Development of Explicit Moving Particle Simulation Framework and Zoom-Up Tsunami Analysis System

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LexADV_EMPS : Explicit Moving Particle Simulation Framework

Objective and Motivation

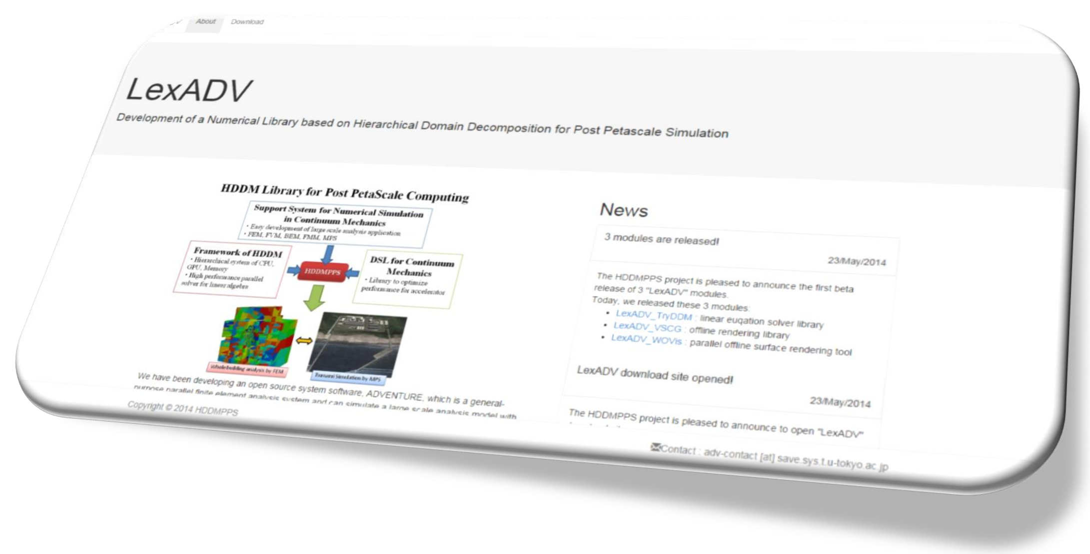
We have been developing the open source CAE software, named ADVENTURE, which is a general-purpose parallel finite element analysis system and can simulate a large-scale analysis model with various supercomputers. Our aim in this research is to develop scientific libraries for the post peta-scale simulation by the "particle methods" for the continuum mechanics.

The particle method regards a continuum as a set of particles, discretizes the physical laws governed by differential equations using interactions between the particles, and calculates the states and motions of the particles. Since the particles, as the calculation points, move on the time-marching processes, the particle method is superior to grid methods in terms of solving dynamic physical phenomena such as free surfaces and large deformations. However, the motion of particles makes it difficult to parallelize the particle method in distributed memory parallel computers.

We adopted the Moving Particle Simulation (MPS) method which is one of the most popular particle method as target solver and have been developing the LexADV_EMPS of the Explicit MPS framework which supports "Domain decomposition", "Halo exchange" and "Dynamic load balance" as functions for parallel computing.

http://adventure.sys.t.u-tokyo.ac.jp/lexadv/

LexADV is free and open source software for large-scale numerical simulations of continuum mechanics problems. Currently, some beta version software was released.

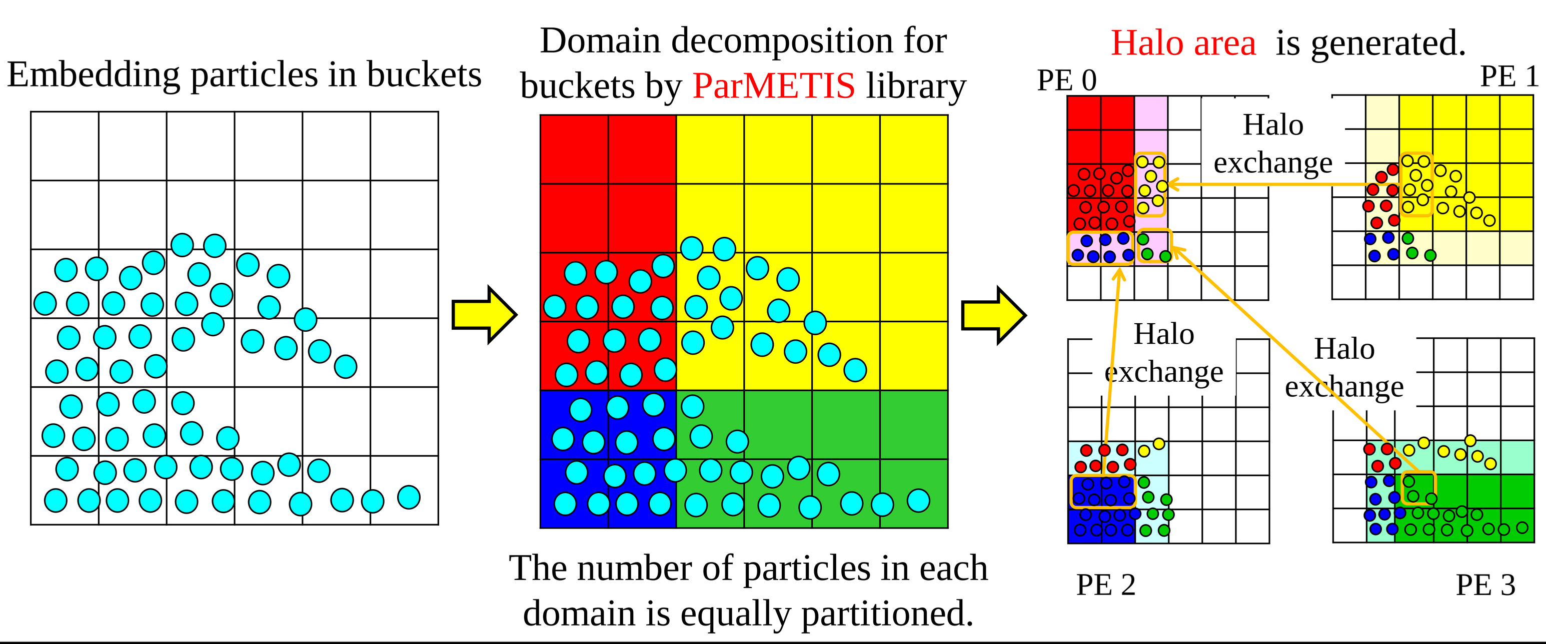


Name	Language	Description
LexADV_TryDDM	C, MPI	DDM-based linear equation solver library
LexADV_EMPS	C, MPI	Explicit MPS solver framework
LexADV_VSCG	C	High-resolution offline rendering library
LexADV_WOVis	C, MPI	Parallel offline surface rendering tool with VSCG

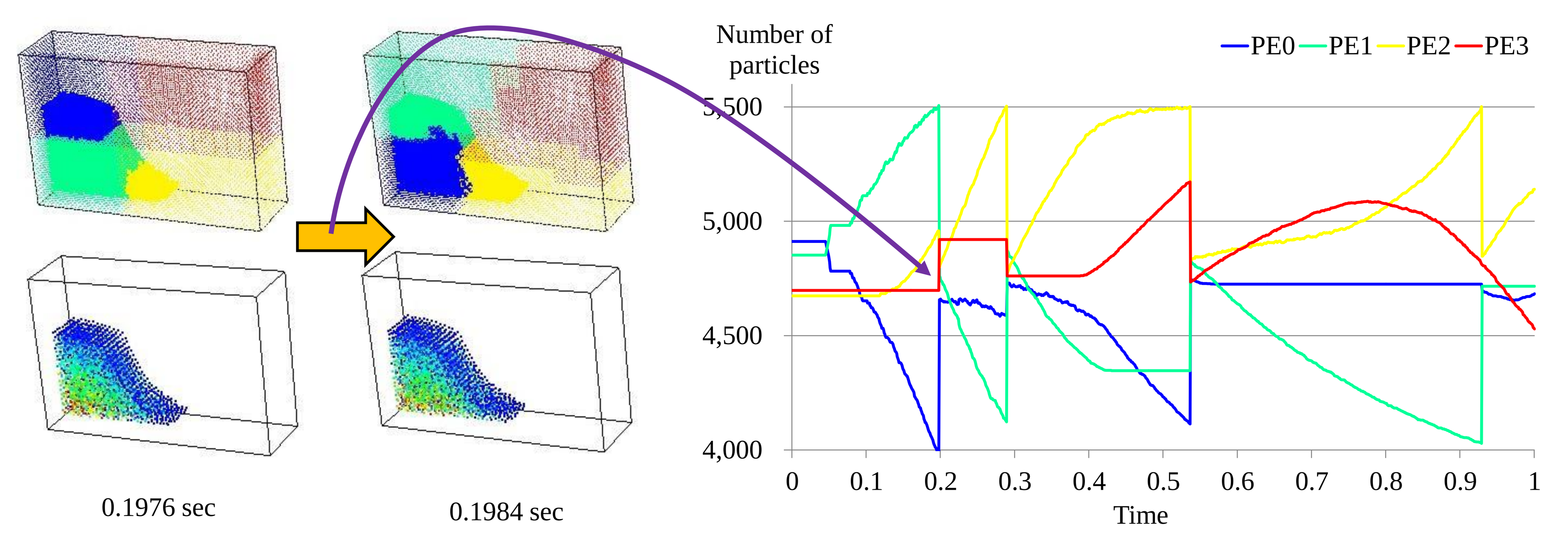
Overview

- LexADV_EMPS v0.1b was released as Open Source Software on Oct. 2014.
- Target problem size
  - 10 million − 1 billion particles
  - Functions for parallel computing
  - Domain decomposition
  - Dynamic load balance
  - Halo exchange
- Hierarchical bucket structure of three levels
  - Domain decomposition on 1st level bucket
  - Halo exchange on 2nd level bucket
  - Neighboring particle search on 3rd level bucket
- Development and operating environment
  - OS : UNIX, Linux
  - Compiler : C
  - Communication library : MPI

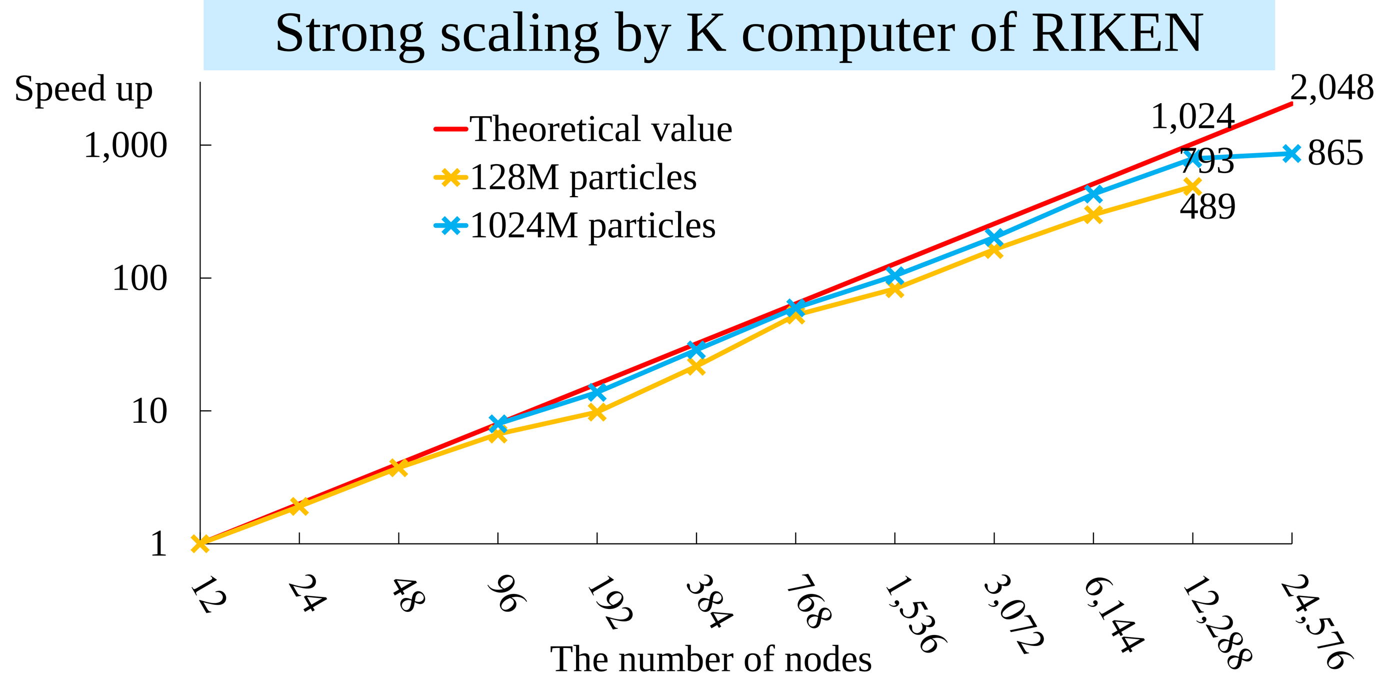
Domain decomposition and Halo exchange



Dynamic load balance



Strong scaling by K computer of RIKEN



Hierarchical bucket structure of three levels

3rd level bucket

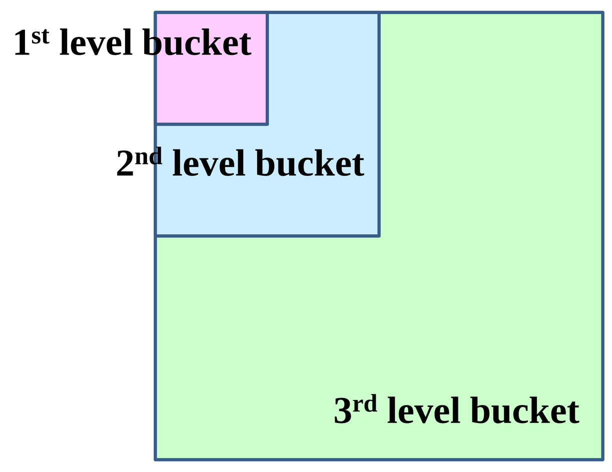
- 3rd level bucket is used for neighboring particle search.
- Various interaction domain are used in particle method.
- For example, small interaction domain in the gradient operator and large interaction domain in the Laplacian operator are often used.
- Bucket length on 3rd level bucket becomes radius of smallest interaction domain.
- 3rd level bucket has finest bucket structure.

2nd level bucket

- 2nd level bucket is used for halo exchange (communication among neighboring nodes).
- Bucket length on 2nd level bucket becomes radius of largest interaction domain.
- Bucket length on 2nd level bucket is 1 ～2 times of 3rd level bucket

1st level bucket

- 1st level bucket is used for domain decomposition.
- ParMETIS v4.0.3 can not partition a graph of more than two billion nodes.
- Less than one billion buckets on 1st level bucket are prepared by LexADV_EMPS.
- Bucket length on 1st level bucket is 1 ～ 4 times of 2nd level bucket.
- 1st level bucket has coarsest bucket structure.



HPC systems used in this research

Machine name	Site	Processor	GFLOPS / Node	Core/Node	Nodes
K computer	RIKEN	Fujitsu SPARC64 VIIIfx	128	8	88,128
FX100	Nagoya Univ.	Fujitsu SPARC64 XIfx	1,126	32	2,880
FX10	Univ. of Tokyo	Fujitsu SPARC64 IXfx	236	16	4,800
CX400	Nagoya Univ.	Intel Xeon E5-2697 v3 (Haswell)	1,164	28 (2 cpus / node)	552

Sample Solver : Distributed Memory Parallel Explicit MPS Implemented by LexADV_EMPS

Overview

- Two kind of sample solvers
  - Dambreak analysis of incompressible fluid analysis with free surface
  - Two floating objects analysis by interaction between fluid and rigid bodies
- Functions for Parallel computing by LexADV_EMPS
  - Domain decomposition
  - Dynamic load balance
  - Halo exchange
- Other function
  - Surface tension model by potential model
  - MPS gradient and Laplacian models
  - 1st, 2nd ,3rd and 4th order spatial derivative models
- Coming soon
  - Semi-implicit MPS method
  - Poisson equation solver with Neumann boundary condition by higher order spatial derivative models

Distributed memory parallel explicit MPS

Governing equations

$$\frac{\partial P}{\partial \rho} = c^2$$

$$\frac{d\vec{v}}{dt} = -\frac{1}{\rho}\nabla P + \nu\Delta\vec{v} + \vec{g}$$

Initialize
- Domain decomposition and Load balance LexADV_EMPS

Calculate viscosity and gravity terms

$$\vec{a} = \nu[\Delta\vec{v}]^k + \vec{g}$$

Update velocity and position

$$\vec{v}^* = \vec{v}^k + \Delta t\,\vec{a} \qquad \vec{r}^* = \vec{r}^k + \Delta t\,\vec{v}^*$$

- Halo exchange by LexADV_EMPS

Calculate pressure

$$P_i^{k+1} = c^2\rho\frac{n_i^* - n_0}{n_0} \Leftarrow \frac{\partial P}{\partial \rho} = c^2$$

c : Sound speed

ρ : Density

- Halo exchange by LexADV_EMPS

Calculate pressure gradient

$$\vec{v}' = -\frac{\Delta t}{\rho}[\nabla P]^{k+1}$$

Correct velocity and position

$$\vec{v}^{k+1} = \vec{v}^* + \vec{v}' \qquad \vec{r}^{k+1} = \vec{r}^* + \Delta t\,\vec{v}'$$

- Halo exchange by LexADV_EMPS

Particle number density

$$n_i^* = \sum_{j\neq i} w\left(\left\|\vec{r}_j^* - \vec{r}_i^*\right\|\right)$$

Check load balances
- If the number of particles is imbalance among each PE, domain decomposition is performed.
- Domain decomposition and Load balance LexADV_EMPS

Finish

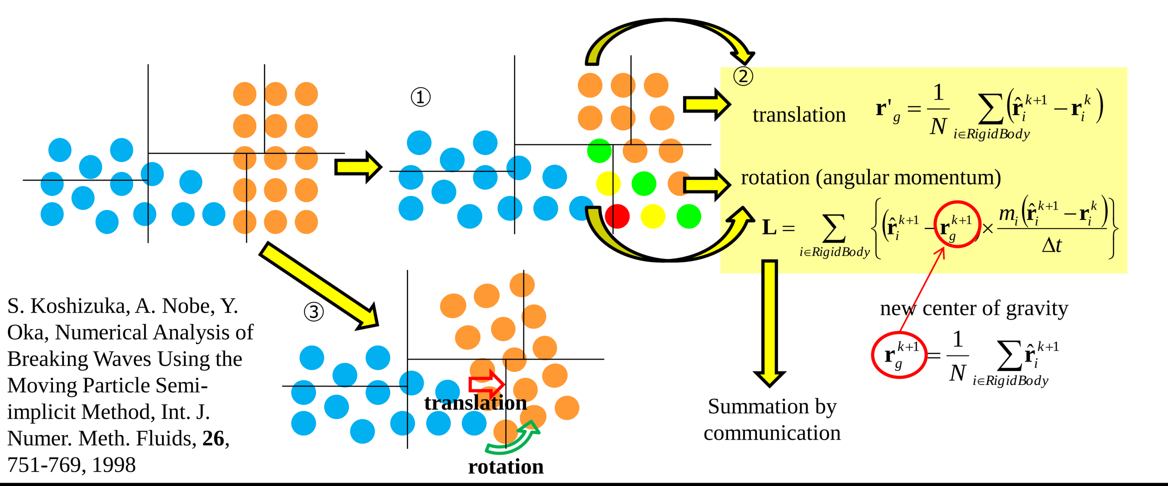
Interaction between fluid and rigid bodies

1. Calculate all particles as fluid particles.
2. Calculate a translation and a rotation of a rigid body from rigid body particles.
3. Perform the translation and the rotation for the rigid body from the original position.

This algorithm corresponds to calculating a volume integral of forces for the rigid body.

Communication for many rigid bodies

- Communication for many rigid bodies occurs in only summation operation. (most important point)
- Summations are done three times for obtaining new center of gravity, translation and angular momentum (rotation) which has 3 components of double type respectively.
- These three values are shared in all nodes by "MPI_Allreduce".
- Communication data size is (9 double type components) x (# of rigid bodies) . (not # of rigid body particles.)
- For example, if 100 rigid bodies, communication size is only 8(size of double)x9x100 byte.



$$\mathbf{r}'_g = \frac{1}{N}\sum_{i\in RigidBody}\left(\hat{\mathbf{r}}_i^{k+1} - \mathbf{r}_i^k\right)$$

$$\mathbf{L} = \sum_{i\in RigidBody}\left\{\left(\hat{\mathbf{r}}_i^{k+1} - \mathbf{r}_g^{k+1}\right)\times\frac{m_i\left(\hat{\mathbf{r}}_i^{k+1} - \mathbf{r}_i^k\right)}{\Delta t}\right\}$$

$$\mathbf{r}_g^{k+1} = \frac{1}{N}\sum_{i\in RigidBody}\hat{\mathbf{r}}_i^{k+1}$$

S. Koshizuka, A. Nobe, Y. Oka, Numerical Analysis of Breaking Waves Using the Moving Particle Semi-implicit Method, Int. J. Numer. Meth. Fluids, **26**, 751-769, 1998

Development of Explicit Moving Particle Simulation Framework and Zoom-Up Tsunami Analysis System

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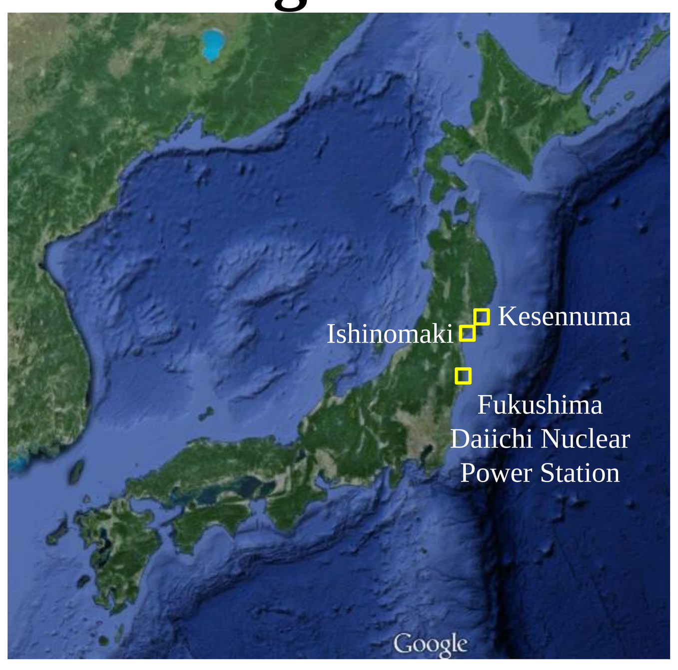
Zoom-Up Tsunami Analysis System

Tohoku area was severely damaged by the tsunami of the Great East Japan Earthquake on 2011. Our target is to simulate impact by three kind of tsunami analyses on urban areas. First, tsunami is running-up in urban area and inundates into a building. Second, floating objects have collisions with each other and buildings. Third, stress of buildings from fluid pressure is estimated.

Zoom-up tsunami analysis system have been built in order to solve our target problems. In our system, zoom-up analysis by three stages analyses is adopted to solve a large area from an epicenter to an urban area. In the first stage, the two-dimensional shallow-water analysis is solved in the area of about 1000 km x 1000 km from the epicenter to the coastal areas. In the second and third stages, the three-dimensional tsunami run-up analyses are solved for the coastal areas using the distributed memory parallel explicit MPS method implemented by LexADV_EMPS. Today, Ishinomaki city, Kesennuma city and Fukushima Daiichi Nuclear Power Station have been successfully solved by our system.

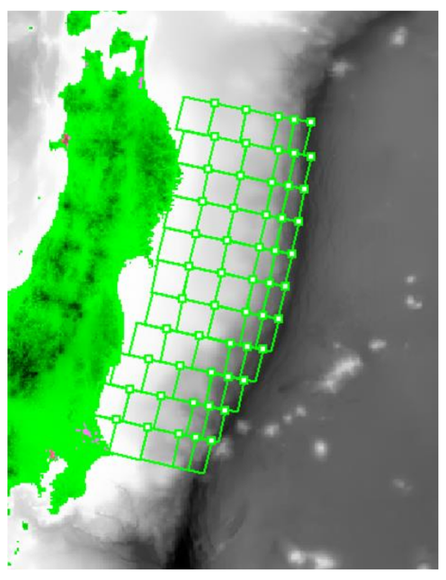
K computer of RIKEN, FX10 of the University of Tokyo, FX100 and CX400 of Nagoya University have been used in our system. For example, in case of Kesennuma city, the tsunami run-up analysis with a large ship of 130 million particles (1m particle spacing) and 1800 seconds has been done by K computer 12000 nodes and total wall-clock time 30 hours.

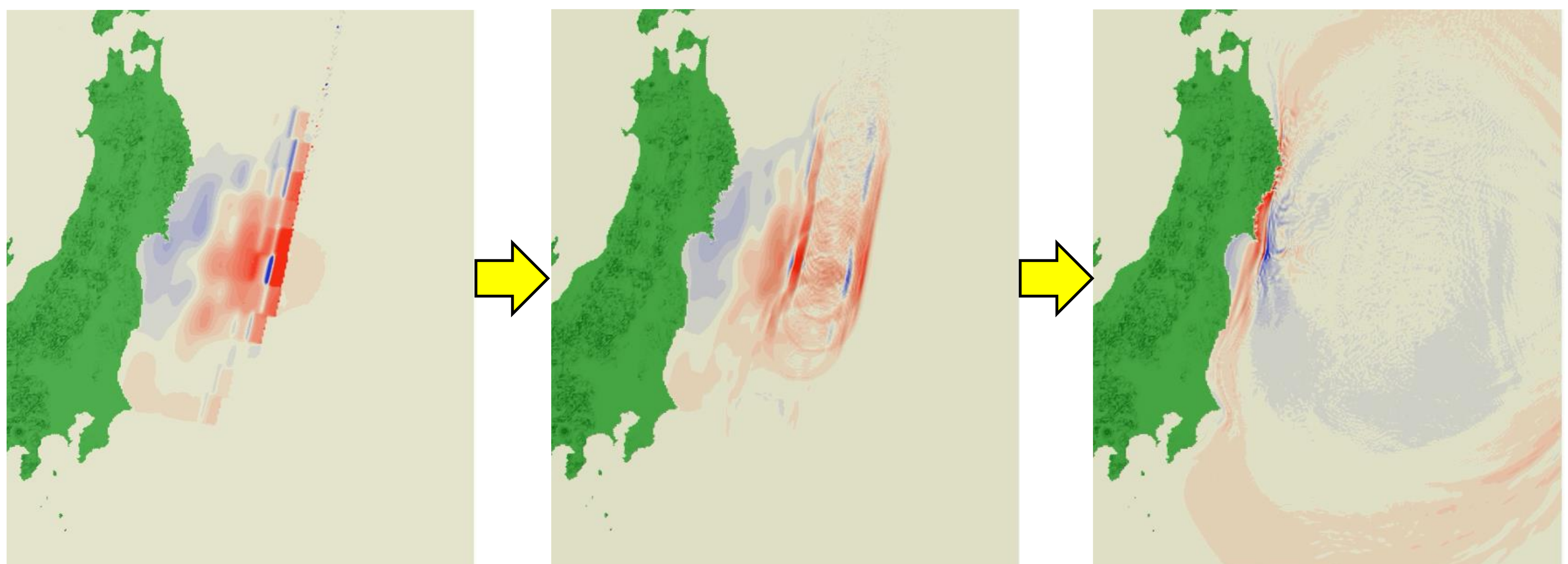
Target areas



First stage analysis by 2D shallow water analysis from epicenter to coast areas

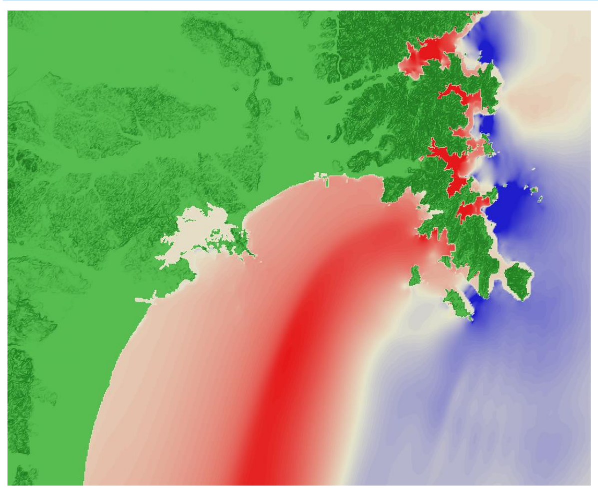
Fault Parameter of Great East Japan Earthquake





Ishinomaki city

First stage analysis by 2D shallow water analysis



Third stage analysis by MPS

Case3

Case1

Case2

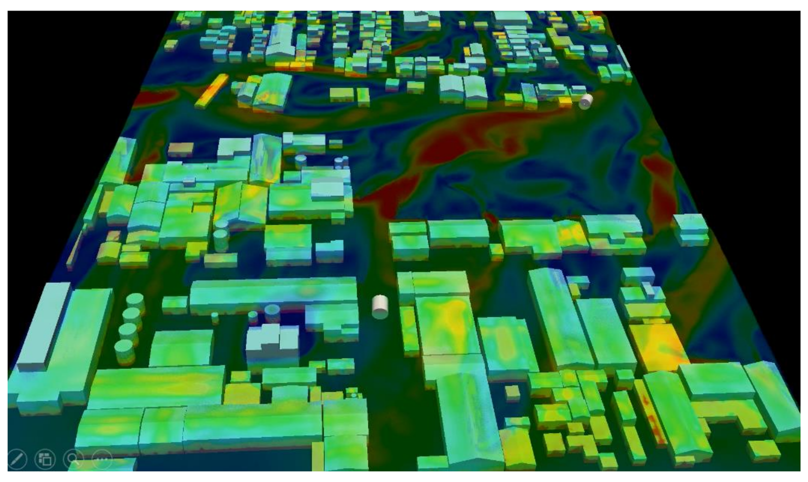
Elastic analysis for buildings by fluid pressure

Fluid analysis

- FX10 600 nodes
- Total wall-clock time: 6 hours
- 40 million particles (0.5m)
- Time: 200 s / 0.1 million step

Structure analysis

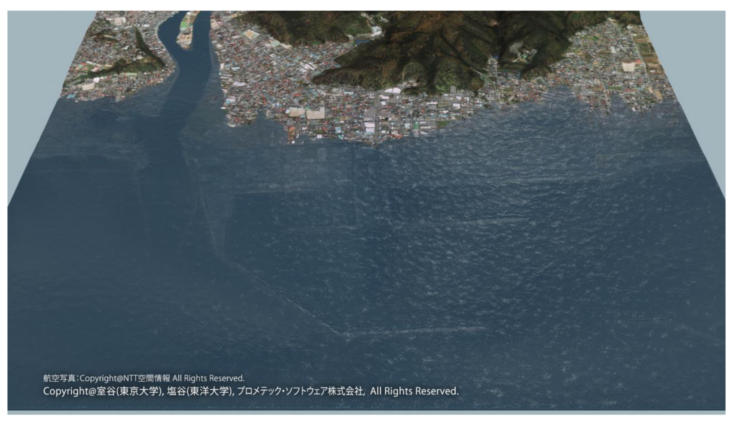
- FX10 120 nodes
- Total wall-clock time: 7 hours
- 10 million elements (2m)
- Time: 200 s / 400 steps



Second stage analysis by MPS

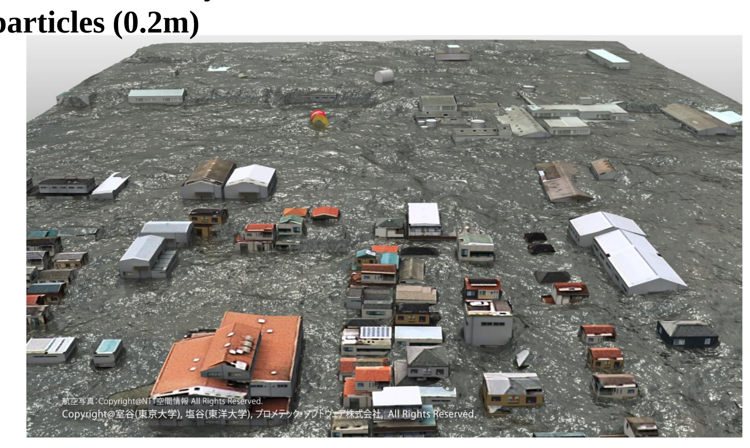
Tsunami run-up analysis

- FX10 144 nodes
- Total wall-clock time: 7 days
- 260 million particles (1m)
- Time: 800 s



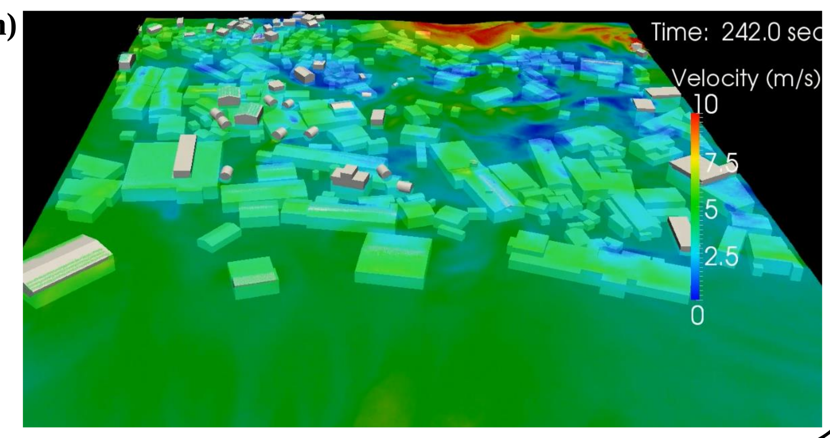
Tsunami run-up analysis with two tanks

- CX400 32 nodes
- Total wall-clock time: 30 days
- 400 million particles (0.2m)
- Time: 200 s



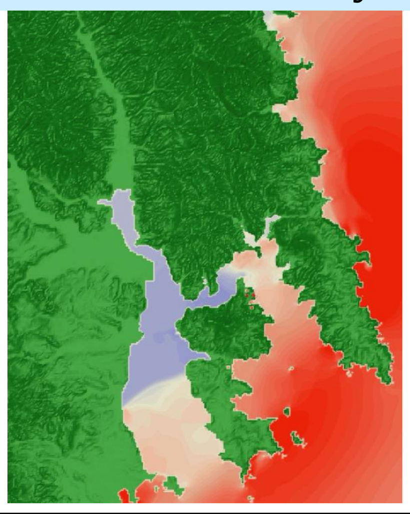
Tsunami run-up analysis with 431 buildings

- CX400 72 nodes
- Total wall-clock time: 40 hours
- 80 million particles (0.5m)
- Time: 400 s



Kesennuma city

First stage analysis by 2D shallow water analysis

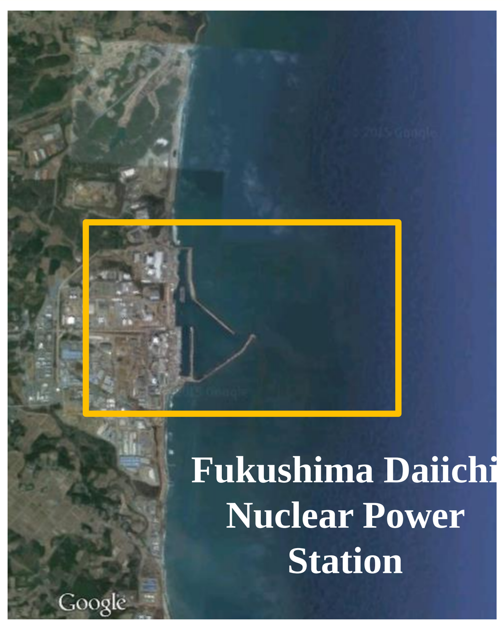


Second stage analysis by MPS

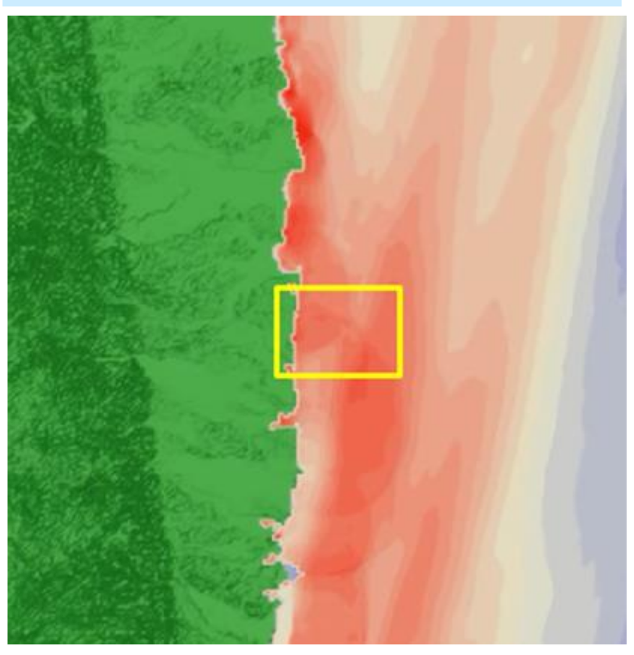
Tsunami run-up analysis with a large ship of 60 m

- K computer 12000 nodes
- Total wall-clock time: 30 hours
- 130 million particles (1m)
- Time: 1800 s

Fukushima Daiichi Nuclear Power Station



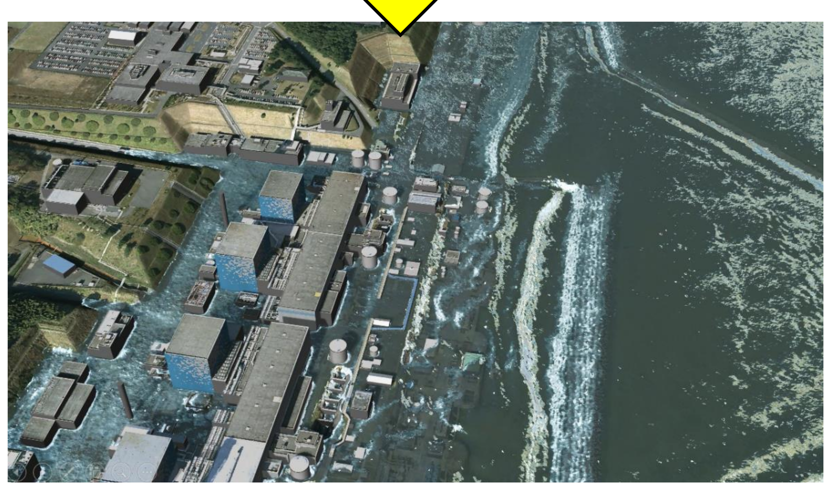
First stage analysis by 2D shallow water analysis



Second stage analysis by MPS

Tsunami run-up analysis

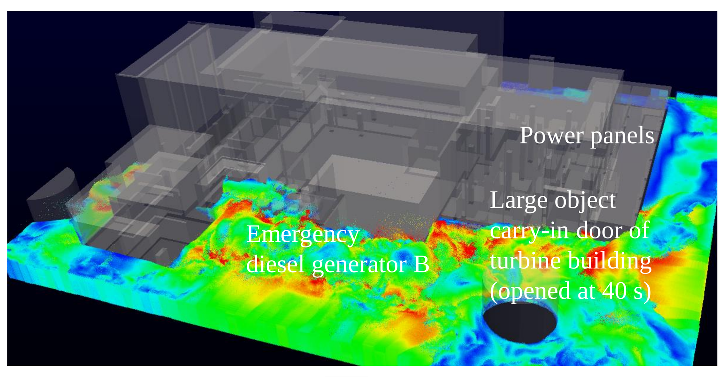
- K computer 4800 nodes
- Total wall-clock time: 40 hours
- 250 million particles (1m)
- Time: 1800 s

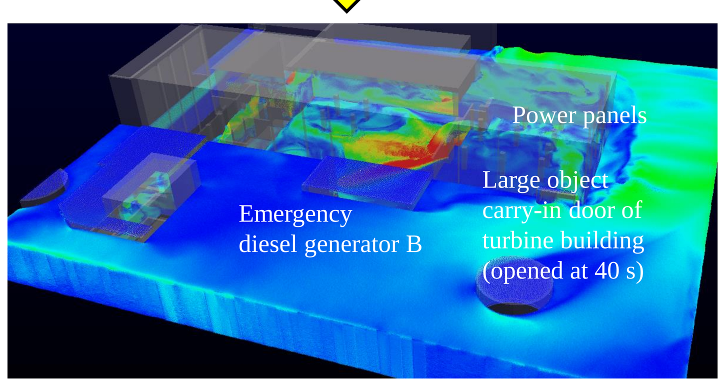


Third stage analysis by MPS

Inundation analysis into Interior of Turbine Building of Fukushima Daiichi Nuclear Power Station Unit 1

- FX100 384 nodes
- Total wall-clock time: 72 hours
- 130 million particles (0.1m)
- Time: 200 s

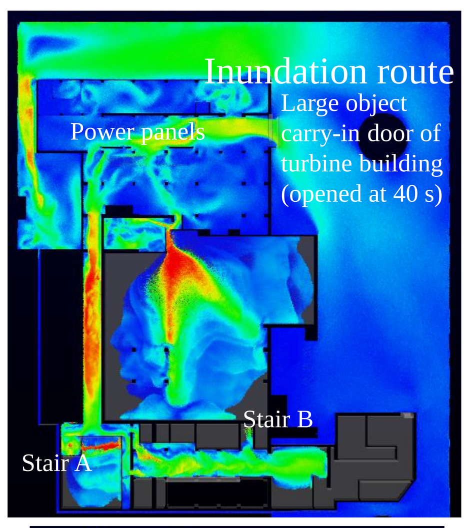




Since the beginning of inundation from the large object carry-in door,

1. The power panels is covered with water after a few second,
2. Inundation on B1 starts from the stair A after 25 s,
3. Emergency diesel generator B is covered with water after 80 s.

1F



B1