High Performance Computing in Computational Mechanics

Kazuo Kashiyama

Department of Civil Engineering, Chuo University, Tokyo, Japan

Outline

- Brief History of Parallel Computing
- Parallel Computing Method for Large Scale Problems
  (Environmental Flow, Composite Materials)
- PC Cluster Parallel Compting

Why do we need parallel computer?

Demand of solution for complex problems in science

Grand Challenge Problems

- Turbulence flow
- Air pollution
- Ocean modeling
- Digital anatomy
- Cosmology

:

Development of computer hardware

circuit element

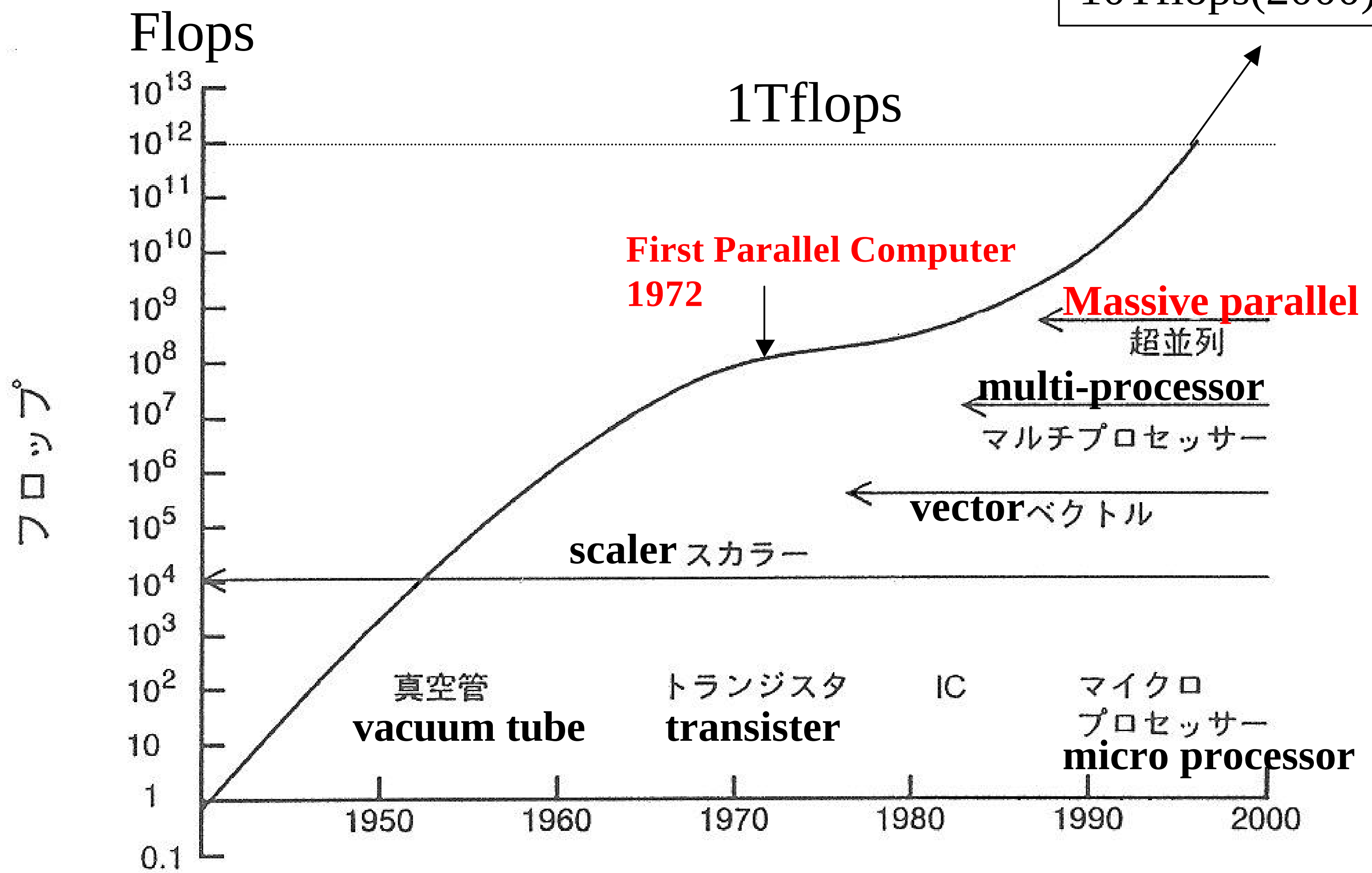
vacuum tube → transistor →IC→VLSI

Limitation of Single Processor

light speed in a vacuum（3×10**8 m/sec)

Performance of Supercomputer

40Tflops(2001)
10Tflops(2000)



Brief History of Parallel Computer

L.F.Richardson(U.K.)

1911: presented a numerical method for non-linear partial differential equations

1922: presented a paper “Weather Prediction by Numerical Processes”

- 3D analysis (5 layers for vertical direction)
- 6 weeks calculation needed for 6 hours prediction by manual calculating machine

Dream of Richardson

- Northern hemisphere are discretized by 2000 blocks
- 32 people are assigned in each block (64,000 people are needed)
- 6 hours prediction carried out by 3 hours

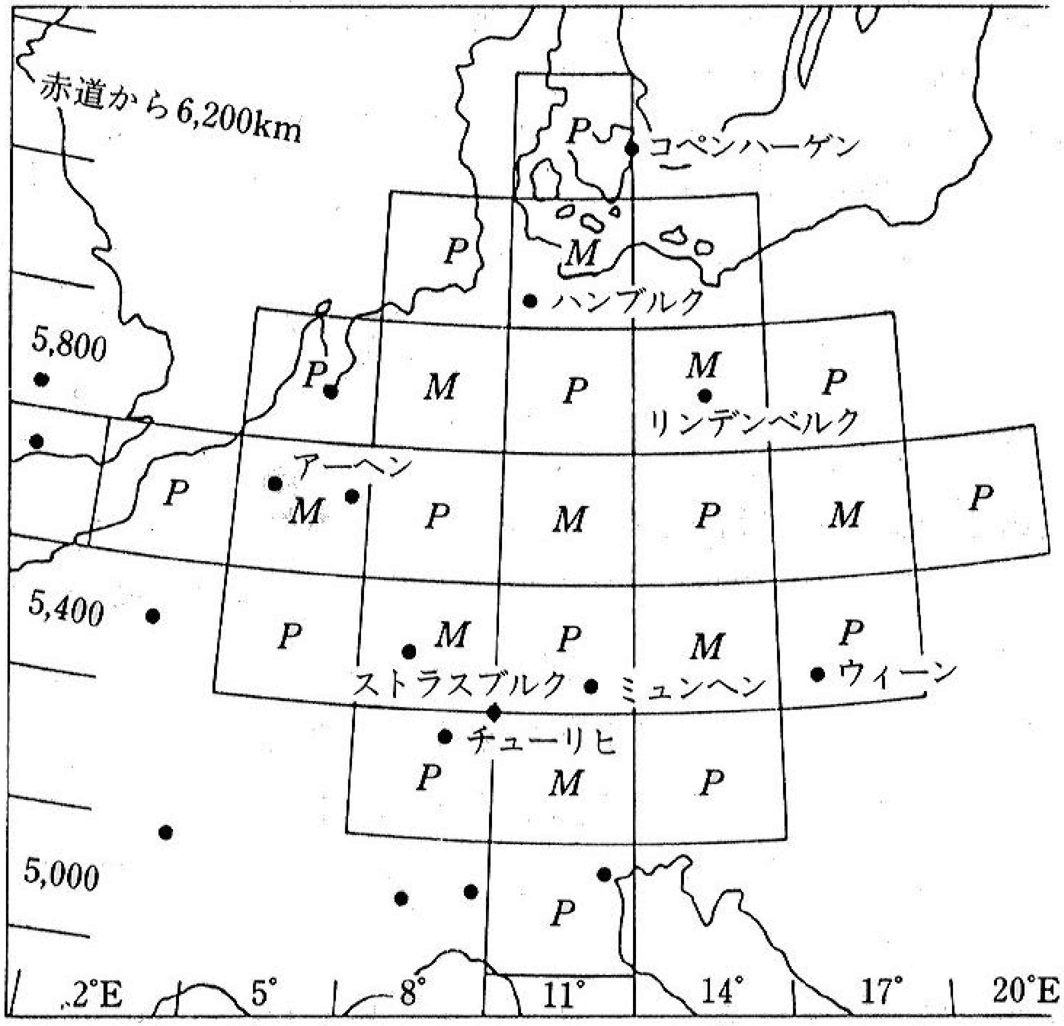
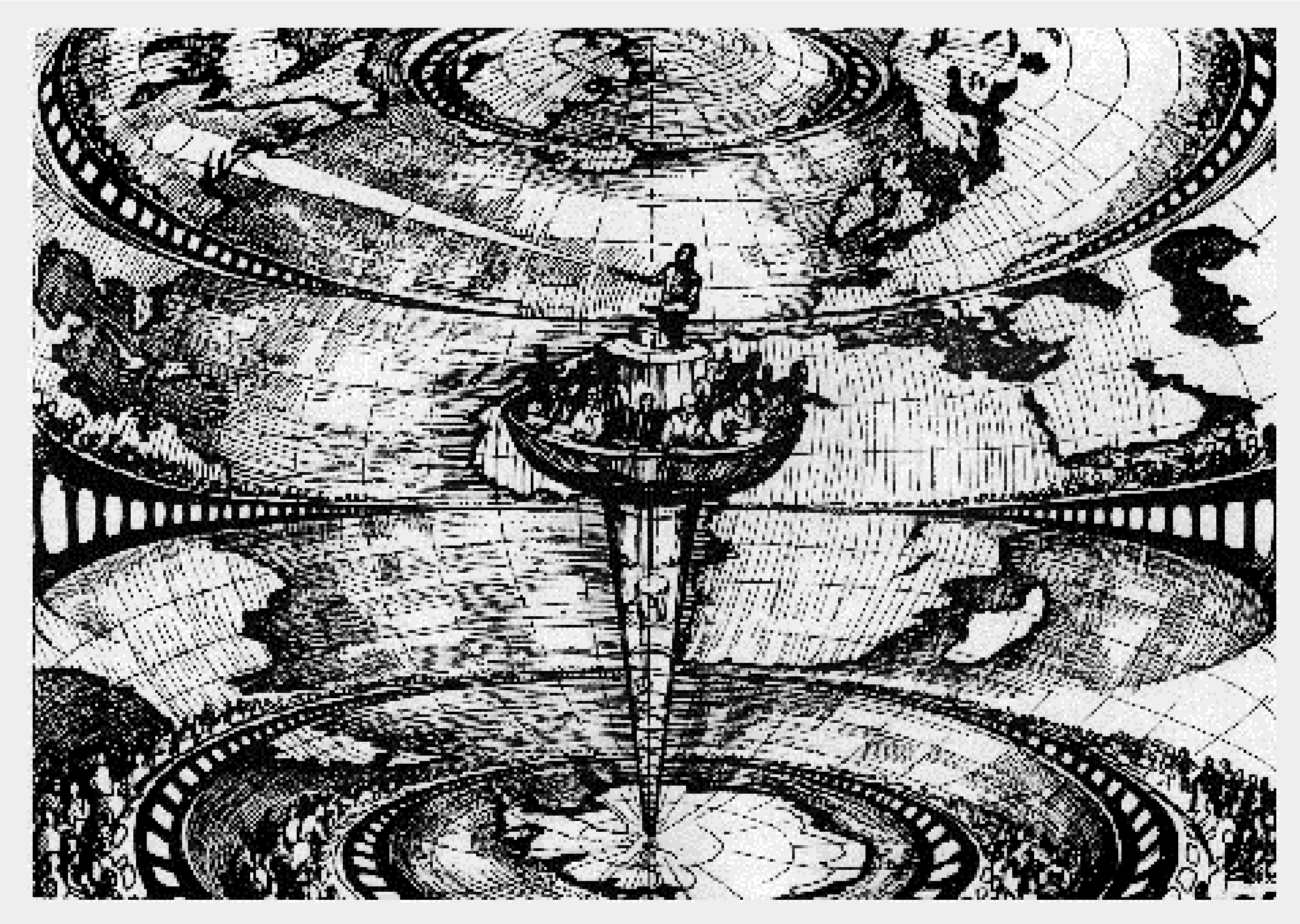


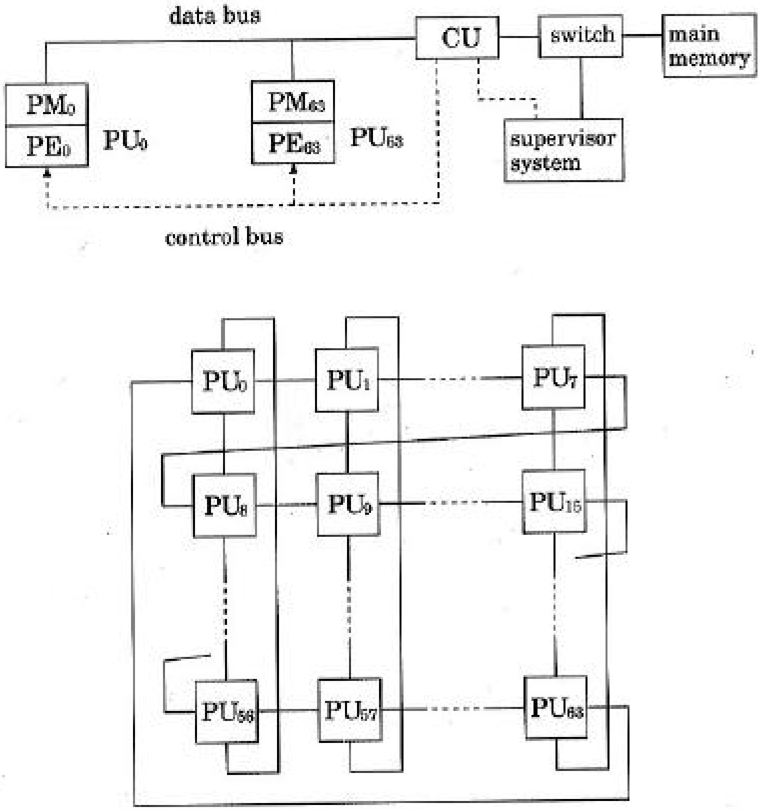
図 1-3 リチャードソンが『数値的方法による天気予測』の中で著したミュンヘン近傍の数値モデルの格子点分布（L. F. Richardson, 1922 : *Weather Prediction by Numerical Processes* より）
M は運動量を与えたボックス，*P* は気圧を与えたボックス．

Dream of Richardson



Birth of Parallel Computer

University of Illinois
(Daniel Slotnic designed two parallel computers)
1972: First parallel computer ILLIAC Ⅳ(Burroughs) was developed
(64 processing element, 1 control unit:SIMD)



Development of Parallel Computer In Japan

1977: PACS/PAX project was started
Tsutomu Hoshino(Kyoto University)

- PACS-9(1978, 0.01Mflops)
- PAX-32(1980, 0.5Mflops)

1980: PACS/PAX project was moved to Tsukuba University

- PAX-128（1983, 4M)
- PAX-64J（1986, 3.2Mflops)
- QCDPAX(1989, 14Gflops)
- CP-PACS（1996, 300Gflops）
  （1997, 600Gflops:2048CPU）

http://www.rccp.tsukuba.ac.jp/

Big Projects in Computer Science

U.S.A.

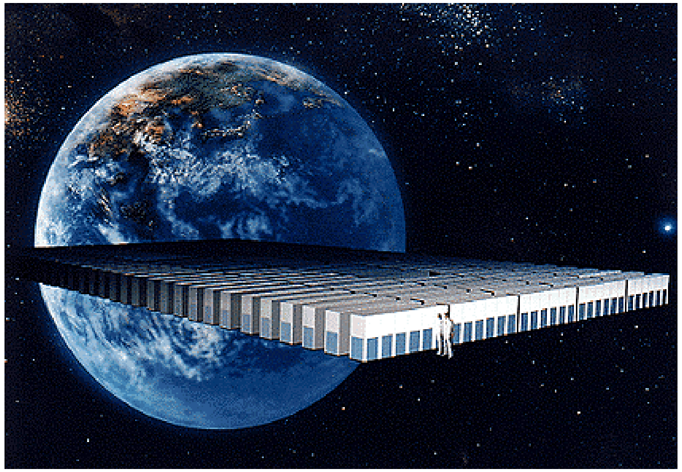
・CIC R&D

(Computing, Information and Communications R&D Program)

ASCI(Accelerated Strategic Computing Initiative) project

White：10Tflops（2000）

Turquoise：30Tflops（2002）



Japan

・「Earth Simulator」 project

(Ministry of Science and Technology)

Peak performance：40Tflops(2001)

Memory：10TB,

Development cost:¥40 billion

・「Computer Science」 project (Ministry of Education)

Support for the development of parallel computer in university

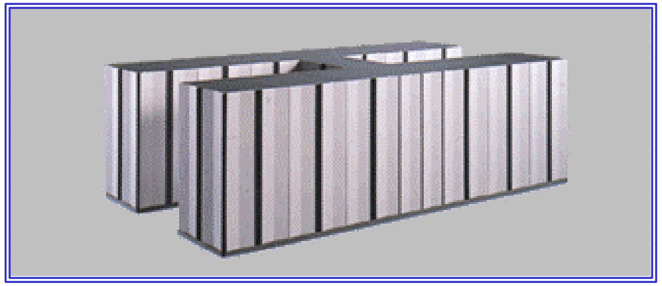
CP-PACS(Tsukuba University),GRAPE(University of Tokyo)

Two Currents for Parallel Computing

Computing using Business Parallel Computer:

Very Large Scale Computing

Expensive



Hitachi SR2201(University of Tokyo)

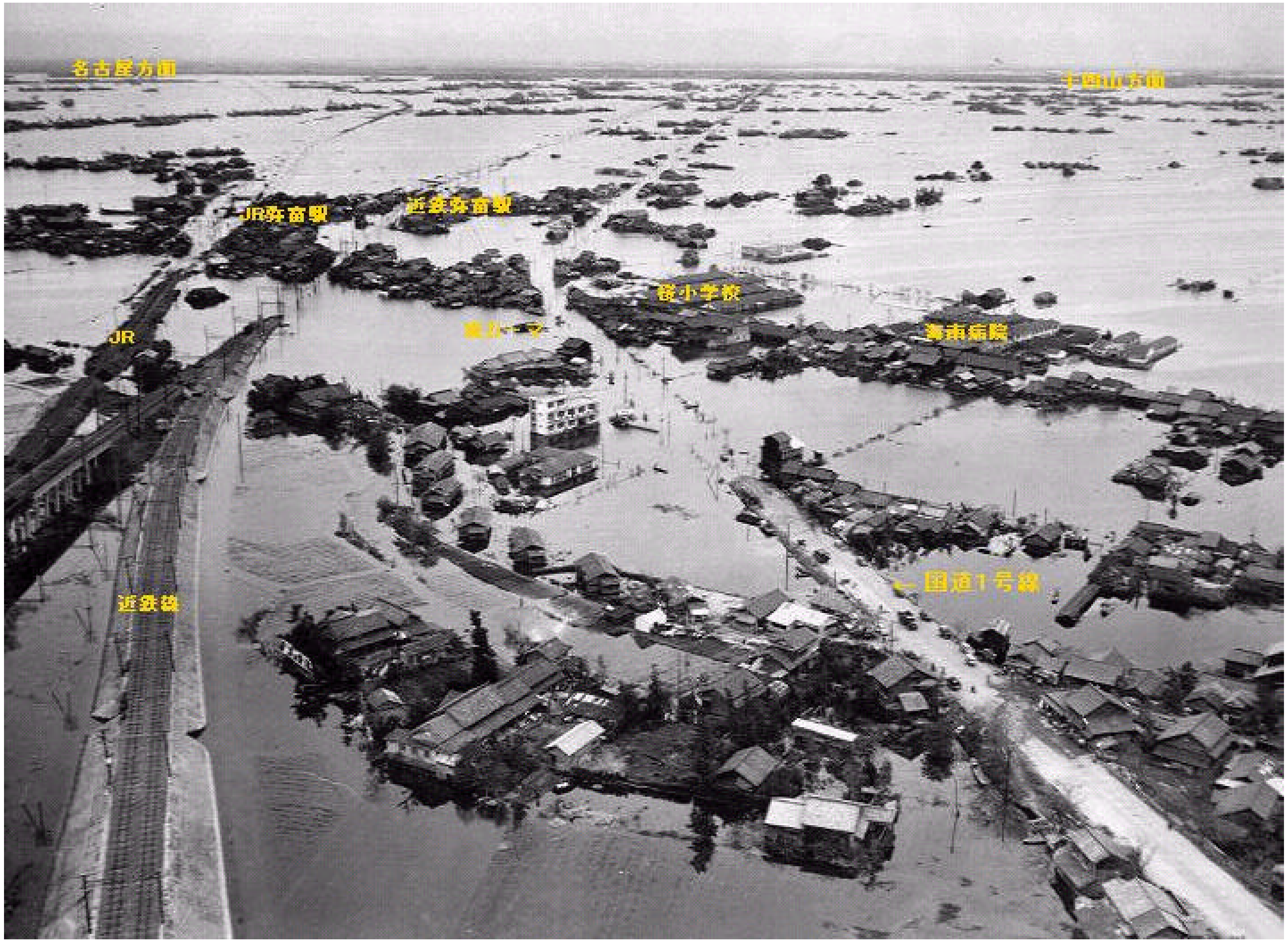
Computing using PC/WS Cluster:

Mediam-Large Scale Computing

Cheap&Flexible

PC Cluster(University of Heidelberg)

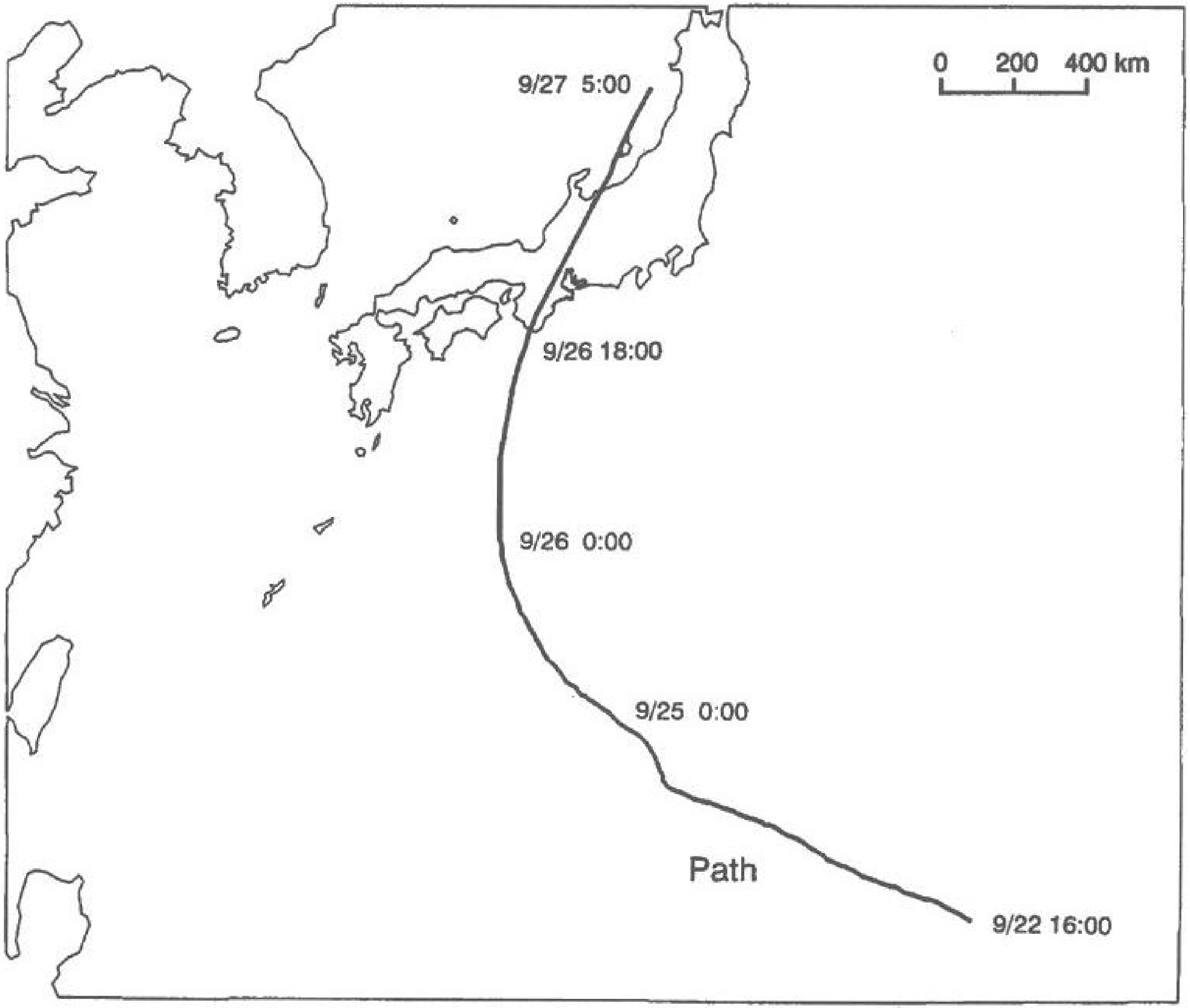
Ise-Bay Typhoon (1959)



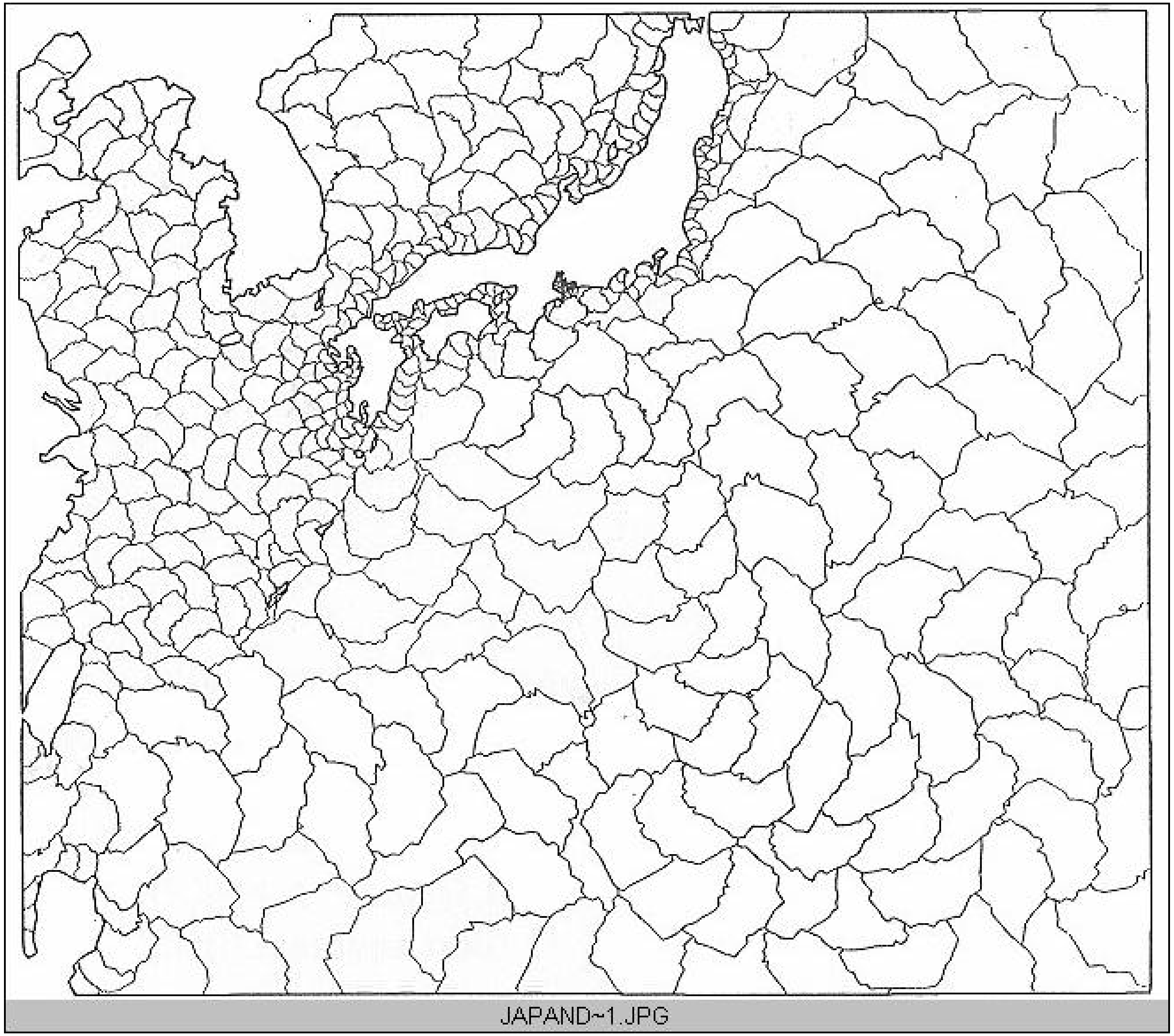
Damage by Ise-Bay Typhoon

Power:929hPa
Number of dead person:5098

Path of Ise-Bay Typhoon



Mesh Partitioning



(512 processors)

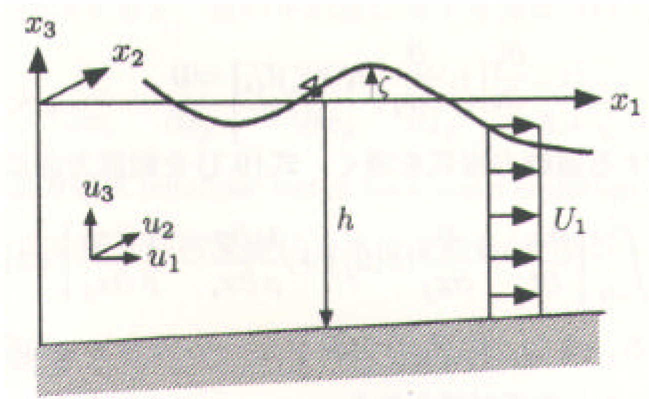
Finite Element Mesh

(elements:206,977, nodes:106,577)

Shallow Water Equations

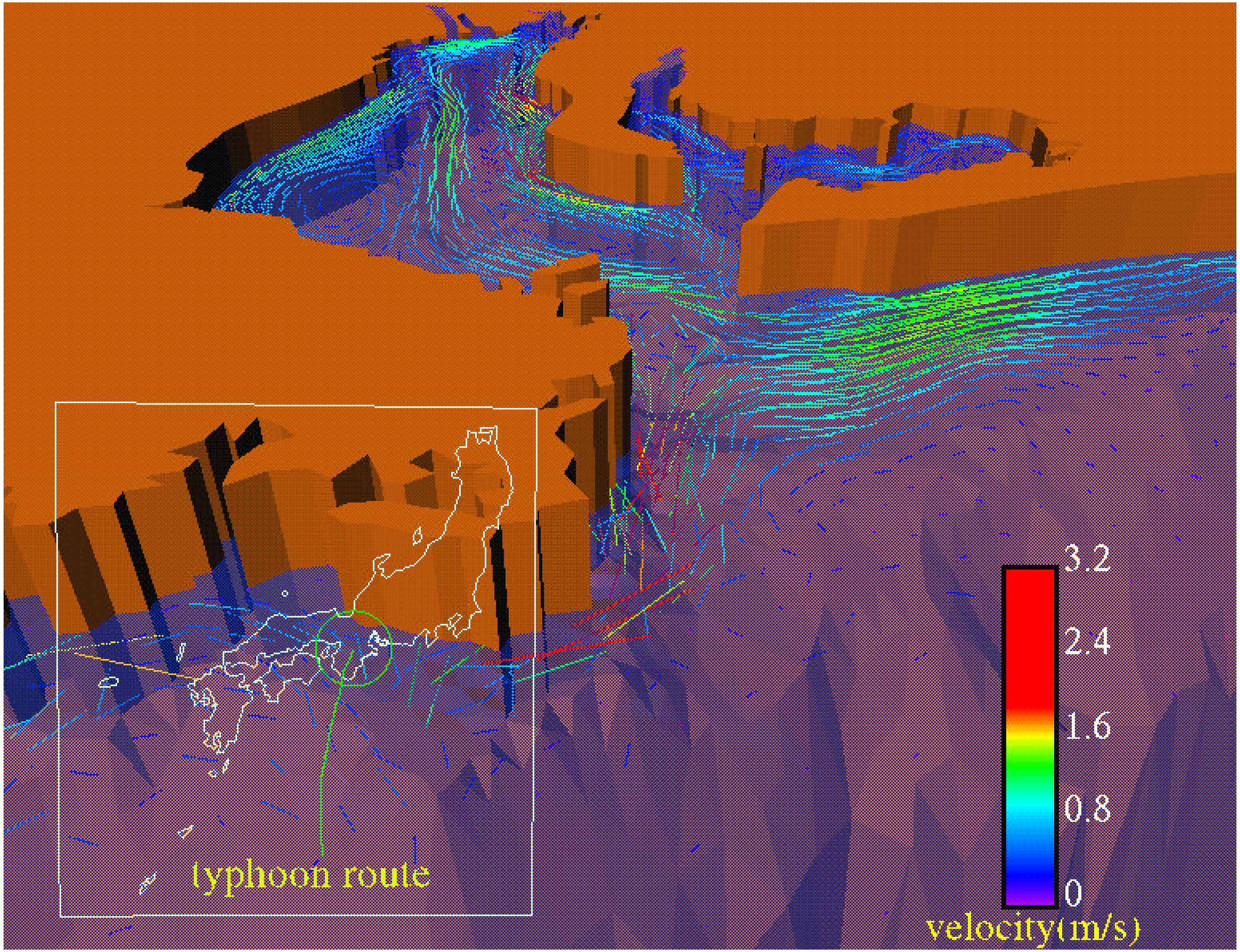
$$\frac{\partial \zeta}{\partial t} + \frac{\partial}{\partial x_i}[(h + \zeta)U_i] = 0$$

$$\frac{\partial U_i}{\partial t} + U_j \frac{\partial U_i}{\partial x_j} + g\frac{\partial \zeta}{\partial x_i} - \frac{\partial}{\partial x_j}\left[A_h\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right)\right] + \frac{\tau_{3i}^{b}}{h + \zeta} - \frac{\tau_{3i}^{s}}{h + \zeta} = 0$$

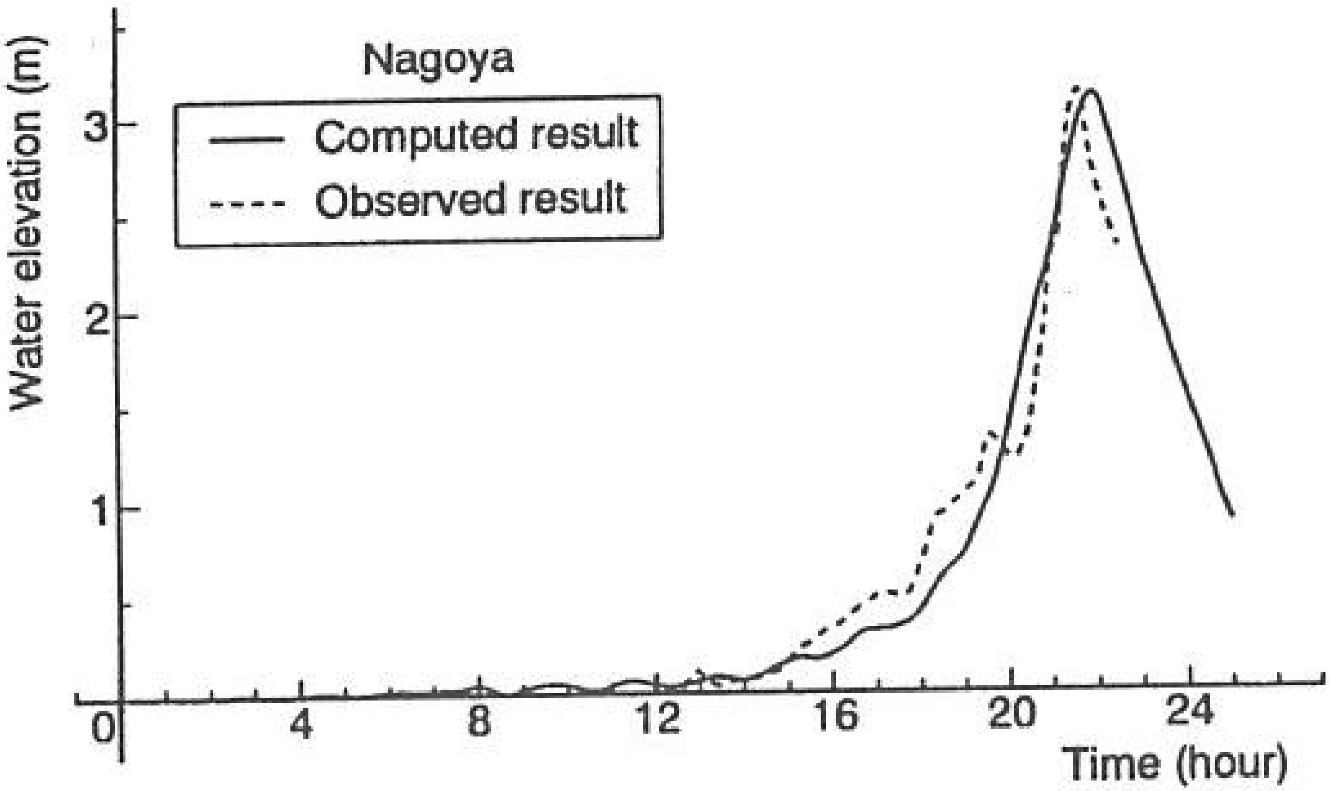


where,

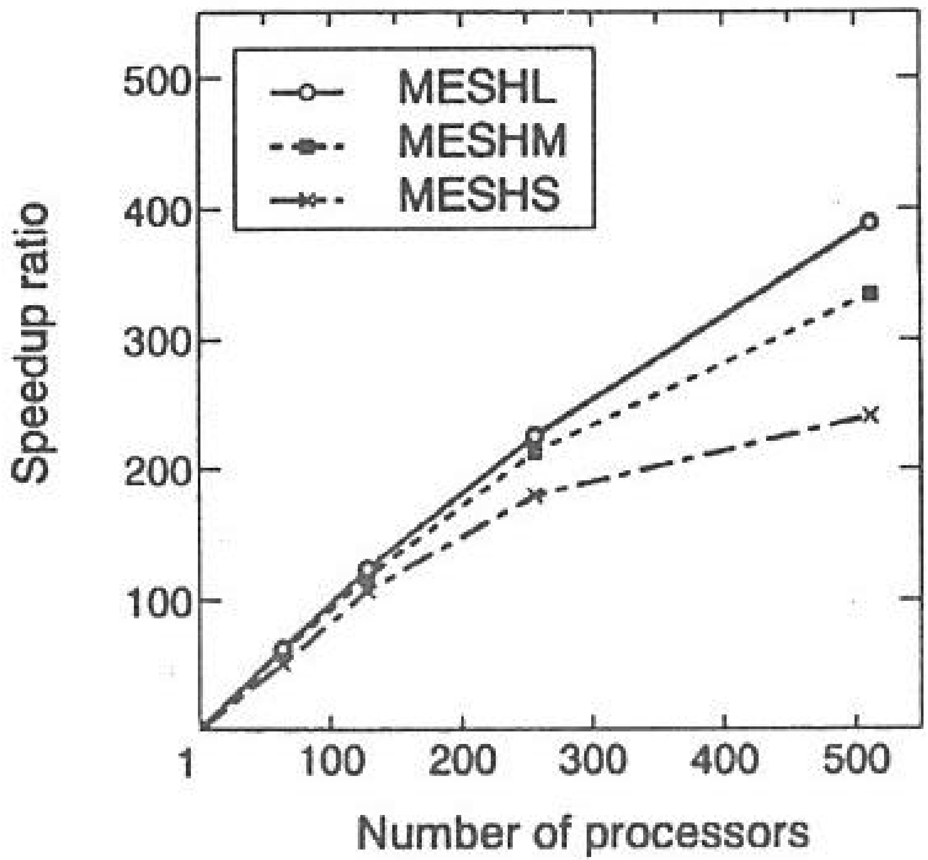
- U_i : mean velocity
- ζ : water elevation
- h : water depth
- g : gravity acceleration
- A_h : horizontal eddy viscosity coefficient
- τ_{3i}^{b} : bottom shear stress
- τ_{3i}^{s} : surface shear stress


typhoon route
3.2
2.4
1.6
0.8
0
velocity(m/s)

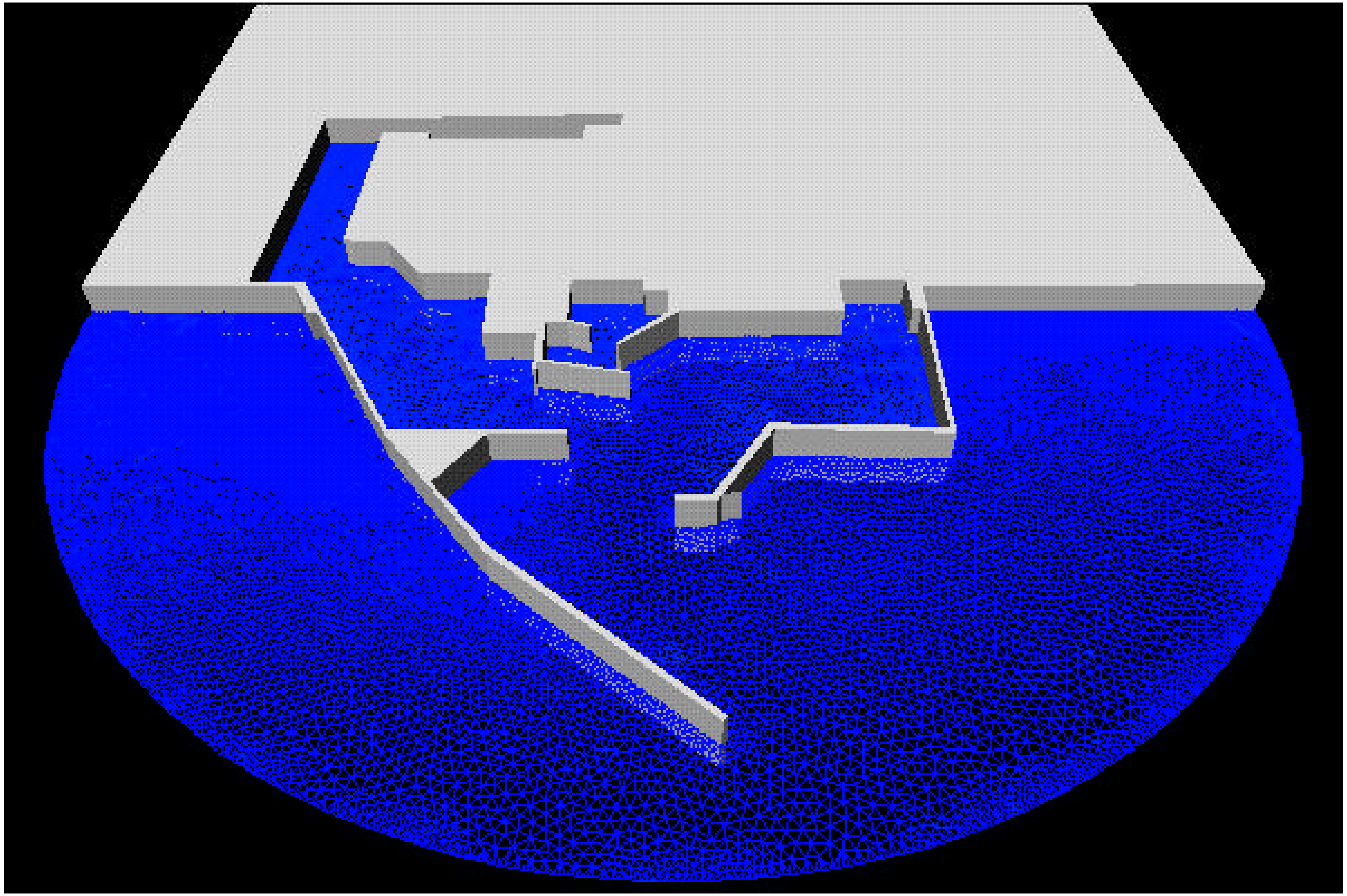
Comparison between computed and observed results at Nagoya

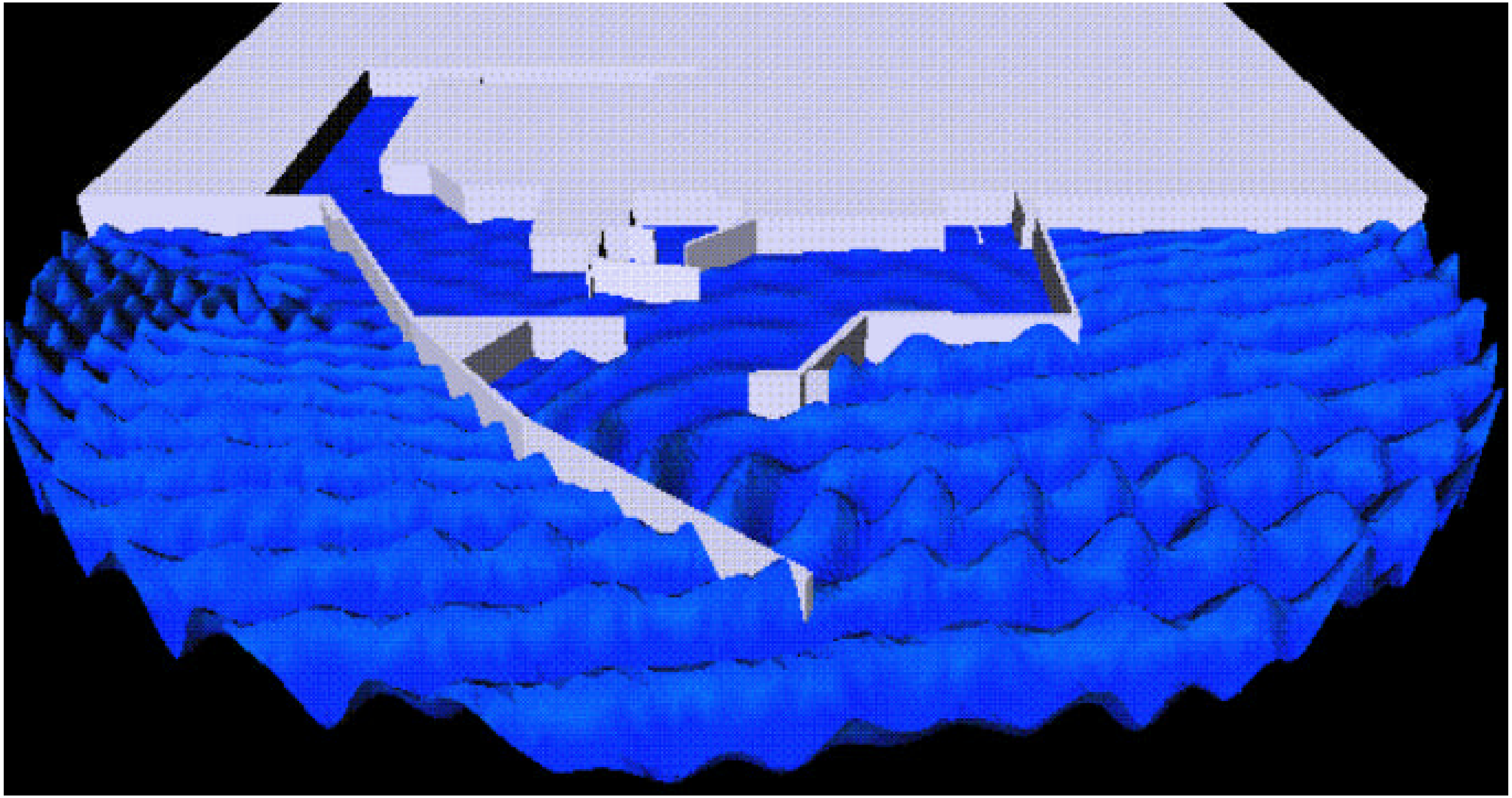


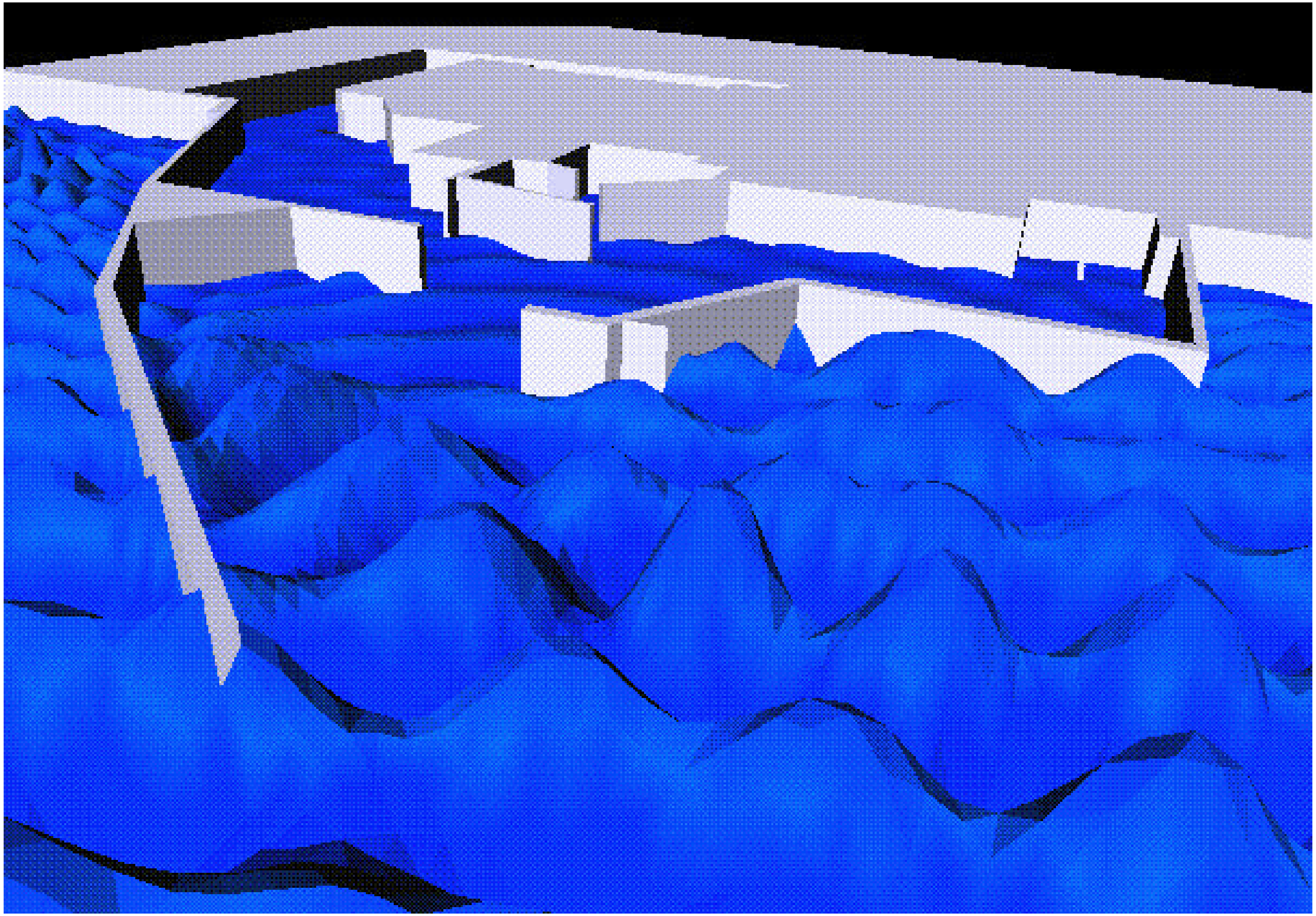
Speed-up ratio



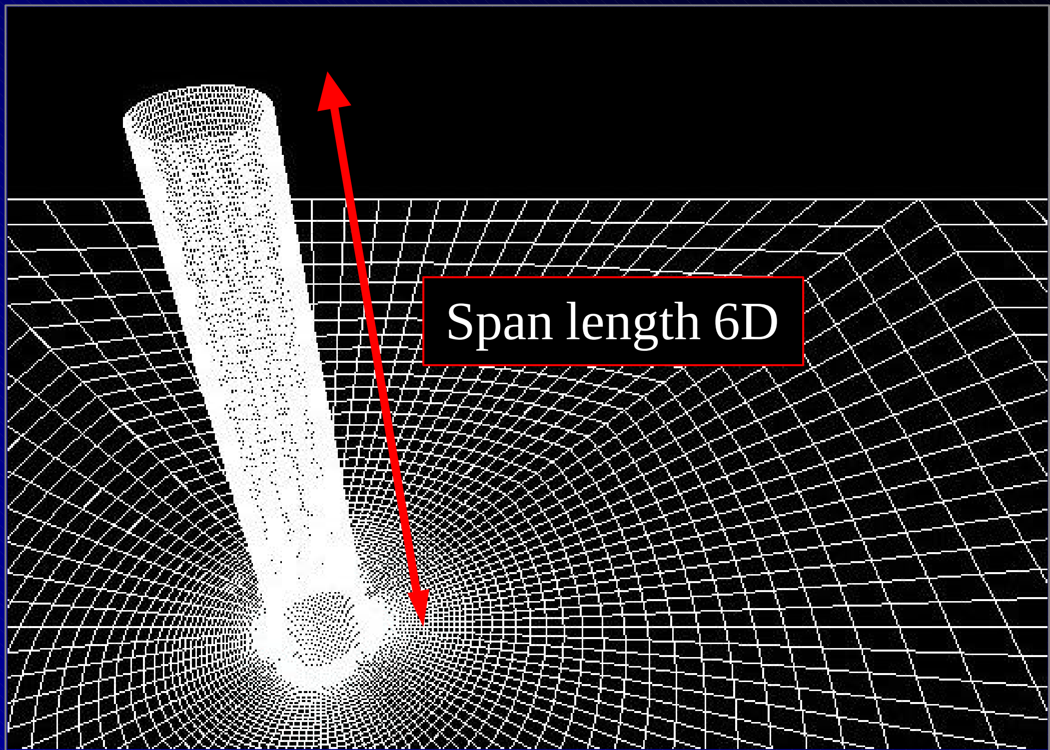
$$\text{Speed-up ratio} = \frac{\text{Computational time for one PE}}{\text{Computational time for N PEs}}$$







Finite Element Mesh



Re=1000

2D-mesh

Elements:7,089
Nodes:7,213
Min. mesh size :0.001D

120 slices

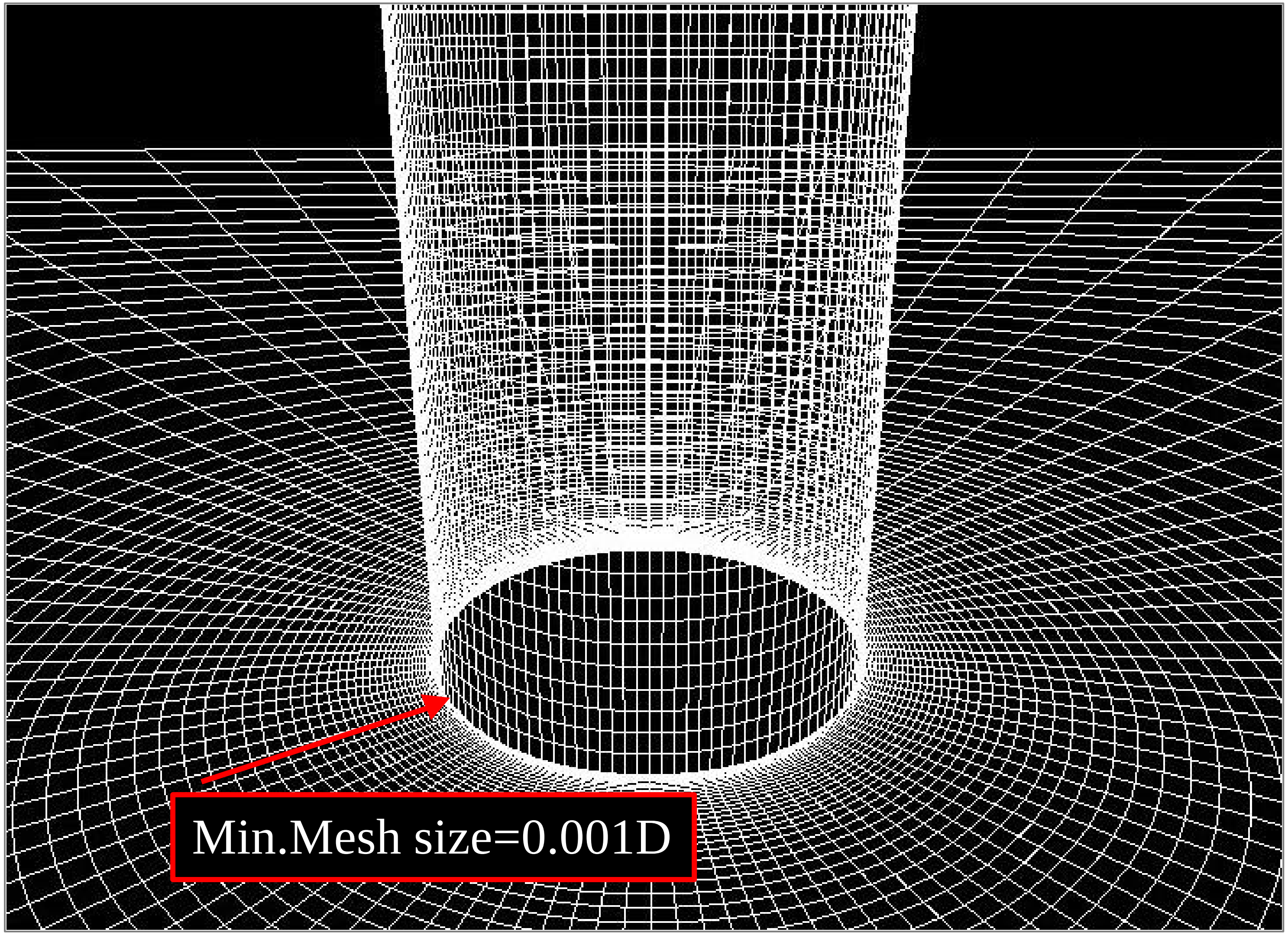
3D-mesh

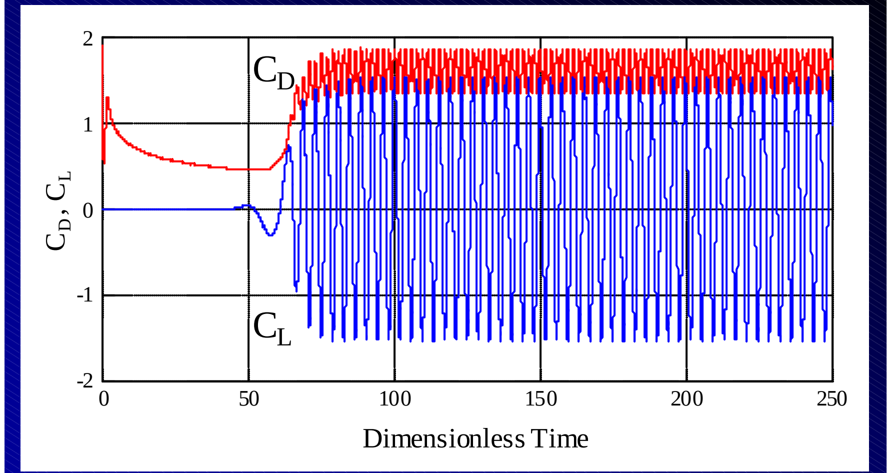
Span length 6D

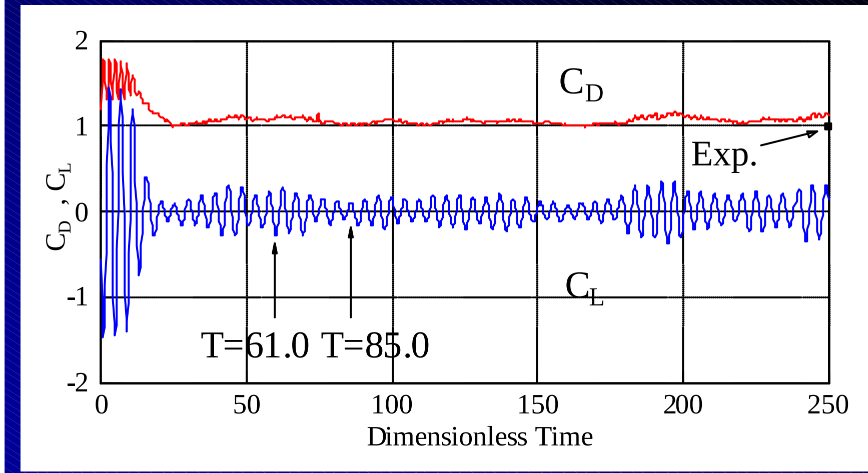
Elements:851,760
nodes:872,773

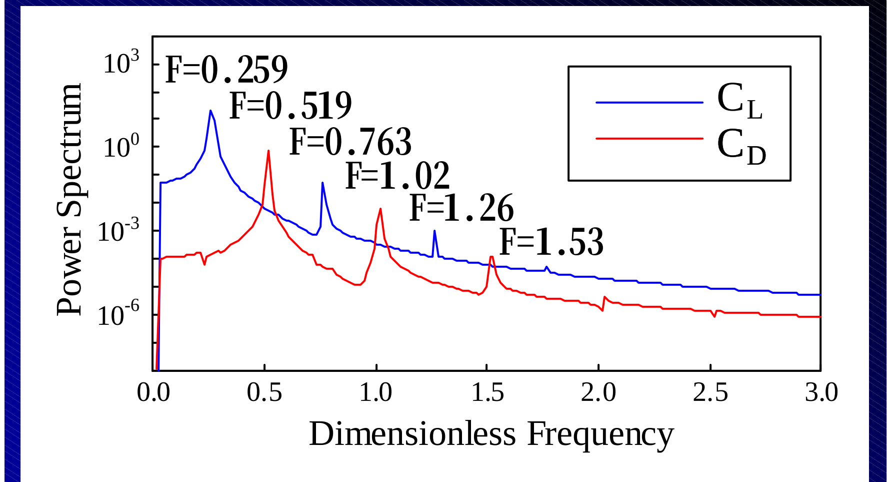
Slice length:0.05D

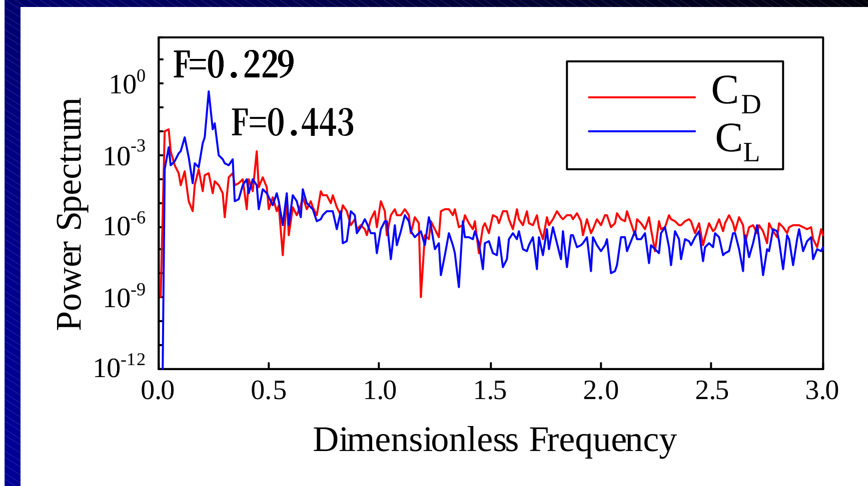
Finite element mesh around a circular cylinder





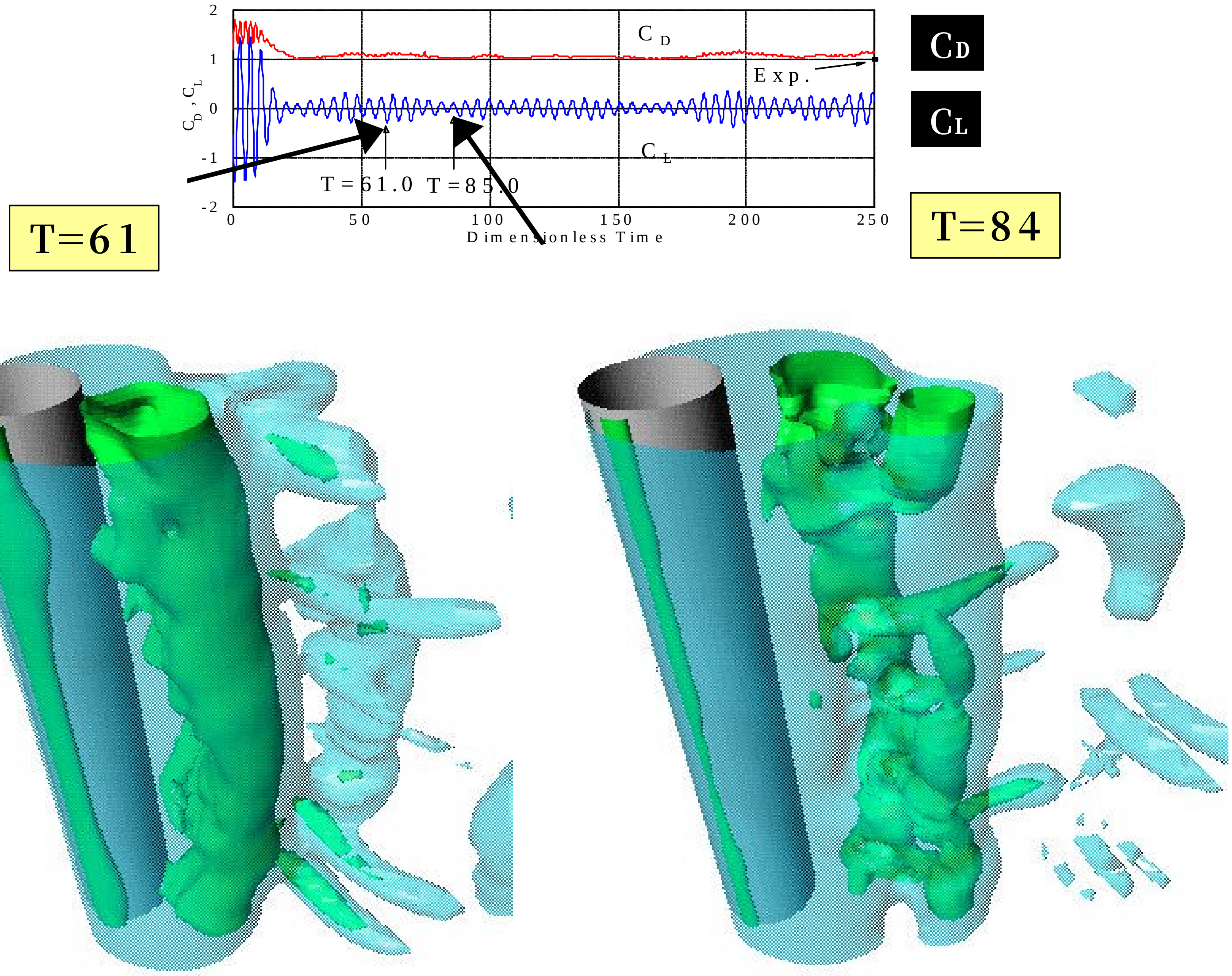






2D analysis

3D analysis



C D
C L
Exp.
T = 61.0
T = 85.0
C D , C L
Dimensionless Time
CD
CL
T=61
T=84

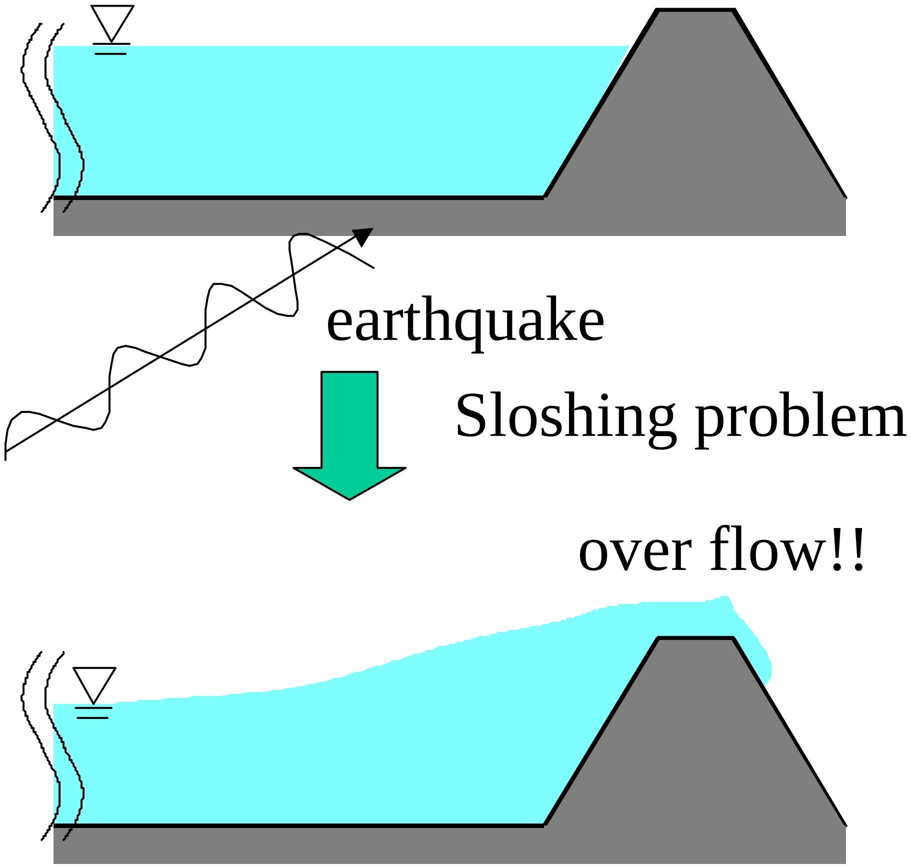
Parallel Finite Element Analysis of Free Surface Flows Using PC Cluster

Kazuo Kashiyama, Seizo Tanaka, Katsuyuki Sue and Masaaki Sakuraba
Chuo University, Tokyo, Japan

Topics

- Introduction
- Governing Equations and Stabilized FEM
- PC Cluster Parallel Computing
- Numerical Examples
  Sloshing of Rectangular Tank and Actual Dam
- Conclusions

Introduction



Purpose:
Development of a useful numerical method to evaluate the safety for sloshing of tank and dam by earthquake

Present Approach:
Navier-Stokes Equation
ALE-Stabilized FEM
PC Cluster Parallel Computing

Governing Equations

$$\rho\left(\frac{\partial u_i}{\partial t} + u_j\frac{\partial u_i}{\partial x_j} - f_i\right) - \frac{\partial \sigma_{ij}}{\partial x_j} = 0$$

$$\frac{\partial u_i}{\partial x_i} = 0$$

$$\sigma_{ij} = -p\delta_{ij} + \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

Boundary Conditions

$$u_i = g \quad \text{on } \Gamma_g$$

$$\sigma_{ij} n_j = h_i \quad \text{on } \Gamma_h$$

Stabilized FEM(SUPG/PSPG)

$$
\begin{aligned}
&\int_{\Omega} w_i \, \rho \left(\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} - f_i \right) d\Omega + \int_{\Omega} \frac{\partial w_i}{\partial x_j} \sigma_{ij} \, d\Omega + \int_{\Omega} q_i \frac{\partial u_i}{\partial x_i} \, d\Omega \\
&+ \sum_{e=1}^{n_{el}} \int_{\Omega^e} \tau_m \left(u_k \frac{\partial w_i}{\partial x_k} + \frac{1}{\rho} \frac{\partial q}{\partial x_i} \right) \cdot \left\{ \rho \left(\frac{\partial u_i}{\partial t} + (u_j) \frac{\partial u_i}{\partial x_j} - f_i \right) - \frac{\partial \sigma_{ij}}{\partial x_j} \right\} d\Omega^e \\
&+ \sum_{e=1}^{n_{el}} \int_{\Omega^e} \tau_c \frac{\partial w_i}{\partial x_i} \, \rho \frac{\partial u_i}{\partial x_i} \, d\Omega^e \\
&= \int_{\Gamma_h} w_i \sigma_{ij} n_j \, d\Gamma_h
\end{aligned}
$$

where

$$
\tau_m = \left[\left(\frac{2}{\Delta t} \right)^2 + \left(\frac{2\|u_i\|}{h_e} \right)^2 + \left(\frac{4\nu}{h_e^2} \right)^2 \right]^{-\frac{1}{2}}
$$

$$
\tau_c = \frac{h}{2} \|u_i\| \xi(Re_e)
$$

Finite Element Equations

$$(M + M_{é})\frac{\partial u_i}{\partial t} + (K(\tilde{u}_j) + K_{é}(\tilde{u}_j))u_i$$

$$- (C - C_{é})\frac{1}{\rho}p + \text{ó}Su_i = (N + N_{é})f_i$$

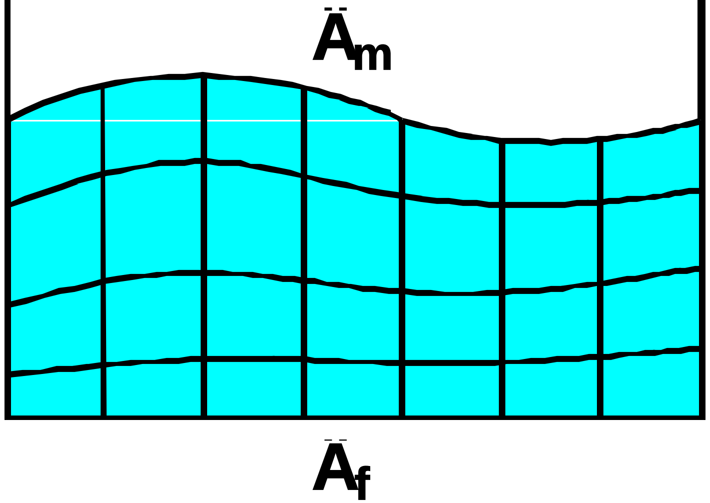
$$C^T u_i + M_{"}\frac{\partial u_i}{\partial t} + K_{"}(\tilde{u}_j)u_i$$

$$- N_{"}f_i + C_{"}\frac{1}{\rho}p = 0$$

↓

$$\begin{bmatrix} \frac{M + M_{é}}{\Delta t} & -(C - C_{é}) \\ C^T + \frac{M_{"}}{\Delta t} & C_{"} \end{bmatrix} \begin{bmatrix} u_i^{n+1} \\ \frac{1}{\rho}p^{n+1} \end{bmatrix} = \begin{bmatrix} b_i^n \\ d_i^n \end{bmatrix}$$

Rezoning and Remeshing



$$\frac{\partial H}{\partial t} = -u_s \frac{n_1}{n_3} - v_s \frac{n_2}{n_3} + w_s$$

$$\frac{\partial^2 \phi}{\partial x_i^2} = 0$$

$$\phi = \Delta H \quad \text{on } \Gamma_m$$

$$\phi = 0 \quad \text{on } \Gamma_f$$

Bi-CGSTAB Method

$$Ax = b$$

Initialization

$$r_0 = b - Ax_0 = b - \underbrace{\sum_e A^{(e)} x_0}_{②}$$

$$p_0 = r_0$$

Iteration

$$q_k = Ap_k = \underbrace{\sum_e A^{(e)} p_k}_{②}$$

$$\alpha_k = \underbrace{(r_0, r_k)}_{①} / \underbrace{(r_0, q_k)}_{①}$$

$$t_k = r_k - \alpha_k q_k$$

$$s_k = At_k = \underbrace{\sum_e A^{(e)} t_k}_{②}$$

$$\omega_k = \underbrace{(s_k, t_k)}_{①} / \underbrace{(s_k, s_k)}_{①}$$

$$x_{k+1} = x_k + \alpha_k p_k + \omega_k t_k$$

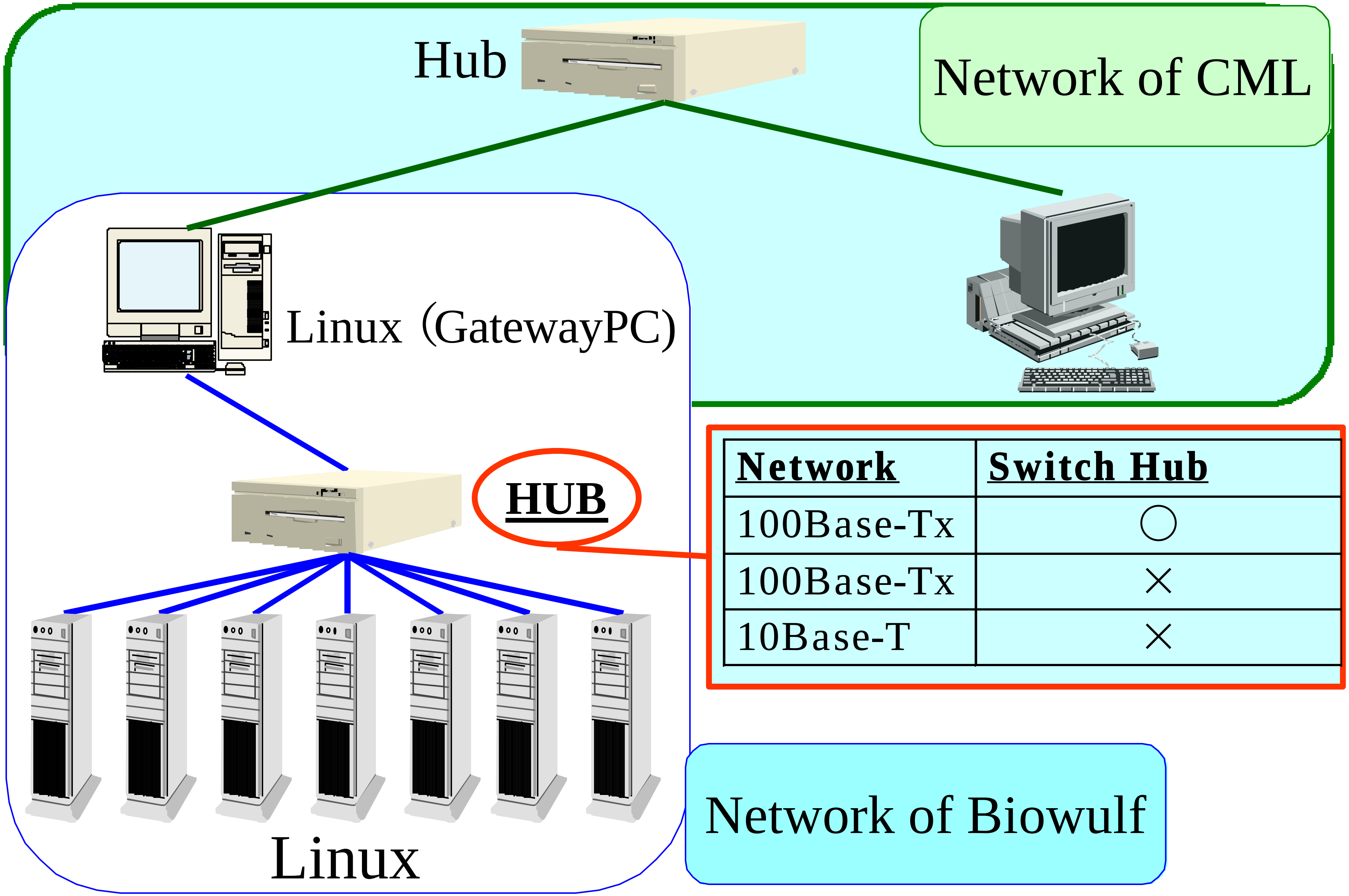
$$r_{k+1} = t_k - \omega_k q_k$$

$$\beta_k = \alpha_k / \omega_k \cdot \underbrace{(r_0, r_{k+1})}_{①} / \underbrace{(r_0, r_k)}_{①}$$

$$p_{k+1} = r_{k+1} + \beta_k (p_k - \omega_k q_k)$$

①:Global communication, ②:Neighboring communication

Network Configuration



Network	Switch Hub
100Base-Tx	○
100Base-Tx	×
10Base-T	×

Development of Parallel Computer

- Hardware

	PC
CPU	PentiumII 400MHz
Cache	512KB
RAM	512MB
NIC	DEC DC21x4x PCI (10/100Base-Tx)

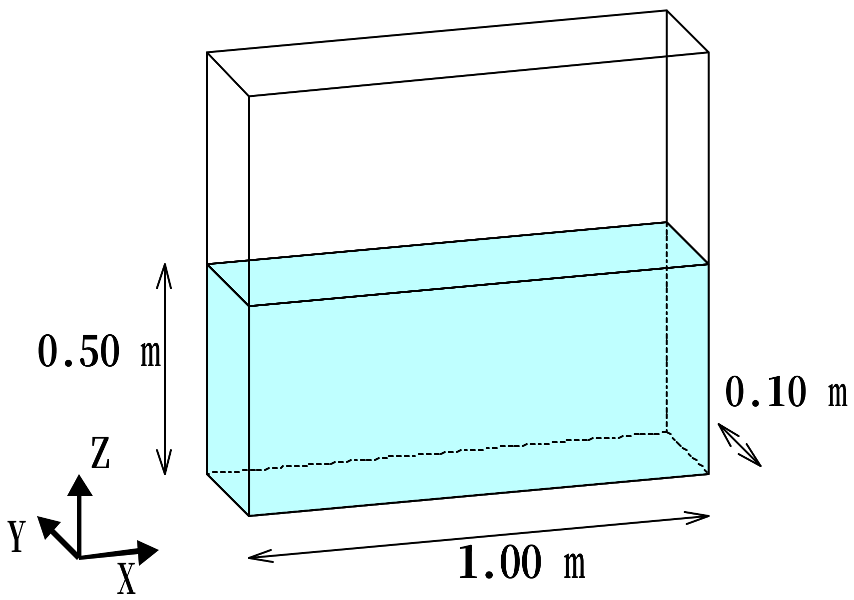
- Software

OS	Linux-2.0.34
Comm. Library	MPICH1.1.1

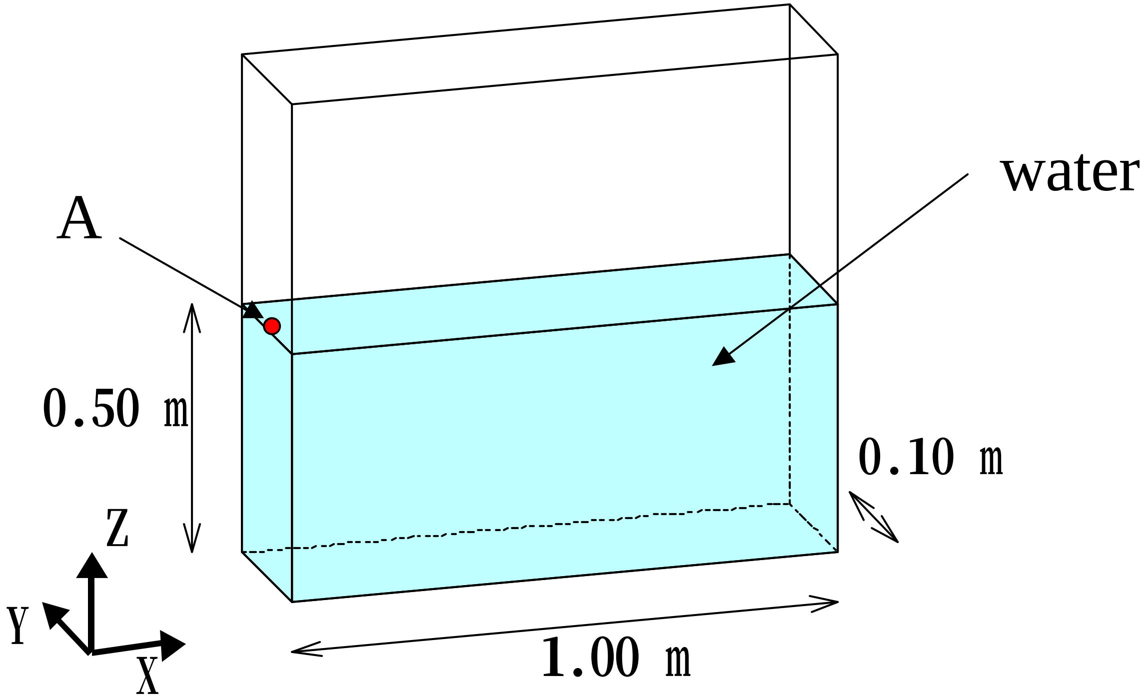
MPICH-A Portable Implementation of MPI（http://www-unix.mcs.anl.gov/mpi/mpich/index.html)

Numerical Examples

・Sloshing analysis of rectangular tank and actual dam
・PC cluster parallel computing



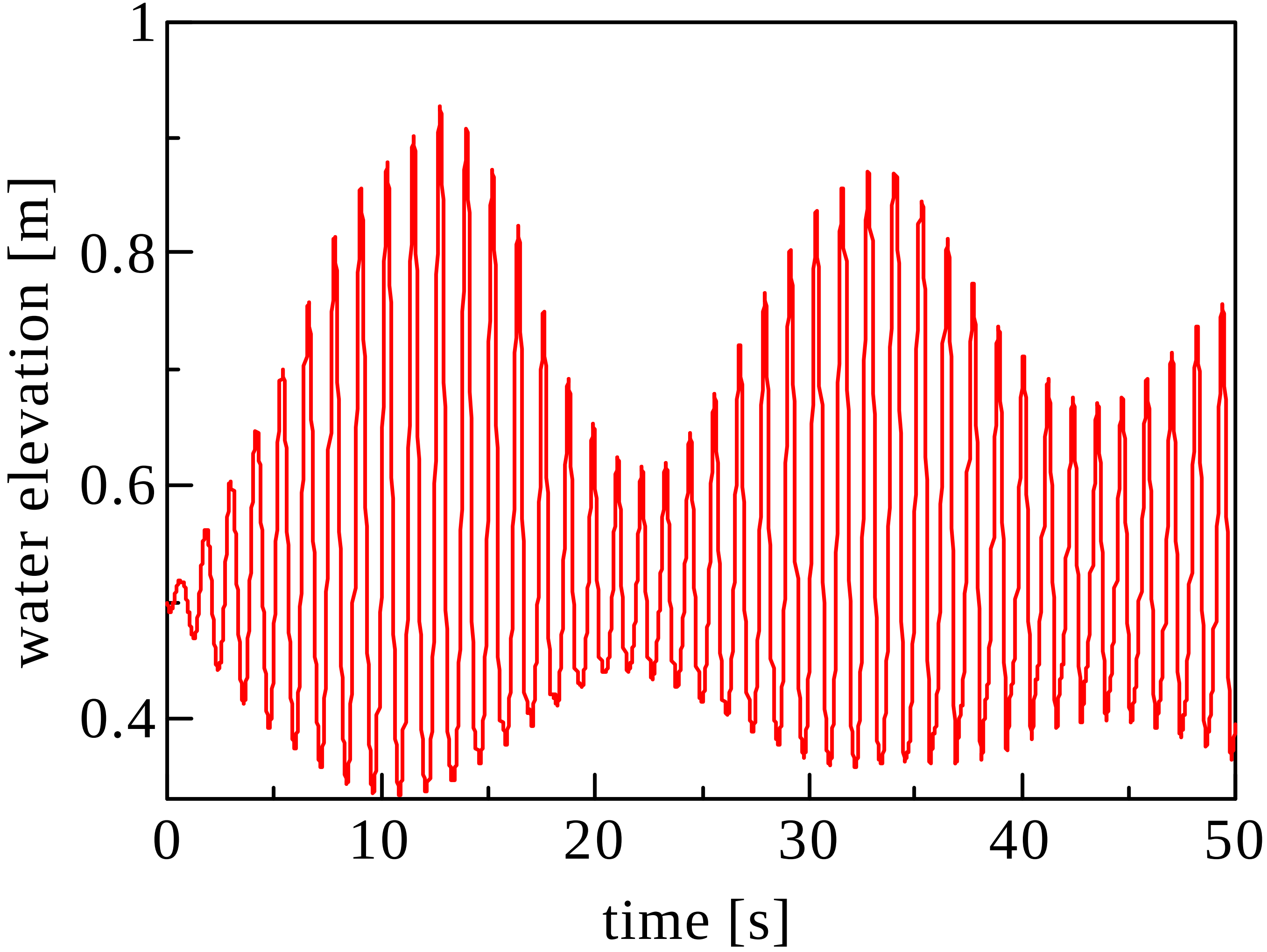
Numerical Example(1)



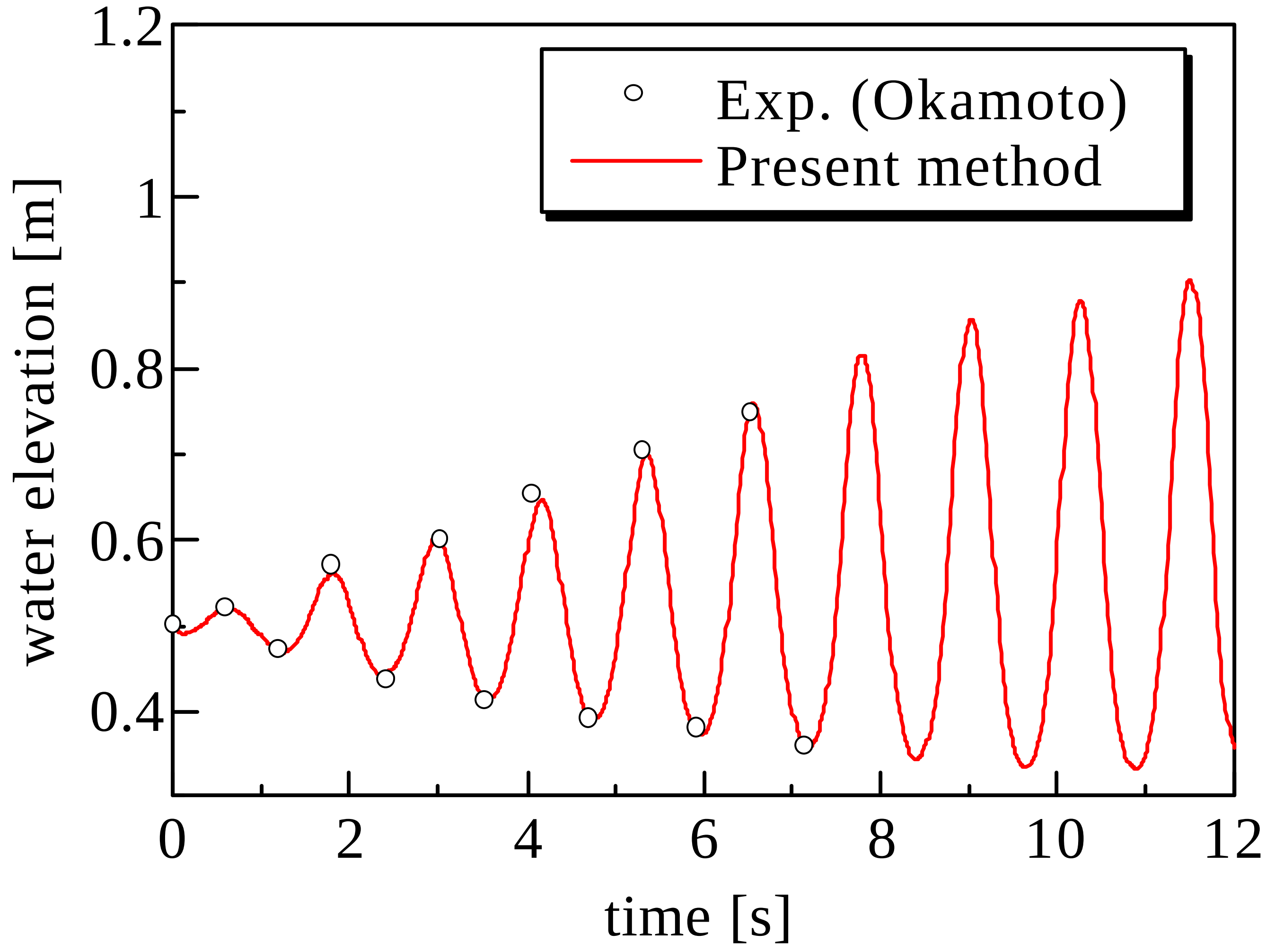
$f_x = A \sin \omega t$ (A=0.0093m, ω=5.311rad/sec)

(4,305 nodes 19,200 elements)

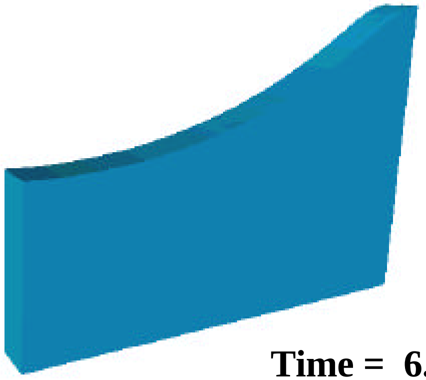
Time History of Water Elevation at Point A



Comparison of Water Elevation



Computed Results



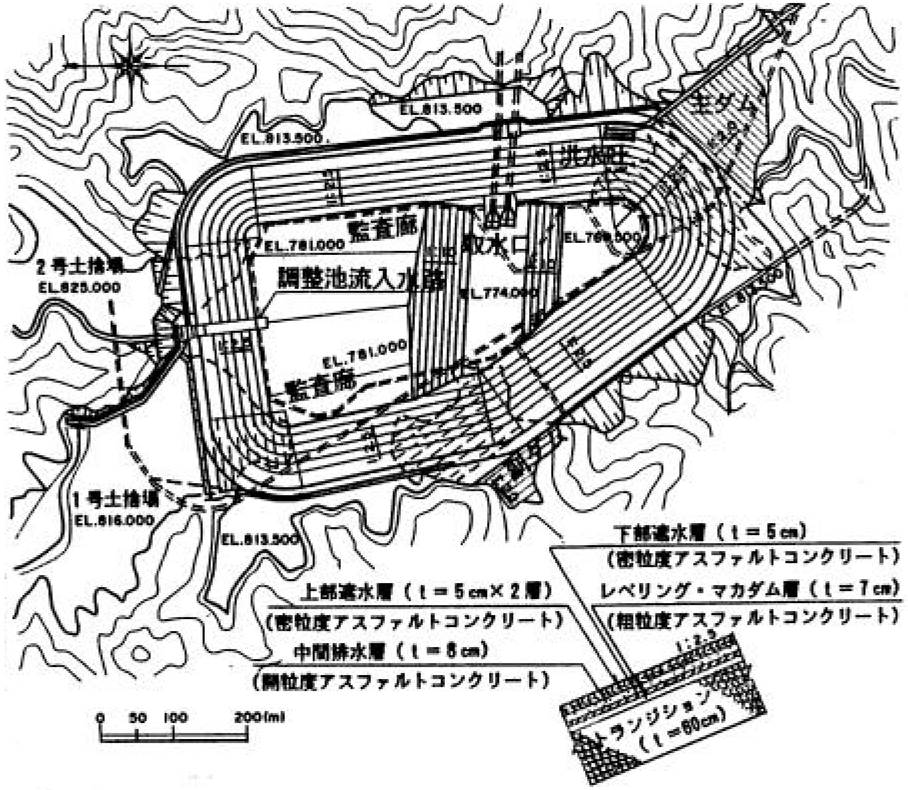
Time = 6.0 [s]

Time = 9.0 [s]

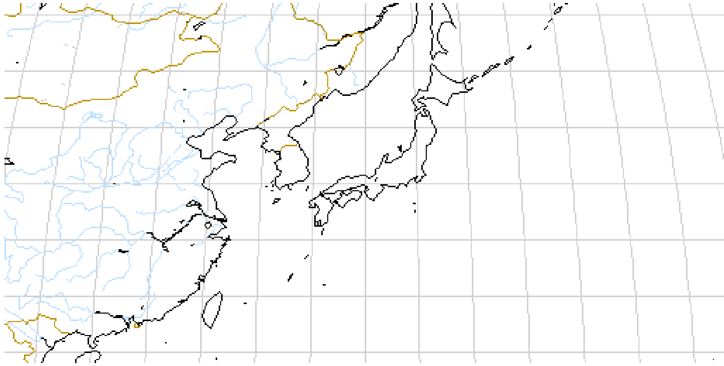
Time = 12.0 [s]

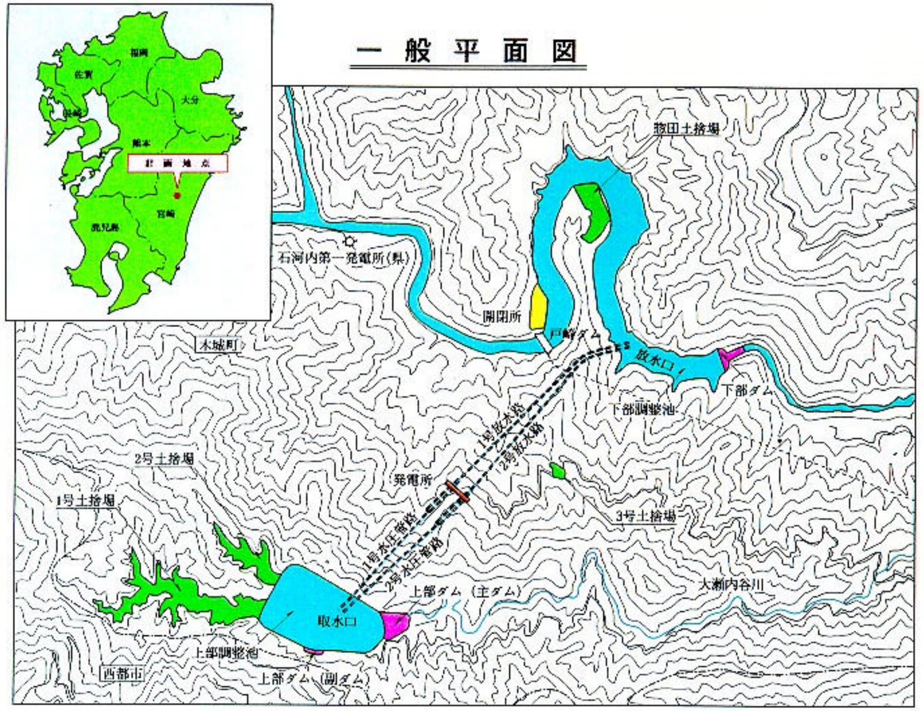
Time = 15.0 [s]

Numerical Example(2)



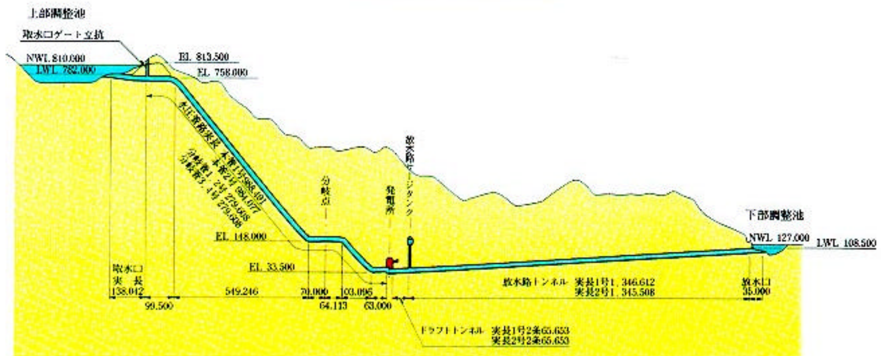
Dam for pumped-storage power generation





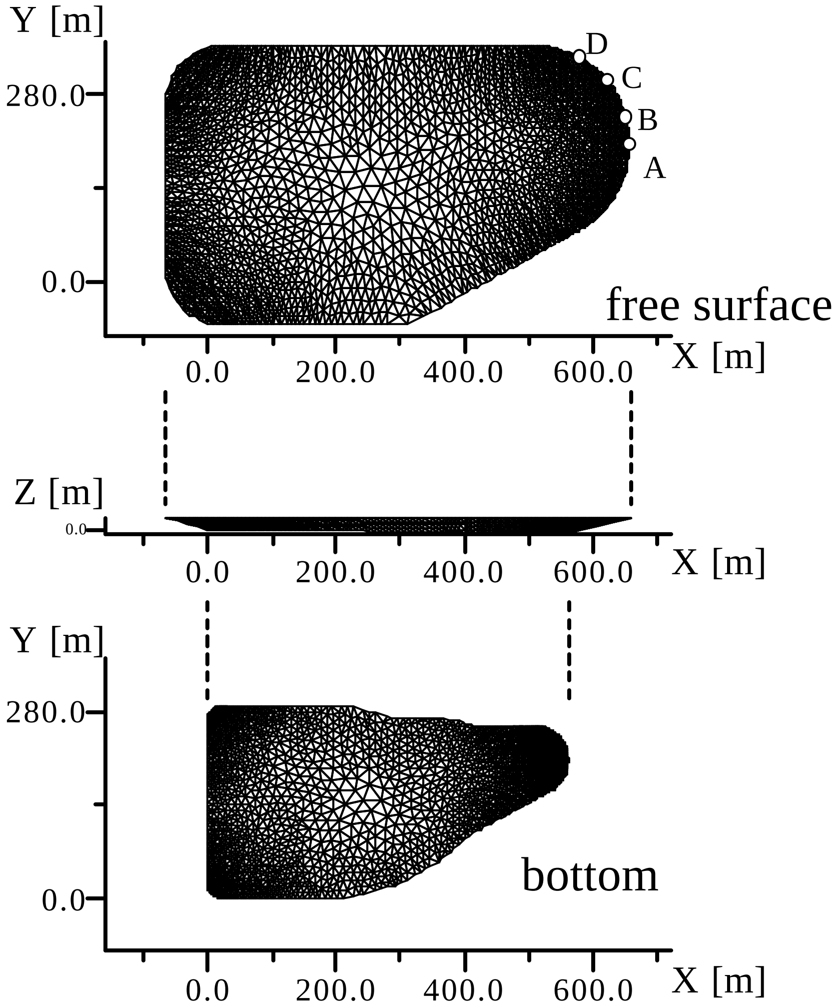
一般平面図
福岡
佐賀
長崎
大分
熊本
計画地点
宮崎
鹿児島
物田土捨場
石河内第一発電所(県)
開閉所
戸崎ダム
木城町
放水口
下部ダム
下部調整池
1号放水路
2号放水路
2号土捨場
発電所
1号土捨場
3号土捨場
1号水圧管路
2号水圧管路
上部ダム（主ダム）
大瀬内谷川
取水口
上部調整池
西都市
上部ダム（副ダム）

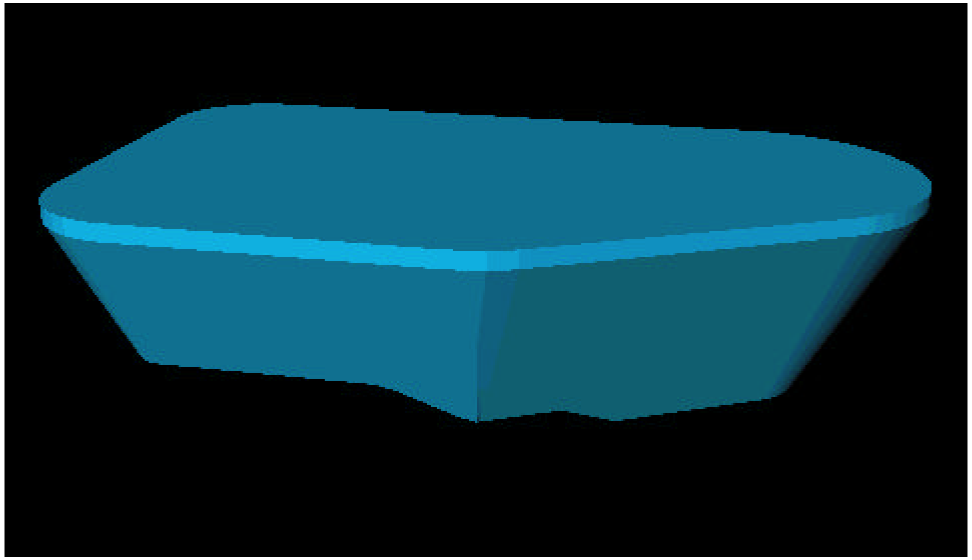
水路縦断面図



上部調整池
取水口ゲート立抗
NWL 810.000
LWL 782.000
EL 813.500
EL 758.000
分岐点
発電所
放水路サージタンク
EL 148.000
EL 33.500
取水口
実長
138.042
99.500
549.246
70.000
64.113
103.095
63.000
放水路トンネル 実長1号1, 346.612
実長2号1, 345.508
ドラフトトンネル 実長1号2条65.653
実長2号2条65.653
下部調整池
NWL 127.000
LWL 108.500
放水口
35.000

Finite Element Model

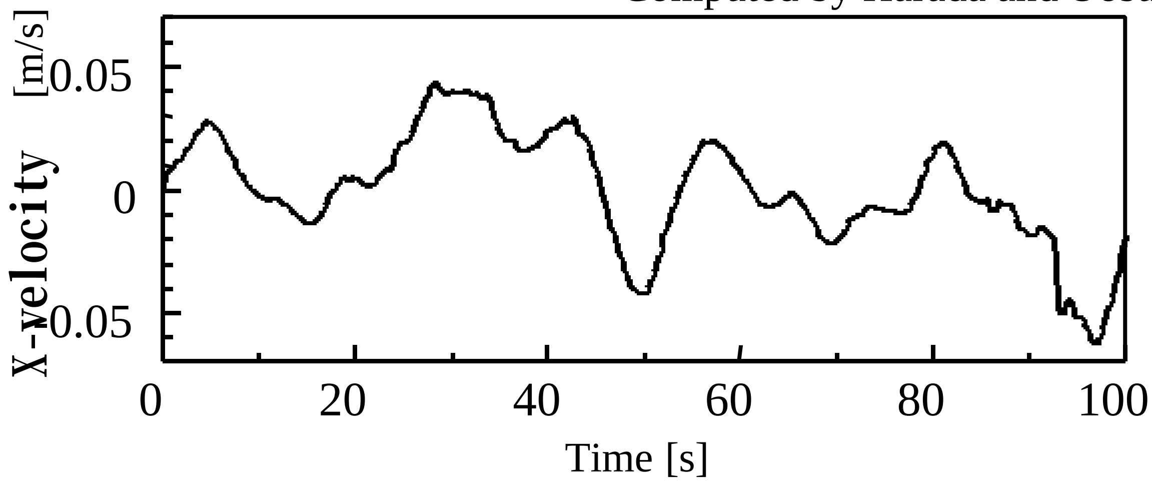


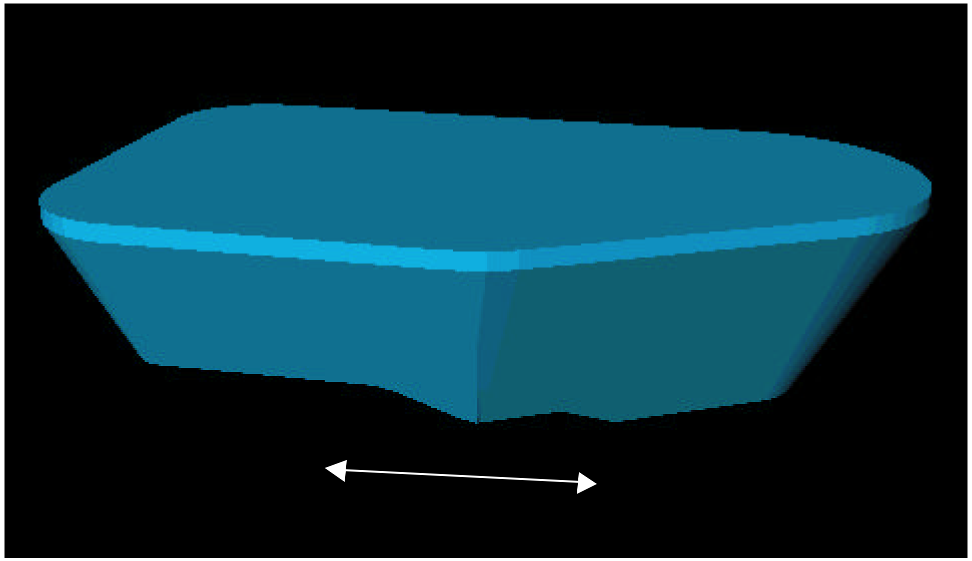


(elements:109,314, nodes:22,610)

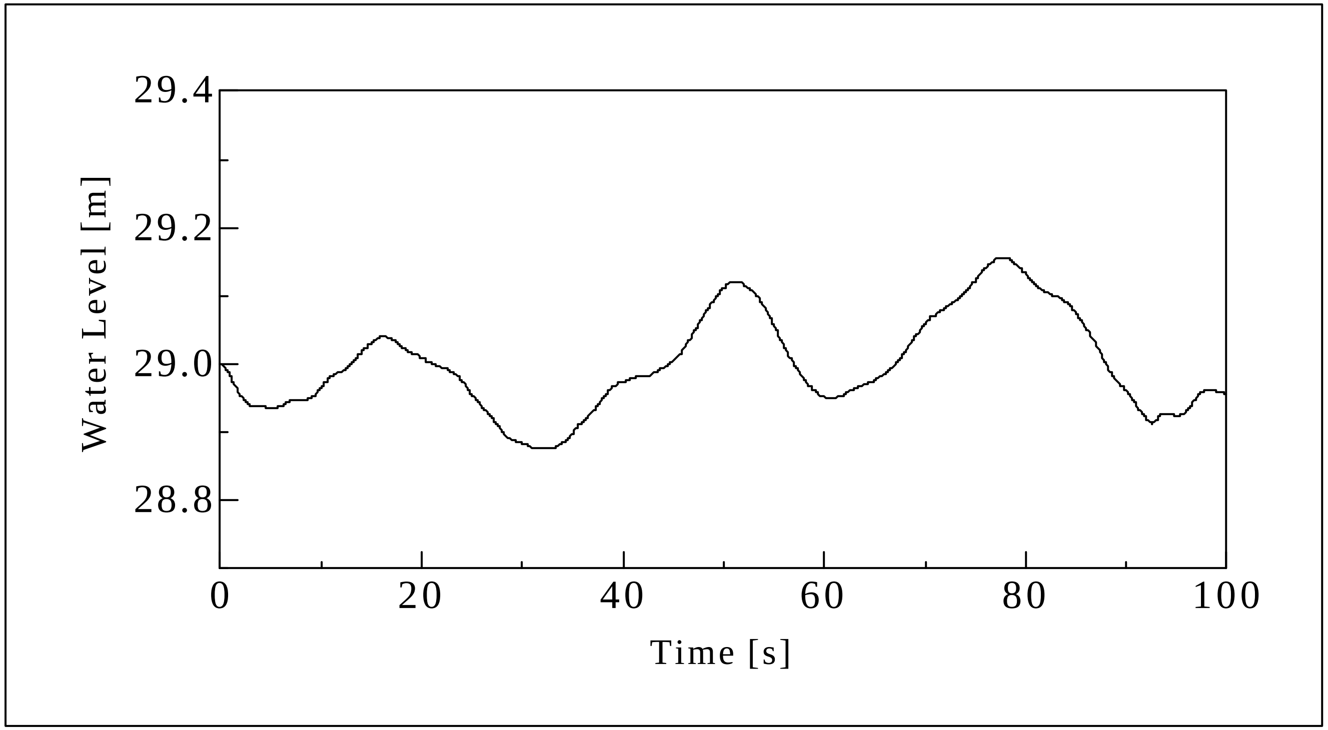
Earthquake Data (Input Ground Motion)

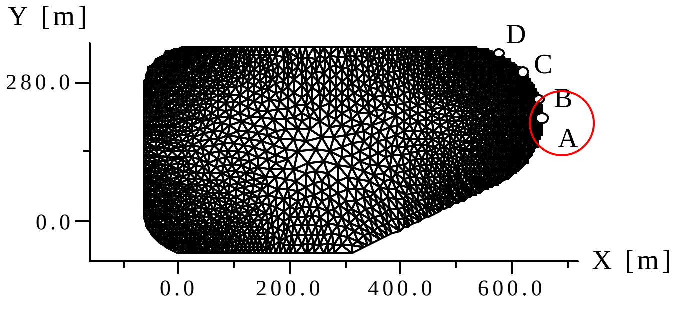
Computed by Harada and Oosumi

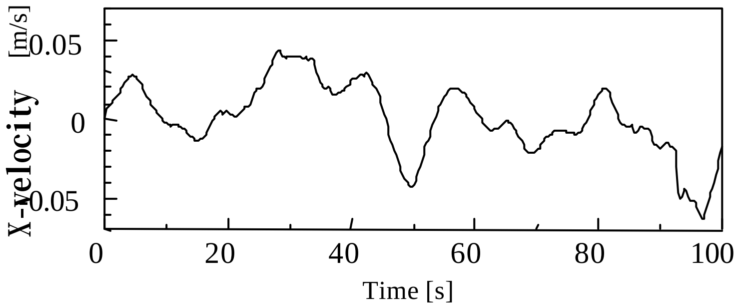




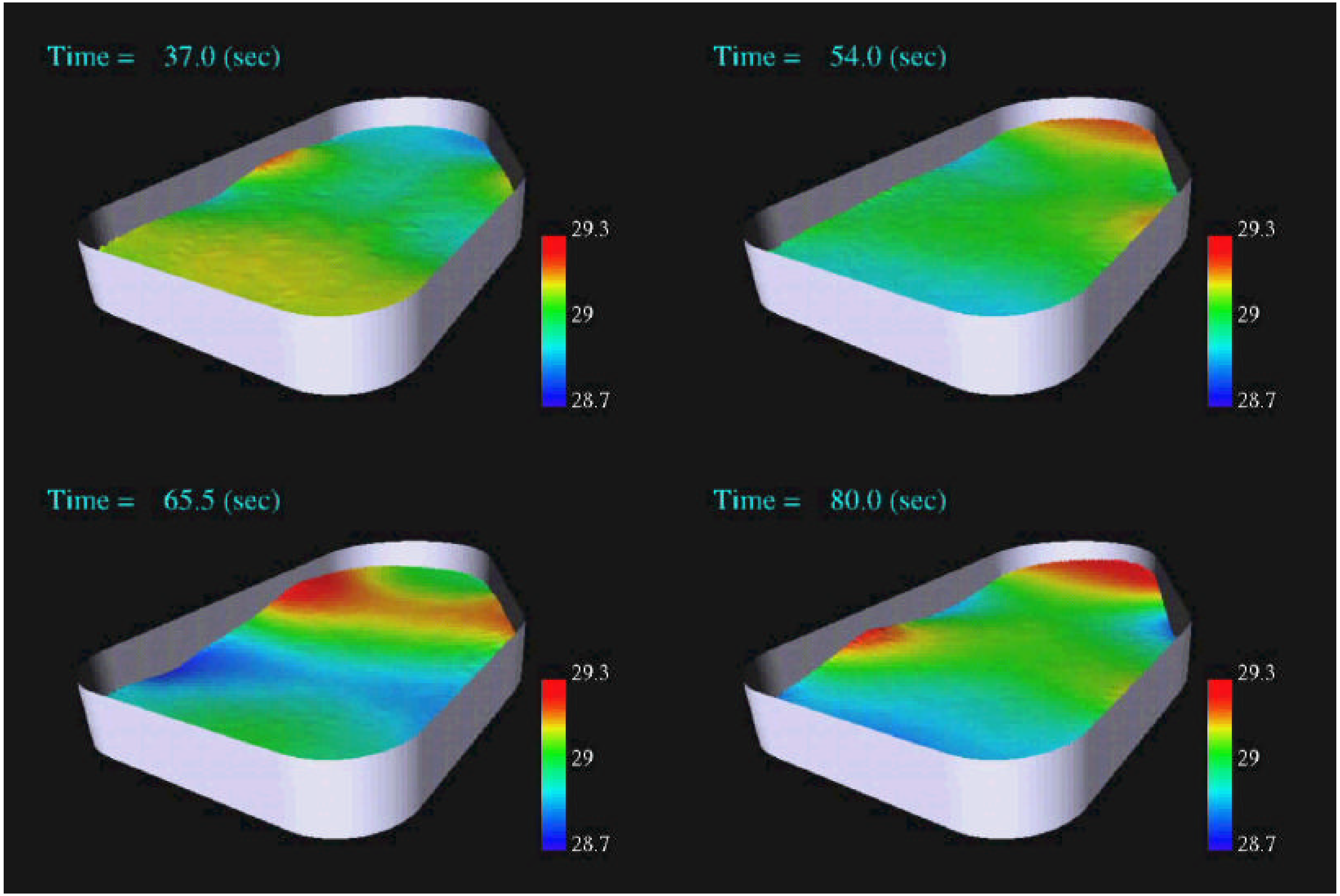
Computed Water Elevation at Point A







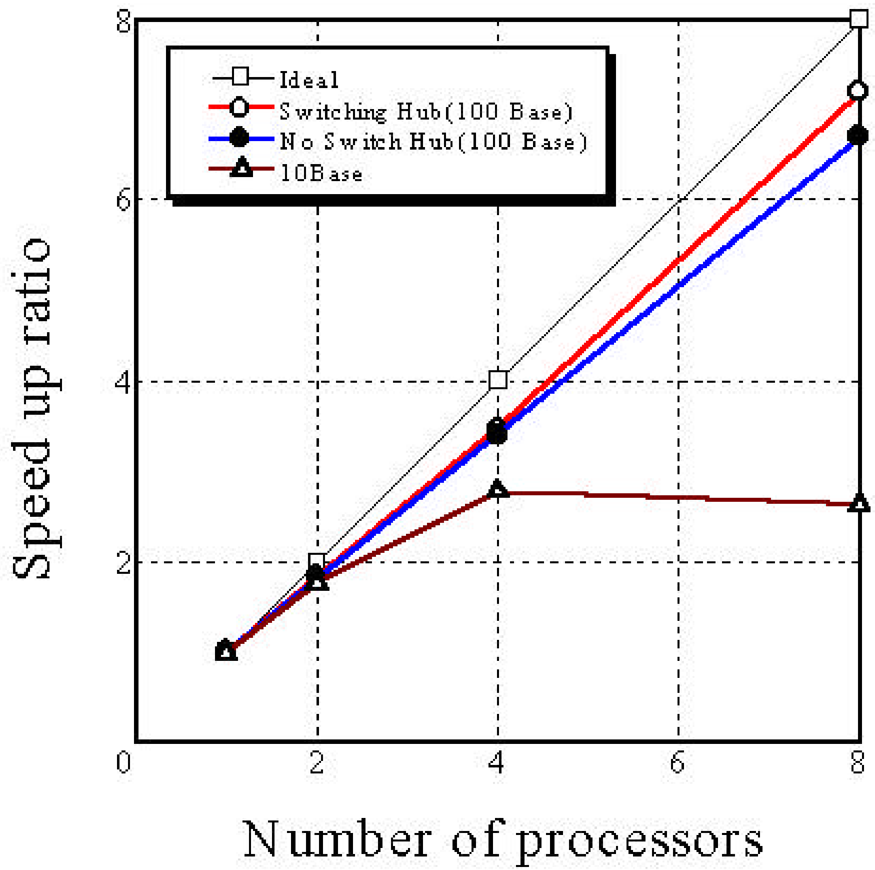
Computed Results

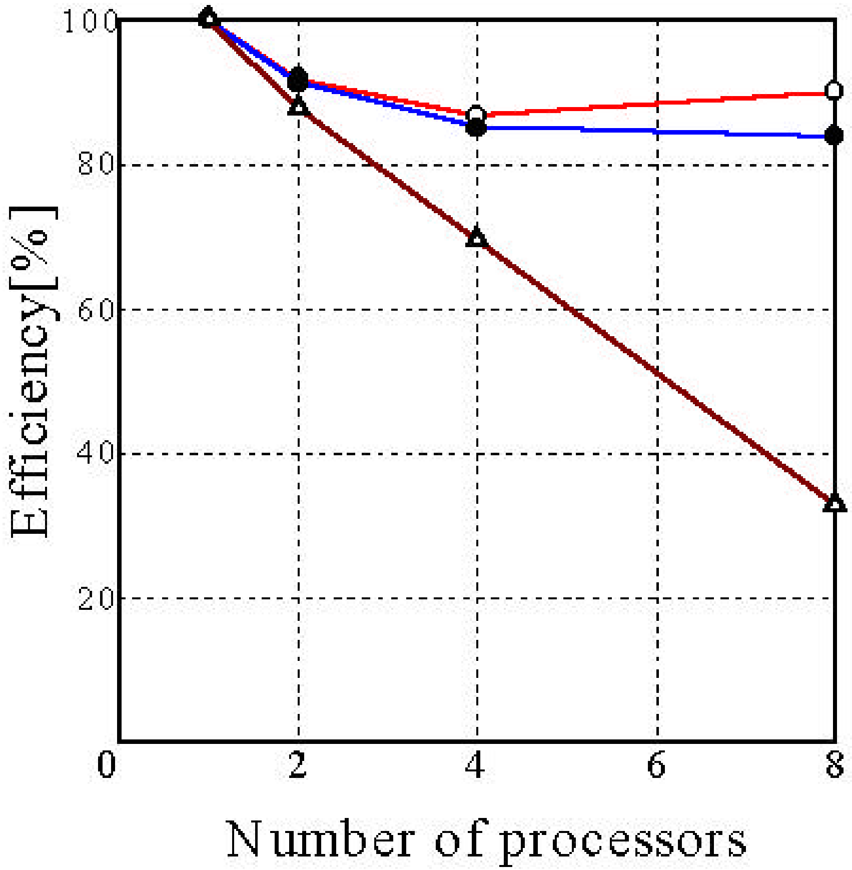


Comparison of Network Environment

	Accton 100Base-TX Switch Hub		Accton 100Base-TX No Switch Hub		Alied Telesis 10Base-T No Switch Hub	
PE	total time	comm.& wait	total time	comm.& wait	total time	comm.& wait
MESH (total number of nodes 22,610, total number of elements 109,314)						
1	3331.3	0.0	3331.3	0.0	3331.3	0.0
2	1812.0	39.1 (2.2%)	1826.1	50.8 (2.8%)	1897.3	121.2 (6.4%)
4	961.1	71.7 (7.5%)	979.1	89.4 (9.1%)	1197.5	287.4 (24.0%)
8	462.4	25.3 (5.5%)	497.0	57.1 (11.5%)	1269.6	698.8 (55.0%)

Performance of Parallel Computing

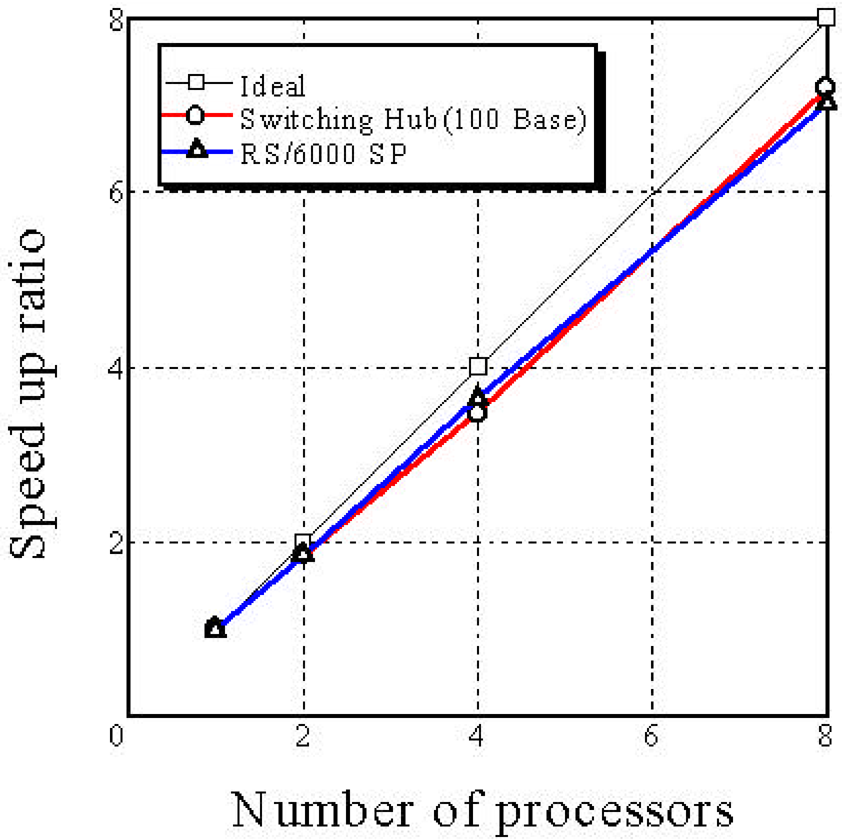


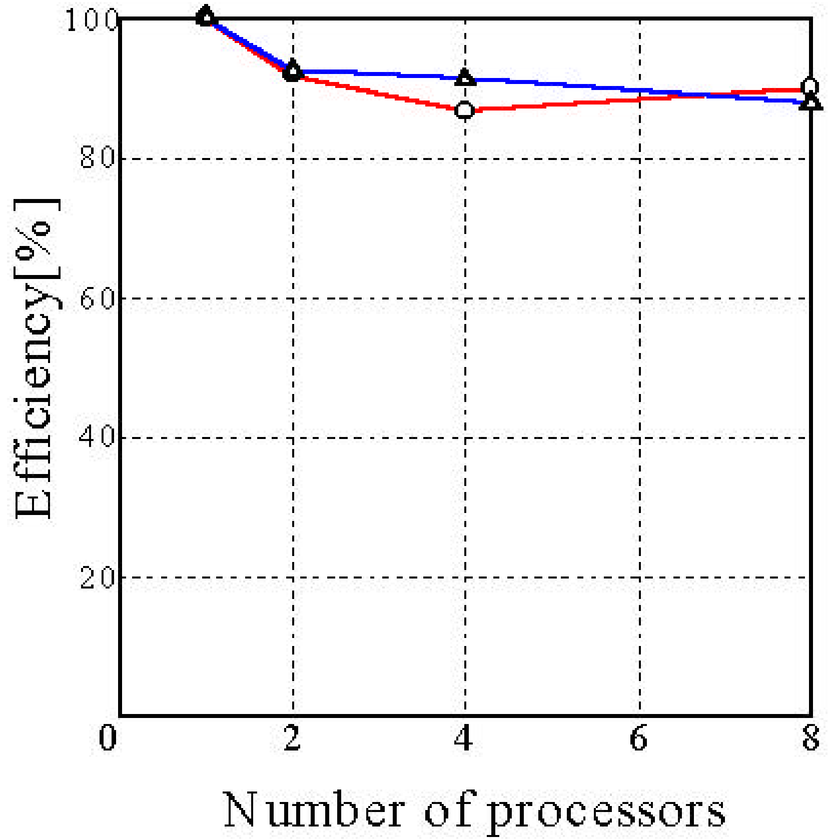


Comparison with RS6000/SP

	Accton 100Base-TX Switch Hub		RS 6000 / SP	
PE	total time	comm.&wait	total time	comm.&wait
MESH (total number of nodes 22,610, total number of elements 109,314)				
1	3331.3	0.0	2935.8	0.0
2	1812.0	39.1 (2.2%)	1586.7	6.6 (0.4%)
4	961.1	71.7 (7.5%)	805.3	56.1 (7.0%)
8	462.4	25.3 (5.5%)	417.8	34.7 (8.3%)

Comparison with IBM RS6000/SP





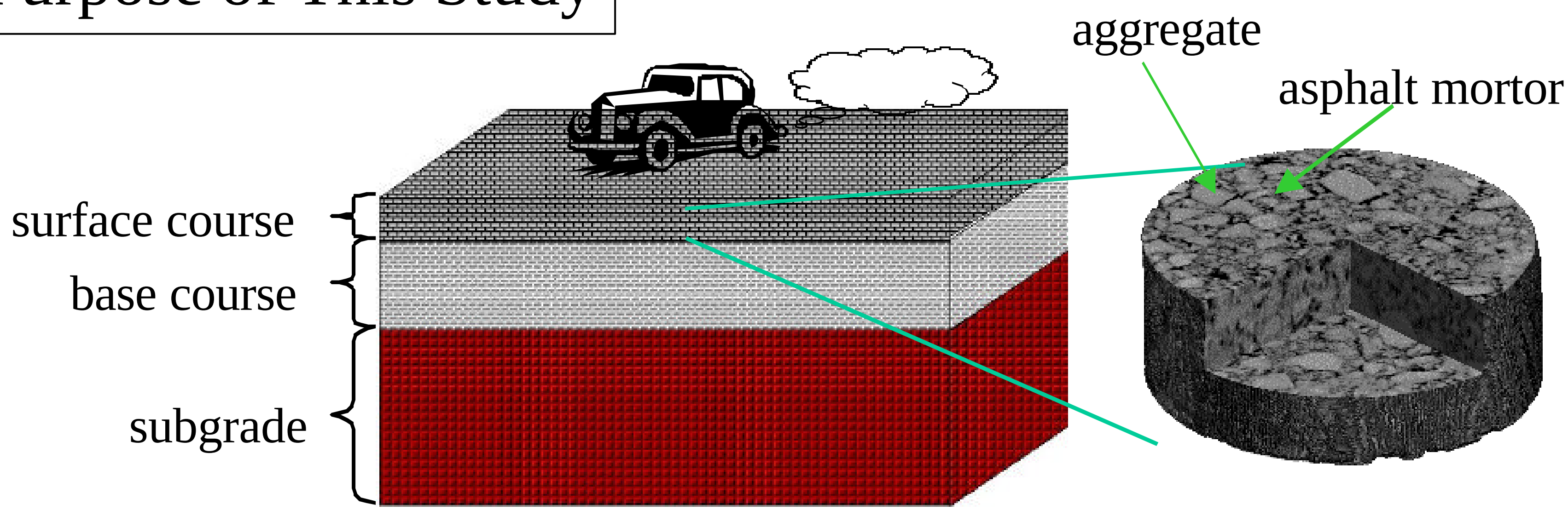
Parallel Finite Element Analysis of Asphalt Concrete Using Image-Base Modeling

Kazuo Kashiyama, Takaaki Kakehi(Chuo University)
Takashi Izumiya(Yachiyo Engineering Corporation)
Tomoyuki Uo(Kajima Corporation)
Kenjiro Terada(Tohoku University)

Outline

- Introduction
- Governing Equation
- Formulation of Homogenization
- Image-Base Modeling Using X-ray CT
- Parallel Implementation
- Numerical Analysis
- Conclusions

Purpose of This Study



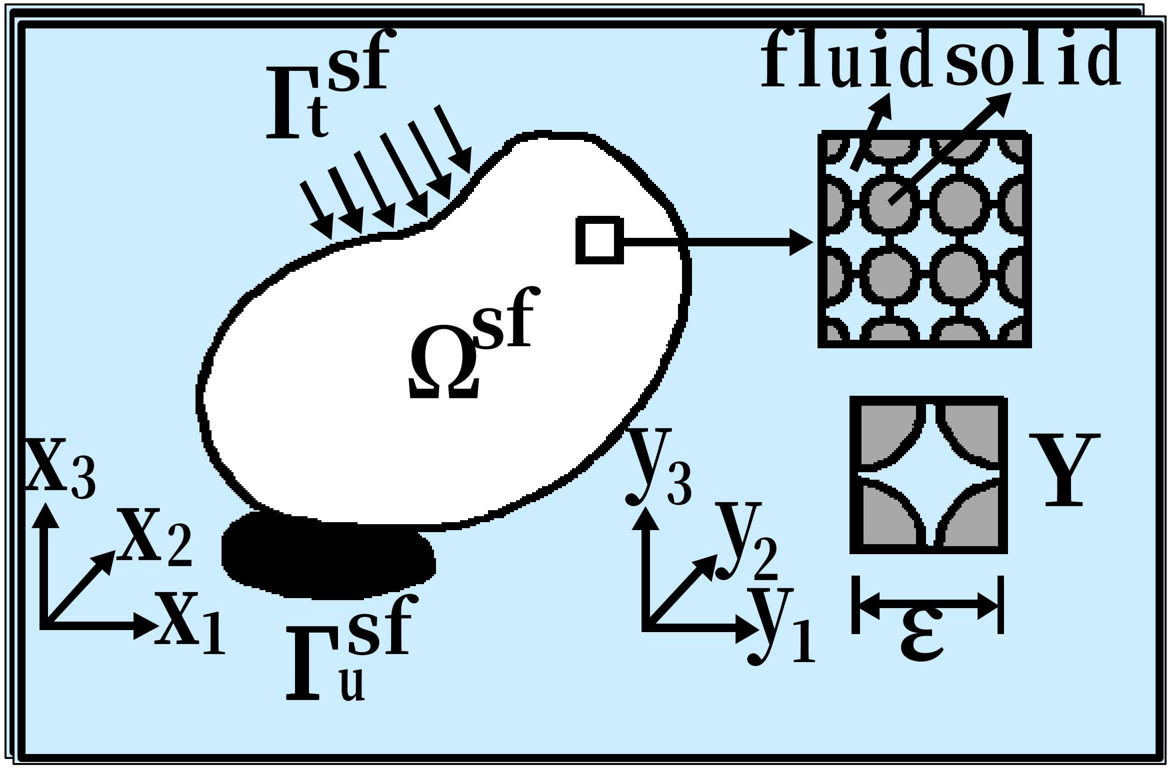
structure of pavement

・A parallel finite element method based on the homogenization theory for the visco-elastic analysis of asphalt concrete is presented.

・The accurate configuration of microstructure is modeled by the digital image obtained by the X-ray CT.

Homogenization Method

Solid-fluid mixtures with periodic microstructure



solid

Elastic body

fluid

Newtonian fluids
(Stokes flow)

Governing Equation

Equilibrium equation:

$$\frac{\partial \sigma^{\varepsilon}_{ij}}{\partial x_i} + \rho^{\varepsilon} b_j = 0 \qquad \text{in}\ \Omega^{\varepsilon}$$

Constitutive equation:

$$\sigma^{\varepsilon}_{ij}(x) = b^{\varepsilon}_{ijkh}(x)\,\varepsilon_{kh}(u^{\varepsilon}) + c^{\varepsilon}_{ijkh}(x)\,\varepsilon_{kh}\left(\frac{\partial u^{\varepsilon}}{\partial t}\right)$$

$$b^{\varepsilon}_{ijkh}(x) = \begin{cases} E_{ijkh}(x) & \text{in} \quad \Omega^{\varepsilon}_{s} \\ \frac{1}{3}K^{f}\,\delta_{ij}\,\delta_{kh} & \text{in} \quad \Omega^{\varepsilon}_{f} \end{cases}$$

$$c^{\varepsilon}_{ijkh}(x) = \begin{cases} 0 & \text{in} \quad \Omega^{\varepsilon}_{s} \\ 2\mu^{\varepsilon}\left(\delta_{ik}\,\delta_{jh} - \frac{1}{3}\delta_{ij}\,\delta_{kh}\right) & \text{in} \quad \Omega^{\varepsilon}_{f} \end{cases}$$

Principle equation of virtual work

$$b^{\varepsilon}(u^{\varepsilon}, \omega^{\varepsilon}) + c^{\varepsilon}\left(\frac{\partial u^{\varepsilon}}{\partial t}, \omega^{\varepsilon}\right) = \int_{\Gamma_t} t \cdot \omega^{\varepsilon}\, d\Gamma + \int_{\Omega^{\varepsilon}} f^{\varepsilon} \cdot \omega^{\varepsilon}\, dx$$

$$\begin{cases} b^{\varepsilon}(u^{\varepsilon}, \omega^{\varepsilon}) = \int_{\Omega^{\varepsilon}} b^{\varepsilon}_{ijkh}(x)\, \varepsilon_{ij}(u^{\varepsilon})\, \varepsilon_{kh}(\omega^{\varepsilon})\, dx \\ c^{\varepsilon}(u^{\varepsilon}, \omega^{\varepsilon}) = \int_{\Omega^{\varepsilon}} c^{\varepsilon}_{ijkh}(x)\, \varepsilon_{ij}(u^{\varepsilon})\, \varepsilon_{kh}(\omega^{\varepsilon})\, dx \end{cases}$$

Two-scale asymptotic expansion

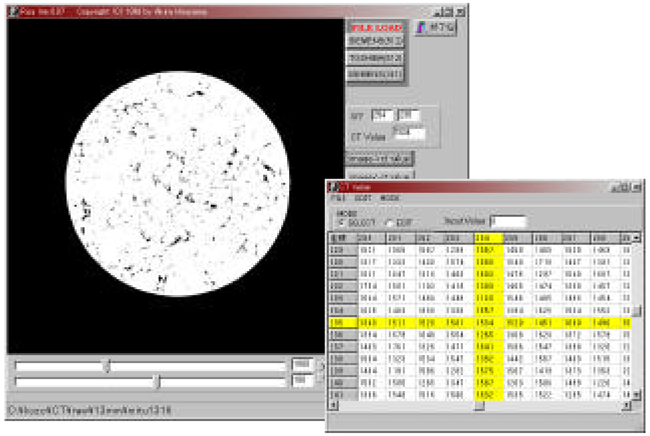
$$u^{\varepsilon}(x) = u^0(x, t) + \varepsilon u^1(x, y, t) + \varepsilon^2 u^2(x, y, t) + \cdots\cdots\cdots + \varepsilon^n u^n(x, y, t)$$

Digital Image Processing for Asphalt Concrete

TOSCANER-23200 (Kumamoto Univ.)

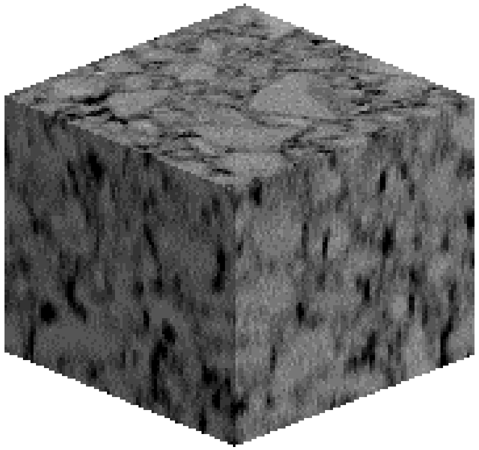
Scann type : Traverse/Rotation
Power of X-ray : 300kV/200kV
Number of detectors : 176 channels
Size of specimen : ϕ400mm × H600mm
Thickness of slice : 0.5mm,1mm,2mm
Spacial resolusion : 0.2mm

Finite Element Model for Microstructure

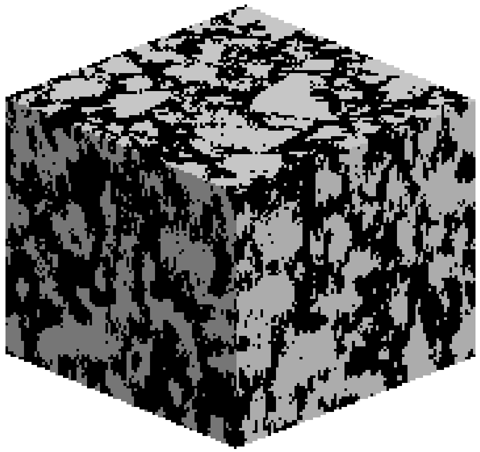


Digital Image (2D)

Digital Image(3D)



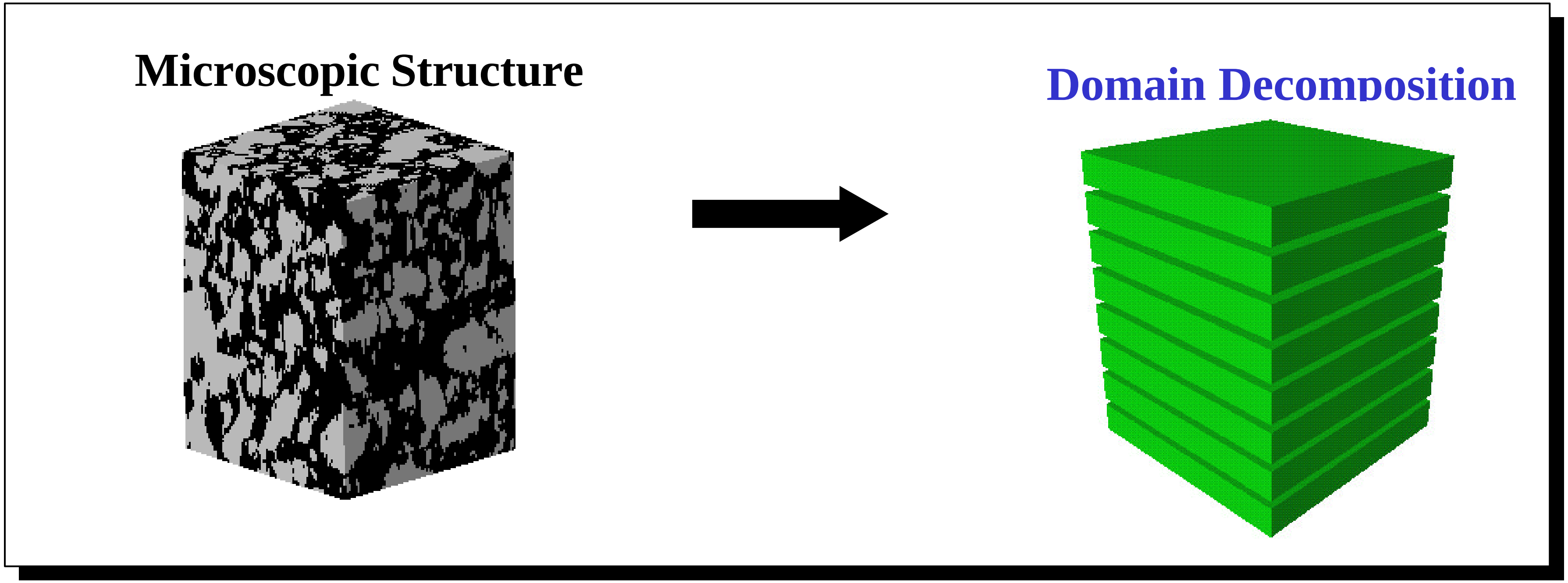
Microscopic Domain



Finite Element Model

Parallel Computing Method based on Domain Decomposition Method

1) Equalize the number of elements in each sub-domain
2) Minimize the number of nodes on the boundary of sub-domain



Element by Element SCG Method for Parallel Computing

Ax=b

$$r_0 = b \text{ Ä } Ax_0 = b \text{ Ä } \overset{\wedge}{\underset{e}{}} A^{(e)}x_0$$

$$p_0 = r_0$$

$$q_k = Ap_k = \overset{X}{\underset{e}{}} A^{(e)}p_k$$

$$\tilde{a}_k = (r_k; r_k)=(p_k; q_k)$$

$$x_{k+1} = x_k + \tilde{a}_k p_k$$

$$r_{k+1} = r_k \text{ Ä } \tilde{a}_k q_k$$

$$\mathring{a}_k = (r_{k+1}; r_{k+1})=(r_k; r_k)$$

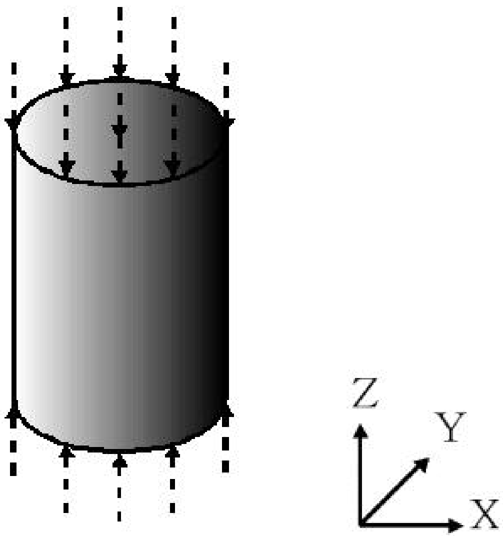
$$p_{k+1} = r_{k+1} + \mathring{a}_k p_k$$

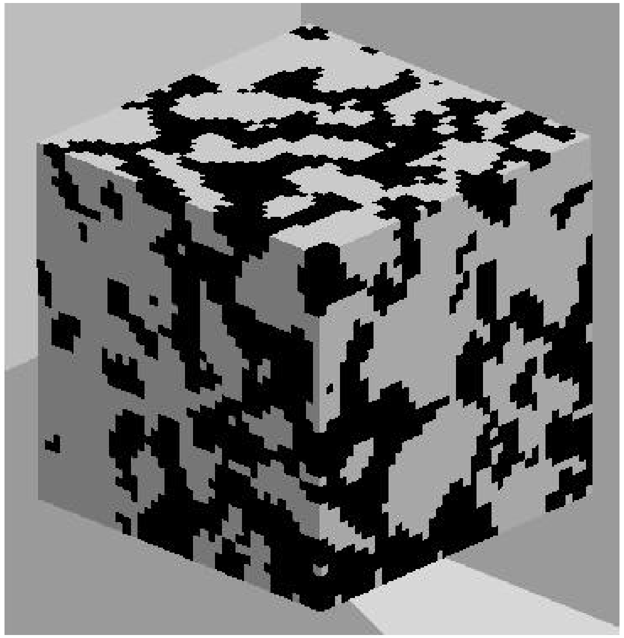
①neighboring communication

②global communication

Numerical Analysis

Macro-microscopic model





(ϕ 10cm , h 20cm) (40mm × 40mm × 40mm)

(nodes 9537,elements 8192)(nodes68921,elements64000)

Macroscopic model Microscopic model

Material constants

Solid

E=61.0GPa

ν=0.21

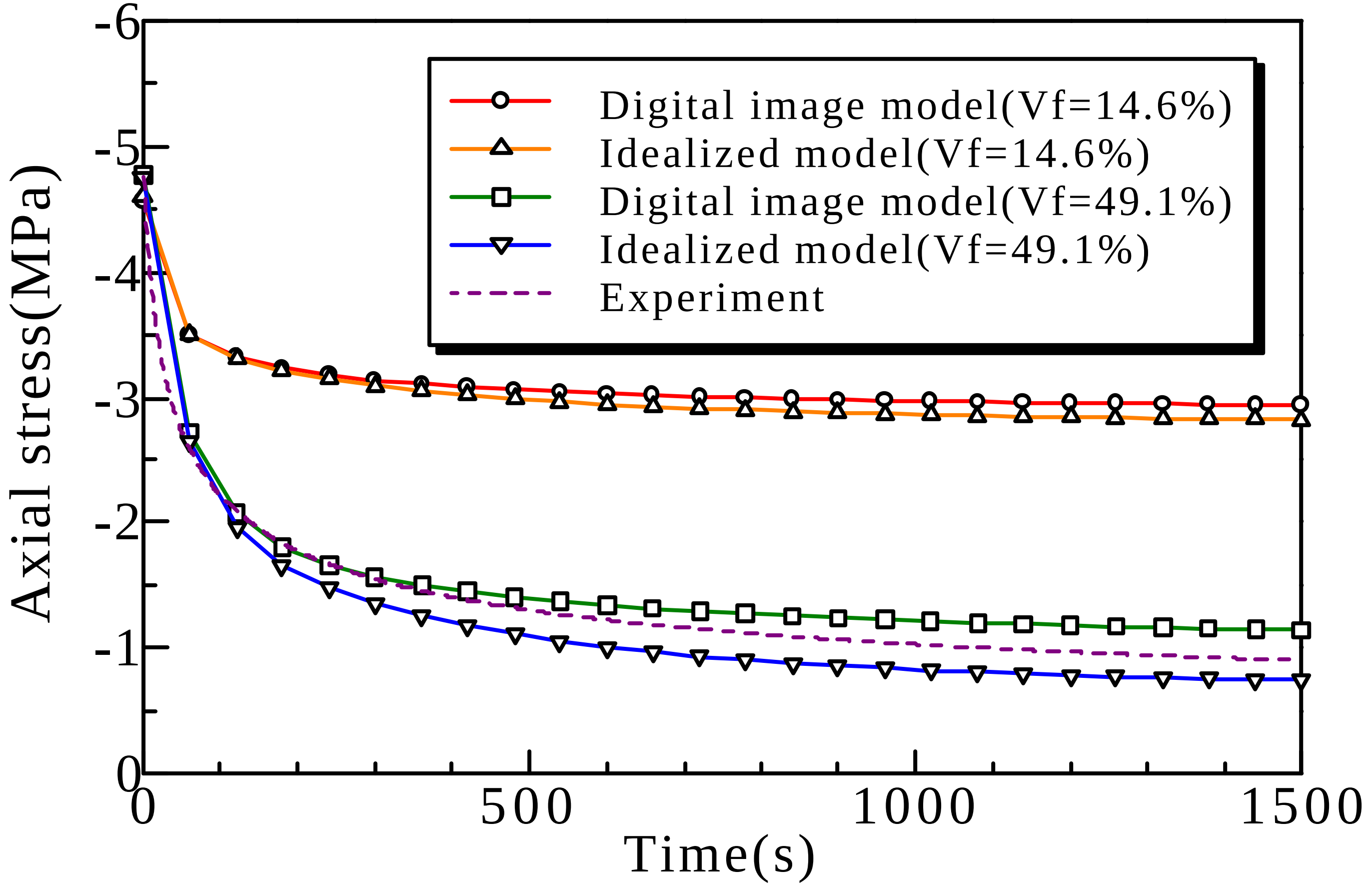
Fluid

K=10.0GPa

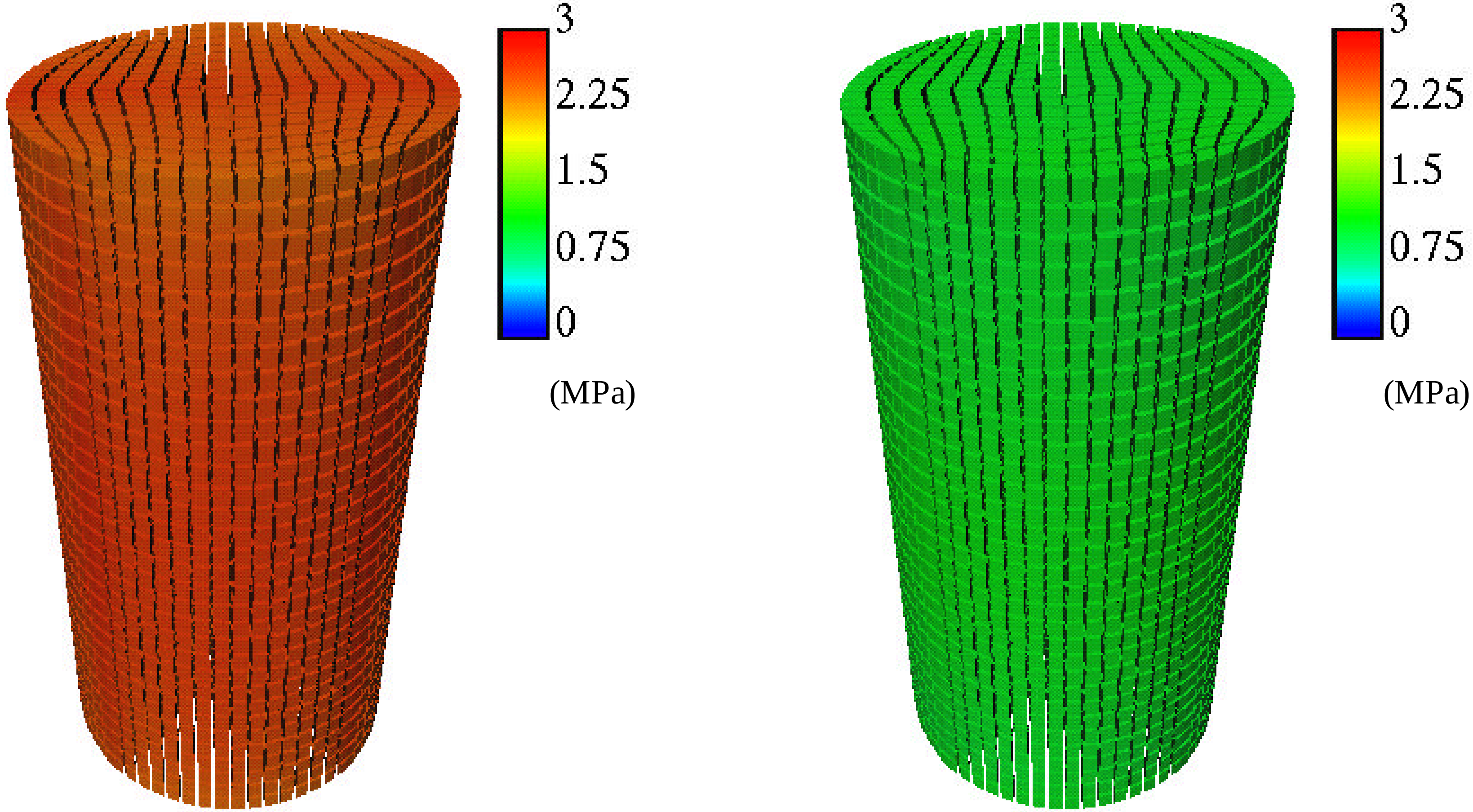
μ=1.0GPas

Vf=49.1%

Time history of axial stress of the macroscopic

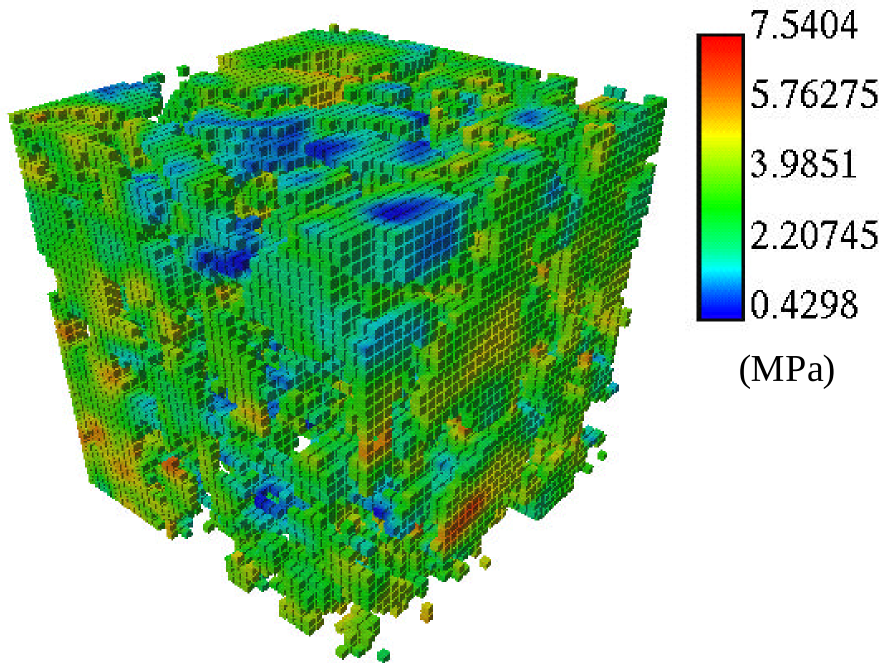


Macroscopic von Mises stress distribution(Vf=49.1%)

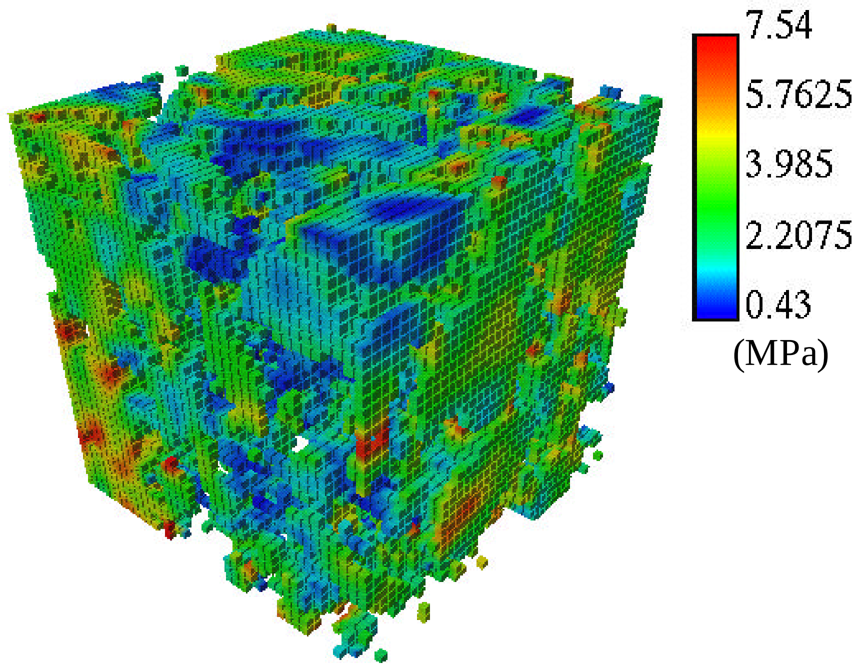


60s 1500s

<u>Microscopic von Mises stress distribution of the solid parts(Vf=49.1%)</u>

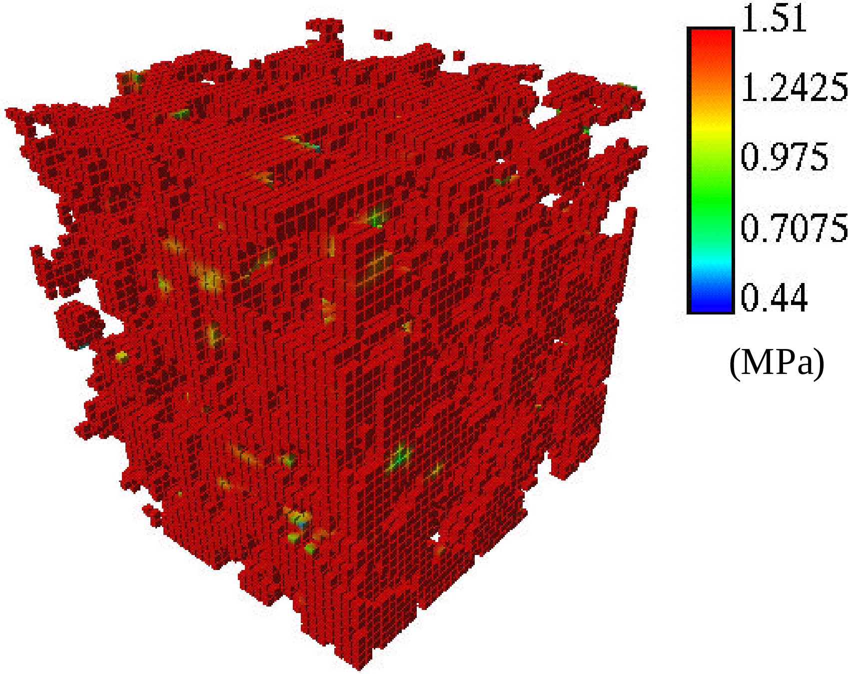


60s

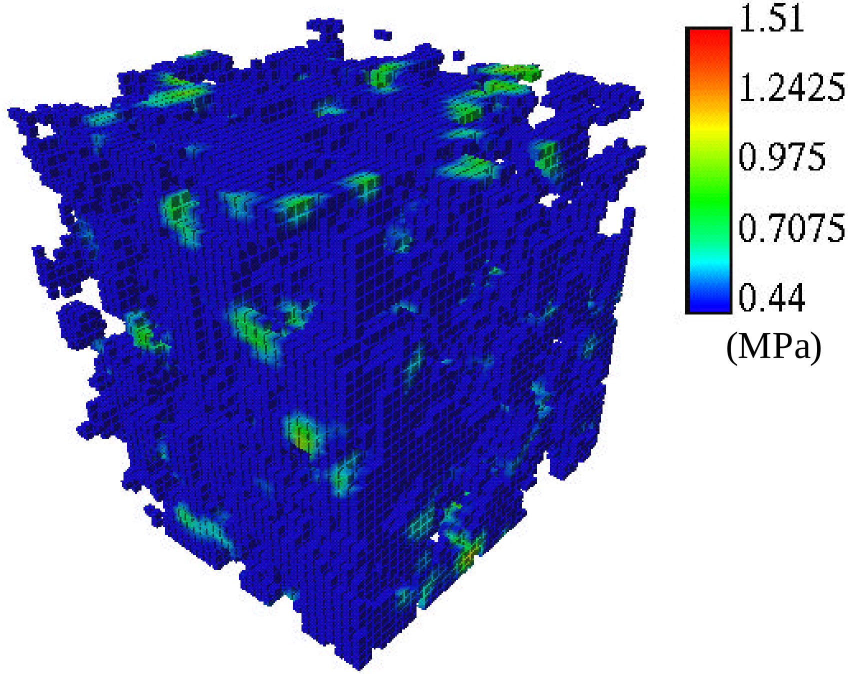


1500s

Microscopic von Mises stress distribution of the fluid parts(Vf=49.1%)

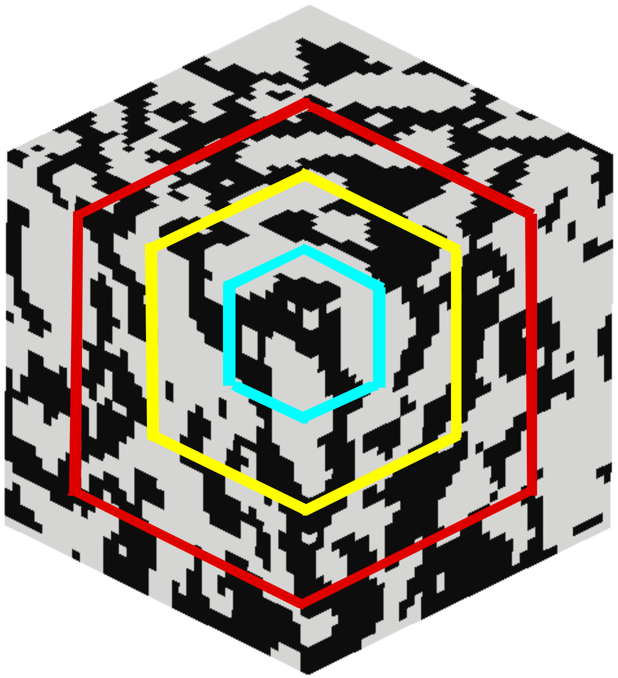


60s



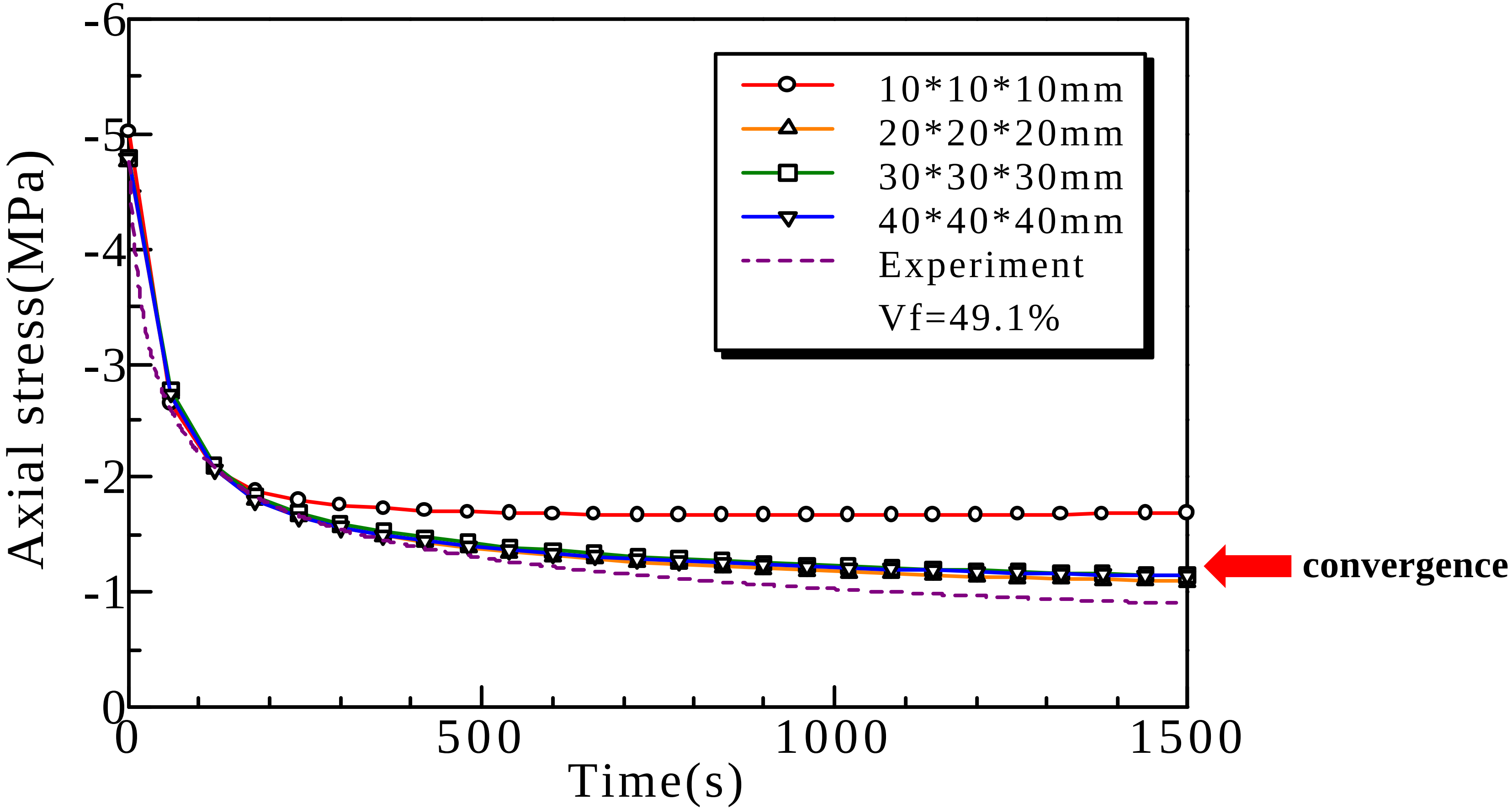
1500s

Effect of the region of unit cell

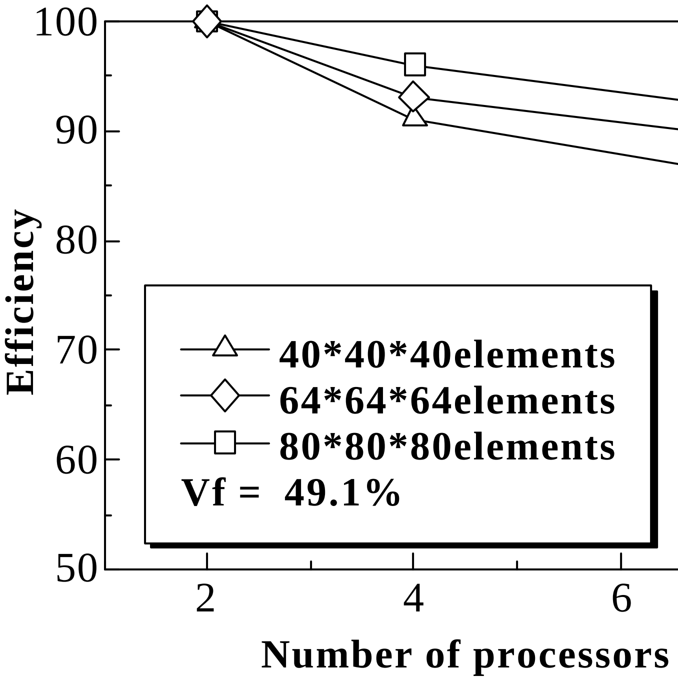


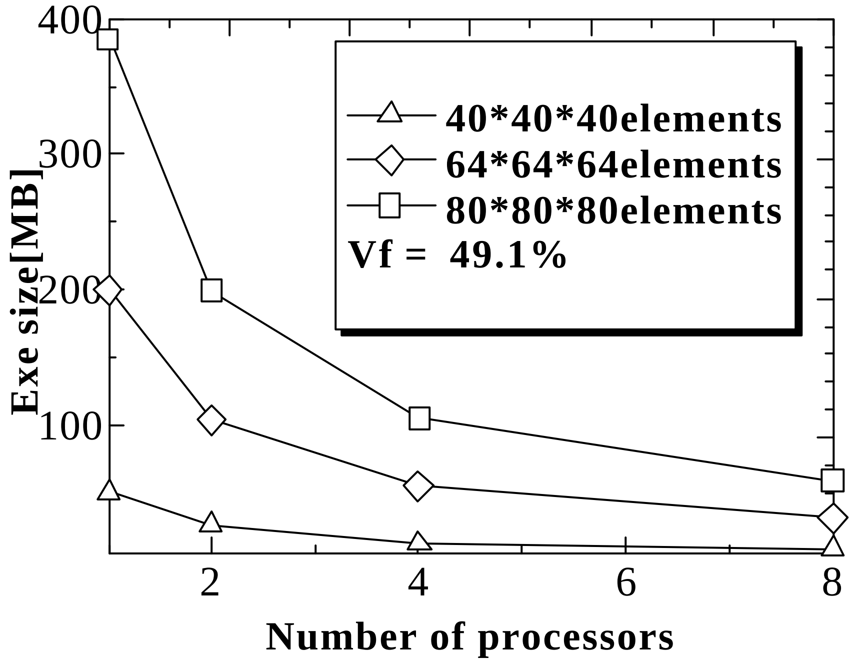
10*10*10mm(1000pixels)
20*20*20mm(8000pixels)
30*30*30mm(27000pixels)
40*40*40mm(64000pixels)

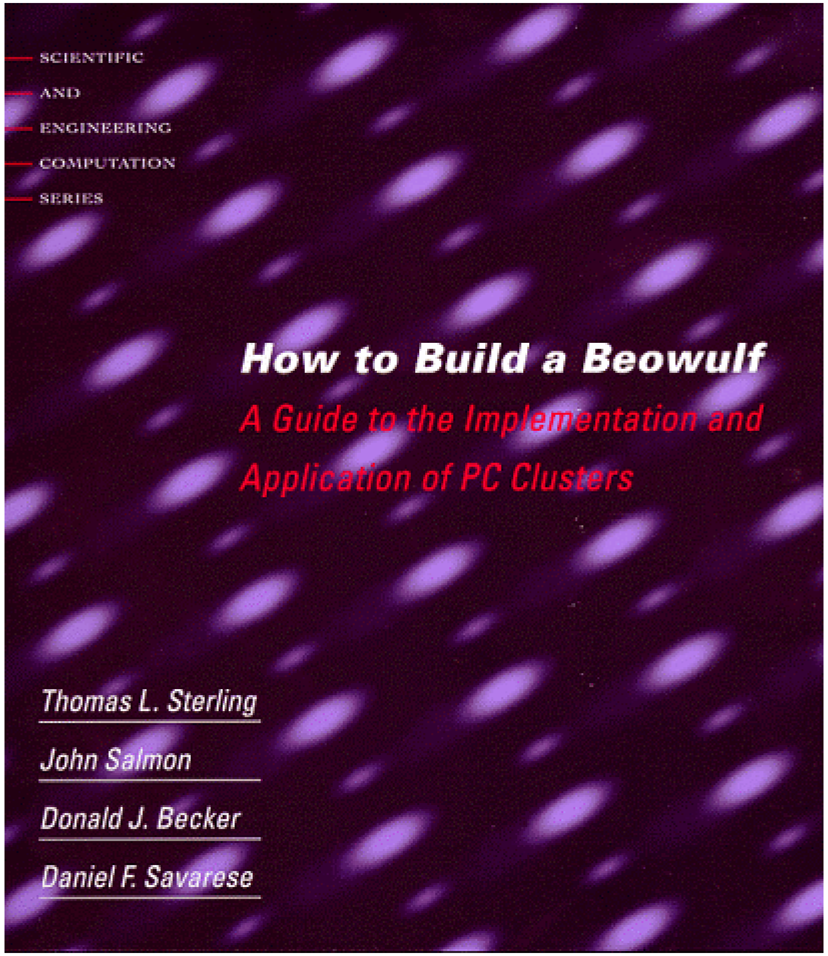
Time history of axial stress of macroscopic(Vf=49.1%)

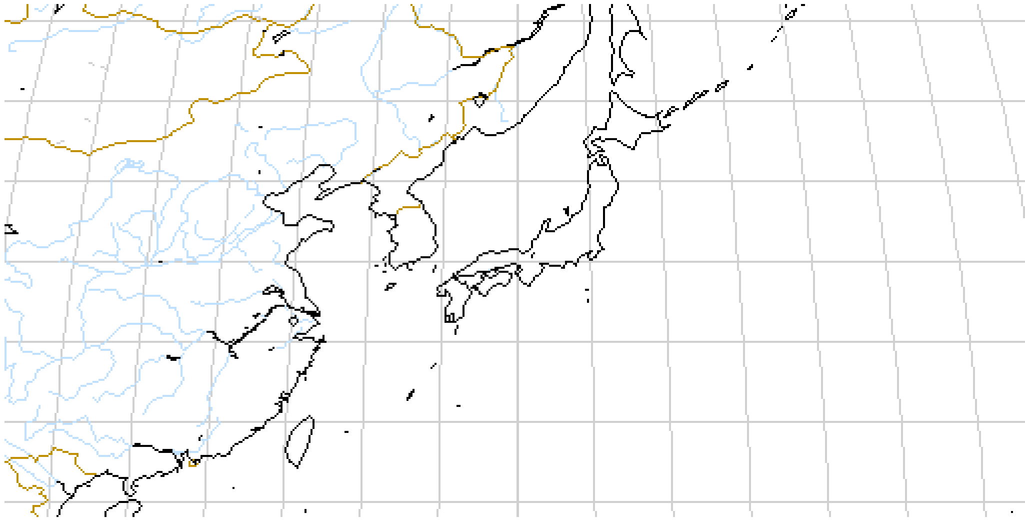


Efficiency of Parallelization





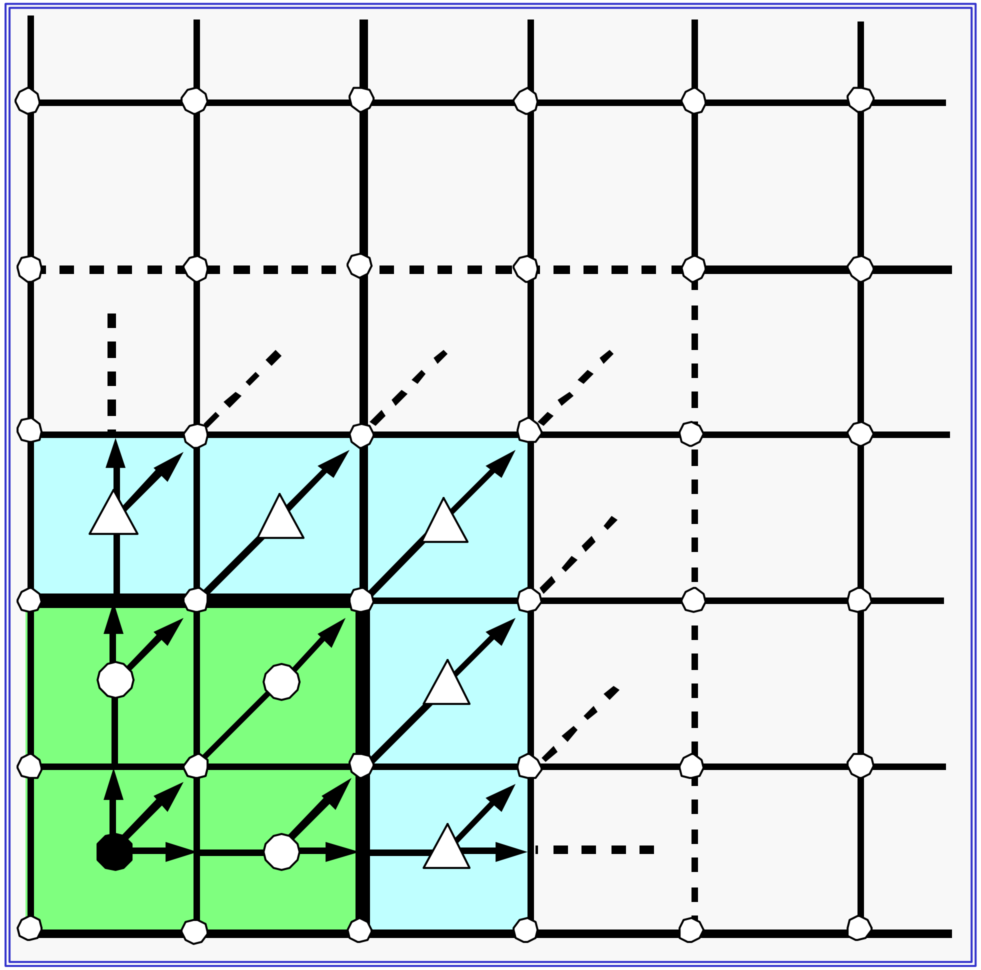

SCIENTIFIC
AND
ENGINEERING
COMPUTATION
SERIES
How to Build a Beowulf
A Guide to the Implementation and
Application of PC Clusters
Thomas L. Sterling
John Salmon
Donald J. Becker
Daniel F. Savarese



Tama Campus
(5 Schools of Liberal Arts)

Korakuen Campus
(School of Science and Engineering)

Domain Decomposition Method



Greedy Algorithm

Farhat,C., A simple and efficient automatic FEM domain decomposer, Computer and Structures, Vol.28, pp.576-602