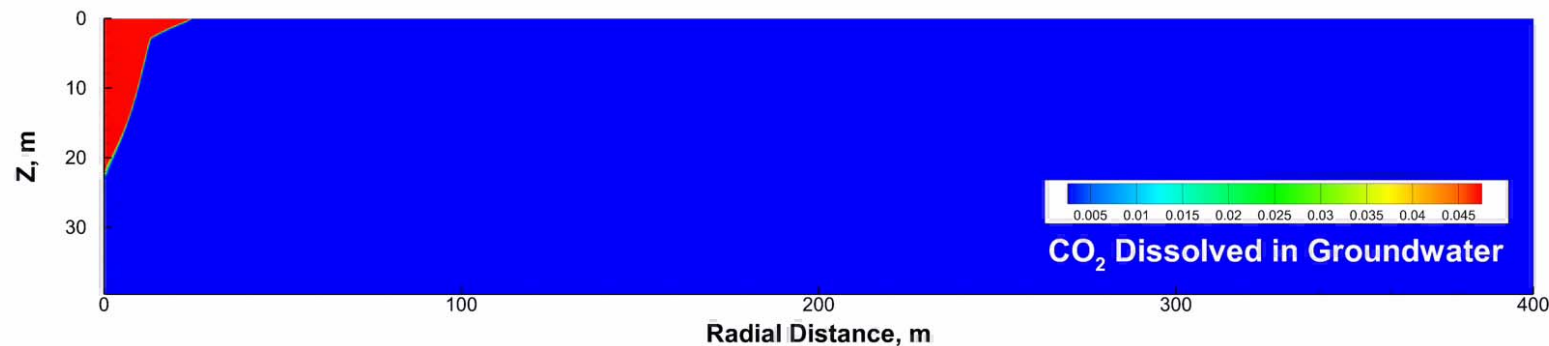
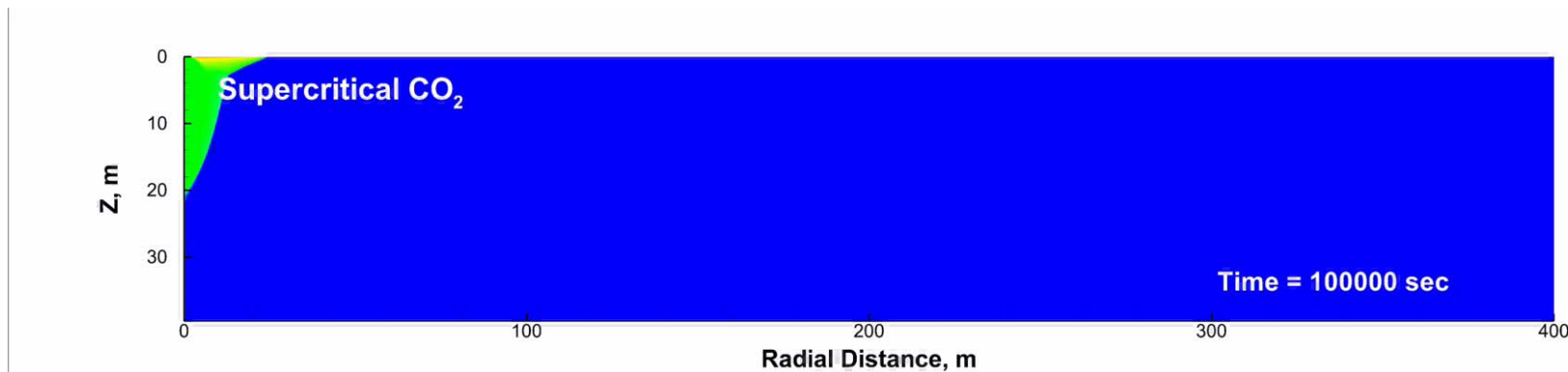
Diffusion-Dissolution-Convection Process

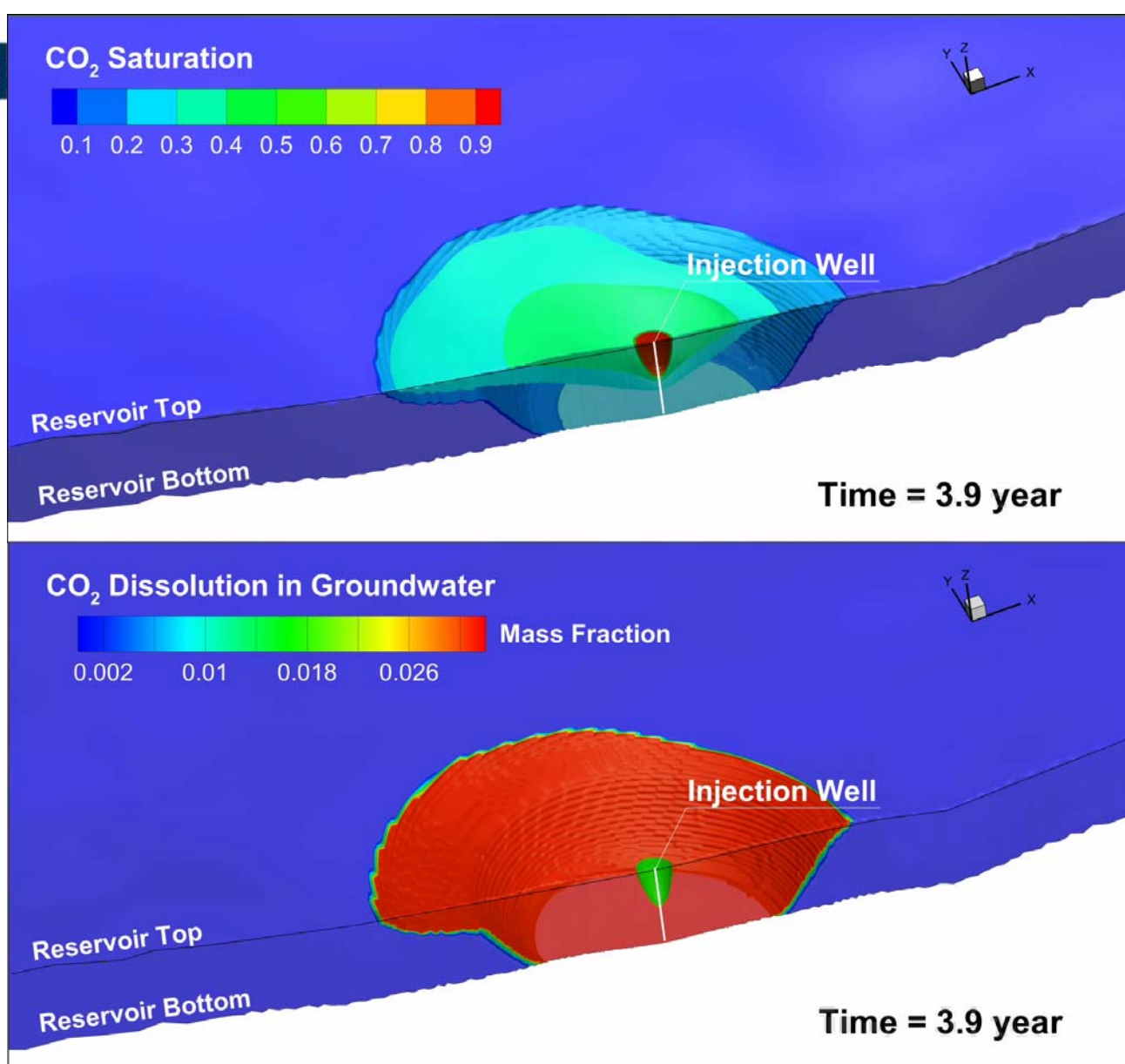


- Buoyant scCO₂ overrides onto groundwater
- Dissolution of CO₂ increases water density
- Denser fluid laid on lighter fluid
- Rayleigh-Taylor instability invokes convective mixing of groundwater

The mixing significantly enhances the CO₂ 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

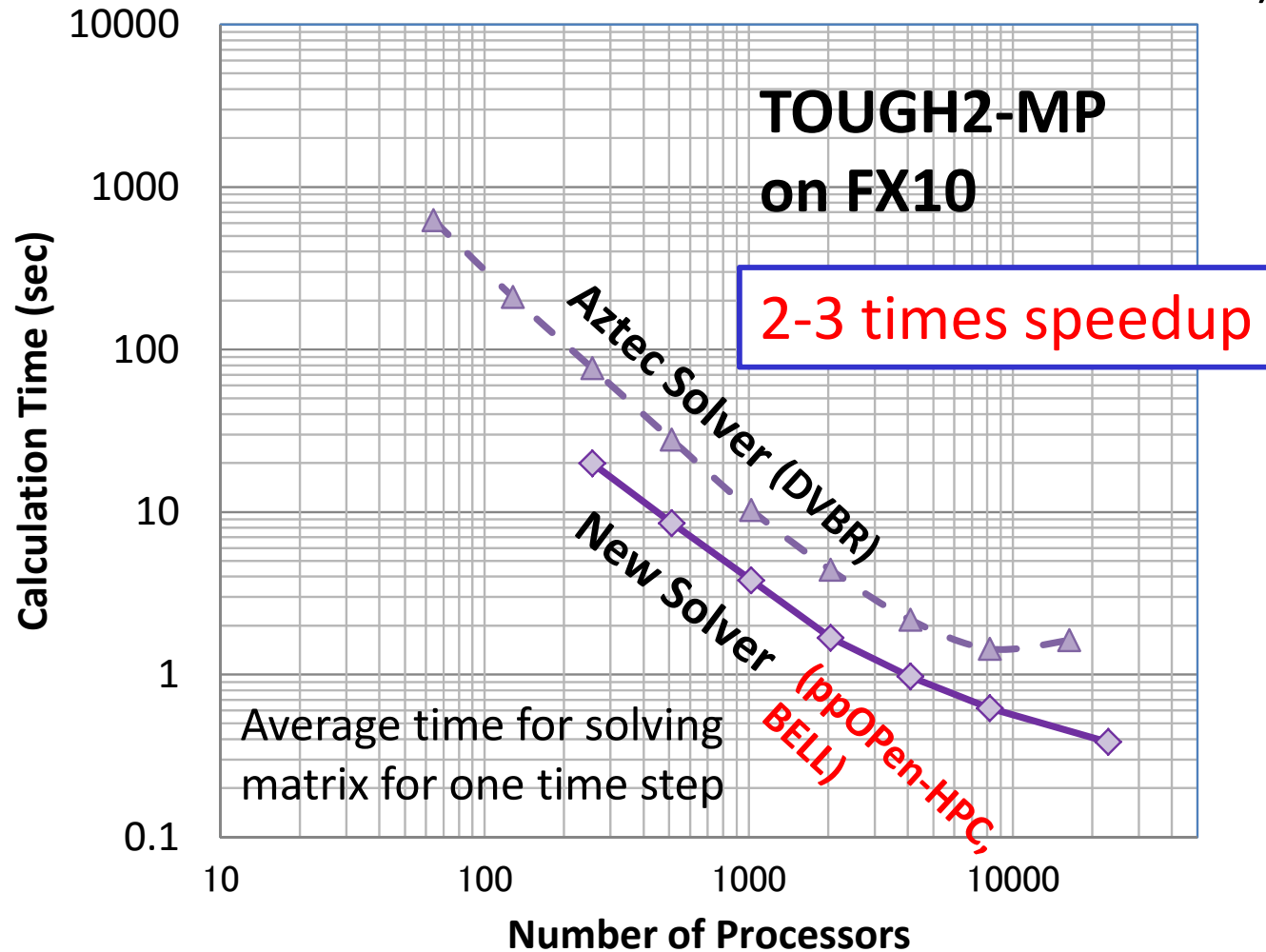
Only the far side of the vertical cross section passing through the injection well is depicted.

[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-yr simulation
- Onset time (10-20 yrs) is comparable to theoretical (linear stability analysis, 15.5yrs)

Simulation of Geologic CO₂ Storage

30 million DoF (10 million grids × 3 DoF/grid node)



**TOUGH2-MP
on FX10**

2-3 times speedup

Average time for solving matrix for one time step

[Dr. Hajime Yamamoto, Taisei]

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

(a) Tokyo Bay Model
–Large scale hydro-geological model–
30 million DoF
Injection Well
Yamamoto et al. (2009) 10km

(b) DDC (Diffusion-Dissolution-Convection)
–Highly non linear process model–
Caprock (Low permeable seal)
Supercritical CO₂
Reservoir
Native Groundwater (Brine)
Local-scale Model
6 million DoF

(c) SPE 10 Model
–Highly heterogeneous reservoir model–
3.3 million DoF
Original Reservoir Model
Producer
Injector
Christie and Blunt (2001)
Qi et al. (2009)
Audigane et al. (2011)
Yamamoto et al. (2013)
CO₂ behavior (No upscaling)
S_{CO2}

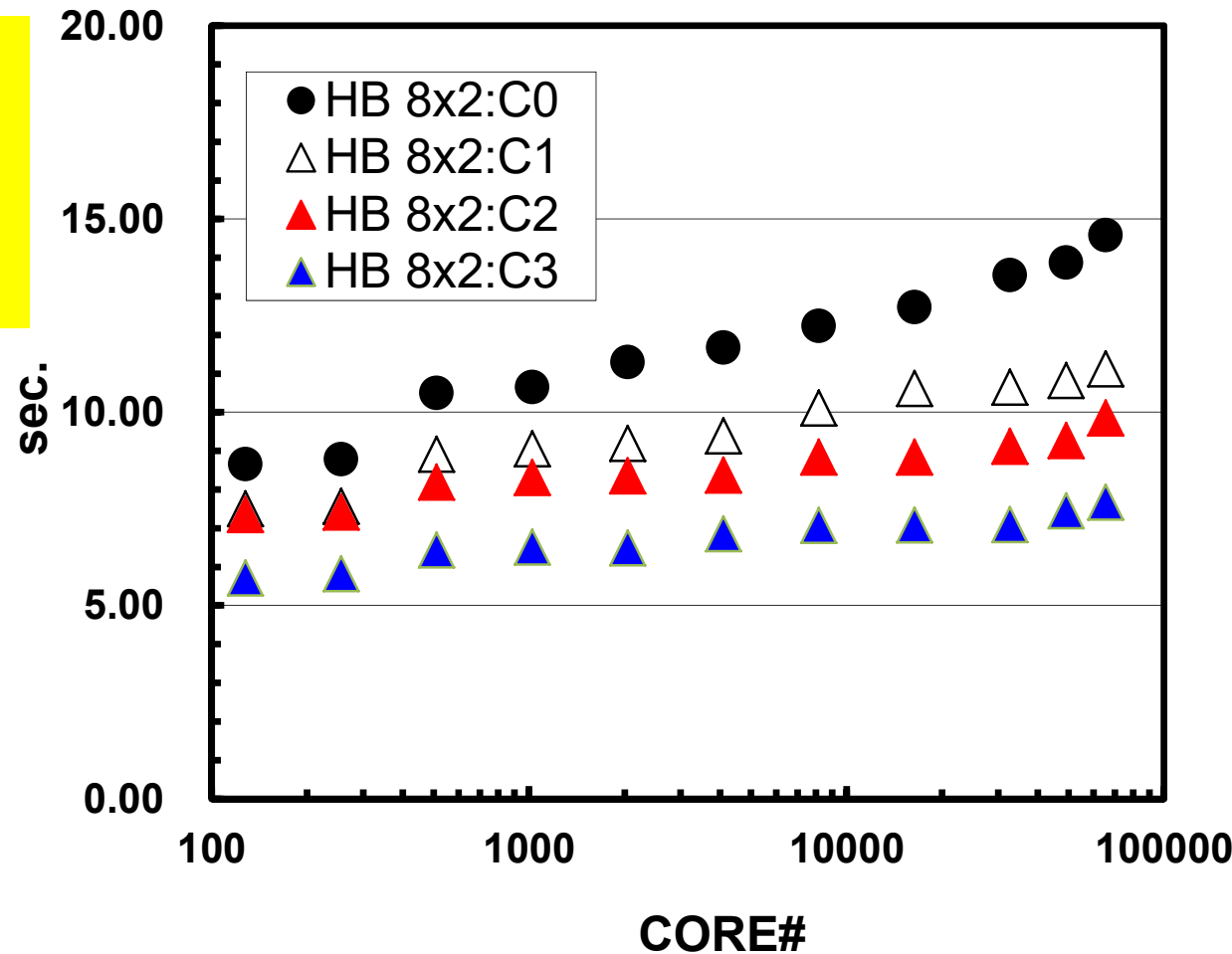
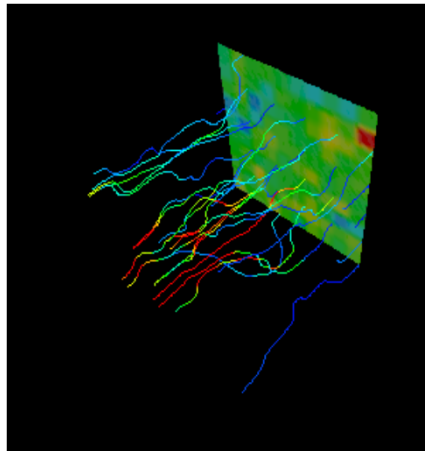
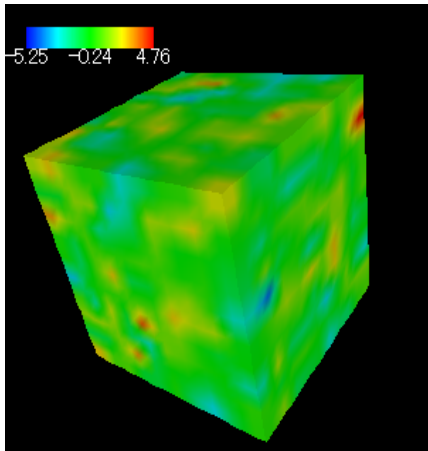
3D Multiphase Flow (Liquid/Gas) + 3D Mass Transfer



3D Ground Water Flow Simulation with up to 4,096 nodes on Fujitsu FX10 (GMG-CG)

up to 17,179,869,184 meshes (64^3 meshes/core)

Linear equations with
17B unknowns can be
solved in 7 sec.



Motivation for Parallel Computing again

- **Large-scale parallel computer enables fast computing in large-scale scientific simulations with detailed models. Computational science develops new frontiers of science and engineering.**
- Why parallel computing ?
 - faster & larger
 - “larger” is more important from the view point of “new frontiers of science & engineering”, but “faster” is also important.
 - + more complicated
 - Ideal: Scalable
 - Solving N^x scale problem using N^x computational resources during same computation time (weak scaling)
 - Solving a fix-sized problem using N^x computational resources in $1/N$ computation time (strong scaling)

- Supercomputers and Computational Science
- **Overview of the Class**

Goal of SC4SC 2017

- **If you want to do something on supercomputers, you have to learn “parallel programming” !!**
- Introduction to MPI & OpenMP
 - MPI: Message Passing Interface
 - “grab” the idea of SPMD (Single-Program Multiple-Data)
 - OpenMP: Multithreading
- Parallel Application
 - **Finite-Volume Method (FVM): We start at this part**
 - Data Structure for Parallel Computing
 - Parallel FVM by OpenMP
 - Parallel FVM by OpenMP/MPI Hybrid

Initial Structure of this Short Course

Feb. 21 (T)	Part-I (Katagiri): Introduction to OpenMP & MPI
Feb. 22 (W)	
Feb. 23 (Th)	Part-II (Nakajima): Parallel FVM
Feb. 24 (F)	

New Structure of this Short Course

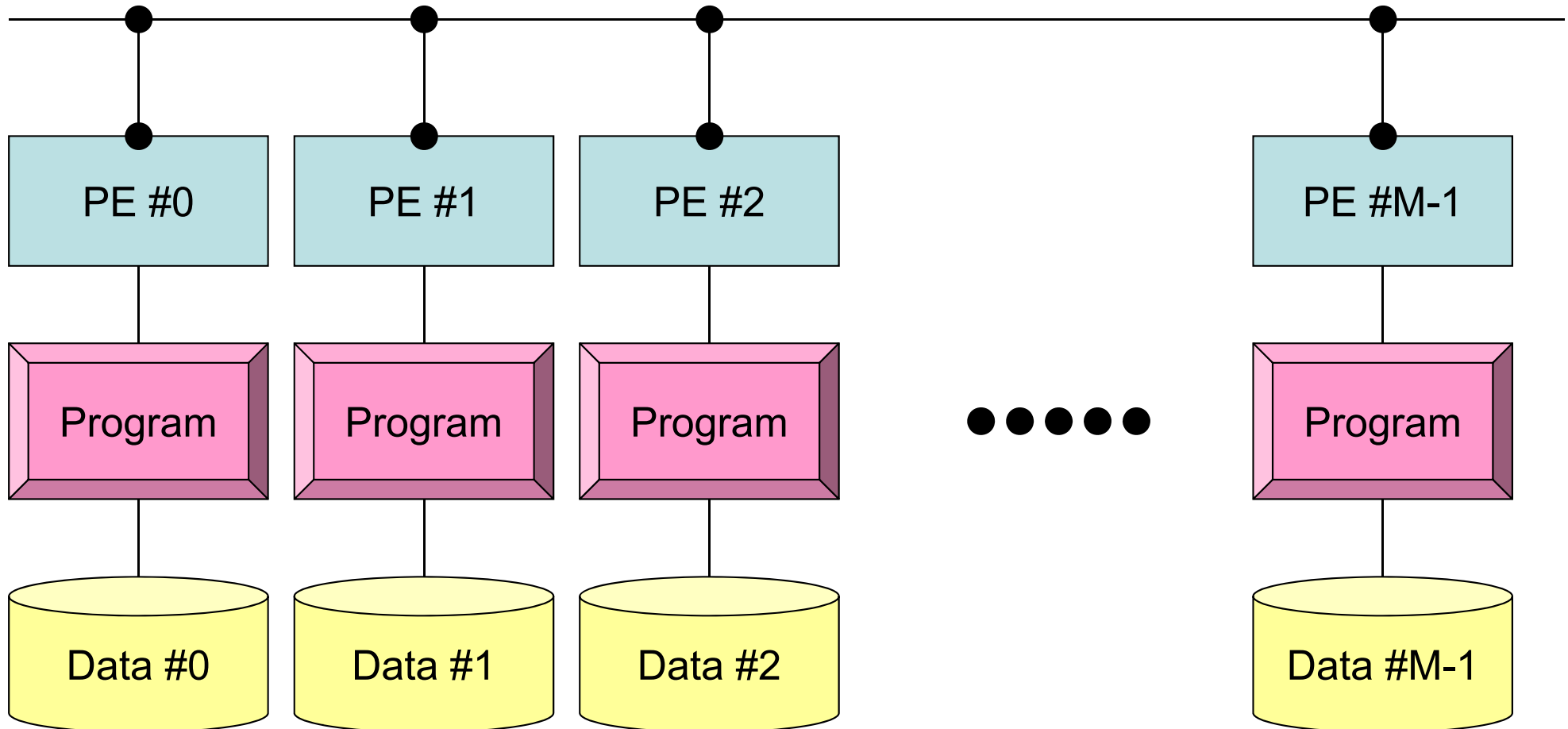
Feb. 21 (T)	Part-II-1 (Nakajima): Introduction to FVM
Feb. 22 (W)	Part-I (Katagiri): Introduction to OpenMP & MPI
Feb. 23 (Th)	
Feb. 24 (F)	Part-II-2 (Nakajima): Parallel FVM FX10 Supercomputer is not available on Feb.24

PE: Processing Element
Processor, Domain, Process

SPMD

You understand 90% MPI, if
you understand this figure.

```
mpirun -np M <Program>
```



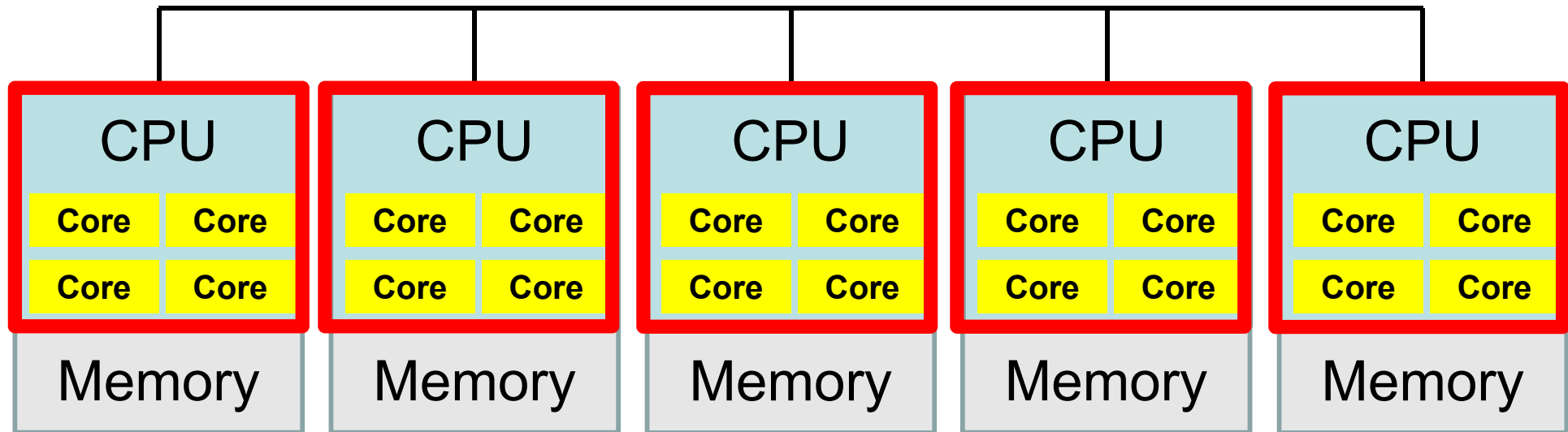
Each process does same operation for different data

Large-scale data is decomposed, and each part is computed by each process

It is ideal that parallel program is not different from serial one except communication.

Our Current Target: Multicore Cluster

Multicore CPU's are connected through network



- OpenMP

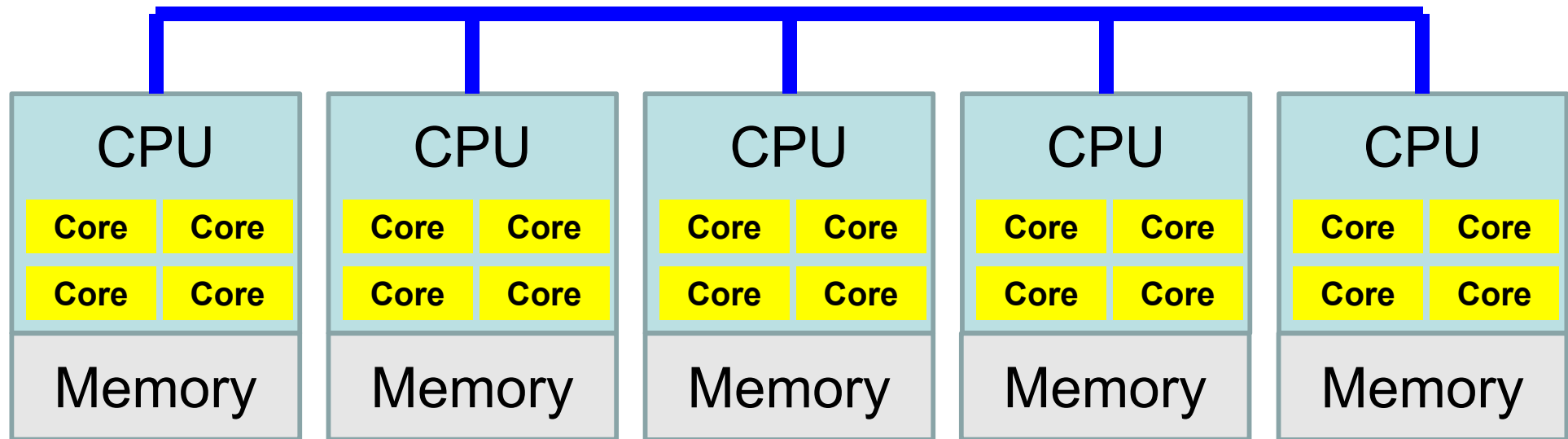
- ✓ Multithreading
- ✓ Intra Node (Intra CPU)
- ✓ Shared Memory

- MPI

- ✓ Message Passing
- ✓ Inter Node (Inter CPU)
- ✓ Distributed Memory

Our Current Target: Multicore Cluster

Multicore CPU's are connected through network

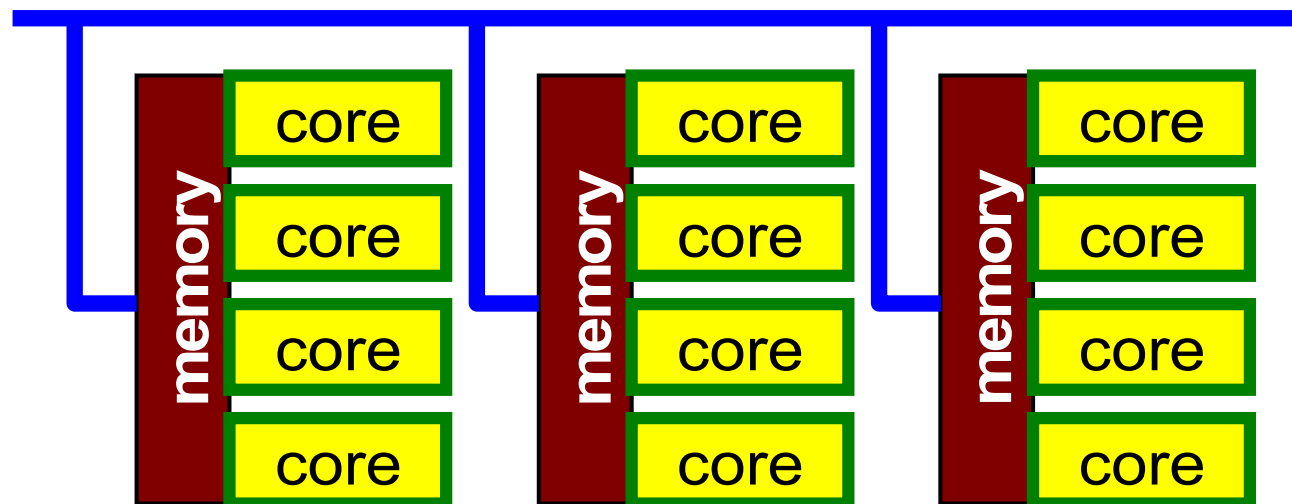


- OpenMP
 - ✓ Multithreading
 - ✓ Intra Node (Intra CPU)
 - ✓ Shared Memory
- MPI
 - ✓ Message Passing
 - ✓ Inter Node (Inter CPU)
 - ✓ Distributed Memory

Flat MPI vs. Hybrid

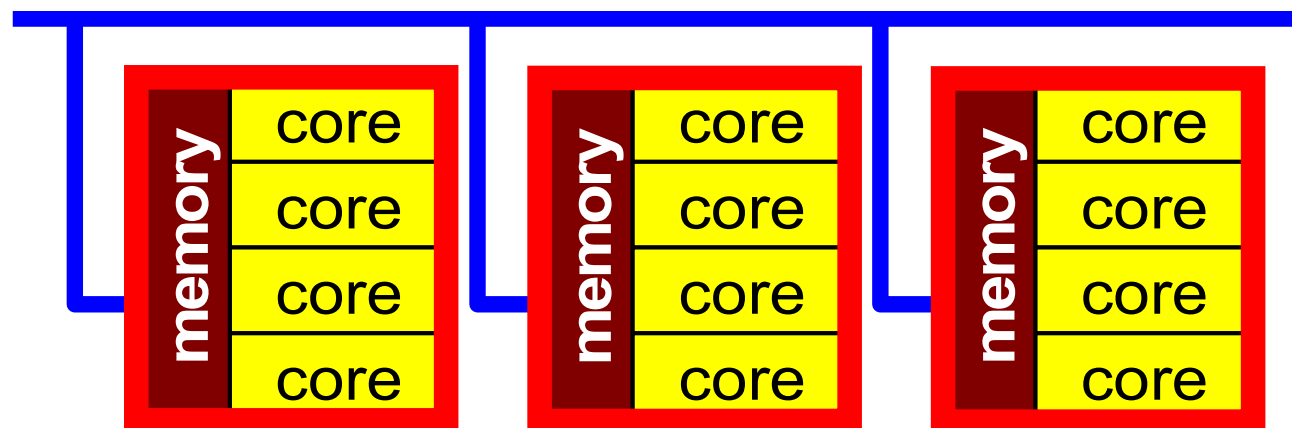
Flat-MPI: Each Core -> Independent

- MPI only
- Intra/Inter Node



Hybrid: Hierarchical Structure

- OpenMP
- MPI



Example of OpenMP/MPI Hybrid

Sending Messages to Neighboring Processes

MPI: Message Passing, OpenMP: Threading with Directives

```
!C
!C- SEND

      do neib= 1, NEIBPETOT
        II= (LEVEL-1)*NEIBPETOT
        istart= STACK_EXPORT(II+neib-1)
        inum  = STACK_EXPORT(II+neib  ) - istart
!$omp parallel do
      do k= istart+1, istart+inum
        WS(k-NE0)= X(NOD_EXPORT(k))
      enddo

      call MPI_Isend (WS(istart+1-NE0), inum, MPI_DOUBLE_PRECISION,   &
&                   NEIBPE(neib), 0, MPI_COMM_WORLD,               &
&                   req1(neib), ierr)
      enddo
```

Prerequisites

- Experiences in Unix/Linux
- Experiences of programming (Fortran or C/C++)
- Fundamental numerical algorithms (Gaussian Elimination, LU Factorization, Jacobi/Gauss-Seidel/SOR Iterative Solvers)
- Experiences in SSH Public Key Authentication Method

Preparation

- Windows
 - Cygwin: Please install gcc (C) or gfortran (Fortran) and SSH !!
 - ParaView
- MacOS, UNIX/Linux
 - ParaView
- Cygwin: <https://www.cygwin.com/>
- ParaView: <http://www.paraview.org/>