Introduction
Overview of the Class

Kengo Nakajima
Information Technology Center

Programming for Parallel Computing (616-2057)
Seminar on Advanced Computing (616-4009)

- Target: Parallel FEM
- Supercomputers and Computational Science
- Overview of the Class
- Future Issues

Programming for Parallel Computing Seminar on Advanced Computing
並列計算プログラミング・先端計算機演習

- Instructor
  - Kengo Nakajima
  - Professor, Information Technology Center, The University of Tokyo
- Topics
  - Finite-Element Method (FEM)
  - Parallel FEM using MPI
  - Multicore Programming for FVM code (Finite-Volume Method) using OpenMP

This 10-day intensive class provides introduction to large-scale scientific computing using the most advanced massively parallel supercomputers. Topics cover:

- Finite-Element Method (FEM)
- Message Passing Interface (MPI)
- Parallel FEM using MPI
- Parallel Numerical Algorithms for Iterative Linear Solvers
- Programming for Multicore Architectures using OpenMP

Several sample programs will be provided and participants can review the contents of lectures through hands-on-exercise/practices using Fujitsu PRIMEHPC FX10 at the University of Tokyo (Oakleaf-FX).

Finite-Element Method is widely-used for solving various types of real-world scientific and engineering problems, such as structural analysis, fluid dynamics, electromagnetics, and etc. This lecture course provides brief introduction to procedures of FEM for 1D/3D steady-state heat conduction problems with iterative linear solvers and to parallel FEM. **Lectures for parallel FEM will be focused on design of data structure for distributed local mesh files, which is the key issue for efficient parallel FEM.** Introduction to MPI (Message Passing Interface), which is widely used method as "de facto standard" of parallel programming, is also provided.

Solving large-scale linear equations with sparse coefficient matrices is the most expensive and important part of FEM and other methods for scientific computing, such as Finite-Difference Method (FDM) and Finite-Volume Method (FVM). Recently, families of Krylov iterative solvers are widely used for this process. In this class, details of implementations of parallel Krylov iterative methods are provided along with parallel FEM.

Moreover, lectures on programming for multicore architectures will be also given along with brief introduction to OpenMP.

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.

Kengo Nakajima (1/2)

- Current Position
  - Professor, Supercomputing Research Division, Information Technology Center　情報基盤センター
  - Professor, Department of Mathematical Informatics, Graduate School of Information Science & Engineering　数理情報学専攻
  - Visiting Senior Researcher, Advanced Institute for Computational Science (AICS), RIKEN
- Research Interest
  - High-Performance Computing
  - Parallel Numerical Linear Algebra (Preconditioning)
  - Parallel Programming Model
  - Computational Mechanics, Computational Fluid Dynamics
  - Adaptive Mesh Refinement, Parallel Visualization

Kengo Nakajima (2/2)

- Education
  - B.Eng (Aeronautics, The University of Tokyo, 1985)
  - M.S. (Aerospace Engineering, University of Texas, 1993)
  - Ph.D. (Quantum Engineering & System Sciences, The University of Tokyo, 2003)
- Professional Background
  - Mitsubishi Research Institute, Inc. (1985-1999)
  - Research Organization for Information Science & Technology (1999-2004)
  - The University of Tokyo
    - Department Earth & Planetary Science (2004-2008)
    - Information Technology Center (2008-)
  - JAMSTEC (2008-2011), part-time
  - RIKEN (2009-), part-time

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): Your Department ?

This Class ...

Science

Modeling

Algorithm

Software

Hardware

- Parallel FEM using MPI

- Science: Heat Conduction
- Modeling: FEM
- Algorithm: Iterative Solvers etc.

- You have to know many components to learn FEM, although you have already learned each of these in undergraduate and high-school classes.

Road to Programming for "Parallel" Scientific Computing

Programming for Parallel Scientific Computing (e.g. Parallel FEM/FDM)

Programming for Real World Scientific Computing (e.g. FEM, FDM)

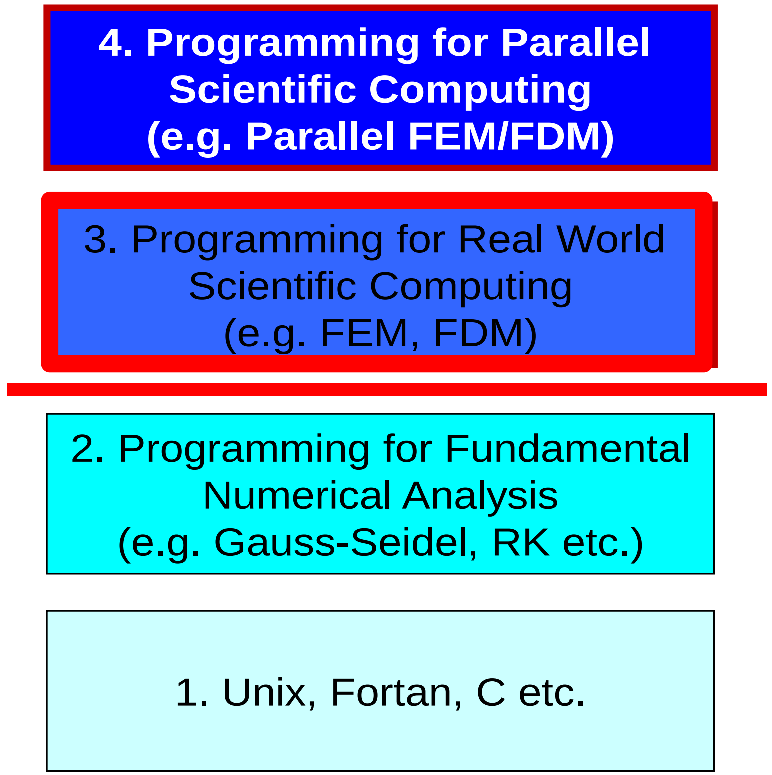
<u>Big gap here !!</u>

Programming for Fundamental Numerical Analysis (e.g. Gauss-Seidel, RK etc.)

Unix, Fortan, C etc.

The third step is important !

- How to parallelize applications ?
  - How to extract parallelism ?
  - If you understand methods, algorithms, and implementations of the original code, it's easy.
  - "Data-structure" is important



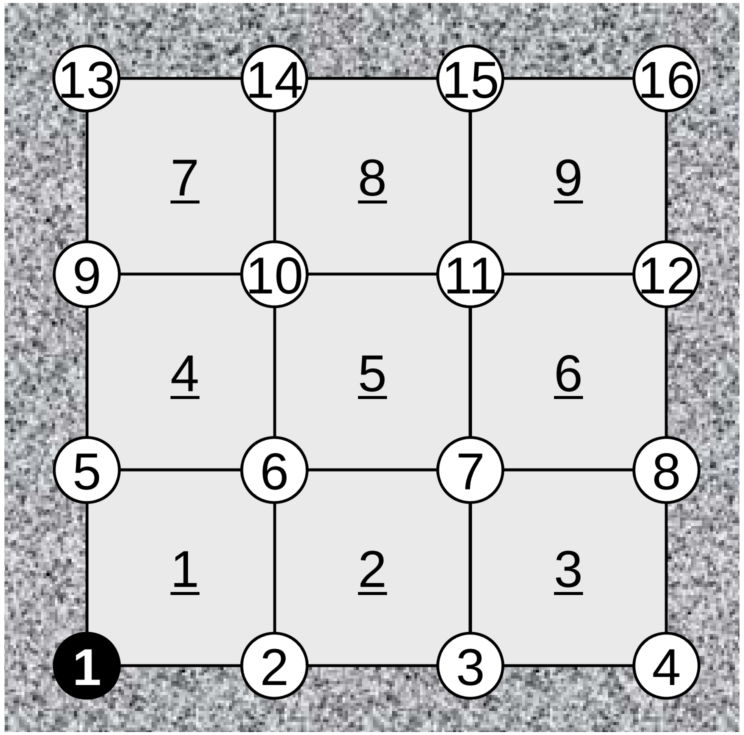
- How to understand the code ?
  - Reading the application code !!
  - It seems primitive, but very effective.
  - In this class, "reading the source code" is encouraged.

Finite-Element Method (FEM)

- One of the most popular numerical methods for solving PDE's.
  - elements (meshes) & nodes (vertices)
- Consider the following 2D heat transfer problem:

$$\lambda\left(\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}\right)+Q=0$$

  - 16 nodes, 9 bi-linear elements
  - uniform thermal conductivity (λ=1)
  - uniform volume heat flux (Q=1)
  - T=0 at node 1
  - Insulated boundaries



Galerkin FEM procedures

- Apply Galerkin procedures to each element:

$$\int_V [N]^T \left\{ \lambda \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) + Q \right\} dV = 0$$

where $T = [N]\{\phi\}$ in each elem.

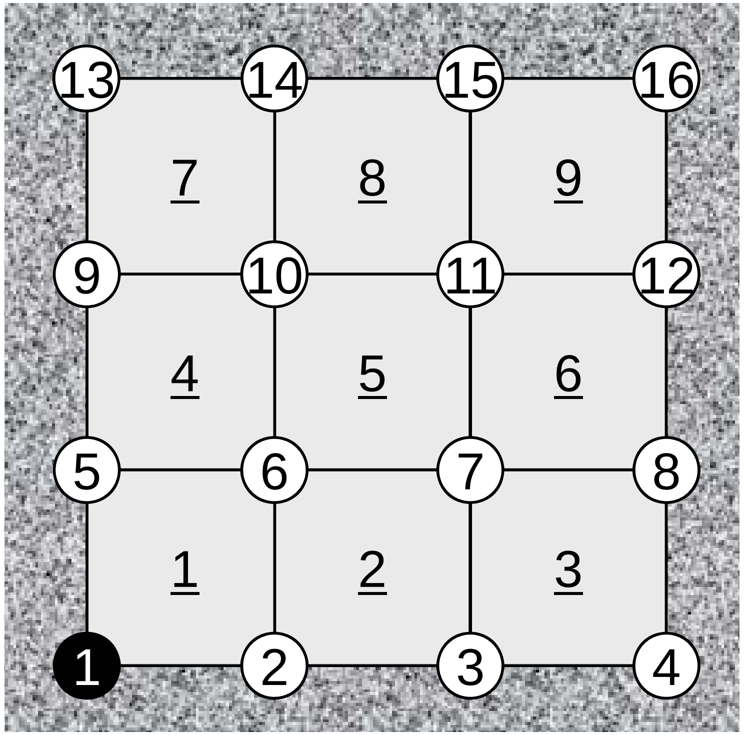
$\{\phi\}$: T at each vertex

$[N]$: Shape function (Interpolation function)

- Introduce the following “weak form” of original PDE using Green’s theorem:

$$-\int_V \lambda \left(\frac{\partial [N]^T}{\partial x} \frac{\partial [N]}{\partial x} + \frac{\partial [N]^T}{\partial y} \frac{\partial [N]}{\partial y} \right) dV \cdot \{\phi\}$$

$$+ \int_V Q [N]^T dV = 0$$

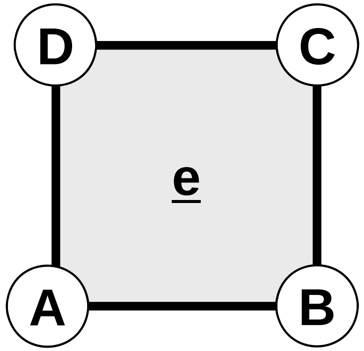


Element Matrix

- Apply the integration to each element and form "element" matrix.

$$-\int_V \lambda \left(\frac{\partial [N]^T}{\partial x} \frac{\partial [N]}{\partial x} + \frac{\partial [N]^T}{\partial y} \frac{\partial [N]}{\partial y} \right) dV \cdot \{\phi\}$$

$$+\int_V Q [N]^T dV = 0$$

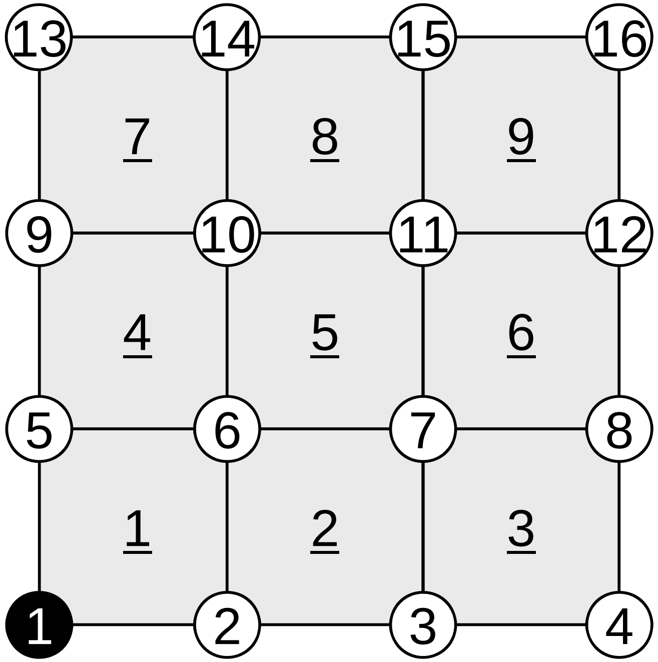


$$[k^{(e)}]\{\phi^{(e)}\} = \{f^{(e)}\}$$

$$\begin{bmatrix} k_{AA}^{(e)} & k_{AB}^{(e)} & k_{AC}^{(e)} & k_{AD}^{(e)} \\ k_{BA}^{(e)} & k_{BB}^{(e)} & k_{BC}^{(e)} & k_{BD}^{(e)} \\ k_{CA}^{(e)} & k_{CB}^{(e)} & k_{CC}^{(e)} & k_{CD}^{(e)} \\ k_{DA}^{(e)} & k_{DB}^{(e)} & k_{DC}^{(e)} & k_{DD}^{(e)} \end{bmatrix} \begin{Bmatrix} \phi_A^{(e)} \\ \phi_B^{(e)} \\ \phi_C^{(e)} \\ \phi_D^{(e)} \end{Bmatrix} = \begin{Bmatrix} f_A^{(e)} \\ f_B^{(e)} \\ f_C^{(e)} \\ f_D^{(e)} \end{Bmatrix}$$

Global (Overall) Matrix

Accumulate each element matrix to “global” matrix.



$$[K]\{\Phi\}=\{F\}$$

$$\begin{bmatrix}
D & X & & & X & X & & & & & & & & & & \\
X & D & X & & X & X & X & & & & & & & & & \\
 & X & D & X & & X & X & X & & & & & & & & \\
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X & X & & & D & X & & & X & X & & & & & & \\
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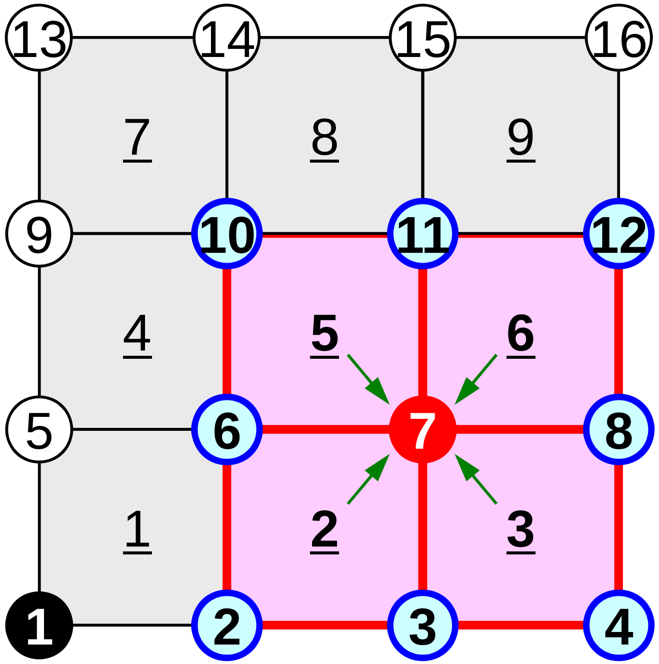
\end{bmatrix}
\begin{Bmatrix}
\Phi_1 \\ \Phi_2 \\ \Phi_3 \\ \Phi_4 \\ \Phi_5 \\ \Phi_6 \\ \Phi_7 \\ \Phi_8 \\ \Phi_9 \\ \Phi_{10} \\ \Phi_{11} \\ \Phi_{12} \\ \Phi_{13} \\ \Phi_{14} \\ \Phi_{15} \\ \Phi_{16}
\end{Bmatrix}
=
\begin{Bmatrix}
F_1 \\ F_2 \\ F_3 \\ F_4 \\ F_5 \\ F_6 \\ F_7 \\ F_8 \\ F_9 \\ F_{10} \\ F_{11} \\ F_{12} \\ F_{13} \\ F_{14} \\ F_{15} \\ F_{16}
\end{Bmatrix}$$

To each node …

Effect of surrounding elem's/nodes are accumulated.



$$[K]\{\Phi\}=\{F\}$$

$$\left[\begin{array}{cccccccccccccccc}
D & X & & & X & X & & & & & & & & & & \\
X & D & X & & X & X & X & & & & & & & & & \\
& X & D & X & & X & X & X & & & & & & & & \\
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X & X & & & D & X & & & X & X & & & & & & \\
X & X & X & & X & D & X & & X & X & X & & & & & \\
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\end{array}\right]
\left\{\begin{array}{c}
\Phi_1 \\ \Phi_2 \\ \Phi_3 \\ \Phi_4 \\ \Phi_5 \\ \Phi_6 \\ \Phi_7 \\ \Phi_8 \\ \Phi_9 \\ \Phi_{10} \\ \Phi_{11} \\ \Phi_{12} \\ \Phi_{13} \\ \Phi_{14} \\ \Phi_{15} \\ \Phi_{16}
\end{array}\right\}
=
\left\{\begin{array}{c}
F_1 \\ F_2 \\ F_3 \\ F_4 \\ F_5 \\ F_6 \\ F_7 \\ F_8 \\ F_9 \\ F_{10} \\ F_{11} \\ F_{12} \\ F_{13} \\ F_{14} \\ F_{15} \\ F_{16}
\end{array}\right\}$$

Solve the obtained global eqn's

under certain boundary conditions (Φ_1=0 in this case)

$$
\begin{bmatrix}
D & X & & & X & X & & & & & & & & & & \\
X & D & X & & X & X & X & & & & & & & & & \\
& X & D & X & & X & X & X & & & & & & & & \\
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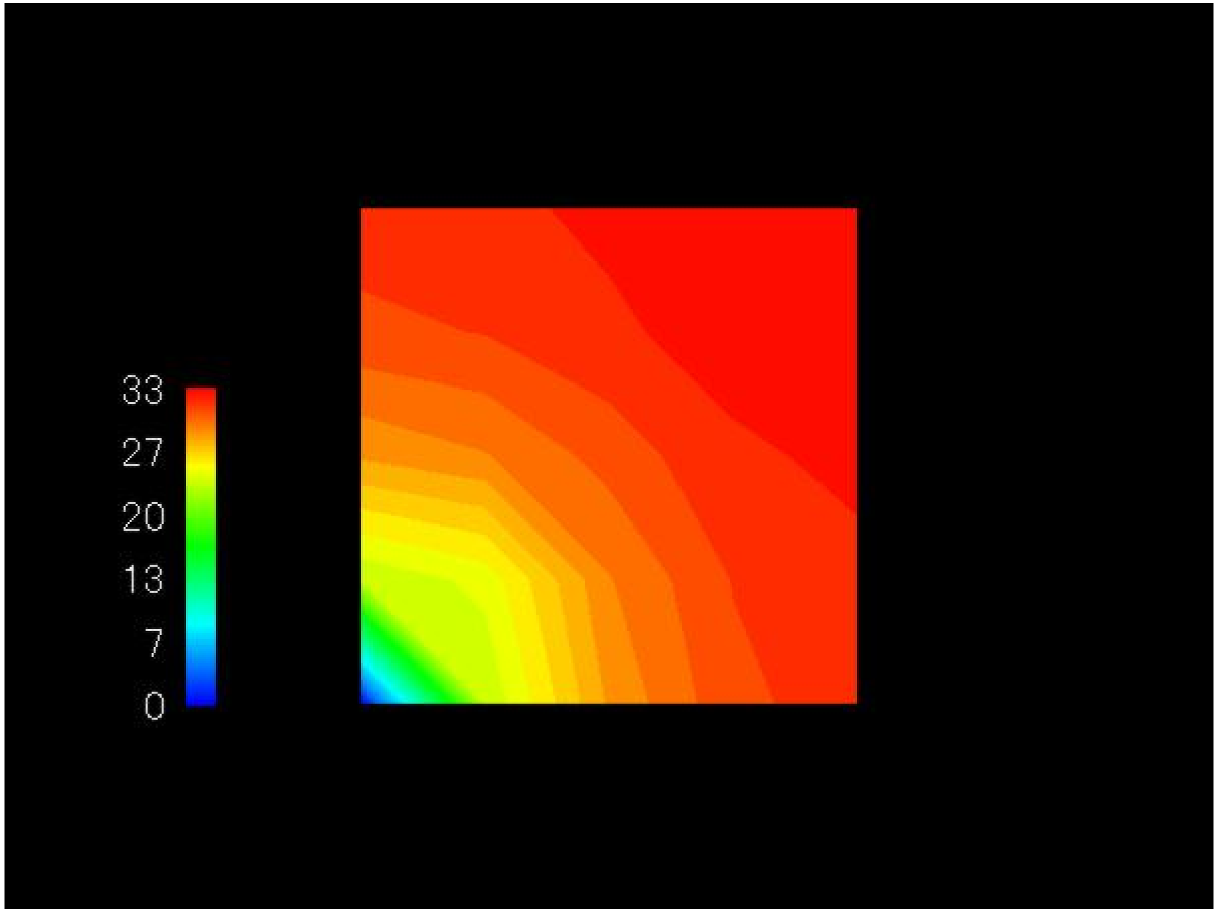
\end{bmatrix}
\begin{Bmatrix}
\Phi_1 \\ \Phi_2 \\ \Phi_3 \\ \Phi_4 \\ \Phi_5 \\ \Phi_6 \\ \Phi_7 \\ \Phi_8 \\ \Phi_9 \\ \Phi_{10} \\ \Phi_{11} \\ \Phi_{12} \\ \Phi_{13} \\ \Phi_{14} \\ \Phi_{15} \\ \Phi_{16}
\end{Bmatrix}
=
\begin{Bmatrix}
F_1 \\ F_2 \\ F_3 \\ F_4 \\ F_5 \\ F_6 \\ F_7 \\ F_8 \\ F_9 \\ F_{10} \\ F_{11} \\ F_{12} \\ F_{13} \\ F_{14} \\ F_{15} \\ F_{16}
\end{Bmatrix}
$$

Result …

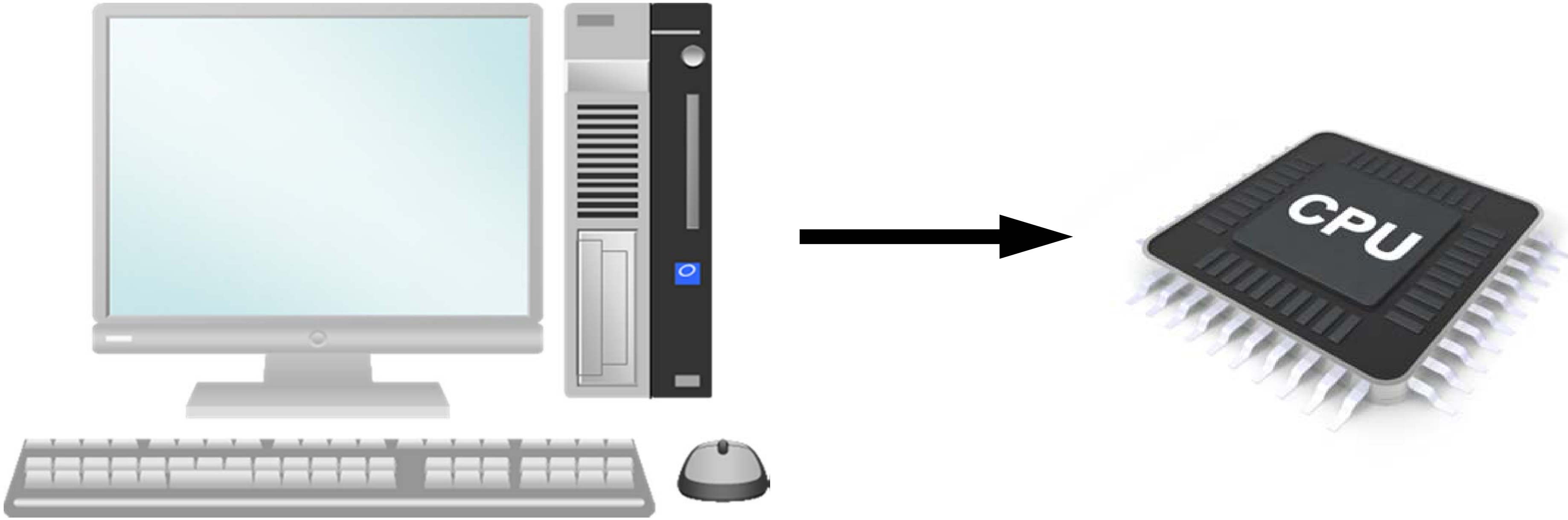


Features of FEM applications

- Typical Procedures for FEM Computations
  - Input/Output
  - Matrix Assembling
  - Linear Solvers for Large-scale Sparse Matrices
  - Most of the computation time is spent for matrix assembling/formation and solving linear equations.
- **HUGE** “indirect” accesses
  - memory intensive
- Local “element-by-element” operations
  - sparse coefficient matrices
  - suitable for parallel computing
- Excellent modularity of each procedure

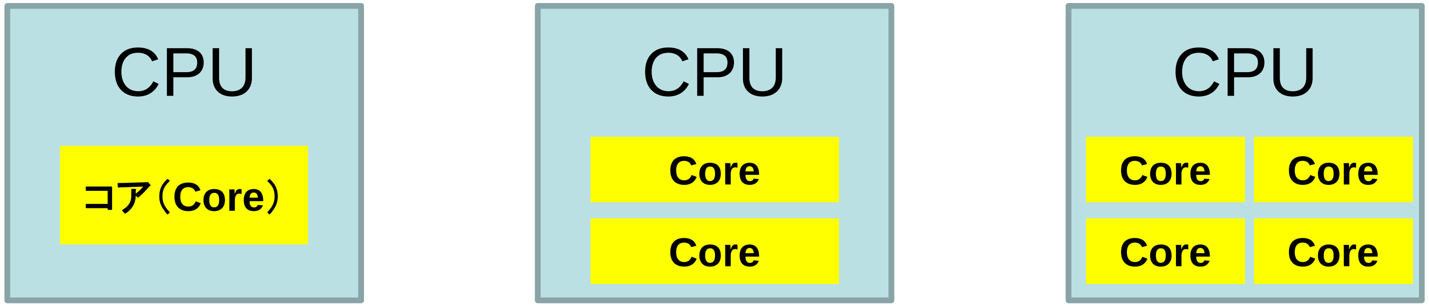
- Target: Parallel FEM
- **Supercomputers and Computational Science**
- Overview of the Class
- Future Issues

Computer & CPU



- Central Processing Unit（中央処理装置）：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

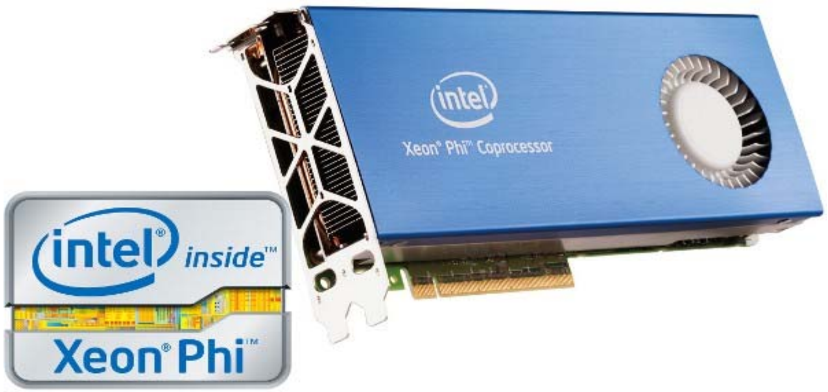
Quad Core
4 cores/CPU

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

- 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

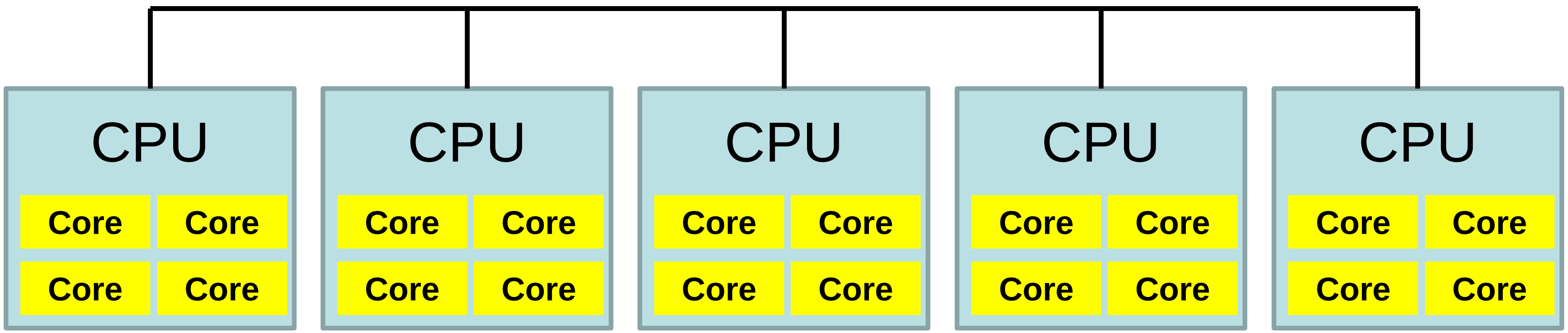
GPU/Manycores

- 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 will be possible soon

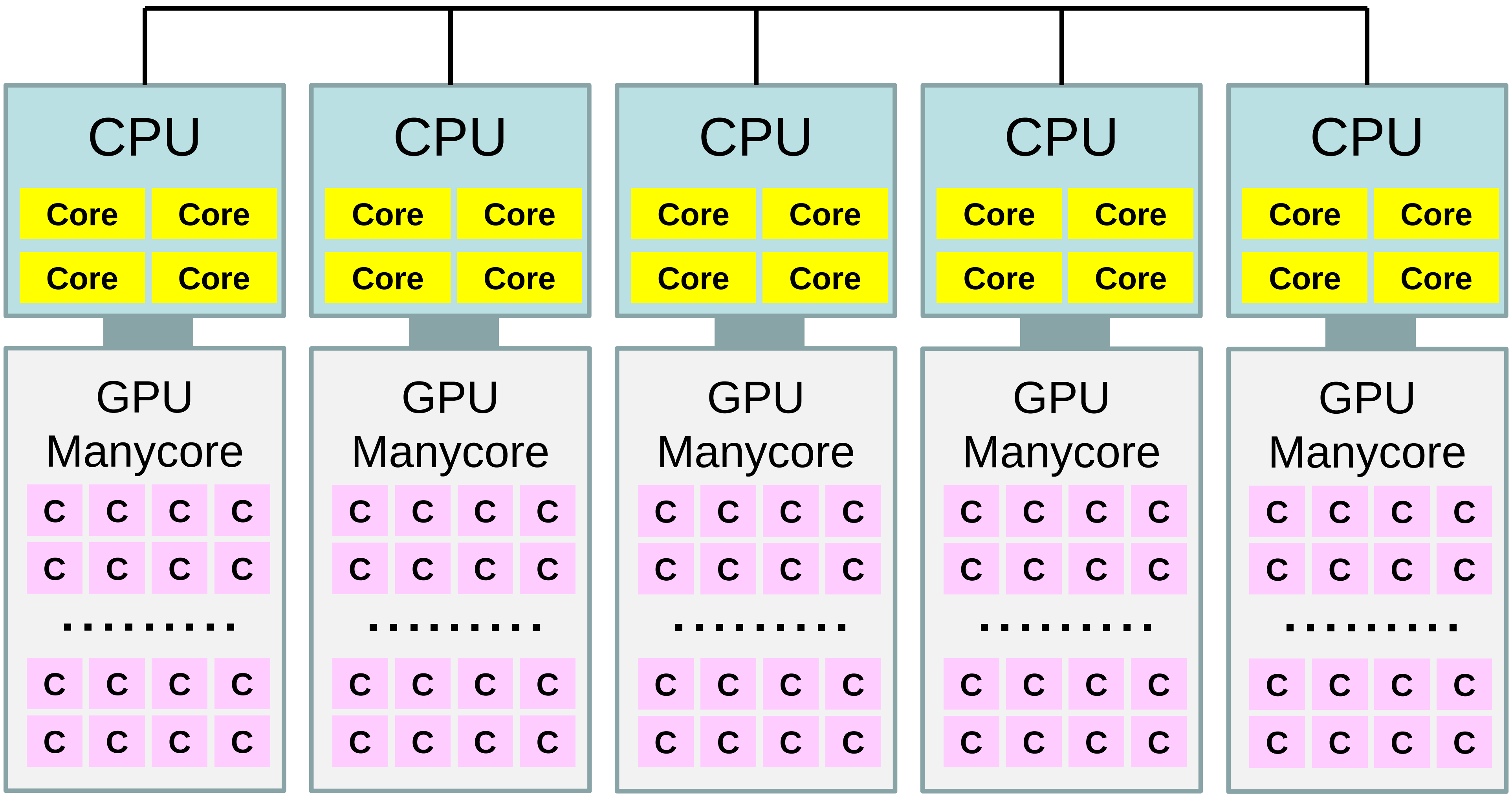


Parallel Supercomputers

Multicore CPU’s are connected through network



Supercomputers with Heterogeneous/Hybrid Nodes



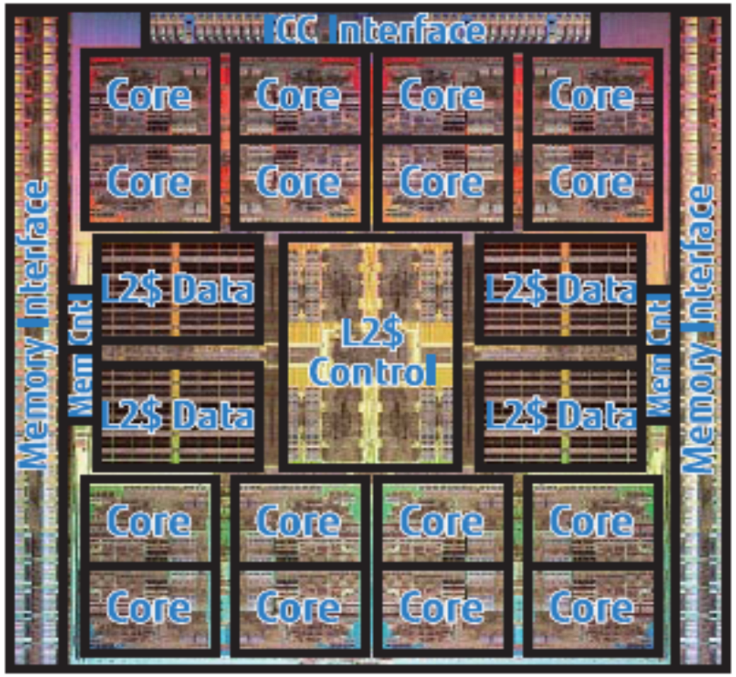
Performance of Supercomputers

- 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
    - $3 \times 10^9 \times 4$(or 8)=12(or 24)$\times 10^9$ FLOPS=12(or 24)GFLOPS

    - 10^6 FLOPS= 1 Mega FLOPS = 1 MFLOPS
    - 10^9 FLOPS= 1 Giga FLOPS = 1 GFLOPS
    - 10^{12} FLOPS= 1 Tera FLOPS = 1 TFLOPS
    - 10^{15} FLOPS= 1 Peta FLOPS = 1 PFLOPS
    - 10^{18} FLOPS= 1 Exa FLOPS = 1 EFLOPS

Peak Performance of Oakleaf-FX

Fujitsu PRIMEHPC FX10 at U.Tokyo

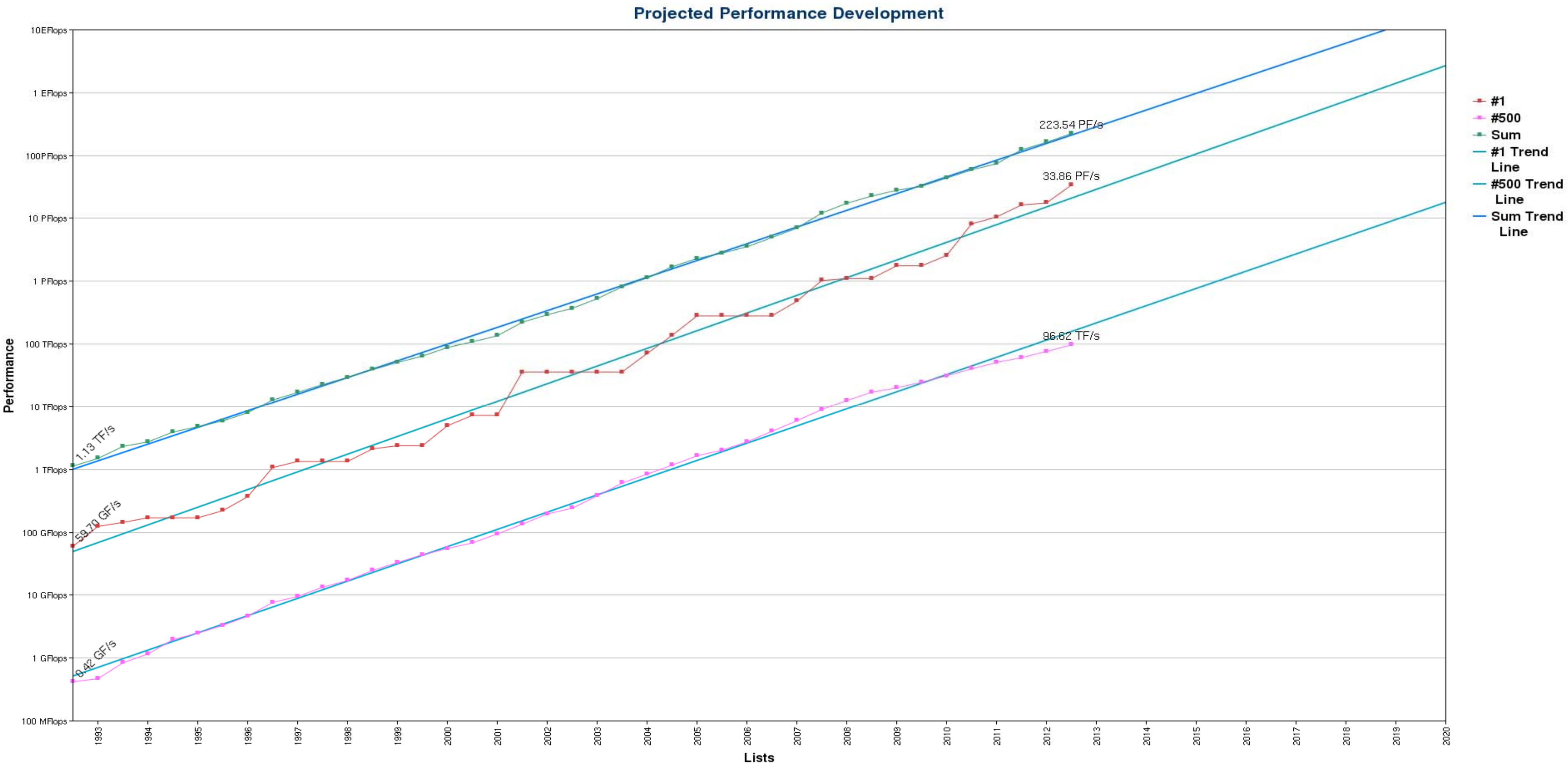


- 1.848 GHz
- 8 FLOP operations per Clock
- Peak Performance (1 core)
  - 1.848 × 8= 14.78 GFLOPS
- Peak Performance (1 node/16 cores)
  - 236.5 GFLOPS
- Peak Performance of Entire Performance
  - 4,800 nodes, 76,800 cores
  - 1.13 PFLOPS

TOP 500 List

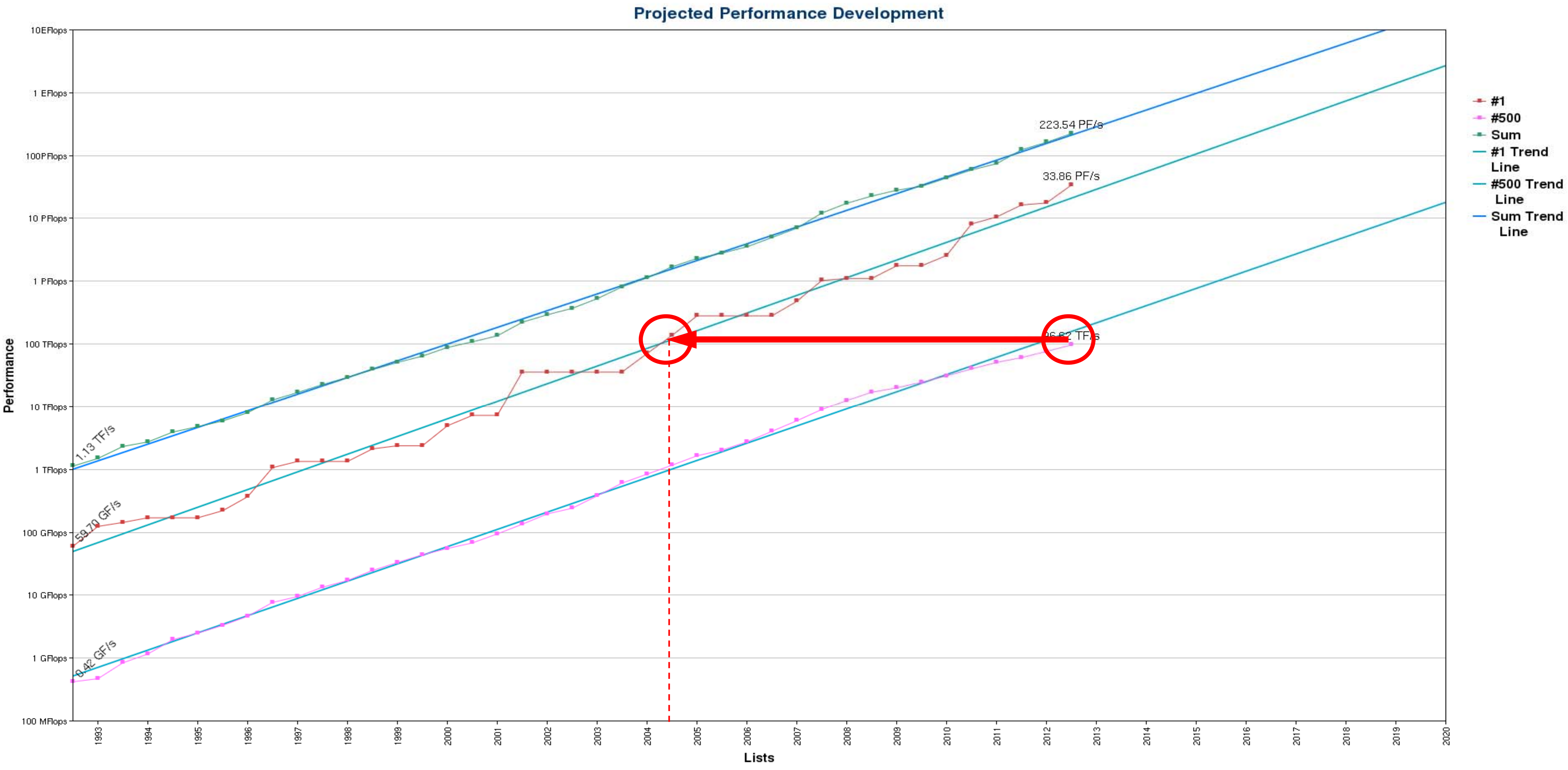
http://www.top500.org/

- 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 in 2020

http://www.top500.org/



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http://www.top500.org/

41^{st} TOP500 List (June, 2013)

	Site	Computer/Year Vendor	Cores	R_{max}	R_{peak}	Power
1	National Supercomputing Center in Tianjin, China	**Tianhe-2** Intel Xeon E5-2692, TH Express-2, IXeon Phi2013 NUDT	3120000	33863 (= 33.9 PF)	54902	17808
2	Oak Ridge National Laboratory, USA	**Titan** Cray XK7/NVIDIA K20x, 2012 Cray	560640	17590	27113	8209
3	Lawrence Livermore National Laboratory, USA	**Sequoia** BlueGene/Q, 2011 IBM	1572864	17173	20133	7890
4	**RIKEN AICS, Japan**	**K computer, SPARC64 VIIIfx , 2011 Fujitsu**	**705024**	**10510**	**11280**	**12660**
5	Argonne National Laboratory, USA	**Mira** BlueGene/Q, 2012 IBM	786432	85867	10066	3945
6	TACC, USA	**Stampede** Xeon E5-2680/Xeon Phi, 2012 Dell	462462	5168	8520	4510
7	Forschungszentrum Juelich (FZJ), Germany	**JuQUEEN** BlueGene/Q, 2012 IBM	458752	5009	5872	2301
8	DOE/NNSA/LLNL, USA	**Vulcan** BlueGene/Q, 2012 IBM	393216	4293	5033	1972
9	Leibniz Rechenzentrum, Germeny	**SuperMUC** iDataPlex/Xeon E5-2680 2012 IBM	147456	2897	3185	3423
10	National Supercomputing Center in Tianjin, China	**Tianhe-1A** Heterogeneous Node 2010 NUDT	186368	2566	4701	4040

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

http://www.top500.org/

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

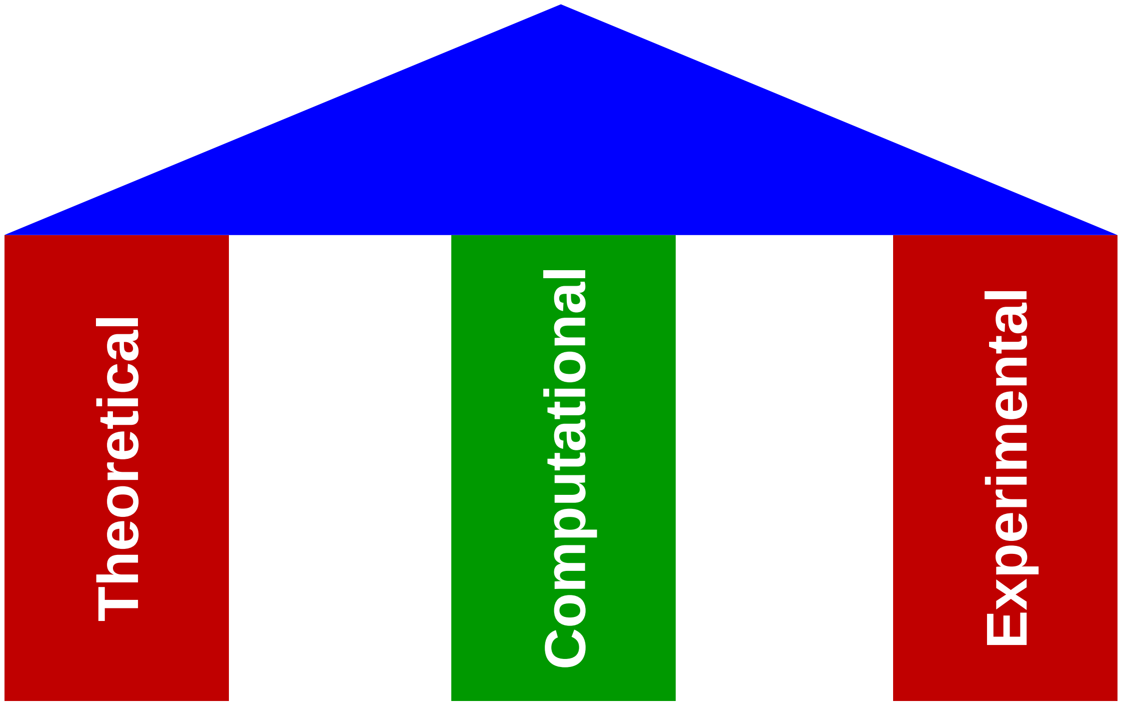
R_{max}: Performance of Linpack (TFLOPS)

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

http://www.top500.org/

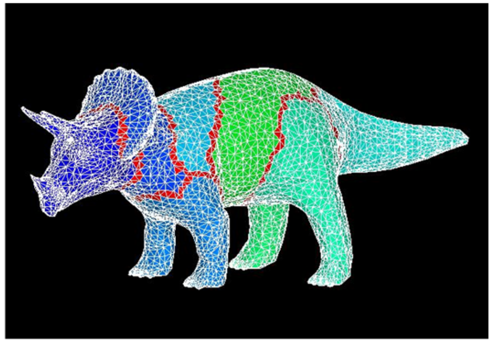
Computational Science
The 3rd Pillar of Science

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

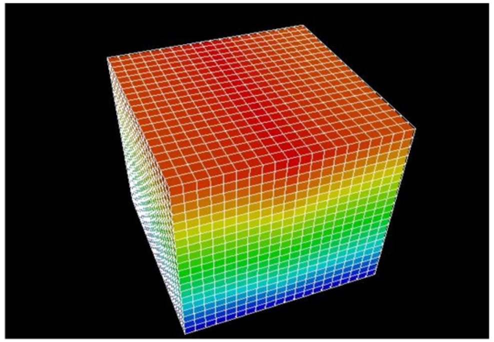


Methods for Scientific Computing

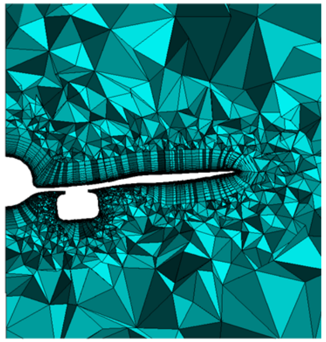
- Numerical solutions of PDE (Partial Diff. Equations)
- Grids, Meshes, Particles
  - Large-Scale Linear Equations
  - Finer meshes provide more accurate solutions



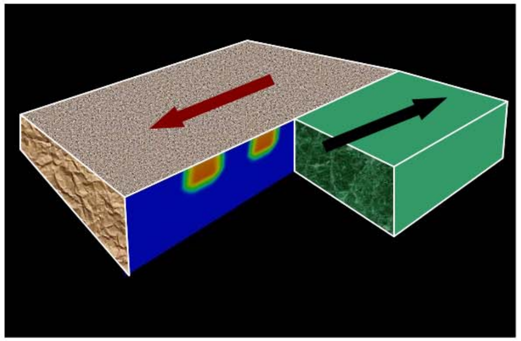
有限要素法
Finite Element Method
FEM



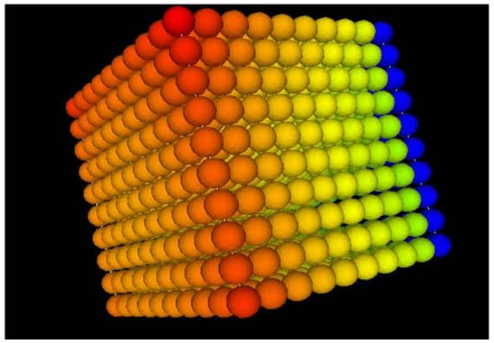
差分法
Finite Difference Method
FDM



有限体積法
Finite Volume Method
FVM



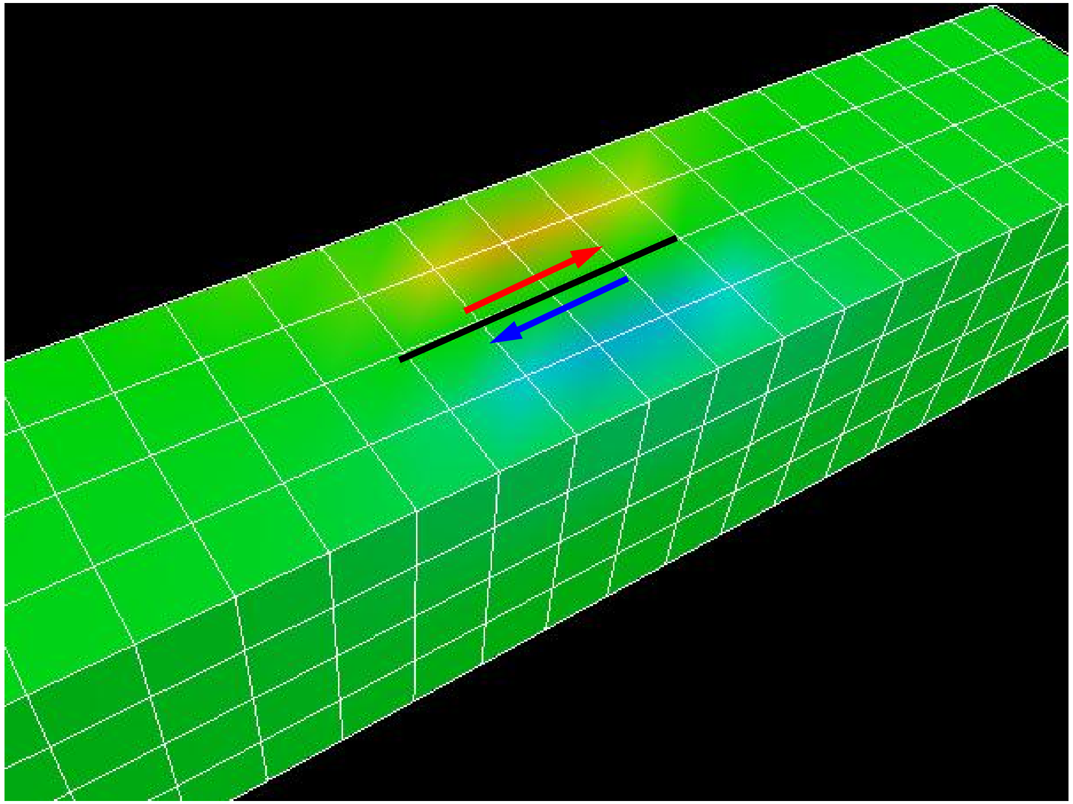
境界要素法
Boundary Element Method
BEM

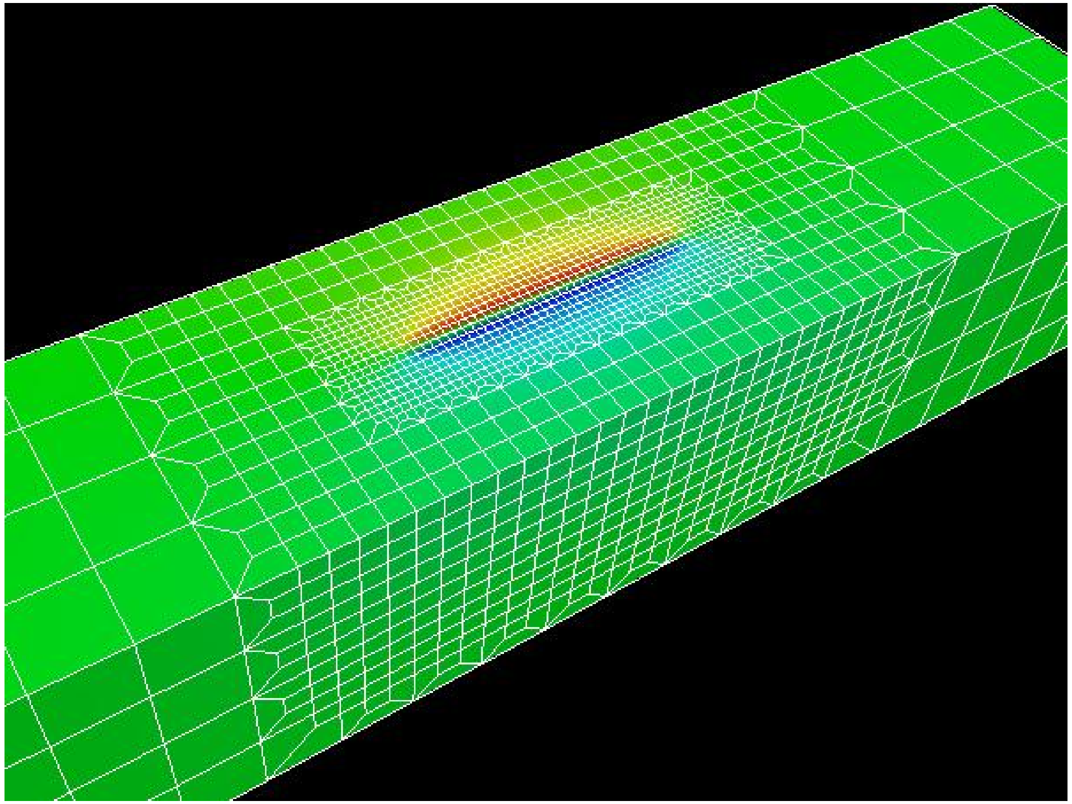


個別要素法
Discrete Element Method
DEM

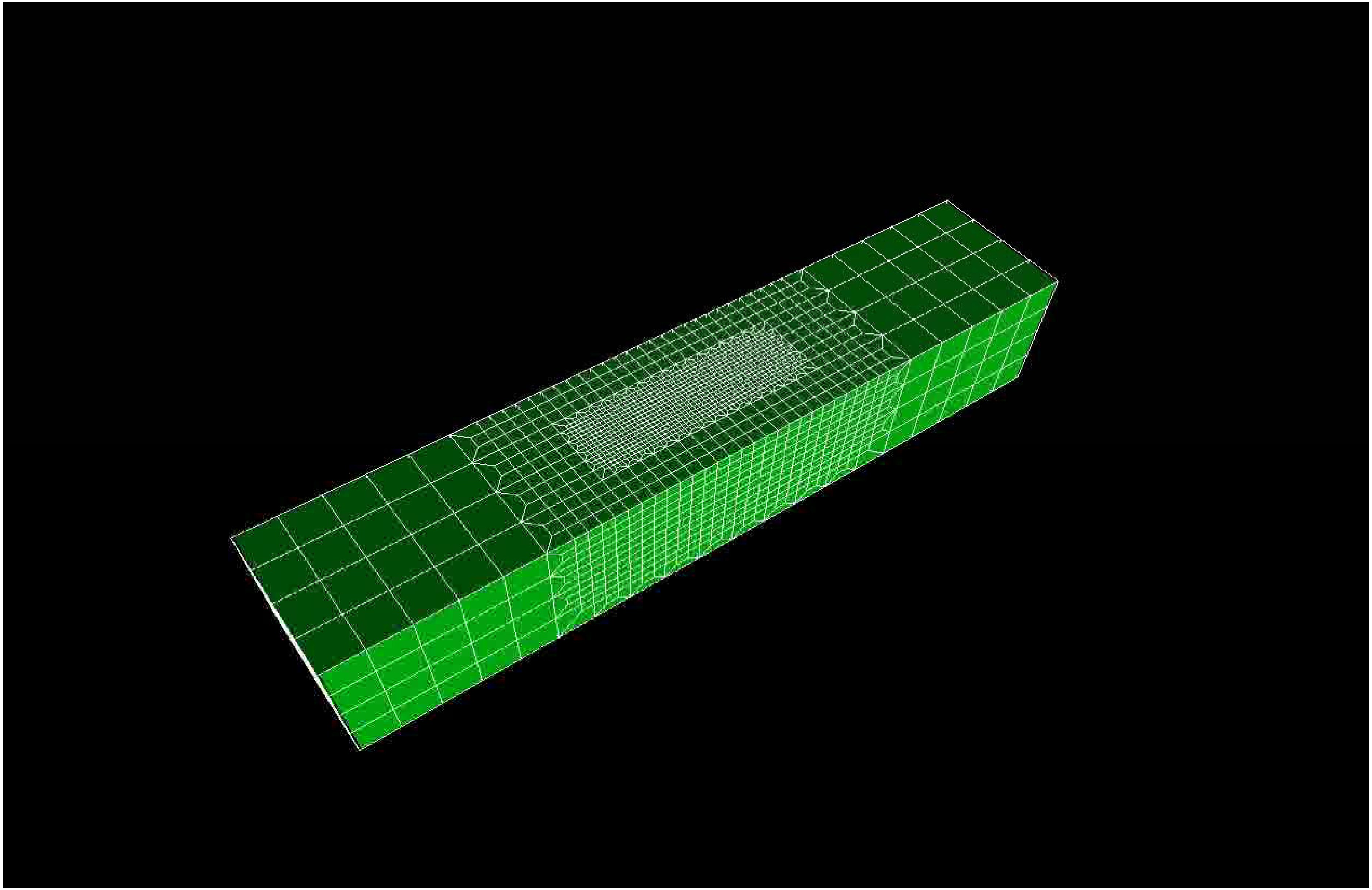
3D Simulations for Earthquake Generation Cycle San Andreas Faults, CA, USA

Stress Accumulation at Transcurrent Plate Boundaries

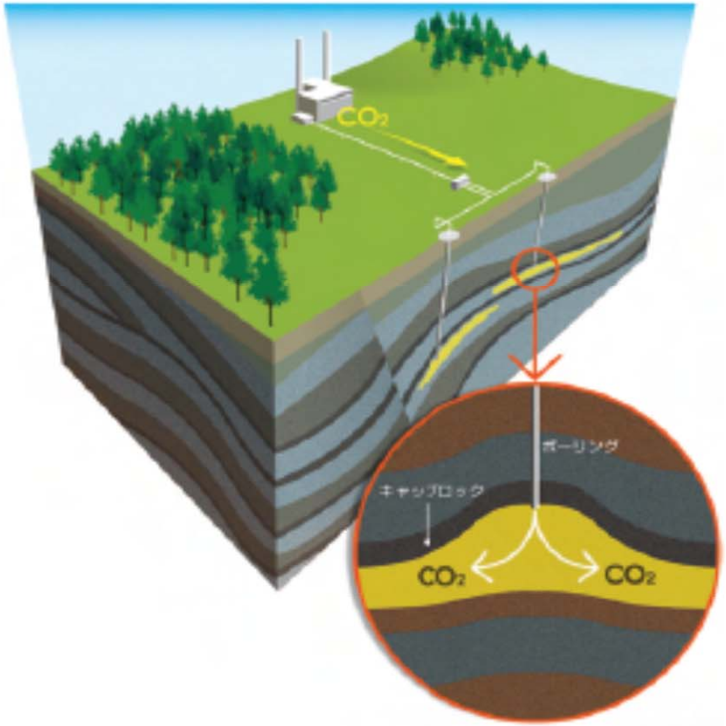




Adaptive FEM: High-resolution needed at meshes with large deformation (large accumulation)



Simulation of Geologic CO_2 Storage



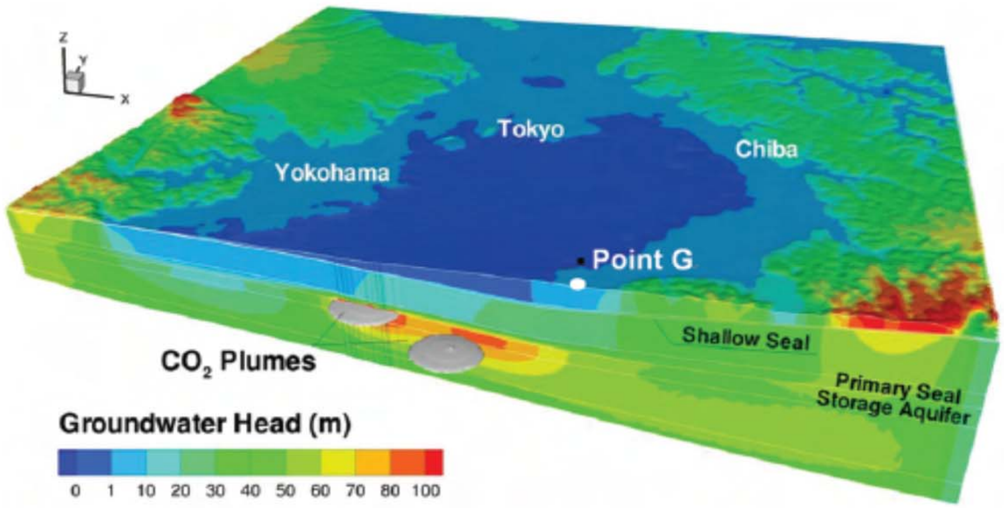
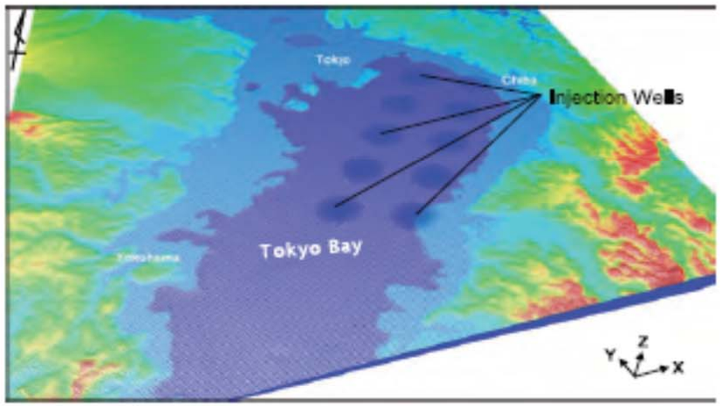
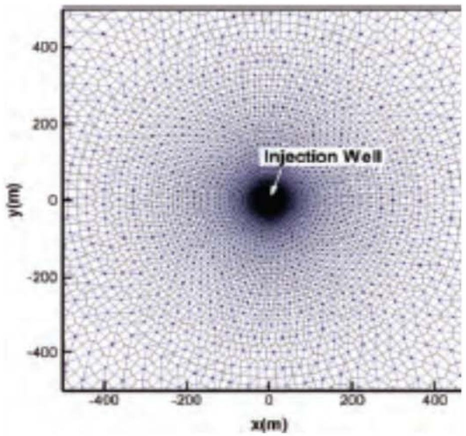
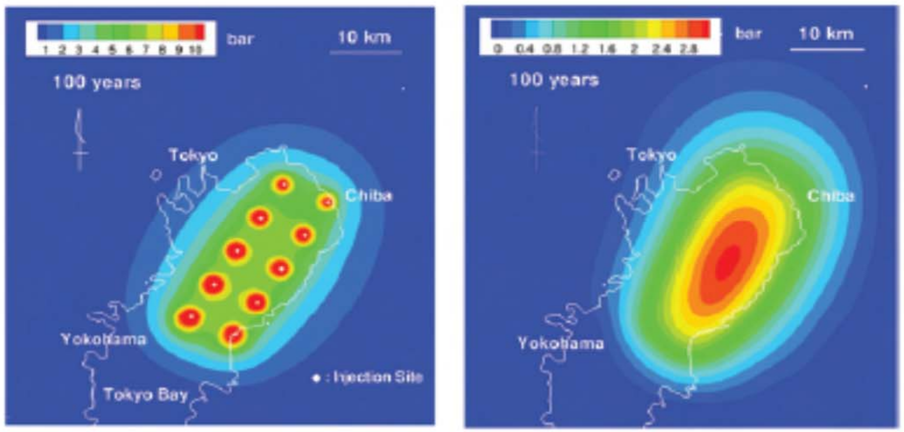


図 -4　CO_2 圧入後の地下水圧（全水頭換算）の分布（100 年後）







(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

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

Science

Modeling

Algorithm

Software

Hardware

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 (Peak Performance: 130 TFLOPS)
    - NEC, JAMSEC

Concentration of CO_2 in Groundwater

Meshes with higher resolution provide more accurate prediction ⇒ Larger Model/Linear Equations

[Dr. Hajime Yamamoto, Taisei]

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.

- Target: Parallel FEM
- Supercomputers and Computational Science
- **Overview of the Class**
- Future Issues

Information of this Class

- Instructor
  - Kengo Nakajima (Information Technology Center)
    - Information Technology Center (Asano) Annex 3F #36 ex: 22719
    - e-mail: nakajima(at)cc.u-tokyo.ac.jp
- Schedule
  - August 26-29, September 2-6, September 9
  - 09:00-10:30, 10:45-12:15, 13:30-15:00, 15:15-16:45
  - No classes on August 30, Sept. 5 (AM)
- Practice
  - Time for exercise
- Lecture Room
  - Information Technology Center (Asano) Seminar Room #2 (1F)
    - No Foods, No Drinks
  - Research Comlex #2, Kashiwa Campus)（柏・第2総合研究棟） on September 9 (M)

Date	Hour	Room	ID	Content
August 26 (M)	0900-1030	ITC-Seminar Room#2	CE01	Introduction
August 26 (M)	1045-1215	ITC-Seminar Room#2	CE02	Introdution to FEM, 1D-FEM (1/3)
August 26 (M)	1330-1500	ITC-Seminar Room#2	CE03	1D-FEM (2/3)
August 26 (M)	1515-1645	ITC-Seminar Room#2	CE04	1D-FEM (3/3)
August 27 (T)	0900-1030	ITC-Seminar Room#2	CE05	3D-FEM (1/4)
August 27 (T)	1045-1215	ITC-Seminar Room#2	CE06	3D-FEM (2/4)
August 27 (T)	1330-1500	ITC-Seminar Room#2	CE07	3D-FEM (3/4)
August 27 (T)	1515-1645	ITC-Seminar Room#2	Practice	Practice (Instructor is not available)
August 28 (W)	0900-1030	ITC-Seminar Room#2	CE08	3D-FEM (4/4)
August 28 (W)	1045-1215	ITC-Seminar Room#2	CE09	Intro. to Parallel FEM, Login to FX10
August 28 (W)	1330-1500	ITC-Seminar Room#2	CE10	Parallel Programming by MPI (I) (1/2)
August 28 (W)	1515-1645	ITC-Seminar Room#2	CE11	Parallel Programming by MPI (I) (2/2)
August 29 (Th)	0900-1030	ITC-Seminar Room#2	CE12	Parallel Programming by MPI (II) (1/3)
August 29 (Th)	1045-1215	ITC-Seminar Room#2	CE13	Parallel Programming by MPI (II) (2/3)
August 29 (Th)	1330-1500	ITC-Seminar Room#2	CE14	Parallel Programming by MPI (II) (3/3)
August 29 (Th)	1515-1645	ITC-Seminar Room#2	Practice	Practice
August 30 (F)	0900-1030	(No Classes)		(No Classes)
August 30 (F)	1045-1215	(No Classes)		(No Classes)
August 30 (F)	1330-1500	(No Classes)		(No Classes)
August 30 (F)	1515-1645	(No Classes)		(No Classes)

Date	Hour	Room	ID	Content
September 2 (M)	0900-1030	ITC-Seminar Room#2	CE15	Report S1
September 2 (M)	1045-1215	ITC-Seminar Room#2	CE16	Introduction to Tuning
September 2 (M)	1330-1500	ITC-Seminar Room#2	CE17	Report S2
September 2 (M)	1515-1645	ITC-Seminar Room#2	Practice	Practice (Instructor is not available)
September 3 (T)	0900-1030	ITC-Seminar Room#2	CE18	Parallel FEM (1/3)
September 3 (T)	1045-1215	ITC-Seminar Room#2	CE19	Parallel FEM (2/3)
September 3 (T)	1330-1500	ITC-Seminar Room#2	CE20	Parallel FEM (3/3)
September 3 (T)	1515-1645	ITC-Seminar Room#2	Practice	Practice
September 4 (W)	0900-1030	ITC-Seminar Room#2	CE21	Multicore Programming (I) (1/2)
September 4 (W)	1045-1215	ITC-Seminar Room#2	CE22	Multicore Programming (I) (2/2)
September 4 (W)	1330-1500	ITC-Seminar Room#2	CE23	Multicore Programming (II) (1/2)
September 4 (W)	1515-1645	ITC-Seminar Room#2	Practice	Practice
September 5 (Th)	0900-1030	(No Classes)		(No Classes)
September 5 (Th)	1045-1215	(No Classes)		(No Classes)
September 5 (Th)	1330-1500	ITC-Seminar Room#2	CE24	Multicore Programming (II) (2/2)
September 5 (Th)	1515-1645	ITC-Seminar Room#2	CE25	Multicore Programming (III) (1/3)
September 6 (F)	0900-1030	ITC-Seminar Room#2	CE26	Multicore Programming (III) (2/3)
September 6 (F)	1045-1215	ITC-Seminar Room#2	CE27	Multicore Programming (III) (3/3)
September 6 (F)	1330-1500	ITC-Seminar Room#2	Practice	Practice
September 6 (F)	1515-1645	ITC-Seminar Room#2	Practice	Practice

Date	Hour	Room	ID	Content
September 9 (M)	1000-1115	ITC-Seminar Room (3F Research Complex #2, Kashiwa Campus)（柏・第2総合研究棟）	CE28	Recent Topics
September 9 (M)	1230-1215	ITC-Machine Room (1F Research Complex #2, Kashiwa Campus)（柏・第2総合研究棟）		Tour to Oakleaf-FX

Prerequisites

- Knowledge and experiences in fundamental methods for numerical analysis (e.g. Gaussian elimination, SOR)
- Knowledge and experiences in UNIX
- Experiences in programming using FORTRAN or C
- “Seminar on Advanced Computing (35616-4009)” should be also registered
- Account for Educational Campuswide Computing System (ECC System) should be obtained in advance:
  - http://www.ecc.u-tokyo.ac.jp/ENGLISH/index-e.html

Grading by Reports ONLY

- MPI (Collective Communication) (S1)
- MPI (1D Parallel FEM) (S2)
- Parallel FEM (S3)
  - If you complete (S1-S3), you get credits of “Programming for Parallel Computing (616-2057)” .
- OpenMP (P1)
  - If you complete (P1), you get credits for “Seminar on Advanced Computing (616-4009)” are graded.

- Sample solutions will be available
- Deadline: October 12th (Sat) 17:00
  - By E-mail: nakajima(at)cc.u-tokyo.ac.jp
  - You can bring hard-copy’s to my office ...

Homepage

- **http://nkl.cc.u-tokyo.ac.jp/13e/**
  - General information is available
  - No hardcopy of course materials are provided (Please print them by yourself)

参考文献(1/2)

- 菊地「有限要素法概説(新訂版)」, サイエンス社, 1999.
- 竹内, 樫山, 寺田(日本計算工学会編)「計算力学:有限要素法の基礎」, 森北出版, 2003.
- 登坂, 大西「偏微分方程式の数値シミュレーション 第2版」, 東大出版会, 2003.
  - 差分法, 境界要素法との比較
- 福森「よくわかる有限要素法」, オーム社, 2005.
  - ヘルムホルツ方程式
- 矢川, 宮崎「有限要素法による熱応力・クリープ・熱伝導解析」, サイエンス社, 1985. (品切)
- Segerlind, L.(川井監訳)「応用有限要素解析 第2版」, 丸善, 1992.(品切)

参考文献（より進んだ読者向け）

- 菊池，岡部「有限要素システム入門」，日科技連，1986.
- 山田「高性能有限要素法」，丸善，2007.
- 奥田，中島「並列有限要素法」，培風館，2004.

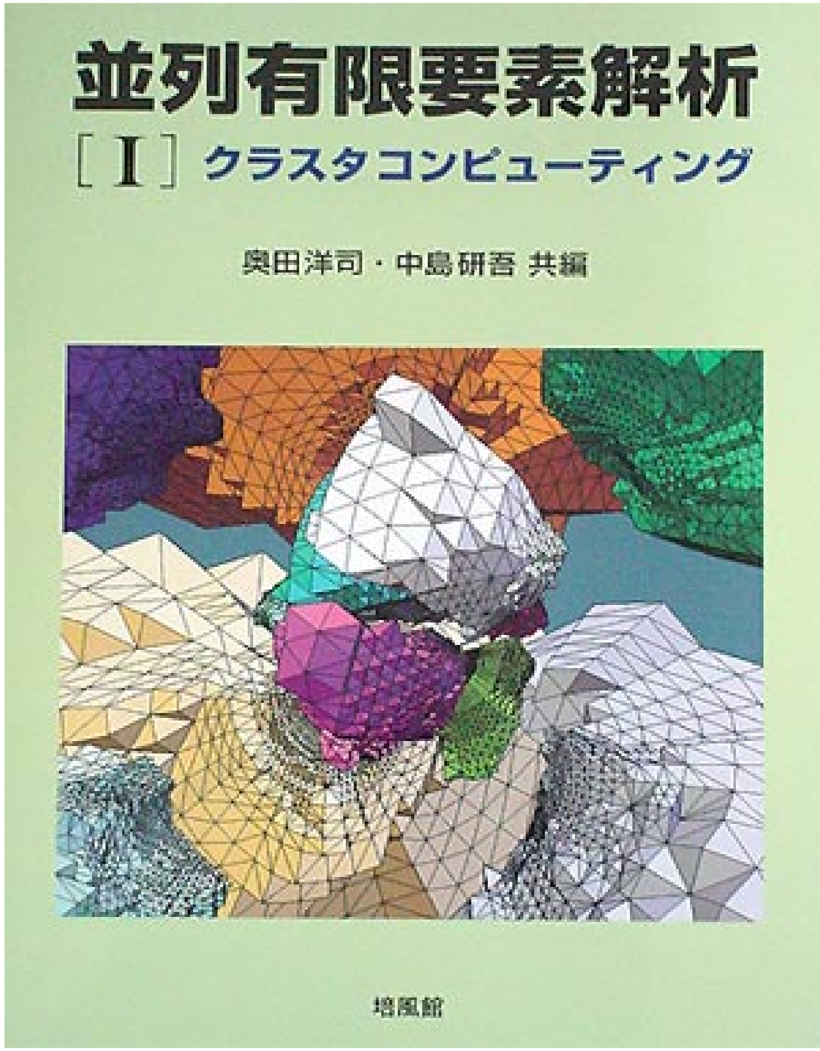
- Smith, I. 他「Programming the Finite Element Method (4th edition)」，Wiley.

奥田，中島編「並列有限要素解析〔I〕クラスタコンピューティング」

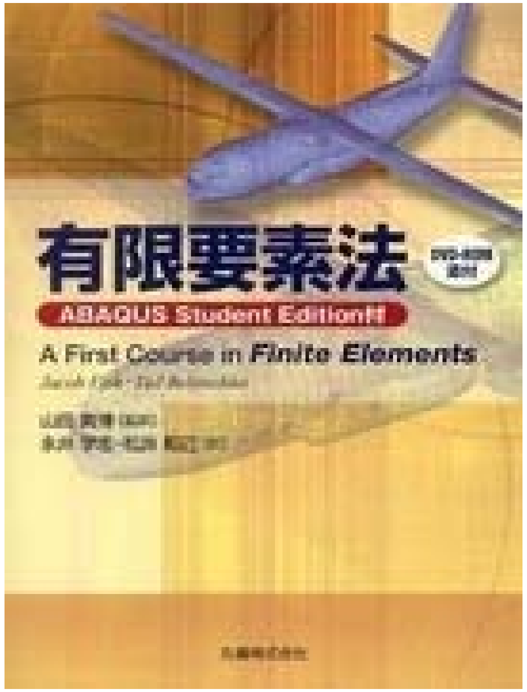
培風館，2004.

- 「GeoFEM」の成果のまとめ
  - http://geofem.tokyo.rist.or.jp
- 「地球シミュレータ」上での最適化，シミュレーション結果を紹介

- 初心者向けでは無い
- 高い・・・
  - 若干残部があるので希望者には貸し出します。



References



- Fish, Belytschko, A First Course in Finite Elements, Wiley, 2007
  - Japanese version is also available
  - “ABAQUS Student Edition” included
- Smith et al., Programming the Finite Element Method (4th edition), Wiley, 2004
  - Parallel FEM
- Hughes, The Finite Element Method: Linear Static and Dynamic Finite Element Analysis, Dover, 2000

- Target: Parallel FEM
- Supercomputers and Computational Science
- Overview of the Class
- **Future Issues**

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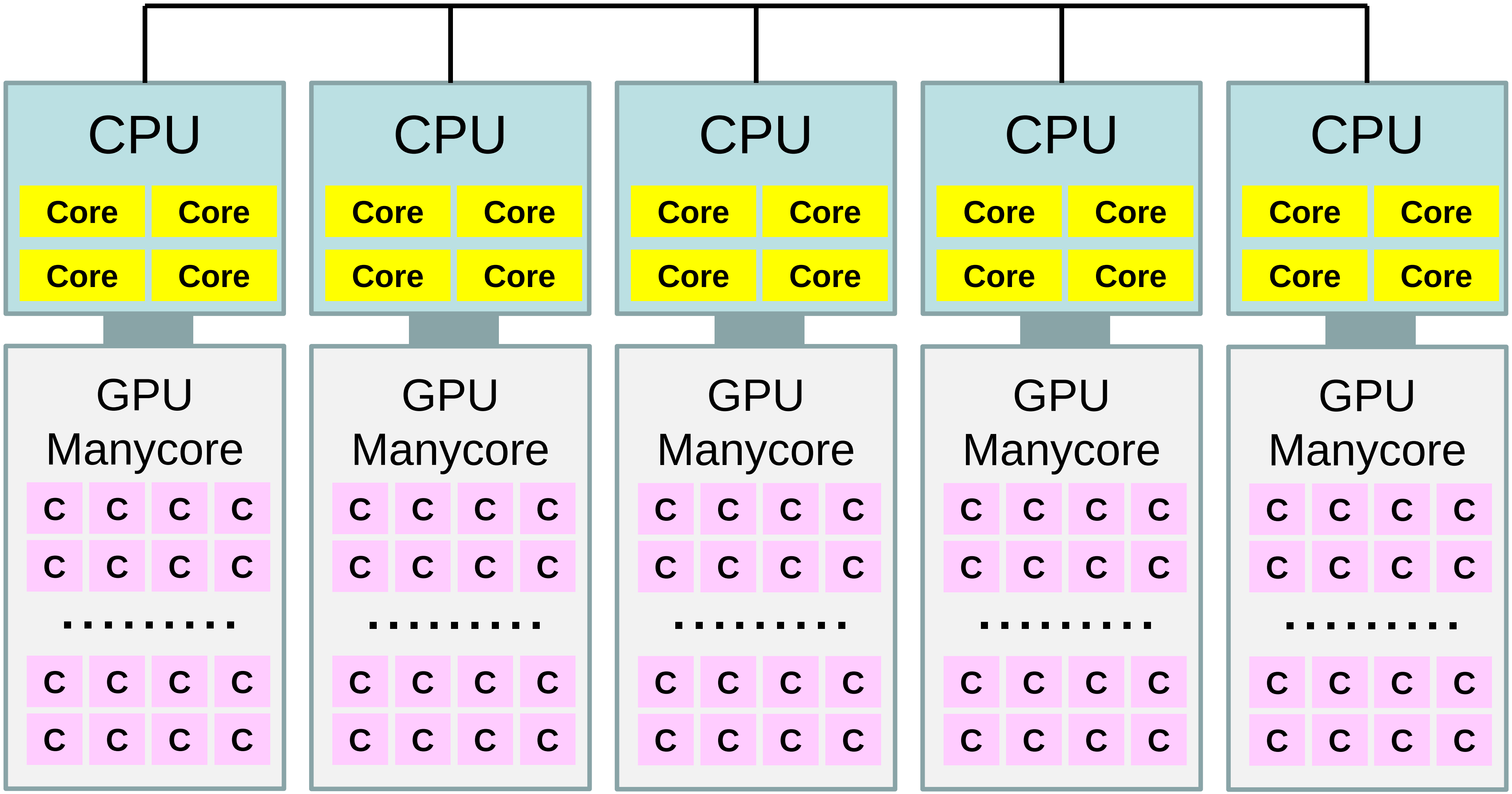
Key-Issues towards Appl./Algorithms on Exa-Scale Systems

Jack Dongarra (ORNL/U. Tennessee) at ISC 2013

- Hybrid/Heterogeneous Architecture
  - Multicore + GPU/Manycores (Intel MIC/Xeon Phi)
    - Data Movement, Hierarchy of Memory
- Communication/Synchronization Reducing Algorithms
- Mixed Precision Computation
- Auto-Tuning/Self-Adapting
- Fault Resilient Algorithms
- Reproducibility of Results

Supercomputers with Heterogeneous/Hybrid Nodes

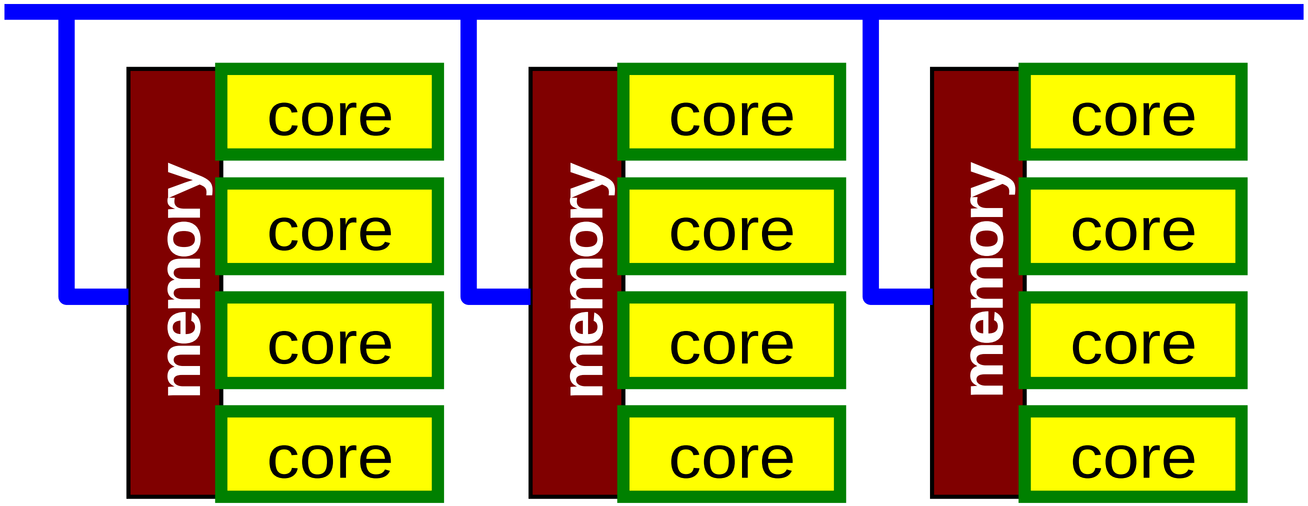


Hybrid Parallel Programming Model is essential for Post-Peta/Exascale Computing

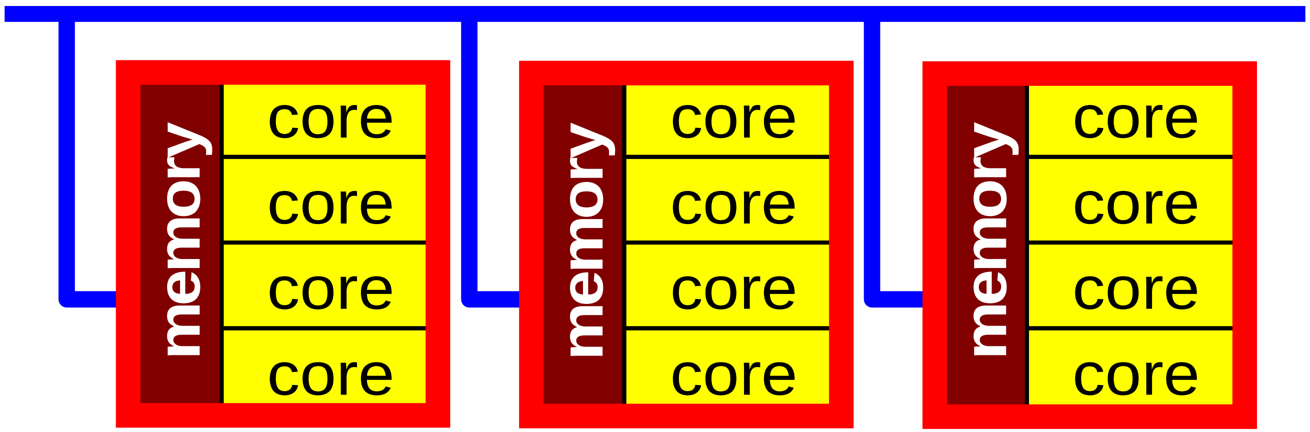
- Message Passing (e.g. MPI) + Multi Threading (e.g. OpenMP, CUDA, OpenCL, OpenACC etc.)
- In K computer and FX10, hybrid parallel programming is recommended
  - MPI + Automatic Parallelization by Fujitsu's Compiler
- Expectations for Hybrid
  - Number of MPI processes (and sub-domains) to be reduced
  - O(10^8-10^9)-way MPI might not scale in Exascale Systems
  - Easily extended to Heterogeneous Architectures
    - CPU+GPU, CPU+Manycores (e.g. Intel MIC/Xeon Phi)
    - MPI+X: OpenMP, OpenACC, CUDA, OpenCL

Flat MPI vs. Hybrid

Flat-MPI：Each PE -> Independent



Hybrid：Hierarchal Structure



In this class...

- You do not have enough time to learn hybrid parallel programming model.
- But you can easily extend the ideas in materials on MPI and OpenMP to hybrid parallel programming models.

- Anyway, MPI is essential for large-scale scientific computing. If you want to something new using supercomputers, you must learn MPI, then OpenMP.
  - You don’t have to be attracted by PGAS (e.g. HPF), automatic parallelization（自動並列化）, etc.

Example of OpnMP/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-NEO)= X(NOD_EXPORT(k))
        enddo

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

Parallel Programming Models

- Multicore Clusters (e.g. K, FX10)
  - MPI + OpenMP and (Fortan/C/C++)
- Multicore + GPU (e.g. Tsubame)
  - GPU needs host CPU
  - MPI and [(Fortan/C/C++) + CUDA, OpenCL]
    - complicated,
  - MPI and [(Fortran/C/C++) with OpenACC]
    - close to MPI + OpenMP and (Fortran/C/C++)
- Multicore + Intel MIC/Xeon-Phi (e.g. Stampede)
  - Xeon-Phi needs host CPU (currently)
  - MPI + OpenMP and (Fortan/C/C++) is possible
    - + Vectorization

Future of Supercomputers (1/2)

- Technical Issues
  - Power Consumption
  - Reliability, Fault Tolerance, Fault Resilience
  - Scalability (Parallel Performancce)
- Petascale System
  - 2MW including A/C, 2M$/year, O($10^5$～$10^6$) cores
- Exascale System (10^3x Petascale)
  - 2018-2020
    - 2GW (2 B$/year !), O($10^8$～$10^9$) cores
  - Various types of innovations are on-going
    - to keep power consumption at 20MW (100x efficiency)
    - CPU, Memory, Network ...
  - Reliability

Future of Supercomputers (2/2)

- Not only hardware, but also numerical models and algorithms must be improved:
  - 省電力アルゴリズム（Power-Aware/Reducing）
  - 耐故障アルゴリズム（Fault Resilient）
  - 通信削減アルゴリズム（Communication Avoiding/Reducing）
- Co-Design by experts from various area (SMASH) is important
  - Exascale system will be a special-purpose system, not a general-purpose one.