



災害・ものづくり系シミュレーションと スパコンからのイノベーション

東京工業大学 学術国際情報センター

青木 尊之

TSUBAME 2.5

System (58 racks)

1442 nodes: 2952 CPU sockets,
4264 GPUs

Performance: 224.7 TFLOPS (CPU) ※ Turbo boost
5.562 PFLOPS (GPU)

Total: 17.1 PFLOPS



Rack (30 nodes)

Performance: 122 TFLOPS
Memory: 2.28 TB

Compute Node (3 Tesla K20X GPUs)

Performance: 4.08 TFLOPS
Memory: 58.0GB(CPU)
+18GB(GPU)

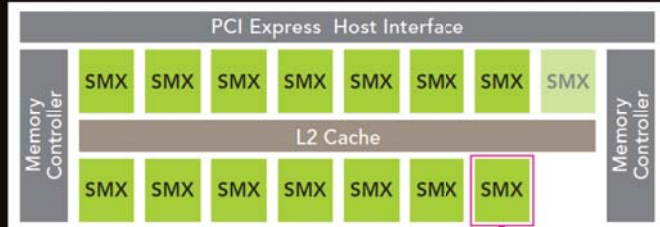




GPU: Kepler core NVIDIA Tesla K20X

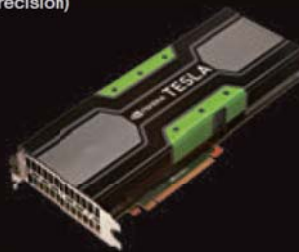
Details of GPU

K20X Architecture (Kepler GK110 Core)

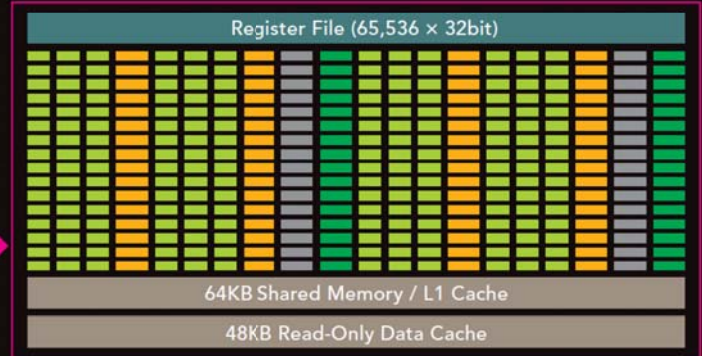


Peak performance : 1.31 TFLOPS (double precision)
3.95 TFLOPS (single precision)

Shader clock : 732 MHz
Number of CUDA cores (SP) : 2,688 cores
Streaming Multiprocessor (SMX) : 14 SMX
Writable L2 cache: 1.5MB
Memory bandwidth : 250GB / sec
Memory clock : 2.6GHz (GDDR5)
ECC support:
internal and external memory
On-board memory: 6GB



Details of SM (Streaming Multiprocessor)



CUDA core (SP) / SMX : 192 cores
DP unit / SMX : 64 SFU / SM : 32 units
Warp scheduler / SMX : 4 units
Shared memory / SMX : 16KB or 32KB or 48KB
Writable L1 cache / SMX : 48KB or 32KB or 16KB
Read-only data cache / SMX: 48KB

Core
DP Unit
LDST
SFU

TOP 500 Ranking 2014 Jun

Rank	Site	System	Cores	Rmax (TFlops)	Rpeak (TFlops)	Power (kW)
1	Northern Super Computer Center in Guangzhou, China	Xeon-2 (Mikkyokyo S1, TH110) / EP Cluster, Intel Xeon E5-2692 12C 2.200GHz, TH Express-2, Intel Xeon Phi 31S1P, NUDT	312000	33502.7	54902.4	17803
2	DOE/SC/Oak Ridge National Laboratory, United States	Titan - Cray XK7 - Opteron 6274 16C 2.200GHz, Cray Gemini Interconnect, NVIDIA K20x, Cray Inc.	560040	17590.0	27112.5	8209
3	DOE/NN/SAILML, United States	Sequoia - BlueGene/Q, Power BQC 16C 1.00 GHz, Custom IBM	157204	17173.2	20132.7	7890
4	Riken Advanced Institute for Computational Science (AICS), Japan	K computer, SPARC64 VIIx2 2.0GHz, Tofu Interconnect, Fujitsu	705014	10510.0	11280.4	12000
5	DOE/SC/Argonne National Laboratory, United States	Mira - BlueGene/Q, Power BQC 16C 1.00GHz, Custom IBM	780412	8580.0	10006.3	3945
6	Swiss National Supercomputing Centre (CSCS), Switzerland	Phi Dante - Cray XC26, Xeon E5-2670 8C 2.600GHz, Arria Interconnect, NVIDIA K20x, Cray Inc.	11584	6271.0	7788.9	2325
7	Texas Advanced Computing Center/Univ. of Texas, United States	Stampede - PowerEdge R620, Xeon E5-2692 8C 2.700GHz, Infiniband FDR, Intel Xeon Phi SE10P, Dell	402402	6106.1	8500.1	4510
8	Forschungszentrum Juelich (FZJ), Germany	JUQUEEN - BlueGene/Q, Power BQC 16C 1.00GHz, Custom Interconnect, IBM	458712	6008.9	5872.0	2301
9	DOE/NN/SAILML, United States	Vulcan - BlueGene/Q, Power BQC 16C 1.00GHz, Custom Interconnect, IBM	393216	4293.3	5033.2	1972
10	Government, United States	Cray XK26, Intel Xeon E5-2697v2 12C 2.70GHz, Arria Interconnect, Cray Inc.	22594	3143.5	4881.3	
11	Exploration & Production - Eni S.p.A., Italy	HPC2 - iDataPlex DX360M4, Intel Xeon E5-2695v2 10C 2.80GHz, Infiniband FDR, NVIDIA K20x, IBM	62548	3003.0	4006.3	1067
12	Leibniz Rechenzentrum, Germany	SuperMUC - iDataPlex DX360M4, Xeon E5-2690 8C 2.70GHz, Infiniband FDR, IBM	147406	2897.0	3185.1	3423
13	ISIC Center, Tokyo Institute of Technology, Japan	TSUBAME 2.5 - Cluster Platform SL390x G7, Xeon X5670 6C 2.80GHz, Infiniband QDR, NVIDIA K20x, NEC/HP	76032	2785.0	5735.7	1389
14	National Supercomputing Center in Tianjin, China	Tianhe-1A - NUDT TH160P, Xeon X5670 6C 2.93 GHz, NVIDIA 2050, NUDT	186368	2506.0	4701.0	4040

MIC Xeon Phi
GPU K20X



GPU K20X
MIC Xeon Phi



GPU K20X

Inexpensive
High Performance

GPU K20X

Low Electronic Consumption

GPU M2050

TOP 500 Ranking

2015 November

RANK	SITE	SYSTEM	CORES	RMAX (TFLOP/S)	RPEAK (TFLOP/S)	POWER (KW)
1	National Super Computer Center in Guangzhou China	Tianhe-2 (MilkyWay-2) - TH-IVB-FEP Cluster, Intel Xeon E5-2692 12C 2.200GHz, TH Express-2, Intel Xeon Phi 3151P NUDT	3,120,000	33,862.7	54,902.4	17,808
2	DOE/SC/Oak Ridge National Laboratory United States	Titan - Cray XK7, Opteron 6274 16C 2.200GHz, Cray Gemini interconnect, NVIDIA K20x Cray Inc.	560,640	17,590.0	27,112.5	8,209
3	DOE/NNSA/LLNL United States	Sequoia - BlueGene/Q, Power BQC 16C 1.60 GHz, Custom IBM	1,572,864	17,173.2	20,132.7	7,890
4	RIKEN Advanced Institute for Computational Science (AICS) Japan	K computer, SPARC64 VIIIfx 2.0GHz, Tofu interconnect Fujitsu	705,024	10,510.0	11,280.4	12,660
5	DOE/SC/Argonne National Laboratory United States	Mira - BlueGene/Q, Power BQC 16C 1.60GHz, Custom IBM	786,432	8,586.6	10,066.3	3,945
6	DOE/NNSA/LANL/SNL United States	Trinity - Cray XC40, Xeon E5-2698v3 16C 2.3GHz, Aries interconnect Cray Inc.	301,056	8,100.9	11,078.9	
7	Swiss National Supercomputing Centre (CSCS) Switzerland	Piz Daint - Cray XC30, Xeon E5-2670 8C 2.600GHz, Aries interconnect, NVIDIA K20x Cray Inc.	115,984	6,271.0	7,788.9	2,325
8	HLRS - Höchstleistungsrechenzentrum Stuttgart Germany	Hazel Hen - Cray XC40, Xeon E5-2680v3 12C 2.5GHz, Aries interconnect Cray Inc.	185,088	5,640.2	7,403.5	
9	King Abdullah University of Science and Technology Saudi Arabia	Shaheen II - Cray XC40, Xeon E5-2698v3 16C 2.3GHz, Aries interconnect Cray Inc.	196,608	5,537.0	7,235.2	2,834
10	Texas Advanced Computing Center/Univ. of Texas United States	Stampede - PowerEdge C8220, Xeon E5-2680 8C 2.700GHz, Infiniband FDR, Intel Xeon Phi SE10P Dell	462,462	5,168.1	8,520.1	4,510

MIC Xeon Phi

GPU K20X

GPU K20X

MIC Xeon Phi



Top500 のうち

69 システムが GPU
27 システムが MIC

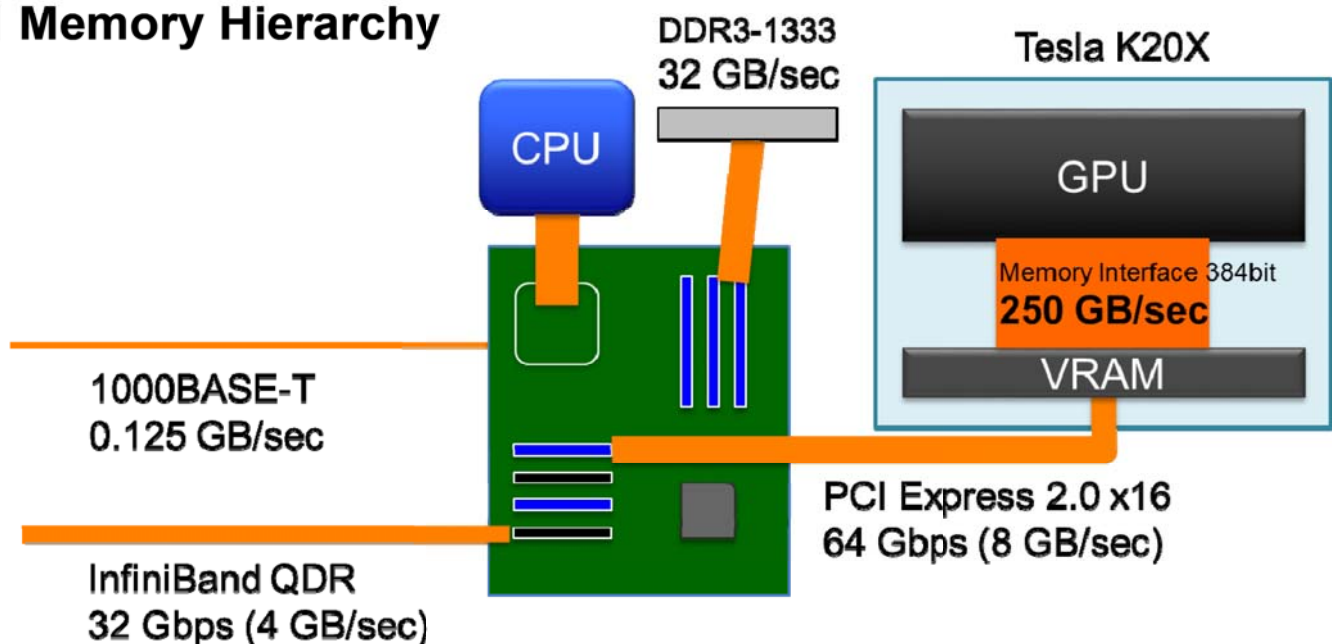
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Bandwidth Bottlenecks



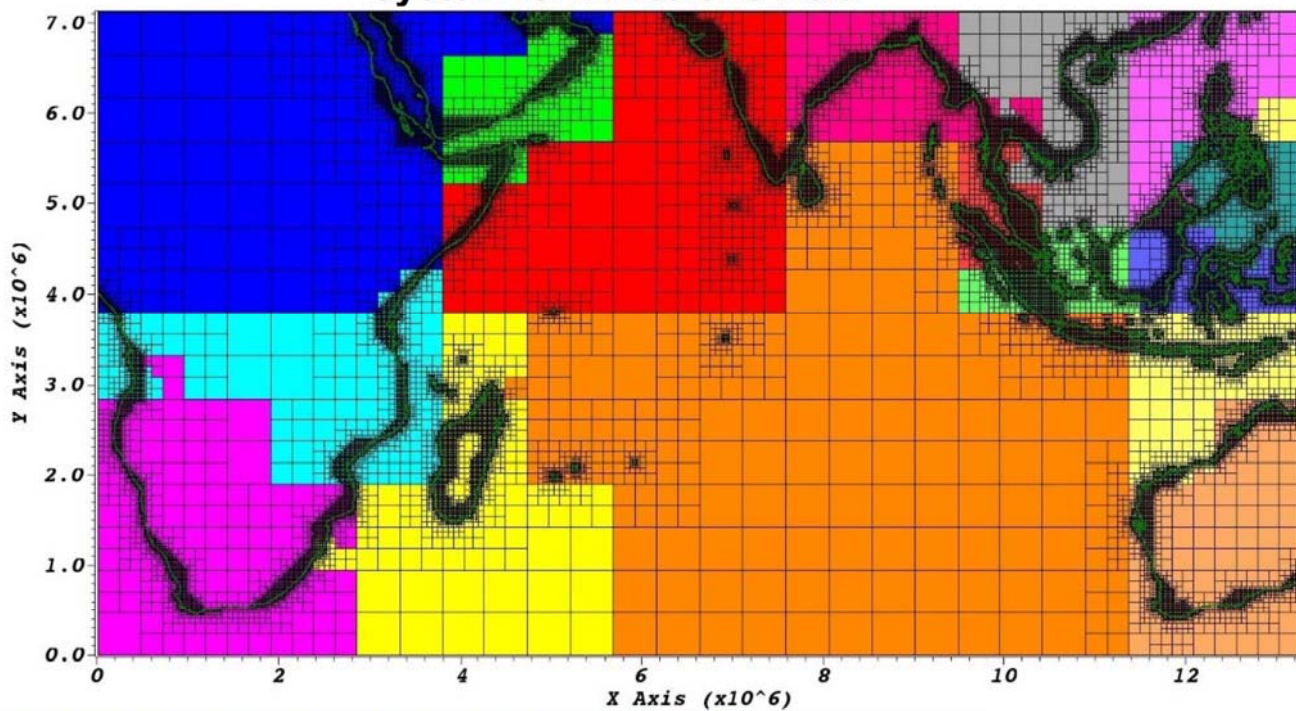
Memory Hierarchy



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6

RIMES Regional Integrated Multi-Hazard Early Warning System for Africa and Asia



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7

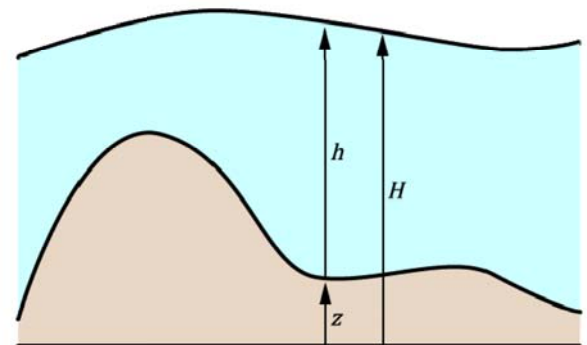
Shallow Water Solver



$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = S \quad U = \begin{bmatrix} h \\ hu \\ hv \end{bmatrix}, \quad F = \begin{bmatrix} hu \\ hu^2 + \frac{1}{2}gh^2 \\ huv \end{bmatrix}, \quad G = \begin{bmatrix} hv \\ huv \\ hv^2 + \frac{1}{2}gh^2 \end{bmatrix}$$

Two GPU kernels:

- Characteristics Method for **Deep Ocean**
Directional splitting (fractional step)
- FVM for the area including **Coastlines**
A lot of exceptional processes



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Characteristics Method

Factorization:

$$\frac{\partial U}{\partial t} + A \frac{\partial U}{\partial x} = 0 \quad A = \frac{\partial F}{\partial U} = \begin{bmatrix} 0 & 1 \\ \Gamma^2 - u^2 & 2u \end{bmatrix}$$

for $\Gamma = \sqrt{gh}$

$$\Gamma^{n+1} = \frac{1}{2} \left\{ \Gamma^{+n+1} + \Gamma^{-n+1} + \frac{1}{2} (u^+ - u^-) \right\}$$

$$u^{n+1} = \frac{1}{2} \left\{ u^+ - u^- + 2(\Gamma^+ - \Gamma^-) \right\}$$

Riemann invariants :

$$\frac{\partial W}{\partial t} + \Lambda \frac{\partial W}{\partial x} = 0 \quad W = \begin{bmatrix} \Gamma + \frac{1}{2}u \\ \Gamma - \frac{1}{2}u \end{bmatrix}, \quad \Lambda = \begin{bmatrix} u + \Gamma & 0 \\ 0 & u - \Gamma \end{bmatrix}$$

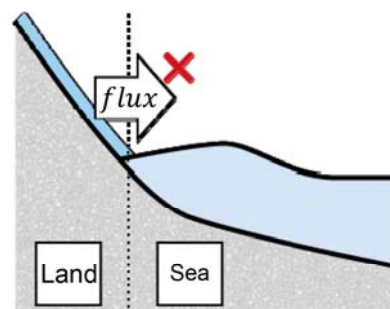
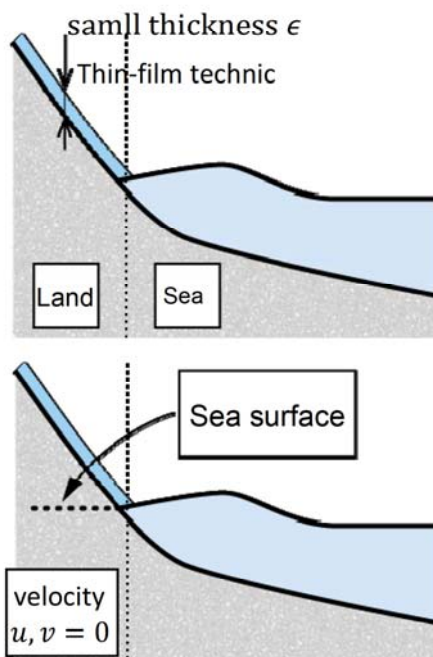
$$\frac{\partial \Gamma^\pm}{\partial t} + \lambda^\pm \frac{\partial \Gamma^\pm}{\partial x} = 0 \quad \Gamma^\pm = \Gamma \pm \frac{1}{2}u$$

Semi-Lagrangian Scheme

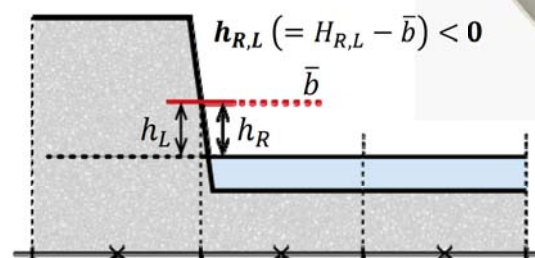
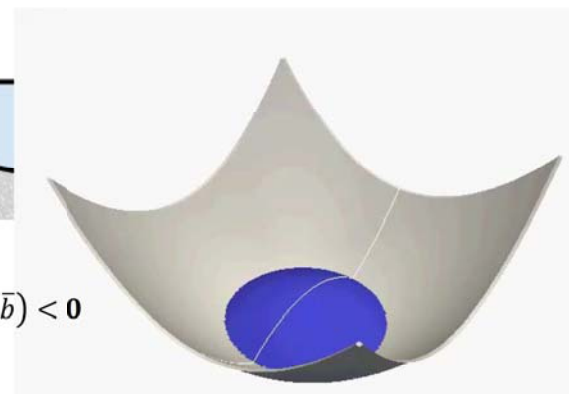
↓

$$h^{n+1}, (hu)^{n+1}$$

Inundation at coastlines



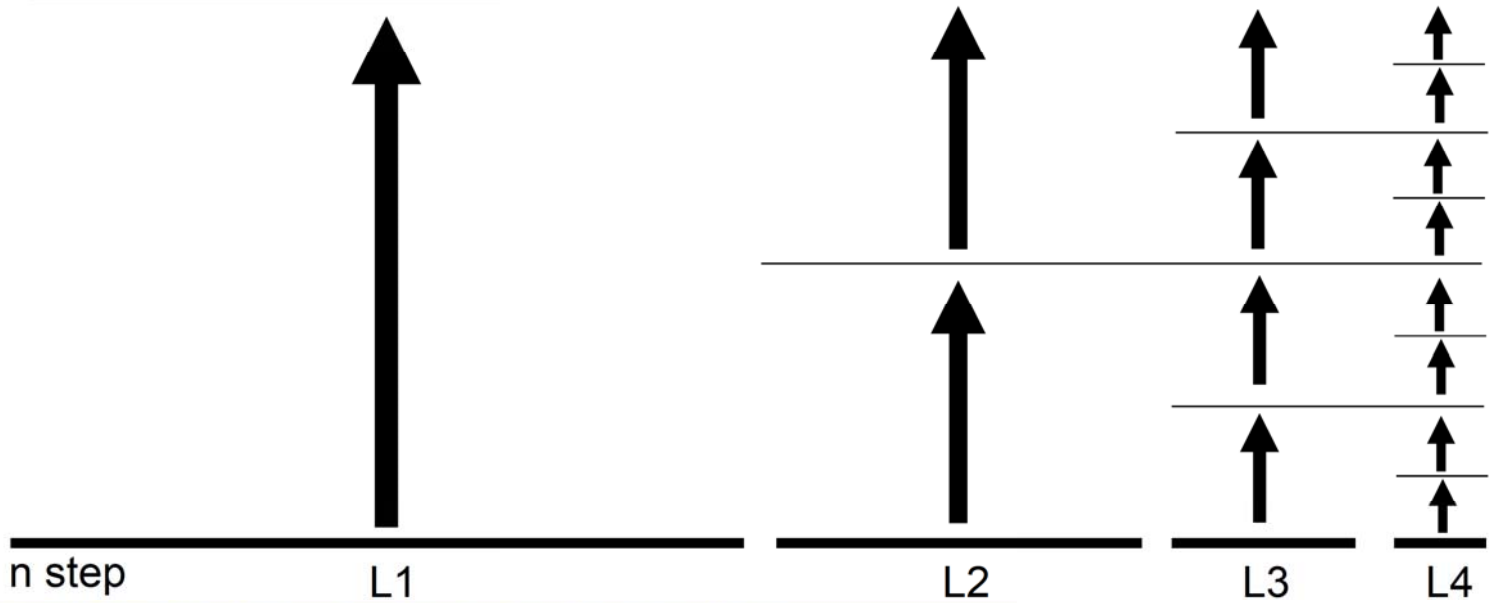
Many exceptional treatments



Time-step Control (Sub-cycling)

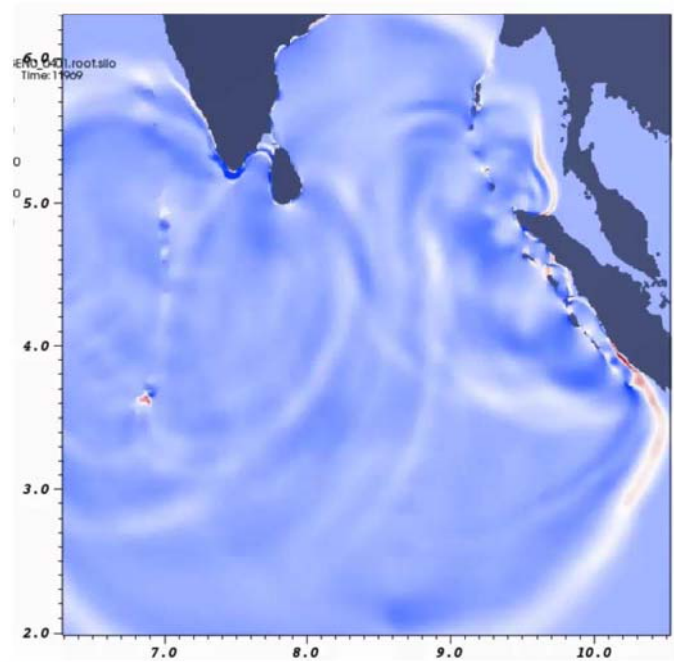
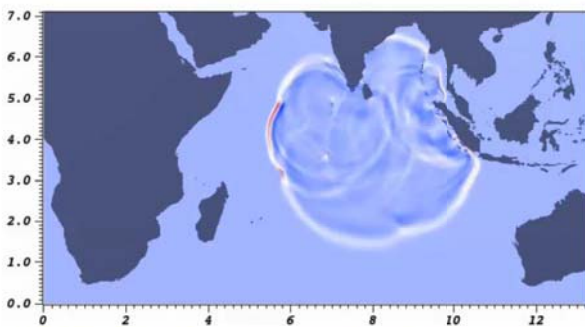
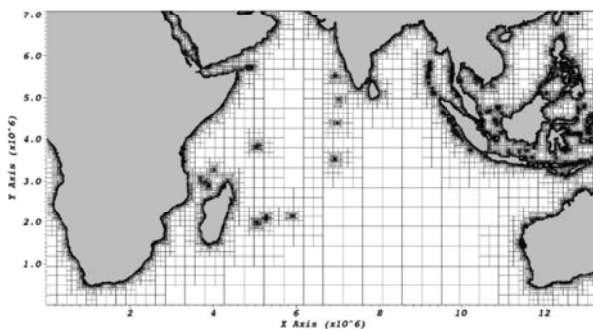


n+1 step



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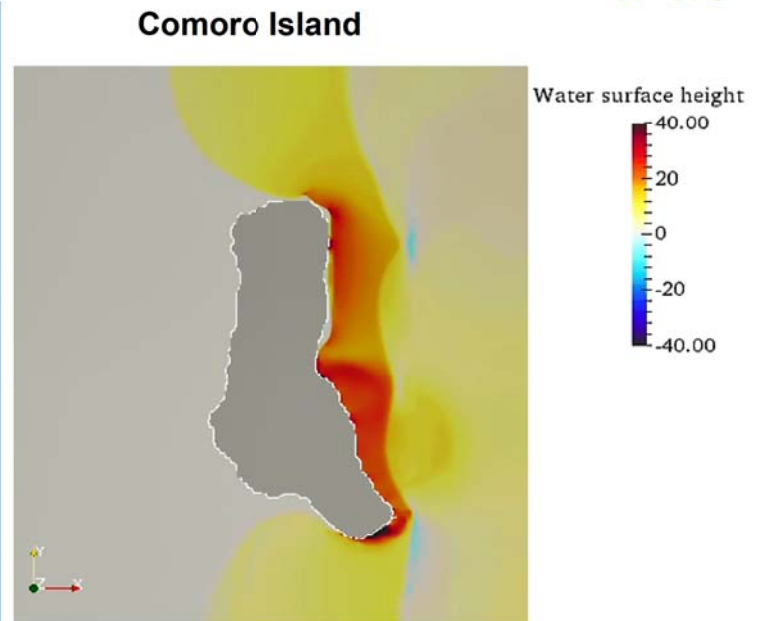
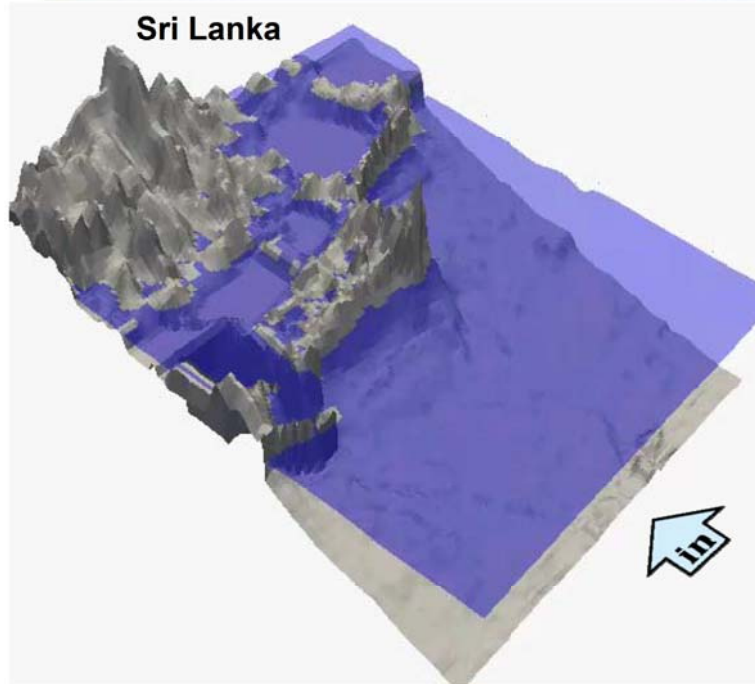
Global Tsunami Simulation



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Inundation Validation



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津波の建物への影響



A Tsunami Shelter Project



**Urgent Electric
Power Supply**

**Vertical Axis
Wind Turbine**

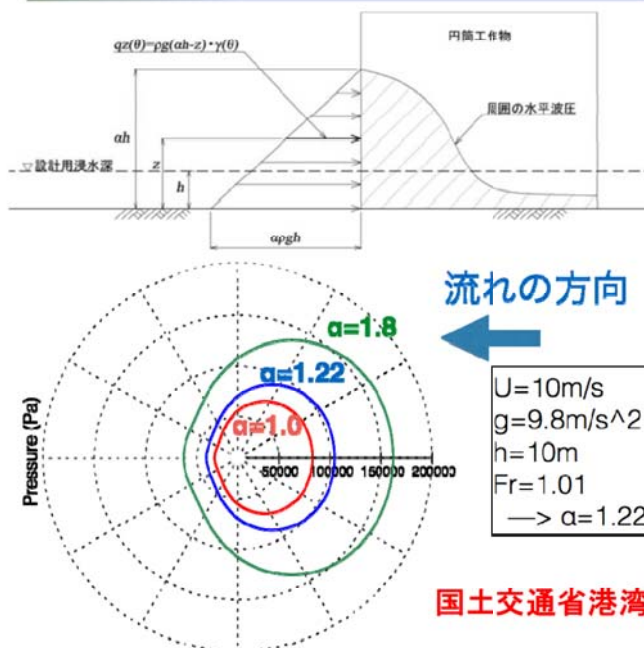
~ 100kW

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円筒形状の構造物への津波の作用



$$qz(\theta) = \rho g(\alpha h - z) \cdot \gamma(\theta)$$

$qz(\theta)$: 構造設計用の円周方向の津波波圧

θ : 津波の来襲方向を0°とした円筒工作物の角度

α : 水深係数

*1.0~3.0が
使用されている

$$\alpha = \begin{cases} 1.0 & (F_r < 0.9) \\ 2.0F_r - 0.8 & (0.9 \leq F_r \leq 1.3) \\ 1.8 & (1.3 \leq F_r) \end{cases}$$

F_r : フルード数 $F_r = U/\sqrt{gh}$ U : 津波の流速 (m/s)

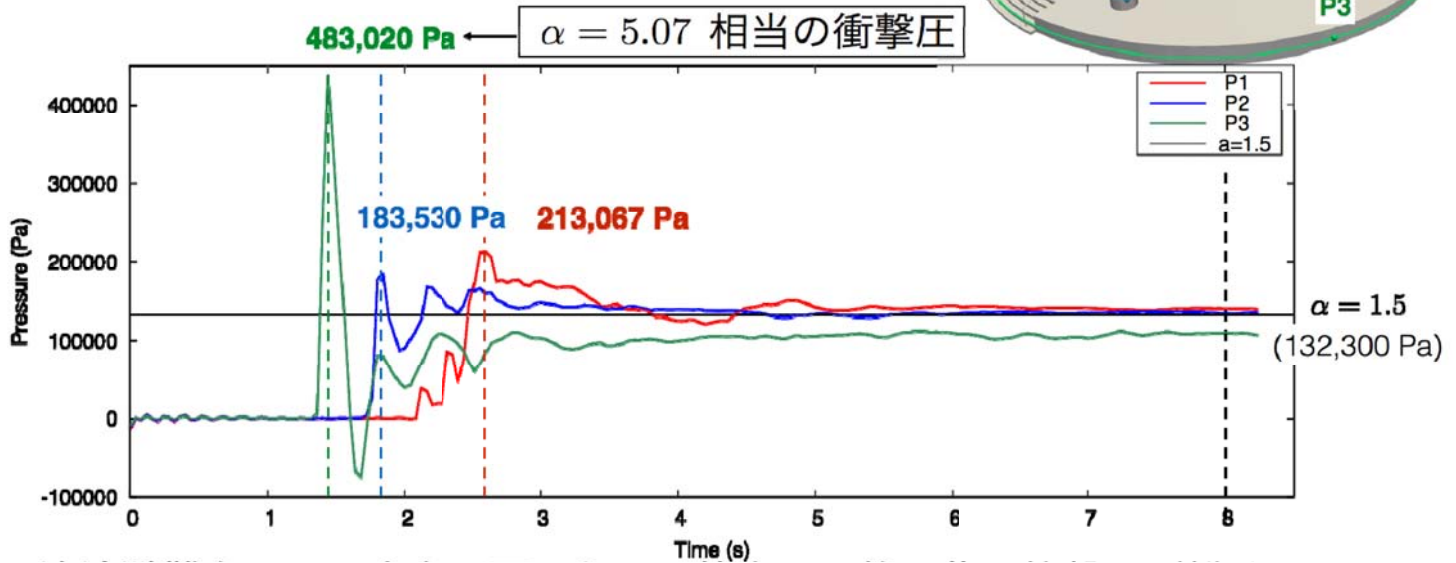
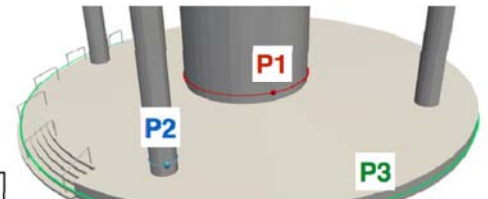
$\gamma(\theta)$: 円周方向の低減係数

$$\gamma(\theta) = \sum_{m=0}^3 p_m \cos(m\theta)$$

$$p_0 = 0.680, p_1 = 0.340, p_2 = 0.015, p_3 = -0.035$$

国土交通省港湾局: 「港湾の津波避難施設の設計ガイドライン(平成25年10月)」

柱にかかる圧力の時間履歴



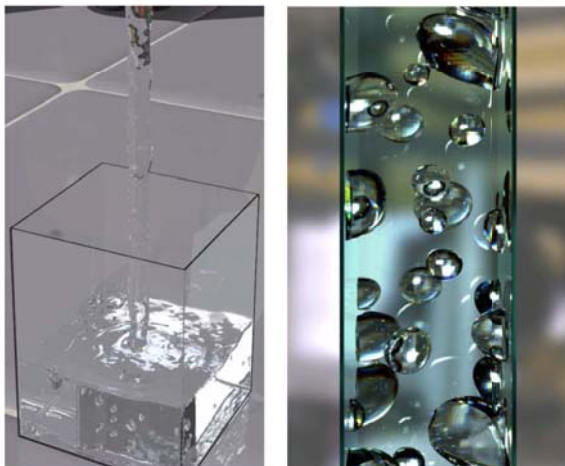
※ 津波避難タワーの土台正面に静水圧の5倍の衝撃圧がかかる

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気液二相流(有限体積法)



Two-Phase Flows



Mesh Method (Surface Capture)
to solve Navier Stokes equation

- Navier-Stokes solver: Fractional Step
- Time integration: 3rd TVD Runge-Kutta
- Advection term: 5th WENO
- Diffusion term: 4th FD
- Poisson: MG-BiCGstab
- Surface tension: CSF model
- Surface capture: CLSVOF(THINC + Level-Set)

Fine meshes should be assigned around
gas-liquid interfaces

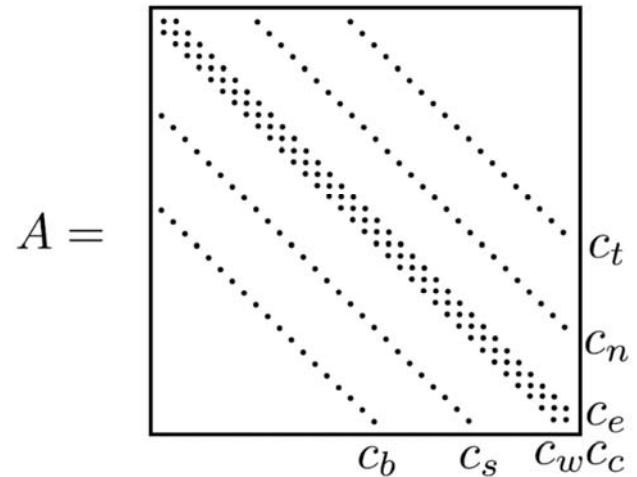
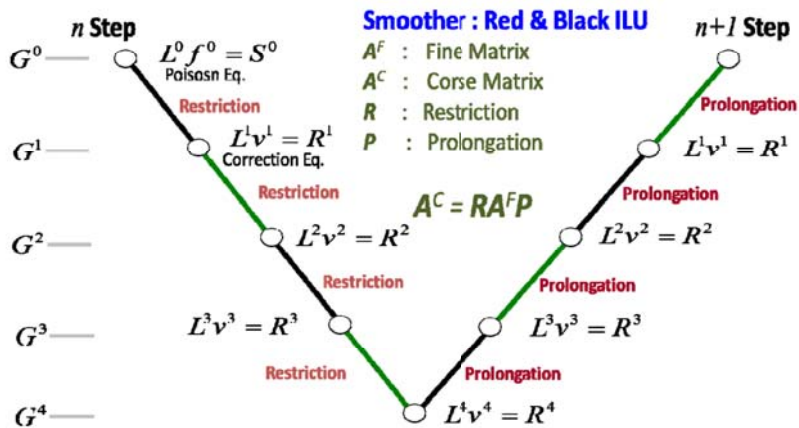
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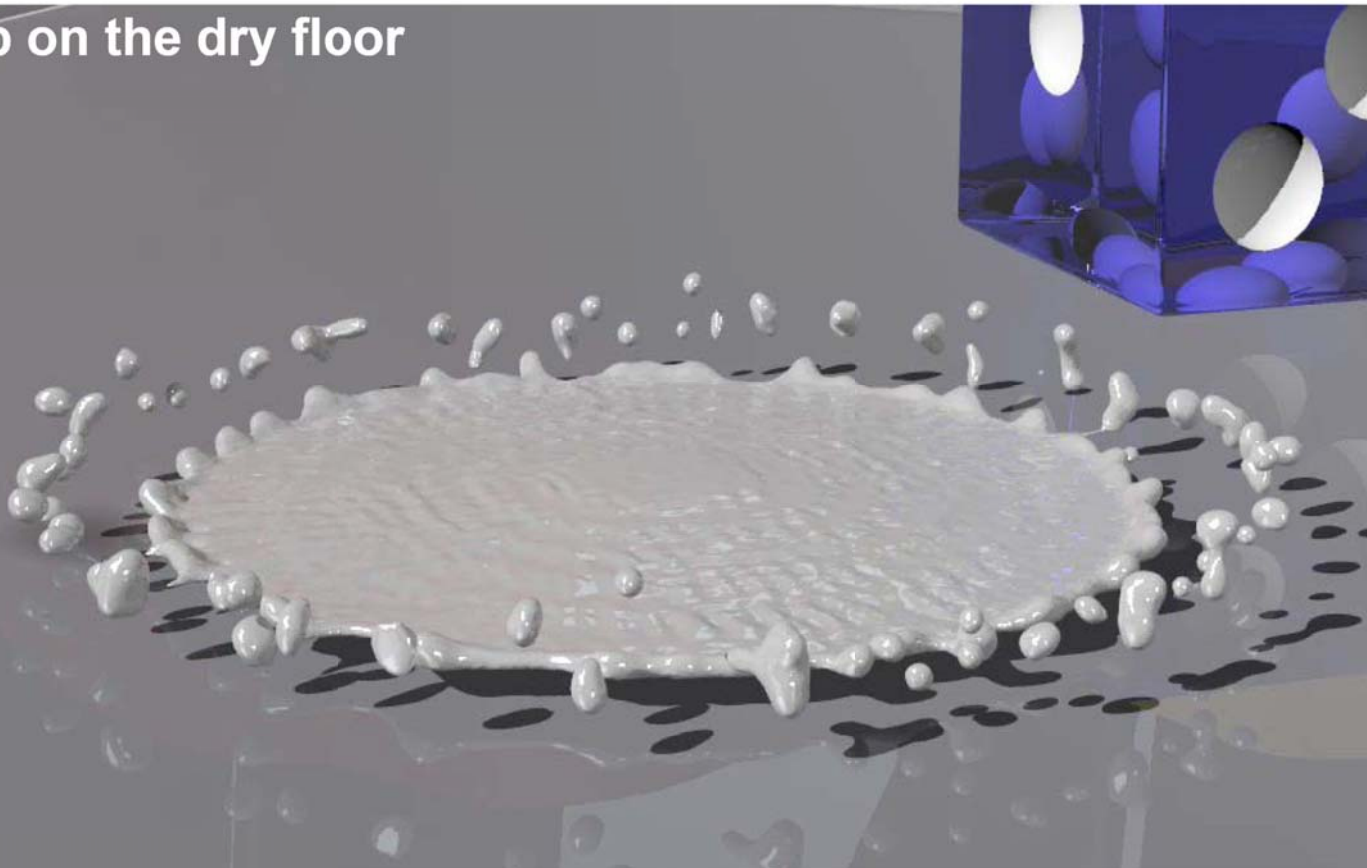
Sparse Matrix Solver

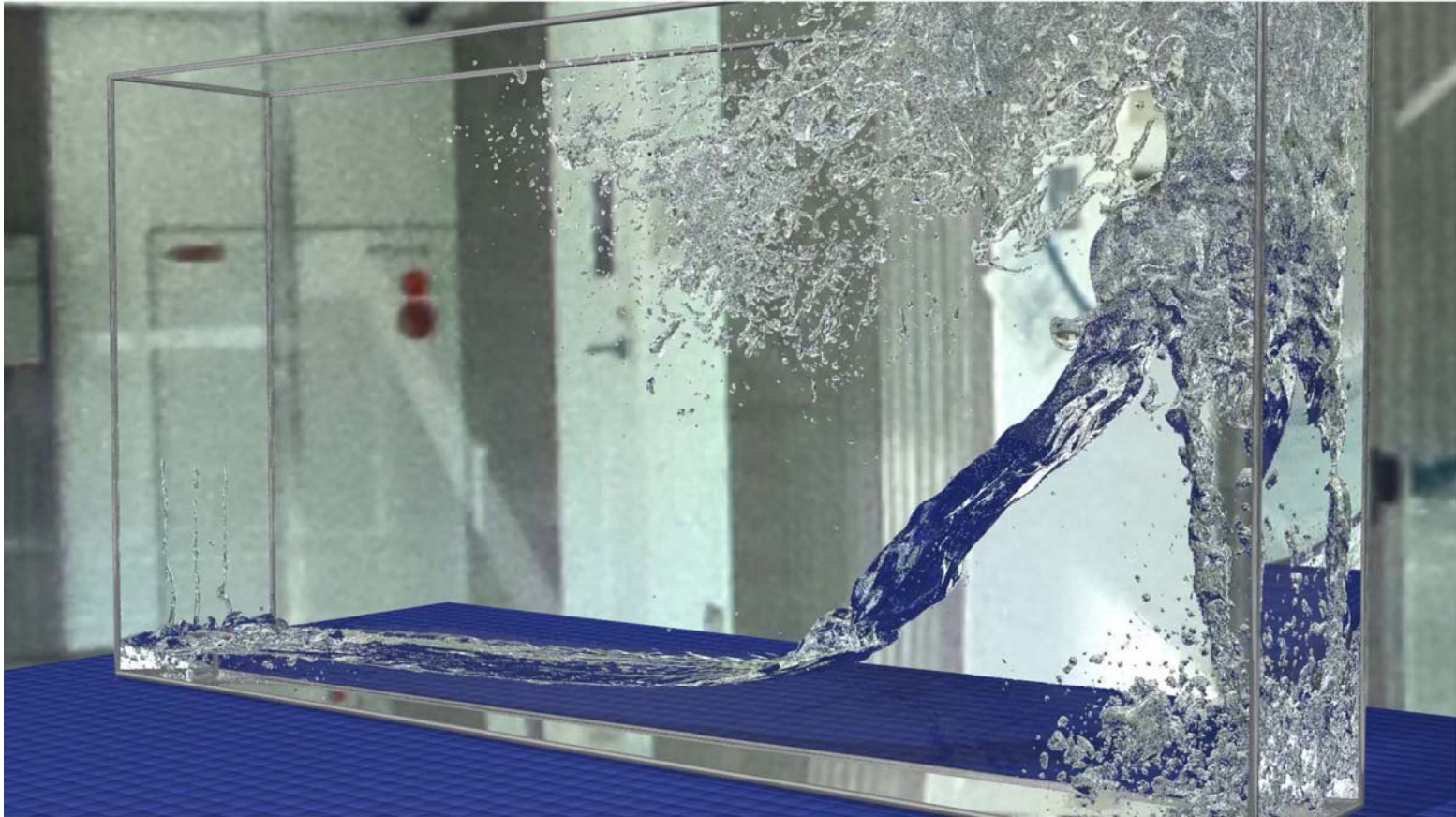
$$\mathbf{Ax} = \mathbf{b} \quad \text{for} \quad \nabla \cdot \left(\frac{1}{\rho} \nabla p \right) = \frac{\nabla \cdot \mathbf{u}}{\Delta t}$$

BiCGStab + MG preconditioner



A drop on the dry floor

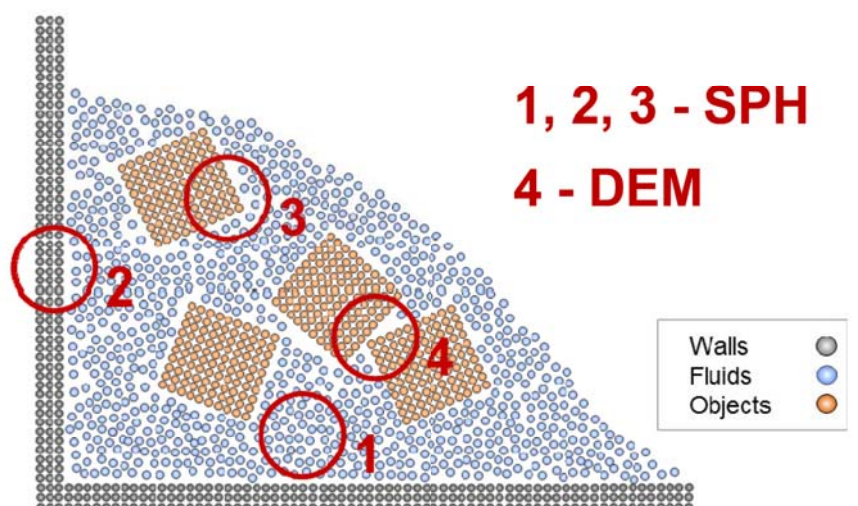




多数の瓦礫を含んだ津波シミュレーション



粒子法によるシミュレーション





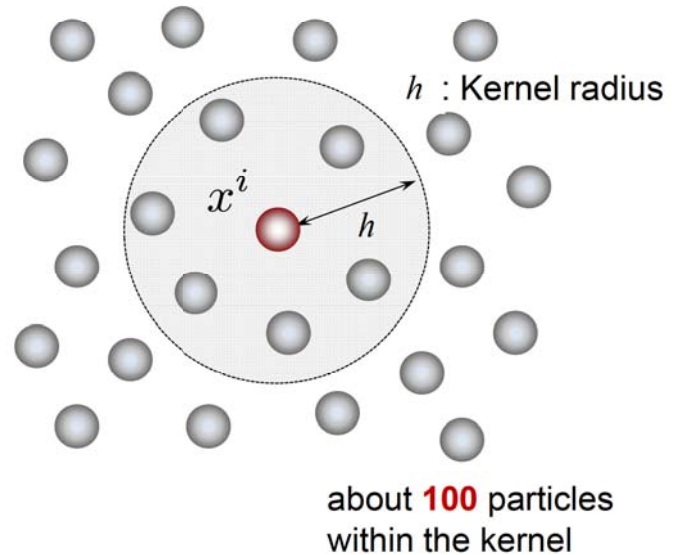
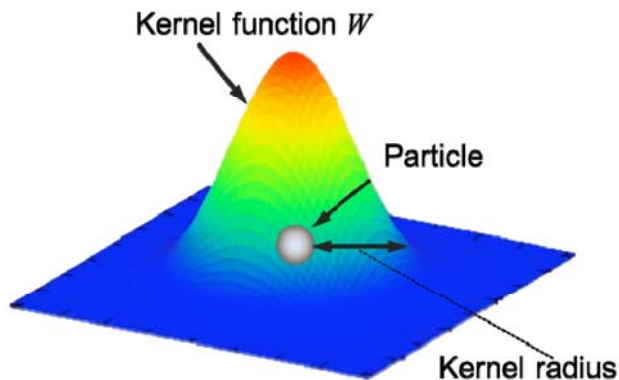
SPH (Smoothed Particle Hydrodynamics)

Improve SPH: Generalization of Finite Difference Operators (Imoto, Tagami 2014)

Physical property

$$\phi(\mathbf{x}) = \sum_j m_j \frac{\phi_j}{\rho_j} W(\mathbf{x} - \mathbf{x}_j)$$

m_j : mass ρ_j : density

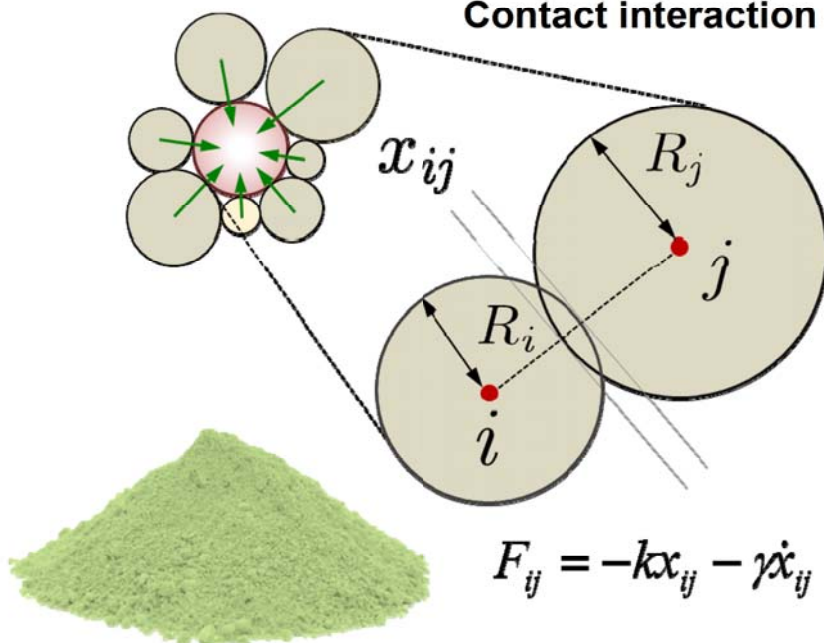


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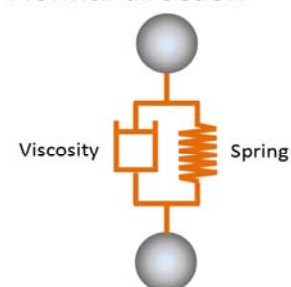
DEM (Discrete Element Method)



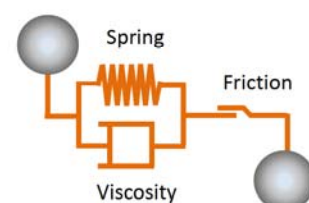
Contact interaction



Normal direction

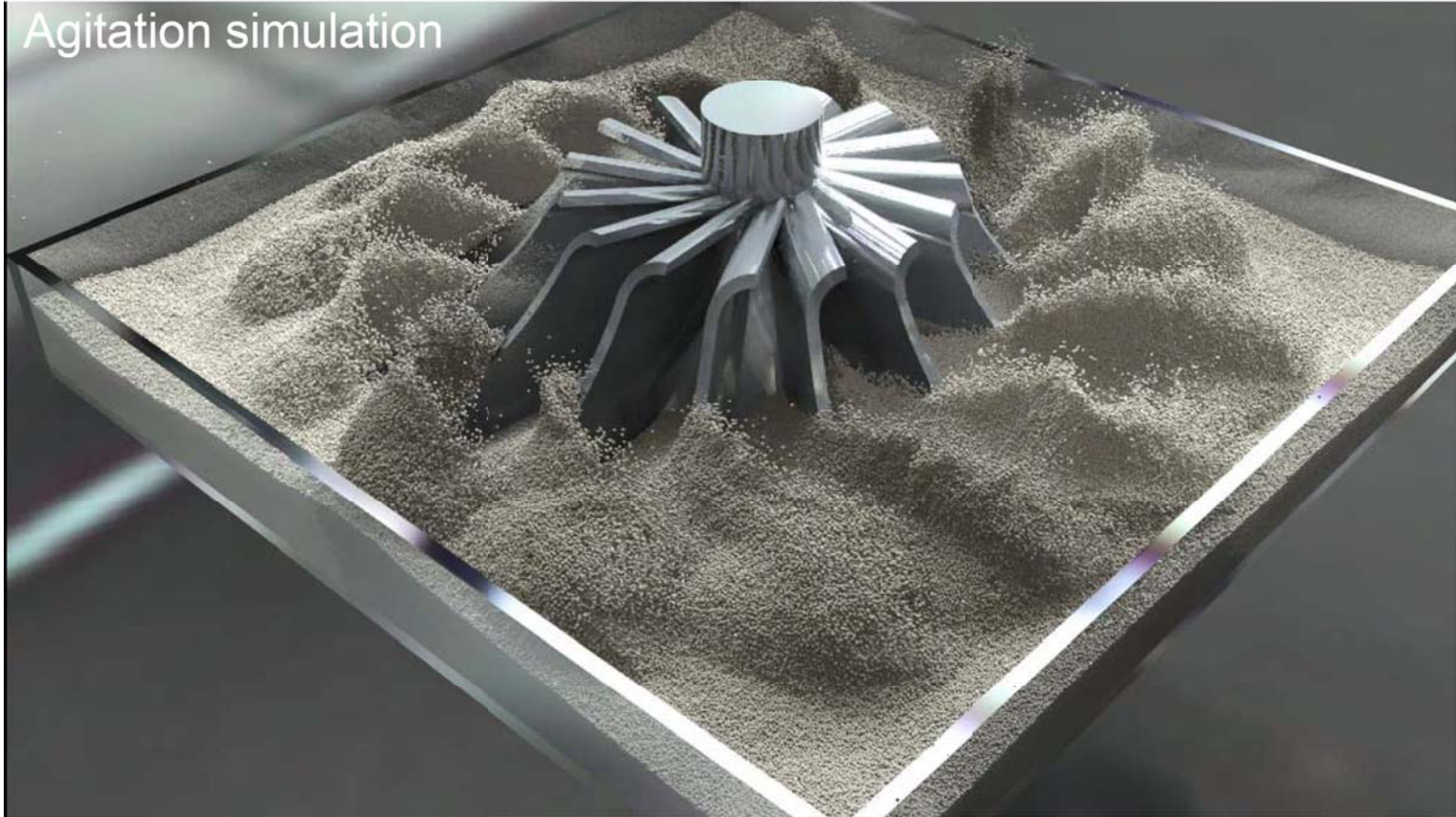


Tangential direction



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Agitation simulation



Golf Bunker shot using 16.7 millions particles
with 64 GPUs





Complex Shape Objects

Non-spherical model described by rigidly connected sphere particles

$$Fg = \sum F \quad Mg = \sum (x - xg) \times F$$

$$vg_{t+\Delta t/2} = vg_{t-\Delta t/2} + (Fg/mg)\Delta t$$

$$xg_{t+\Delta t} = xg_t + vg_{t+\Delta t/2}\Delta t$$

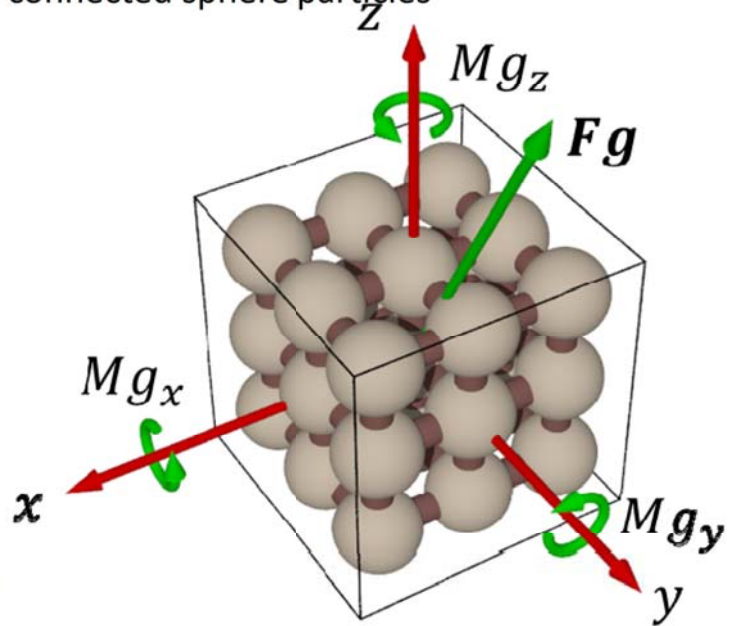
$$\omega g_{t+\Delta t/2} = \omega g_{t-\Delta t/2} + (Ig^{-1}Mg)\Delta t$$

$$Qg_{t+\Delta t} = \Delta Qg_{t+\Delta t/2}Qg_t$$

$$Ig_{t+\Delta t} = R_{t+\Delta t}^{-1}Ig_{init}R_{t+\Delta t}$$

$$x_{t+\Delta t} = xg_{t+\Delta t} + Qg_{t+\Delta t}r_{init}(Qg_{t+\Delta t})^T$$

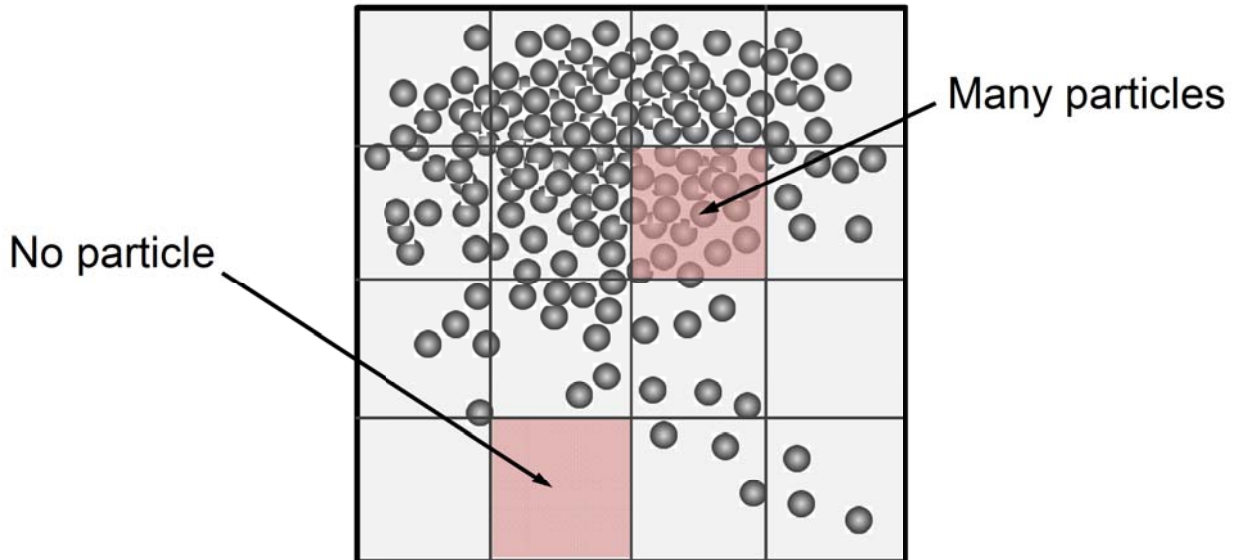
$$v_{t+\Delta t/2} = vg_{t+\Delta t/2} + \omega g_{t+\Delta t/2} \times (x_{t+\Delta t} - xg_{t+\Delta t})$$





Particle Distribution

- The load imbalance problem among subdomains

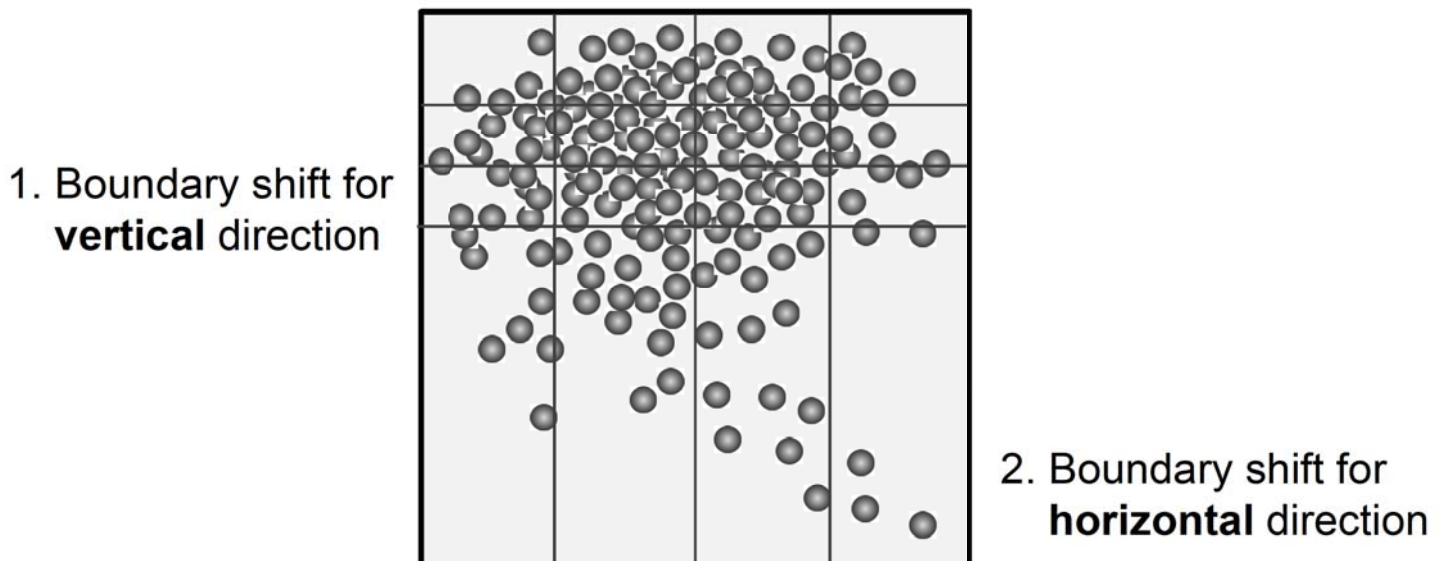


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Dynamic Domain Decomposition



- 2-dimensional slice-grid method



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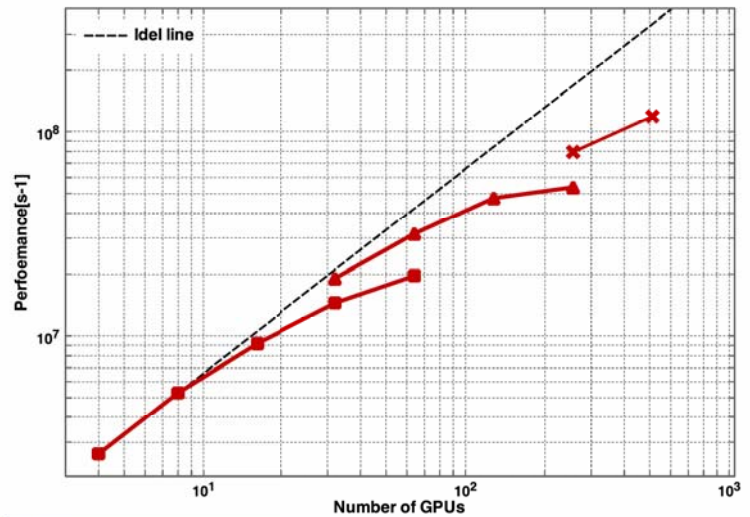
Multiple GPU Scalability

• Conditions

Particles : $2 \times 10^6, 1.6 \times 10^7, 1.29 \times 10^8$

Domain Decomposition : Dynamic load Balance using Slice Grid Method

Time-Integration : 2-stage
Runge-Kutta

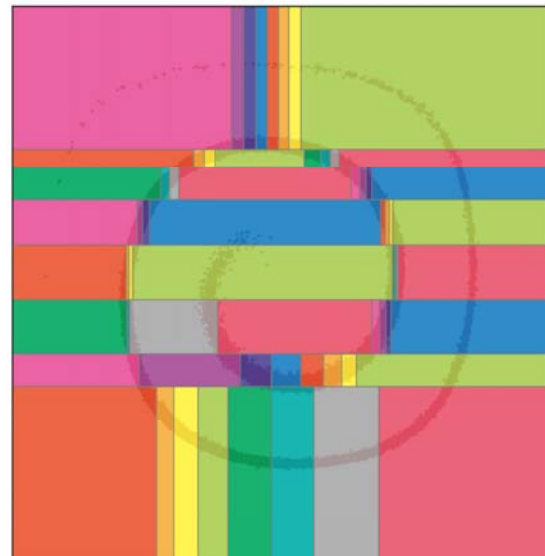
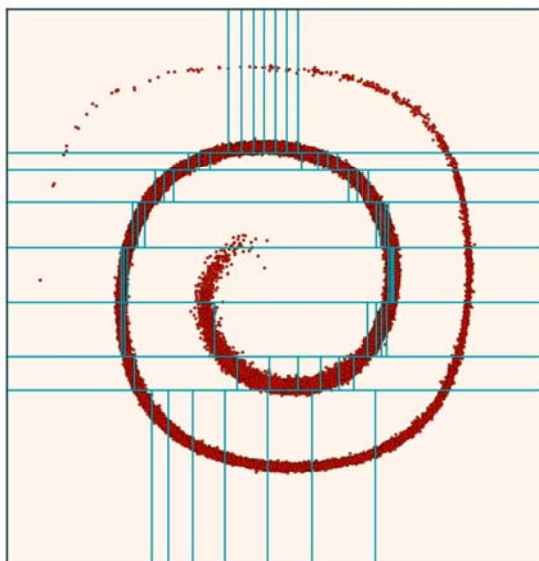


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Sub-domains with High Aspect ratio



Slice Grid Method



- The passive particles under vortex velocity field using 64 GPUs

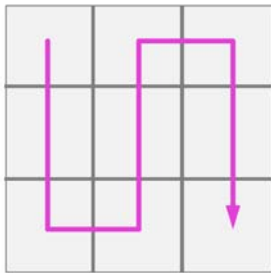
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Space Filling Curves

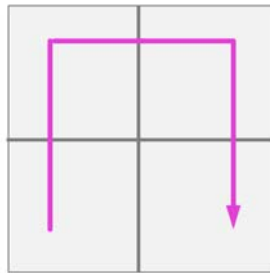
- ✓ Construction of a tree so that each leafs contain minimum number of particles
- ✓ Each leafs is numbered by following the rules of space filling curves.

Peano



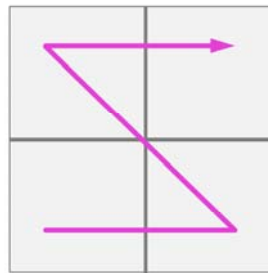
9 Cells

Hilbert

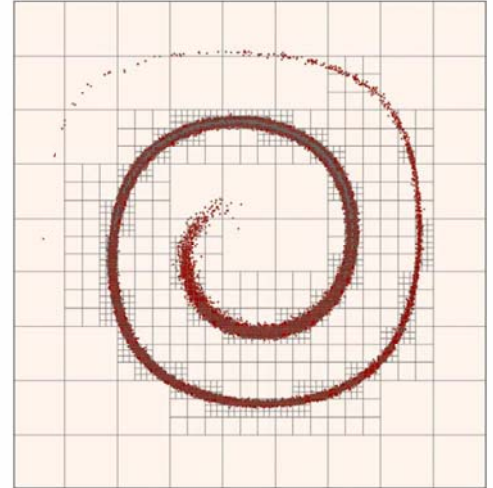


4 Cells

Morton



4 Cells



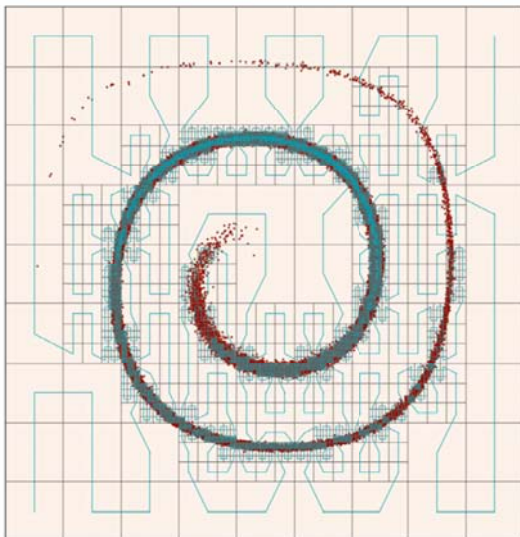
A tree-base cell refinement

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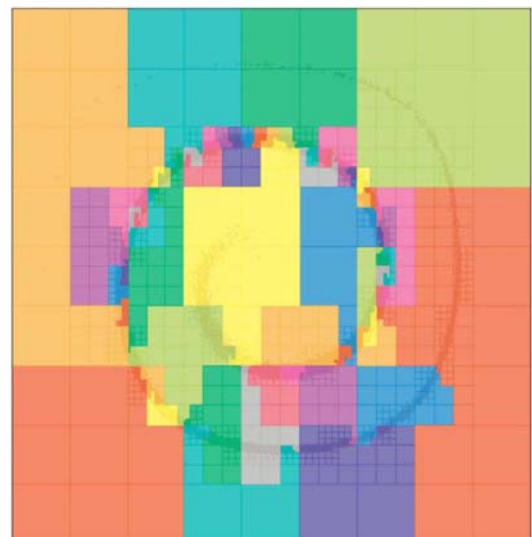
Space Filling Curves



- The connections of leafs by Peano curve



- The domain decomposition by Peano curve

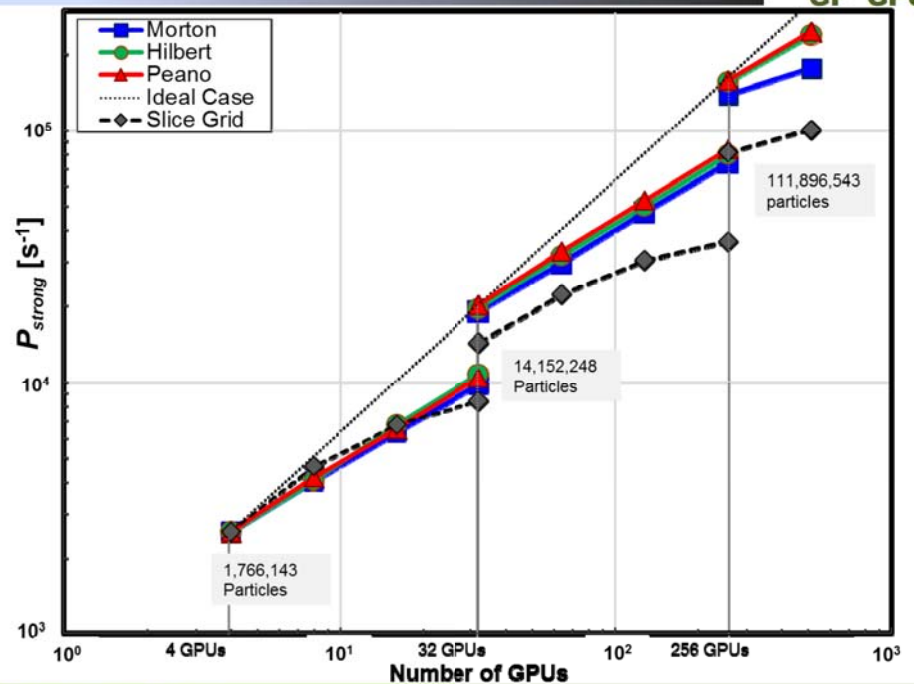
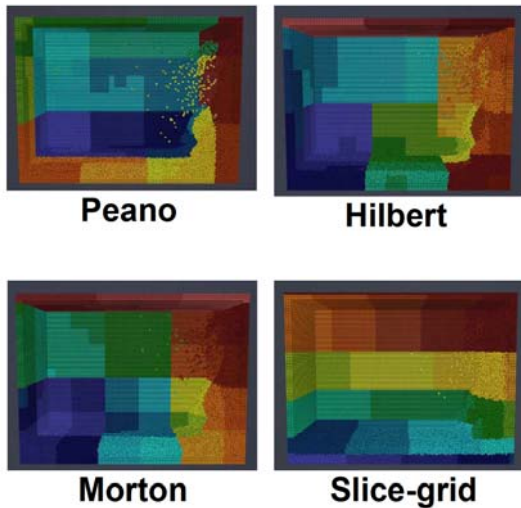


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Scalability on TSUBAME2.5



Comparison of 3 different SFC
with slice-grid method



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Tsunami Debris Flow

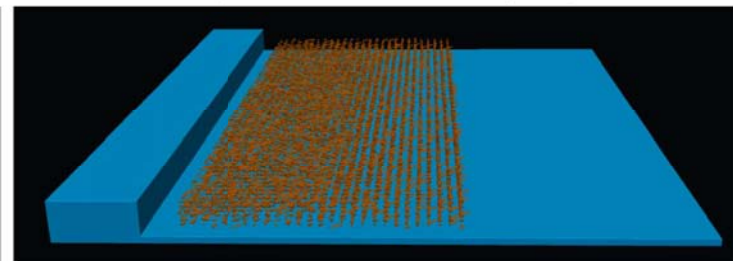


■ Including a lot of floating objects

Computational conditions

- Simulation area : 180 m × 160 m × 20 m
- Total particles : **117,561,285**
- Particles / object : 19 ~ 472
- Objects : **10368**
- Physical time (s) : 10.0
- Steps : 20,000
- GPUs : 256
- Simulation (h) : 100
- Initial height (m) : 10.0

Initial state of each objects

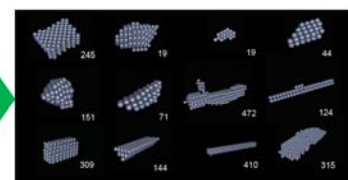


Representation of object shapes

CAD Data



Particles



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Dynamic Domain Decomposition



- Using the improved SPH with 87Million particles with 256 GPUs





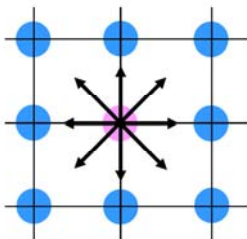
東京都心部の10km四方の1m格子解像度による 大規模気流シミュレーション

LBM (Lattice Boltzmann Method)

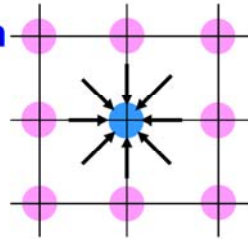


$$\frac{\partial f_i}{\partial t} + \mathbf{e}_i \cdot \nabla f_i = -\frac{1}{\lambda} (f_i - f_i^{eq})$$

**Streaming
step:**

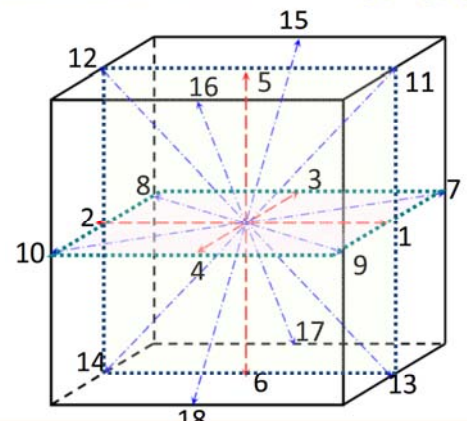


**Collision
step:**



SRT: Memory Bound, MRT: Compute Intensive

$$f_i^{eq} = \rho w_i \left[1 + \frac{3}{c^2} (\mathbf{e}_i \cdot \mathbf{u}) + \frac{9}{2c^4} (\mathbf{e}_i \cdot \mathbf{u})^2 - \frac{3}{2c^2} (\mathbf{u} \cdot \mathbf{u}) \right]$$



i is the value in the direction of i th discrete velocity
 $\mathbf{e}_i$ is the discrete velocity set;
 w_i is the weighting factor
 $\mathbf{u}$ is the macroscopic velocity

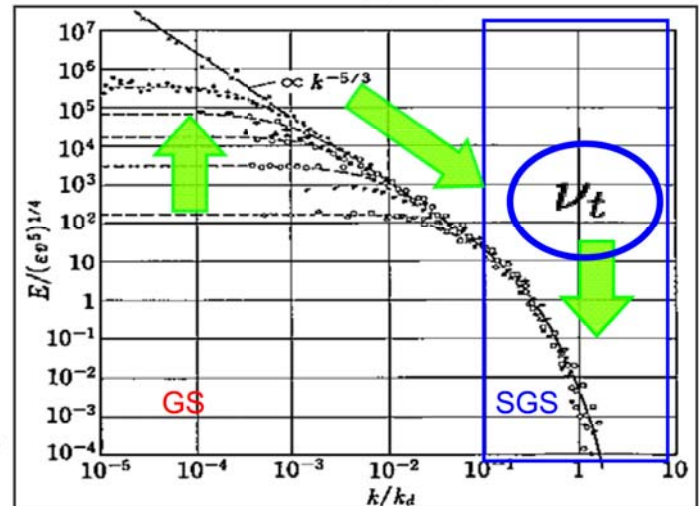
$$f_\alpha(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) - f_\alpha(\mathbf{x}, t) = -M_{\alpha\beta}^{-1} \hat{S}_{\beta\beta'} M_{\beta'\alpha'} (f_{\alpha'}(\mathbf{x}, t) - f_{\alpha'}^{eq}(\mathbf{x}, t))$$



LES (Large-Eddy Simulation)

$$f_i(\mathbf{x} - \mathbf{c}_i \Delta t, t + \Delta t) = f_i(\mathbf{x}, t) - \frac{1}{\tau_*} (f_i(\mathbf{x}, t) - f_i^{eq}(\mathbf{x}, t)) + F_i$$

Energy spectrum



Relaxation time
for LES model

$$\tau_* = \frac{1}{2} + \frac{3\nu_*}{c^2 \Delta t}$$

$$\nu_* = \nu_0 + \nu_t$$

Molecular viscosity and Eddy viscosity

コヒーレント構造スマゴリンスキーモデル

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Computational Area



Major part of Tokyo

Including Shinjuku-ku,
Chiyoda-ku, Minato-ku,
Meguro-ku, Chuo-ku,

10km × 10km

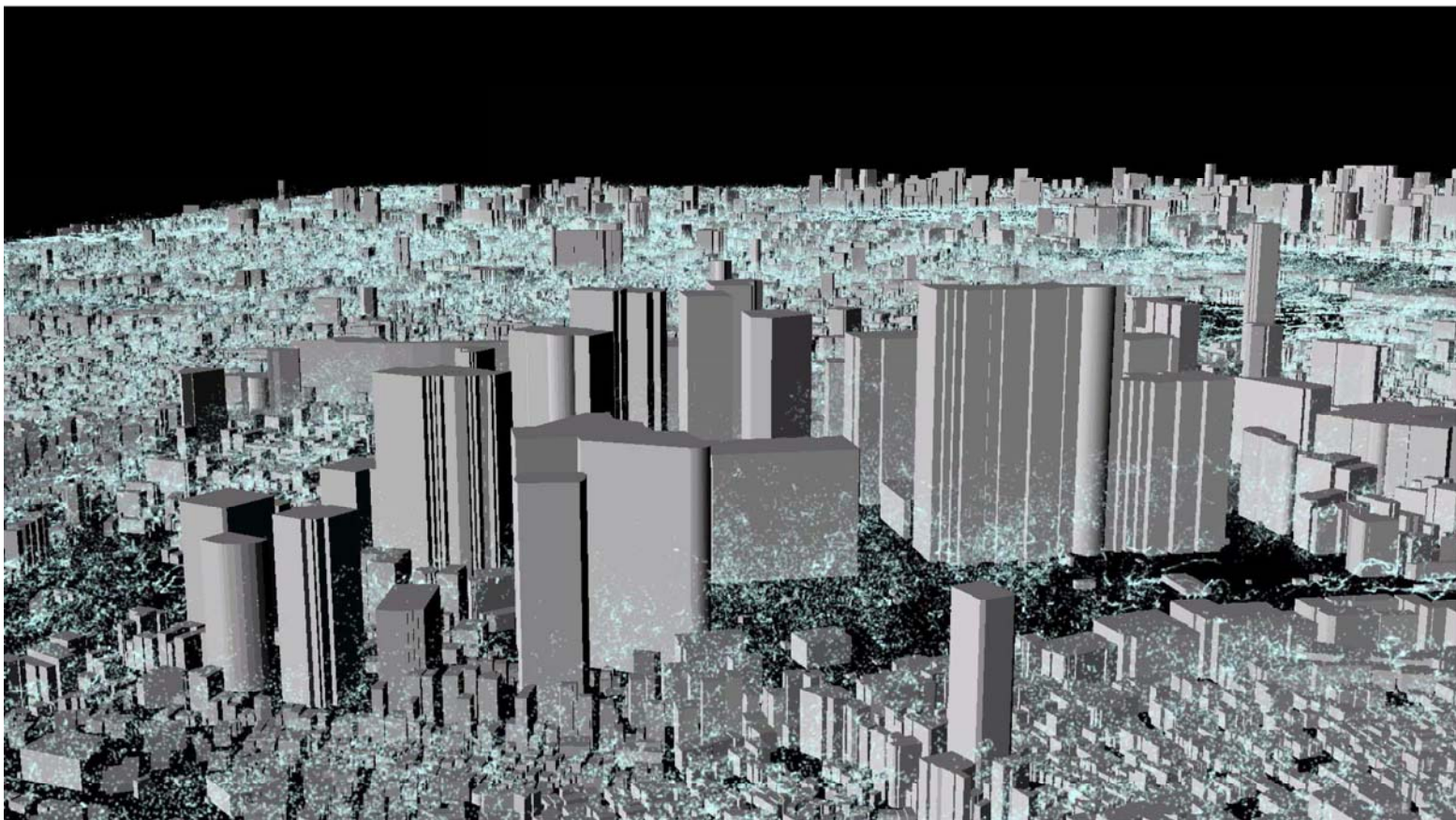
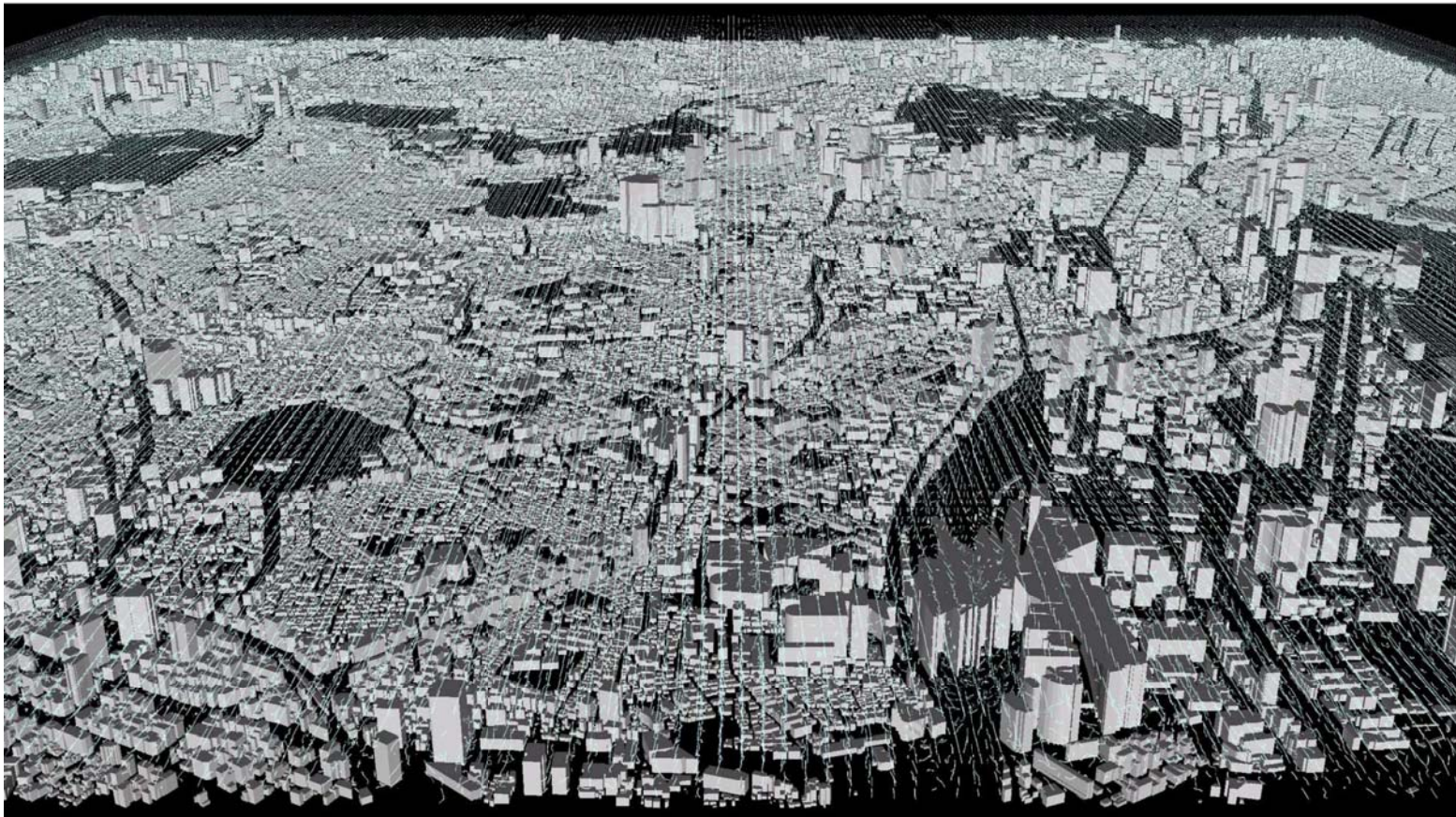
Building Data:

Pasco Co. Ltd.
TDM 3D



Map ©2012 Google, ZENRIN

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LBM-DEM coupled method

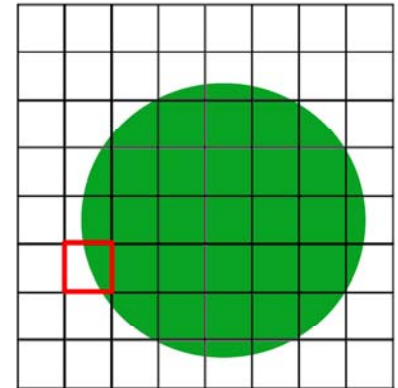
- Solid fraction in each cell: β_n
- Bounce back boundary condition f^m

$$f(x + c_i \Delta t, t + \Delta t) = f(x, t) - (I - \beta) M^{-1} S(m(x, t) - m^{eq}(x, t)) + \beta f^m$$

$$\beta_n = \frac{\text{Area of solid in cell}}{\text{Cell area}} \quad \beta: \beta_n \text{ diagonal matrix}$$

$$f_i^m = [f_{-i}(x, t) - f_{-i}^{eq}(\rho, u)] - [f_i(x, t) - f_i^{eq}(\rho, v_{\text{wall}})]$$

$$v_{\text{wall}} = v_{\text{particle}} + \omega_{\text{particle}} \times \left(x + \frac{c_i \Delta t}{2} - x_{\text{particle}}\right)$$



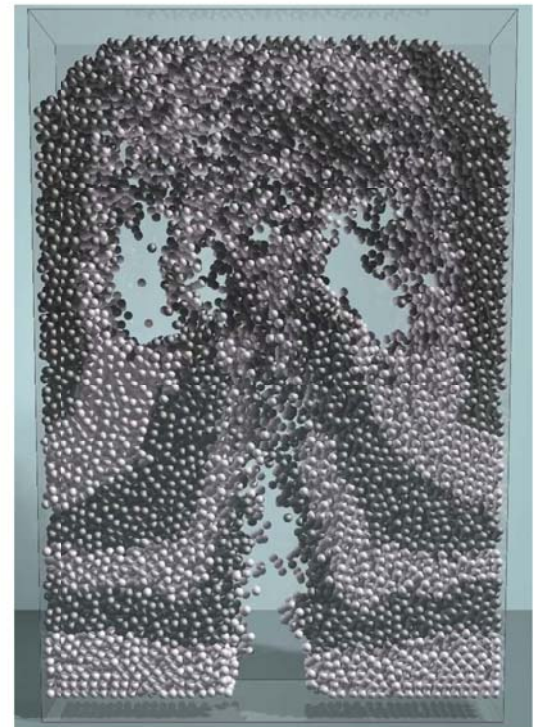
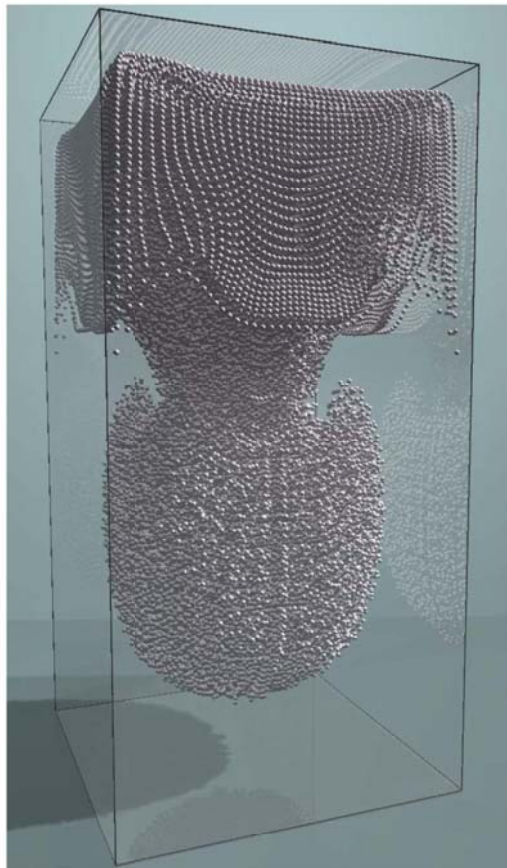
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DEM

68,921 particles

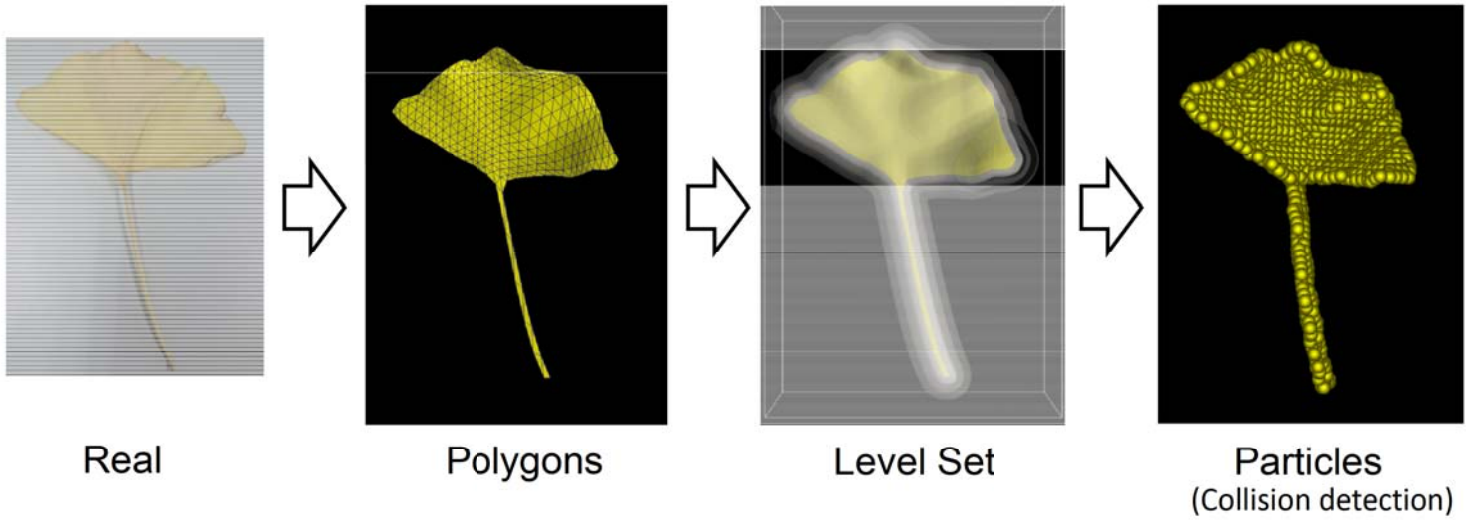
LBM

288x288x576 mesh



Falling Ginkgo leaves

Modeling of Ginkgo leaf



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爆風飛散シミュレーション

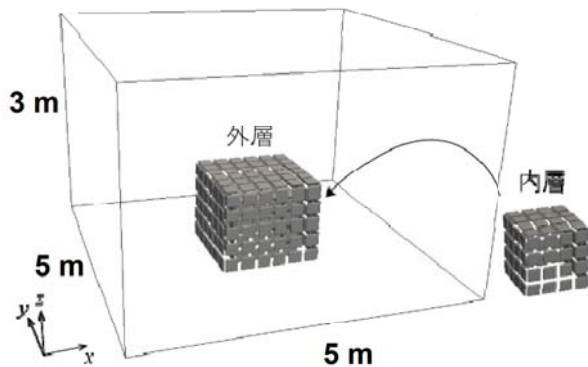


Compressible Fluid

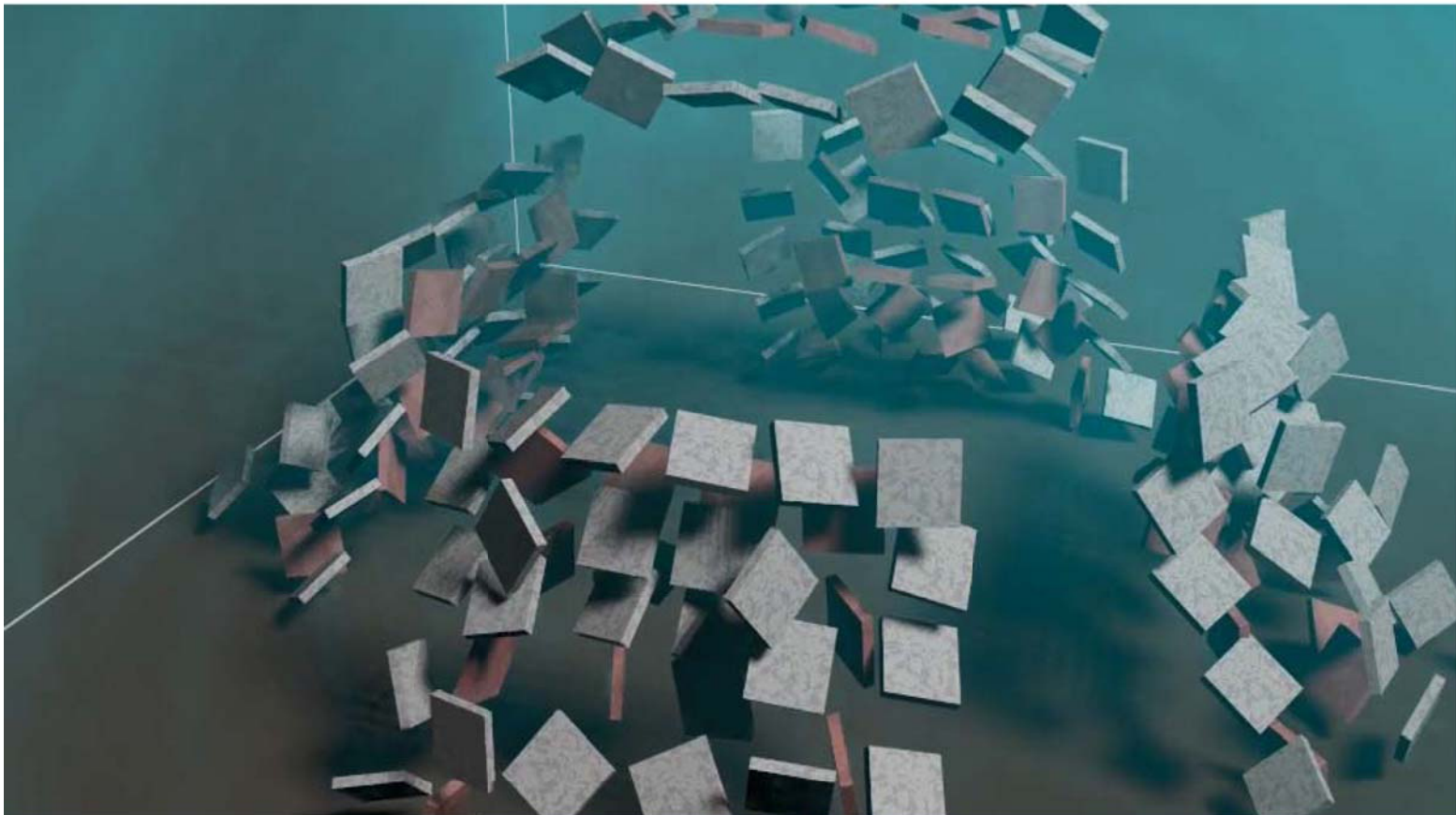
$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} + \frac{\partial H}{\partial z} = \frac{\partial F_v}{\partial x} + \frac{\partial G_v}{\partial y} + \frac{\partial H_v}{\partial z}$$

$$U = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho e \end{bmatrix} \quad F = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho vu \\ \rho wu \\ u(\rho e + p) \end{bmatrix} \quad G = \begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ \rho wv \\ v(\rho e + p) \end{bmatrix} \quad H = \begin{bmatrix} \rho w \\ \rho uw \\ \rho vw \\ \rho w^2 + p \\ w(\rho e + p) \end{bmatrix}$$

Immersed Boundary Method

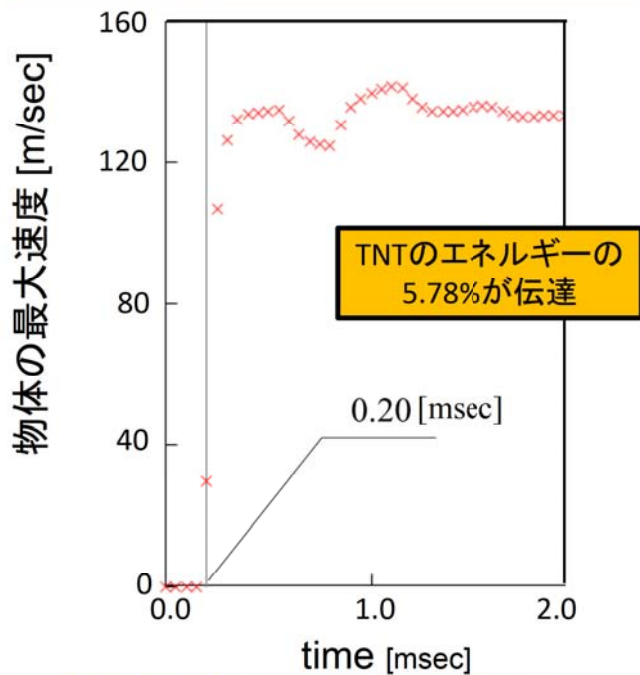


内側に TNT 1kg

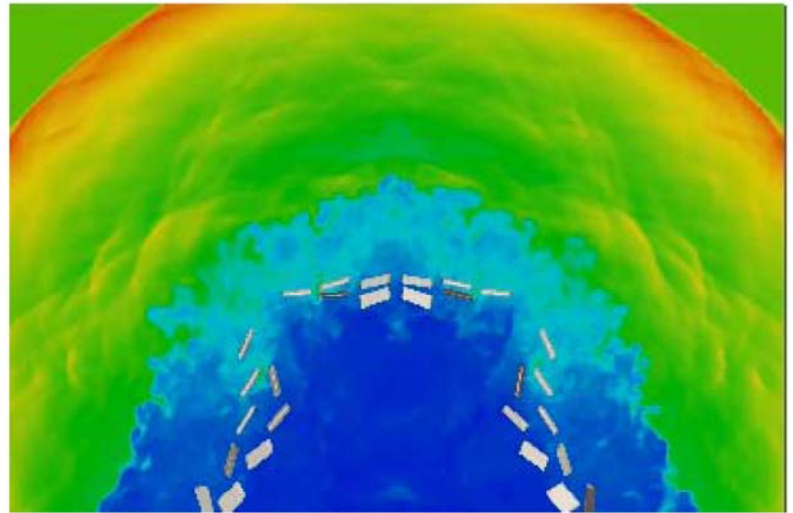




飛散挙動



物体の加速開始

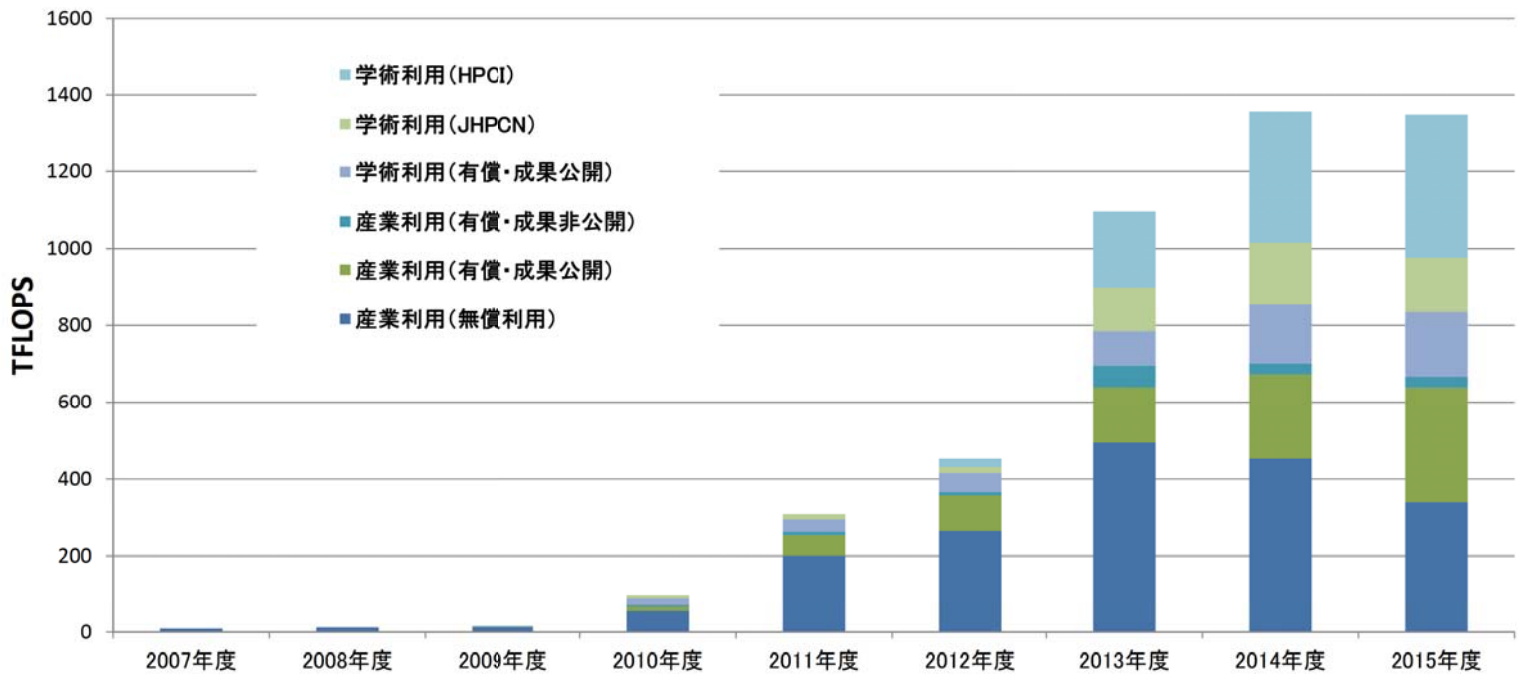


スパコンからのイノベーション

東京工業大学 学術国際情報センター 共同利用推進室

学外利用に供するTSUBAMEの資源量の推移

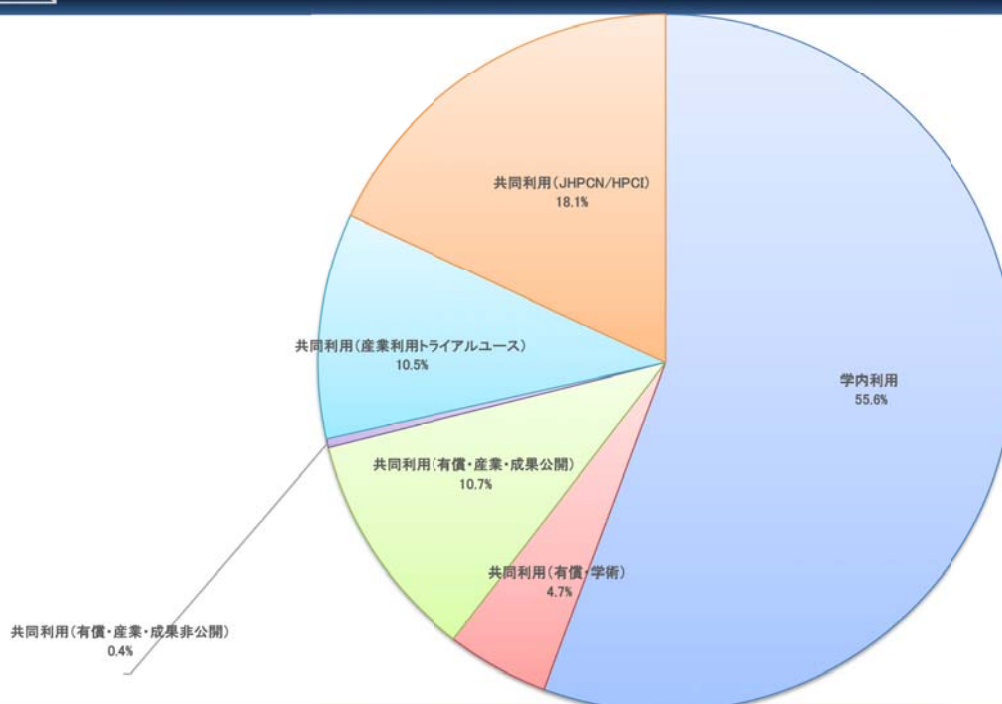
55



東京工業大学 学術国際情報センター

TSUBAME利用種別利用ノード時間積割合(2015年度実績)

56

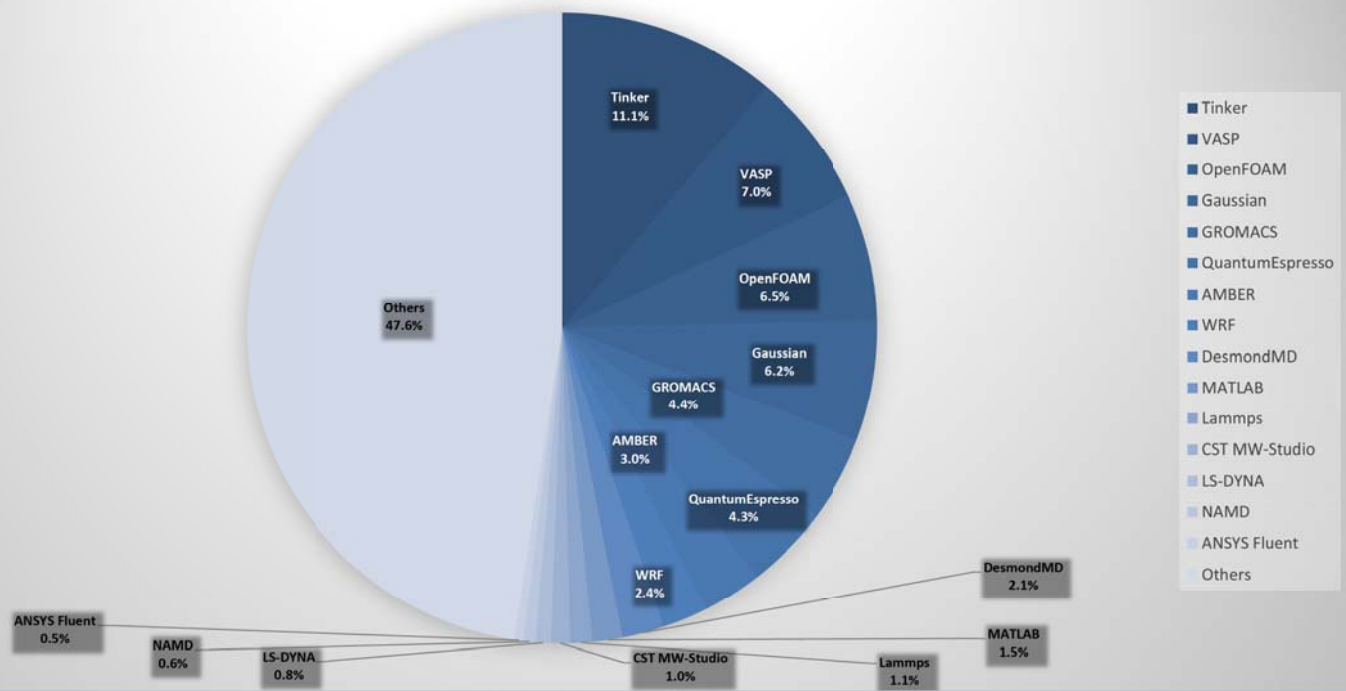


東京工業大学 学術国際情報センター



アプリケーション別利用ノード時間積割合(2015年12月実績)

57

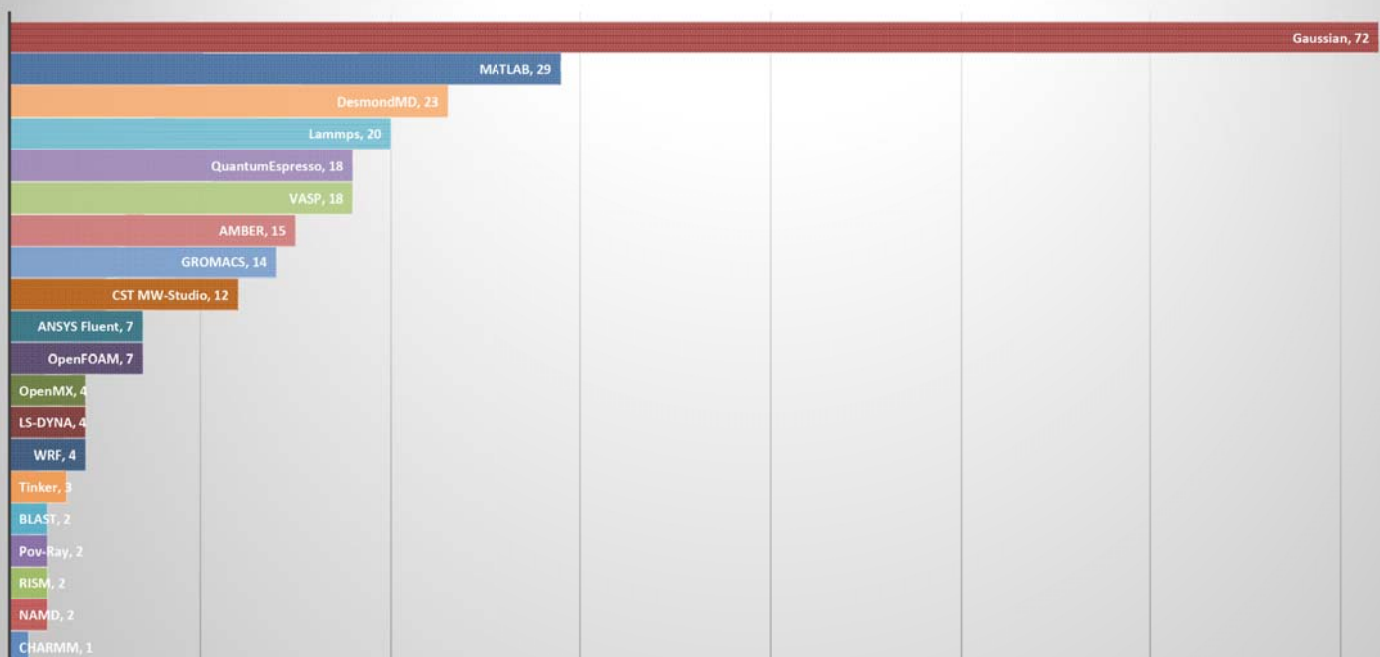


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アプリケーション別利用ユーザ数(2015年12月実績)

58



東京工業大学 学術国際情報センター



TOTO株式会社様の事例

59

利用企業:

TOTO株式会社 技術開発センター

利用課題名:

衛生陶器設計のための並列GPGPU気液二相流シミュレーション

課題区分:

トライアルユース(戦略分野:アクセラレータ利用技術の推進)

利用期間:

平成23年10月～トライアルユース継続利用中

解析プログラム:

自社開発プログラム(GPU化も自社で実施)

可視化プログラム:

POV-Ray(TSUBAME上で可視化)

使用目的:

大容量高精細な格子により高精度なシミュレーションを実現

従来の1/3の格子 解像度として81倍

成果

約1.5億格子の解析において、100GPUで80倍以上の速度向上、150GPUで100倍の速度向上



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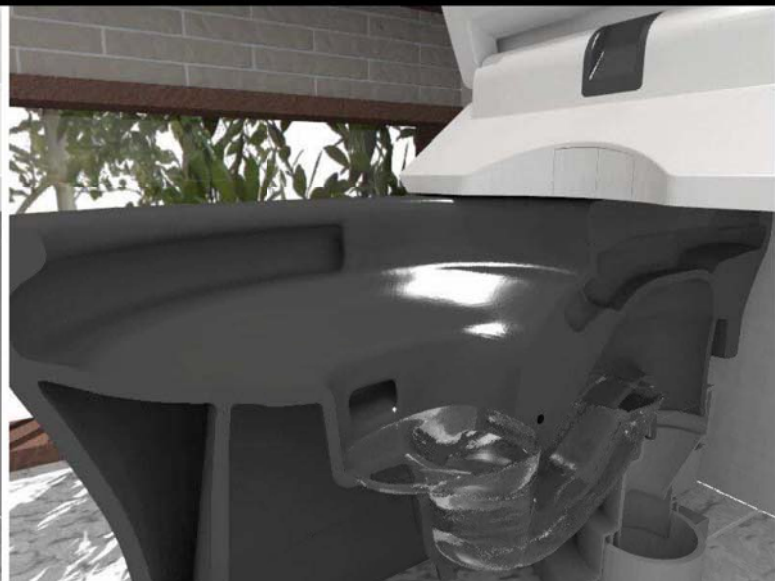
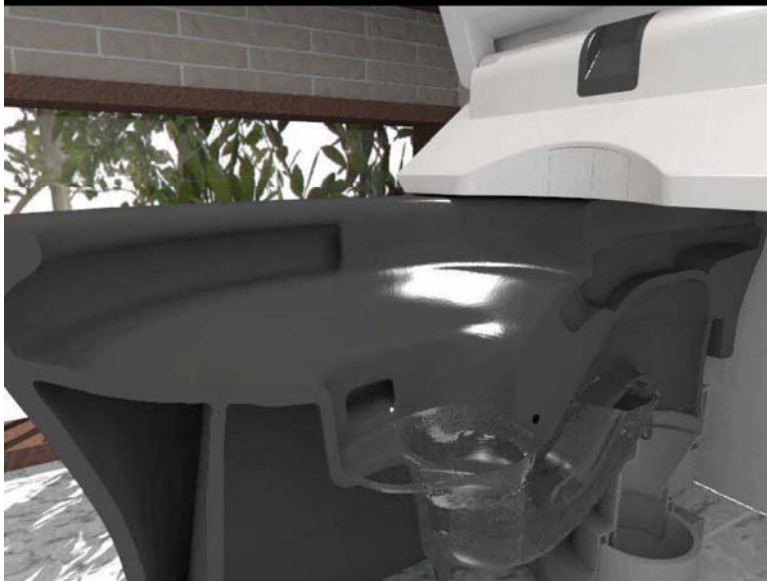


衛生陶器シミュレーション

60

TSUBAMEでの解析結果

自社のクラスタでの解析結果



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シミュレーション結果の精度検証

61

1.5mm /mesh
(従来: 自社クラスタ)



0.5mm /mesh
(TSUBAME)



実機流れ



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最後に



スパコンは計算資源や解析ツールを提供するだけです。

イノベーションを起こすのは、**利用者の方々です。**



Thank you