GP GPU

Tsunami Simulation on GPUs

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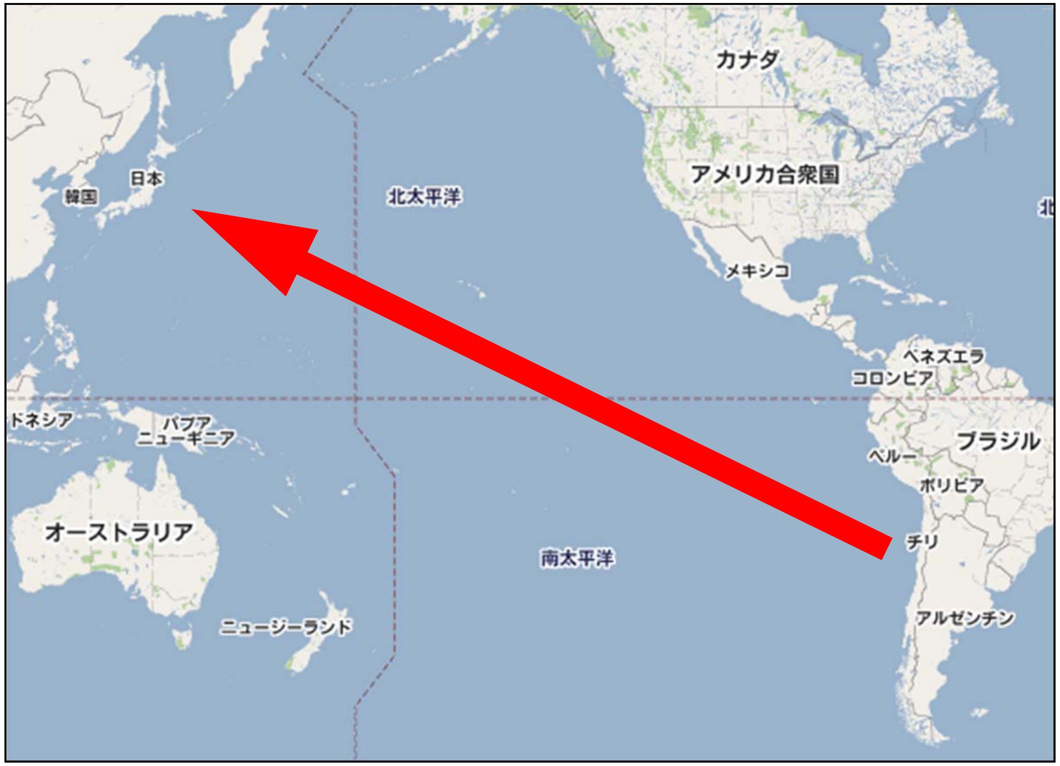
Valdivia Earthquake, 1960

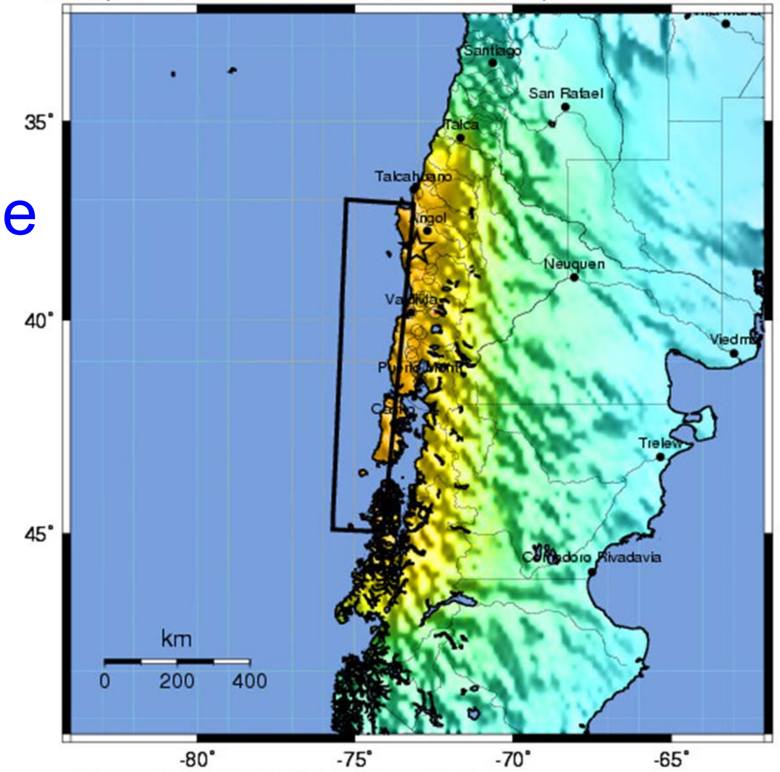
GP GPU

The Biggest earthquake:
several times M7～M8

142 died in Japan　1743 died in Chile



USGS ShakeMap : Concepcion, Chile
Sun May 22, 1960 19:11:17 GMT M 9.5 S38.23 W73.05 Depth: 35.0km ID:196005221911



Map Version 1.1 Processed Sun Nov 9, 2008 09:23:34 AM MST

PERCEIVED SHAKING	Not felt	Weak	Light	Moderate	Strong	Very strong	Severe	Violent	Extreme
POTENTIAL DAMAGE	none	none	none	Very light	Light	Moderate	Moderate/Heavy	Heavy	Very Heavy
PEAK ACC.(%g)	<.17	.17-1.4	1.4-3.9	3.9-9.2	9.2-18	18-34	34-65	65-124	>124
PEAK VEL.(cm/s)	<0.1	0.1-1.1	1.1-3.4	3.4-8.1	8.1-16	16-31	31-60	60-116	>116
INSTRUMENTAL INTENSITY	I	II-III	IV	V	VI	VII	VIII	IX	X+

TSUNAMI Disaster

GP GPU

Real-time
TSUNAMI Simulation

GP GPU

ADPC : Asian Disaster Preparedness Center

Early Warning System:

Data Base → **Real-time CFD**

high accuracy

Shallow-Water Eq.

Conservative Form:

$$\frac{\partial h}{\partial t}+\frac{\partial hu}{\partial x}+\frac{\partial hv}{\partial y}=0$$

Assuming
hydrostatic balance
in the vertical direction,

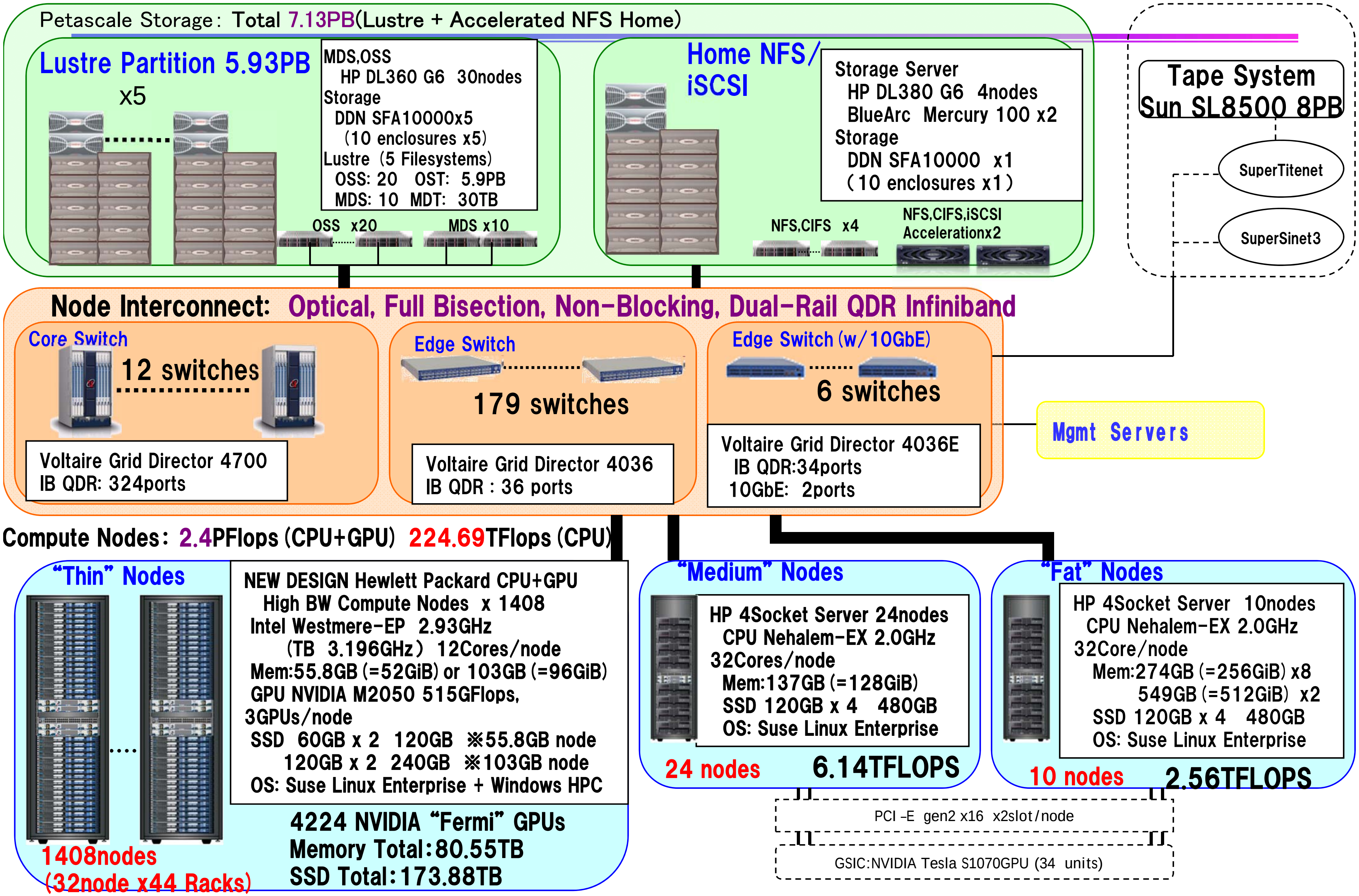
$$\frac{\partial hu}{\partial t}+\frac{\partial}{\partial x}\left(hu^2+\frac{1}{2}gh^2\right)+\frac{\partial huv}{\partial y}=-gh\frac{\partial z}{\partial x}$$

$$\frac{\partial hv}{\partial t}+\frac{\partial huv}{\partial x}+\frac{\partial}{\partial y}\left(hv^2+\frac{1}{2}gh^2\right)=-gh\frac{\partial z}{\partial y}$$

3D → **2D equation**

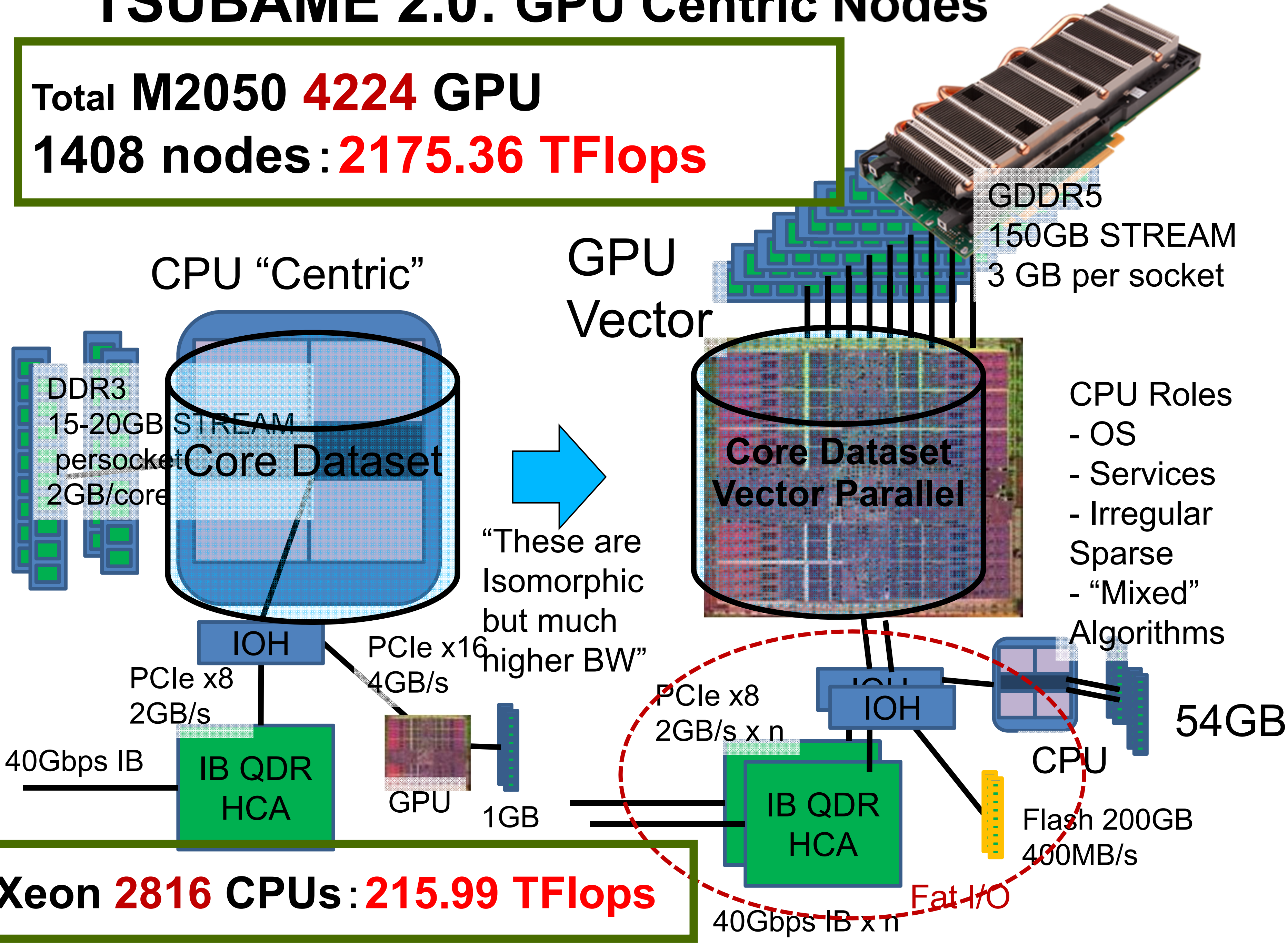

TSUBAME 2.0

TSUBAME2.0 System Overview（2.4 Pflops/15PB）

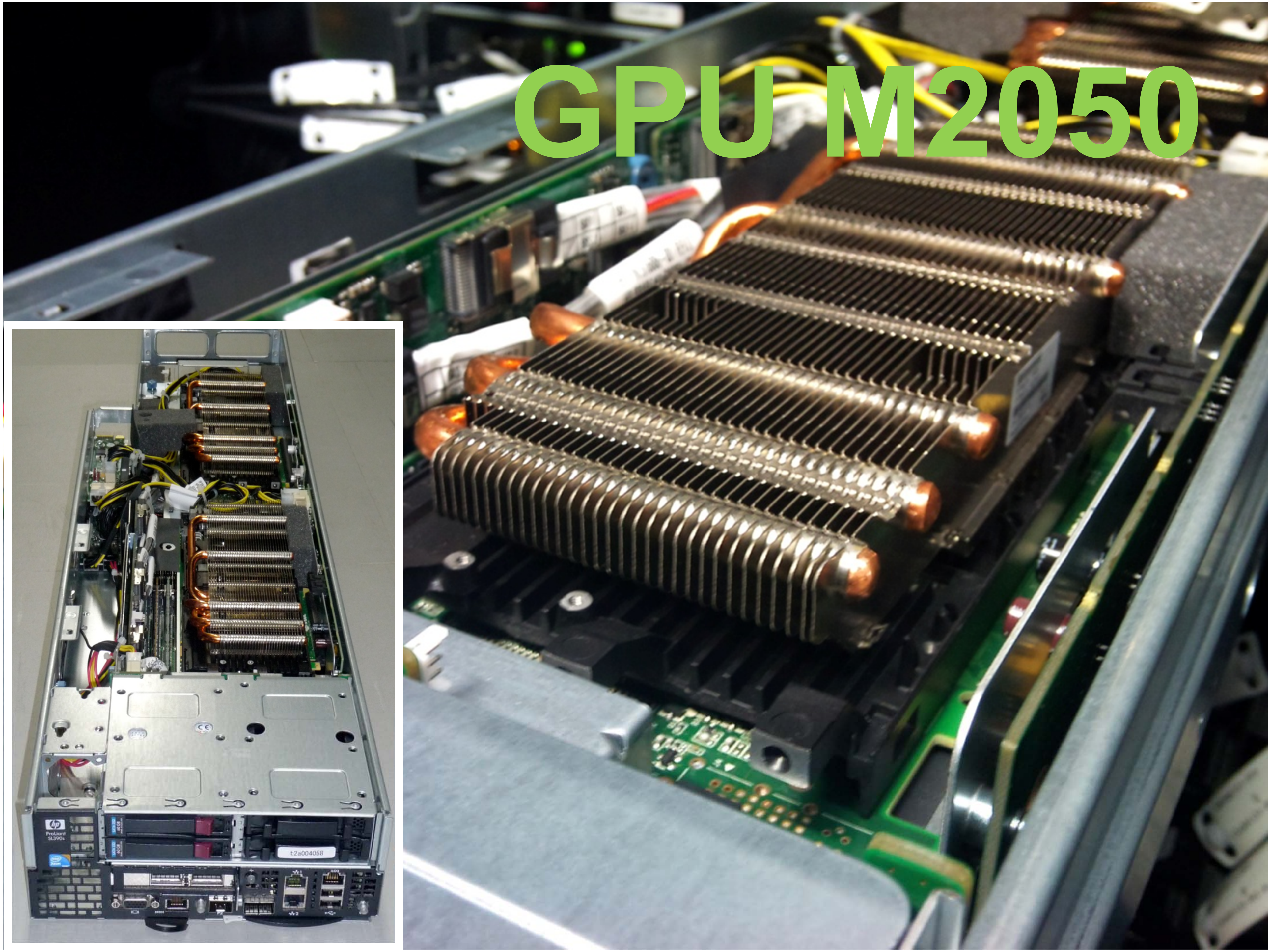


TSUBAME 2.0: GPU Centric Nodes

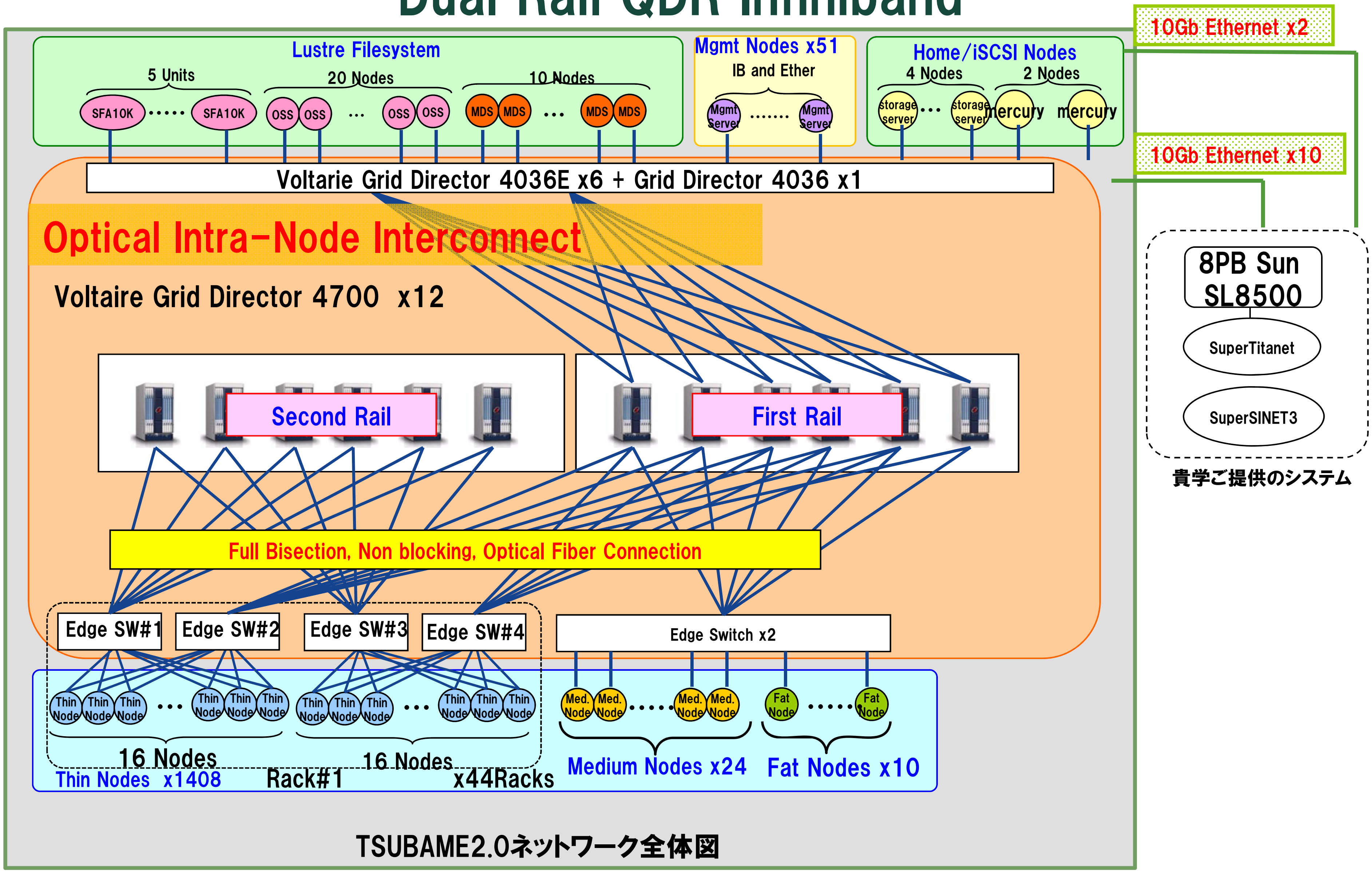
Total M2050 4224 GPU
1408 nodes : 2175.36 TFlops

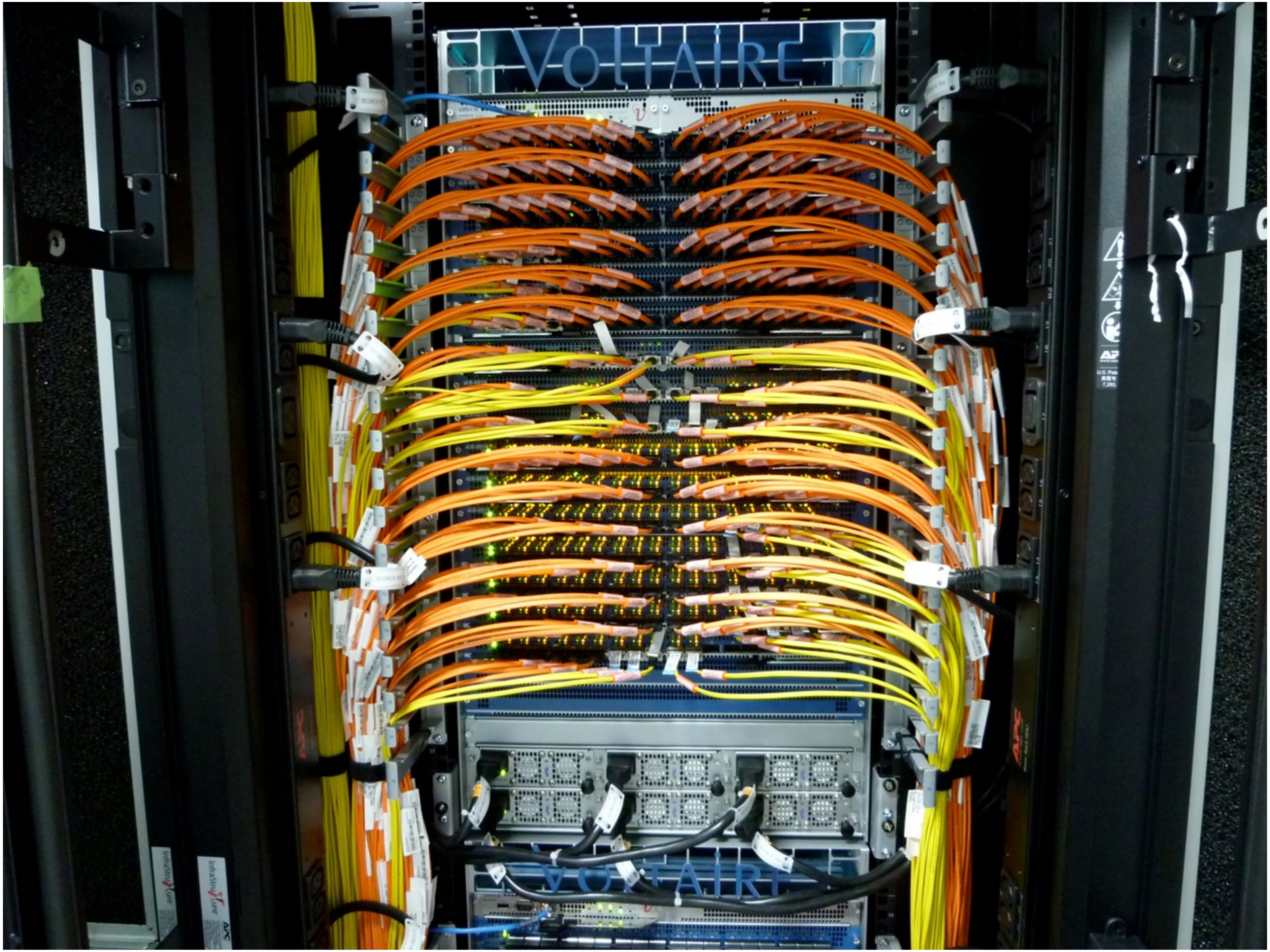


Xeon 2816 CPUs : 215.99 TFlops


GPU M2050

TSUBAME 2.0 Full Bisection Fat Tree, Optical, Dual Rail QDR Infiniband



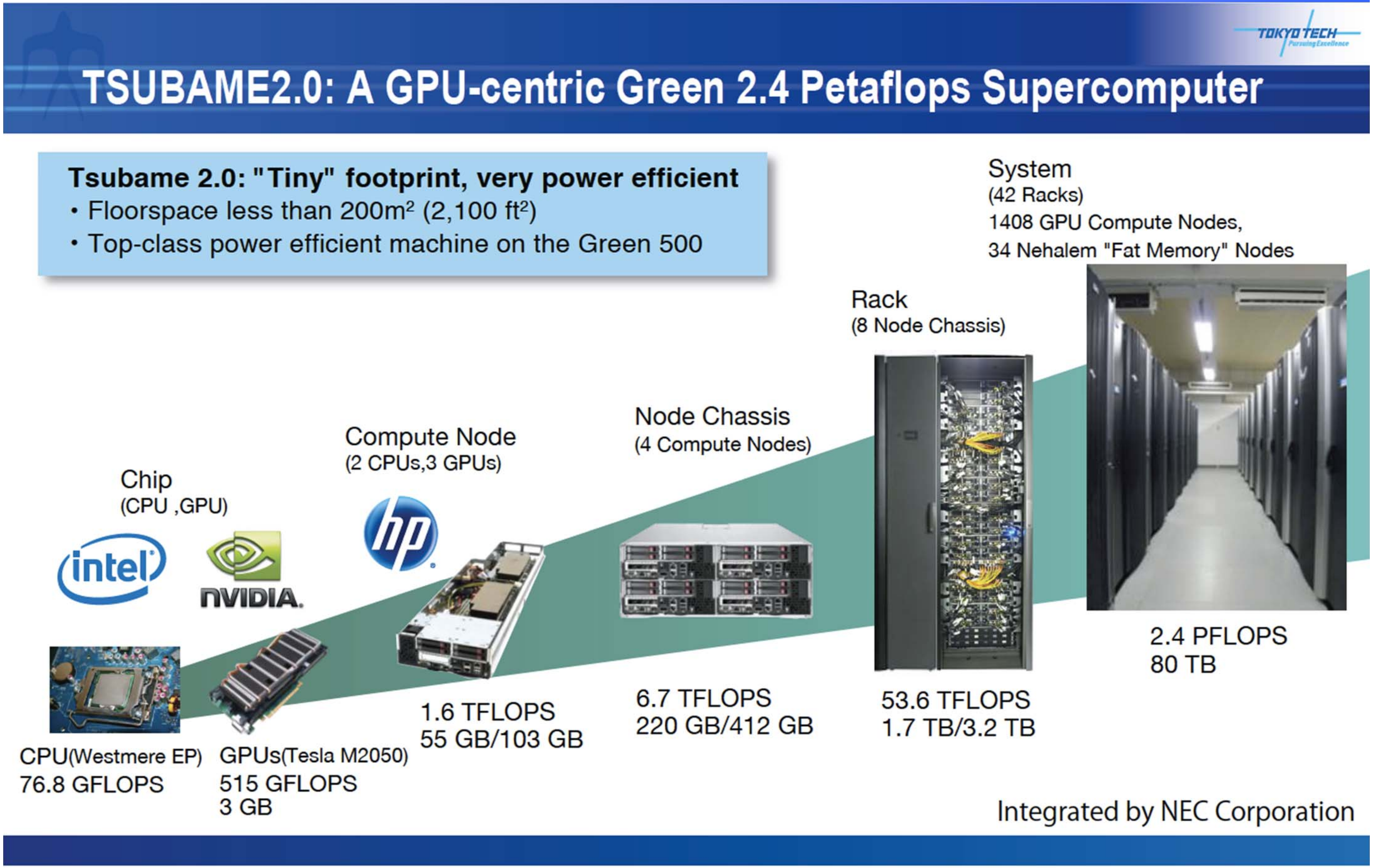

VOLTAIRE


DataDirect


StorageTek


StorageTek

TSUBAME2.0 Nov 1st, 2010



Supercomputer in the world

2010 November

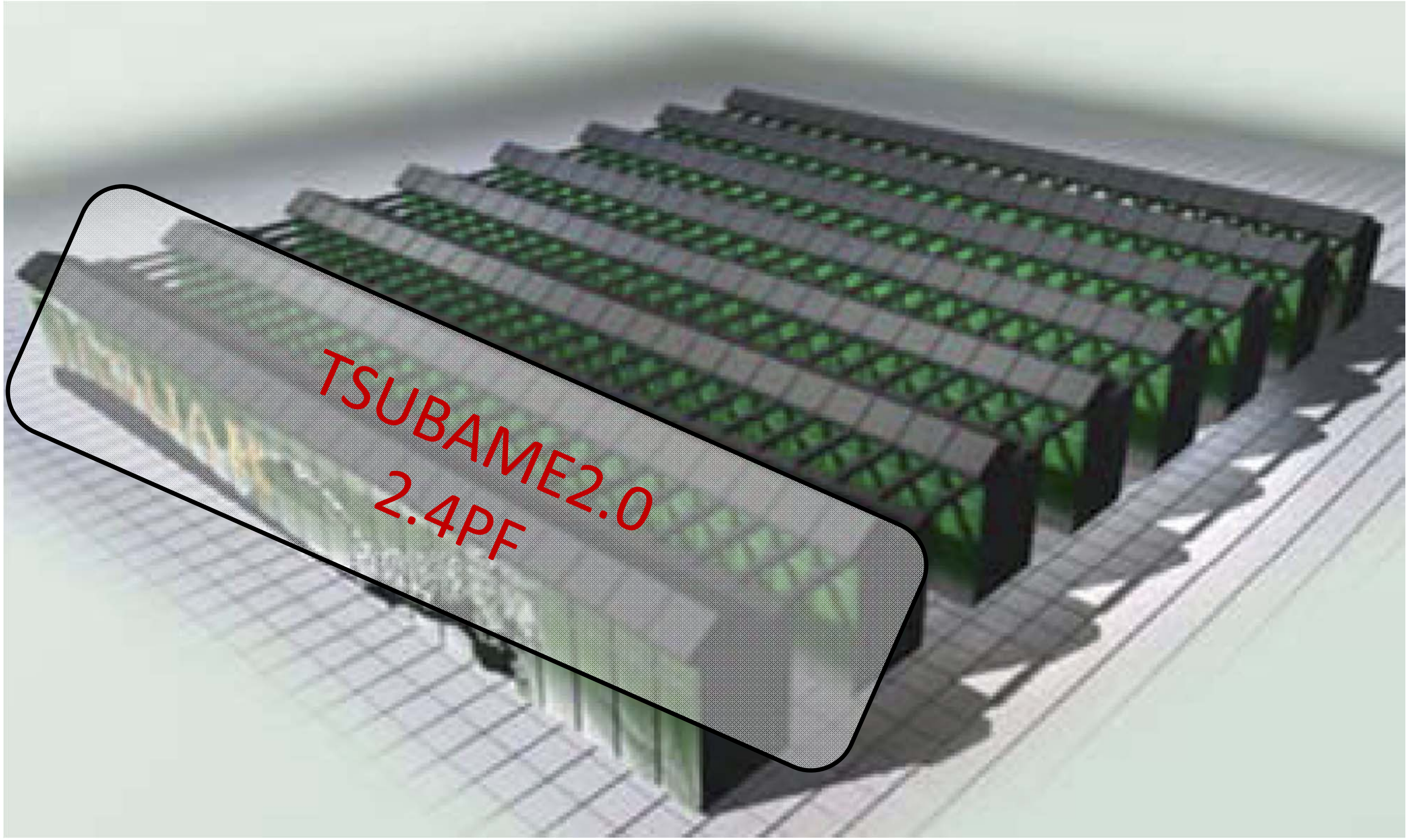
TOP500 SUPERCOMPUTER SITES

Rank	Site	Computer/Year Vendor	Cores	R_{max}	R_{peak}	Power
1	National Supercomputing Center in Tianjin China	Tianhe-1A - NUDT YH Cluster, X5670 2.93Ghz 6C, NVIDIA GPU, FT-1000 8C / 2010 NUDT	186368	2566.00	4701.00	4040.00
2	DOE/SC/Oak Ridge National Laboratory United States	Jaguar - Cray XT5-HE Opteron 6-core 2.6 GHz / 2009 Cray Inc.	224162	1759.00	2331.00	6950.60
3	National Supercomputing Centre in Shenzhen (NSCS) China	Nebulae - Dawning TC3600 Blade, Intel X5650, NVidia Tesla C2050 GPU / 2010 Dawning	120640	1271.00	2984.30	2580.00
4	GSIC Center, Tokyo Institute of Technology Japan	TSUBAME 2.0 - HP ProLiant SL390s G7 Xeon 6C X5670, Nvidia GPU, Linux/Windows / 2010 NEC/HP	73278	1192.00	2287.63	1398.61
5	DOE/SC/LBNL/NERSC United States	Hopper - Cray XE6 12-core 2.1 GHz / 2010 Cray Inc.	153408	1054.00	1288.63	2910.00

ORNL Jaguar vs Tsubame 2.0

Similar Peak Performance, 1/4 the Size and Power

GP GPU



Supercomputer in the world

The Green500 list -- November 2010

Green500 Rank	MFLOPS/W	Site*	Computer*	Total Power (kW)
1	1684.20	IBM Thomas J. Watson Research Center	NNSA/SC Blue Gene/Q Prototype	38.80
2	958.35	GSIC Center, Tokyo Institute of Technology	HP ProLiant SL390s G7 Xeon 6C X5670, Nvidia GPU, Linux/Windows	1243.80
3	933.06	NCSA	Hybrid Cluster Core i3 2.93Ghz Dual Core, NVIDIA C2050, Infiniband	36.00
4	828.67	RIKEN Advanced Institute for Computational Science	K computer, SPARC64 VIIIfx 2.0GHz, Tofu interconnect	57.96
5	773.38	Forschungszentrum Juelich (FZJ)	QPACE SFB TR Cluster, PowerXCell 8i, 3.2 GHz, 3D-Torus	57.54
5	773.38	Universitaet Regensburg	QPACE SFB TR Cluster, PowerXCell 8i, 3.2 GHz, 3D-Torus	57.54
5	773.38	Universitaet Wuppertal	QPACE SFB TR Cluster, PowerXCell 8i, 3.2 GHz, 3D-Torus	57.54
8	740.78	Universitaet Frankfurt	Supermicro Cluster, QC Opteron 2.1 GHz, ATI Radeon GPU, Infiniband	385.00

Power Efficiency

6600x
Faster

3x efficient

<<

Laptop: SONY Vaio type Z (VPCZ1)
CPU: Intel Core i7 620M (2.66GHz)
MEMORY: DDR3-1066 4GBx2
OS: Microsoft Windows 7 Ultimate 64bit
HPL: Intel(R) Optimized LINPACK Benchmark for Windows (10.2.6.015)
256GB HDD

18.1 Gflops

369 MFlops/Watt

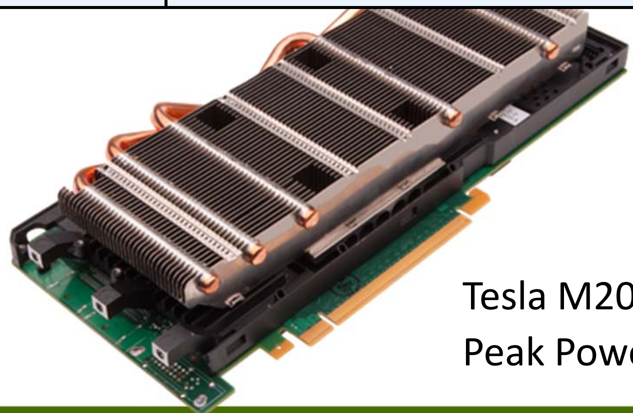
Supercomputer: TSUBAME 2.0
CPU: 2714 Intel Westmere 2.93 Ghz
GPU: 4071 nVidia Fermi M2050
MEMORY: DDR3-1333 80TB + GDDR5 12TB
OS: SuSE Linux 11 + Windows HPC Server R2
HPL: Tokyo Tech Heterogeneous HPL
11PB Hierarchical Storage

1.192 Pflops

1037 MFlops/Watt

NVIDIA GPU

		Intel Core i7 Extreme	Tesla C2050 /M2050	GeForce GTX 580 Fermi
GPU	Peak Performance [GFlops]	**51.2*,102.4**	**515*,1030**	**197*,1576**
	Number of Processor	4	448	512
	Core Clock [MHz]	3200	1476	1544
Memory	Bandwidth[GB/s]	**32**	**148.8**	**192.1**
	Memory Interface [bit]	64	384	384
	Memory Clock [GHz]	1.333 (DDR3)	1.55 (GDDR5)	2.00 (GDDR5)
B_{peak}/F_{peak}	Bandwidth/Performance	**0.624**	**0.289**	**0.974**

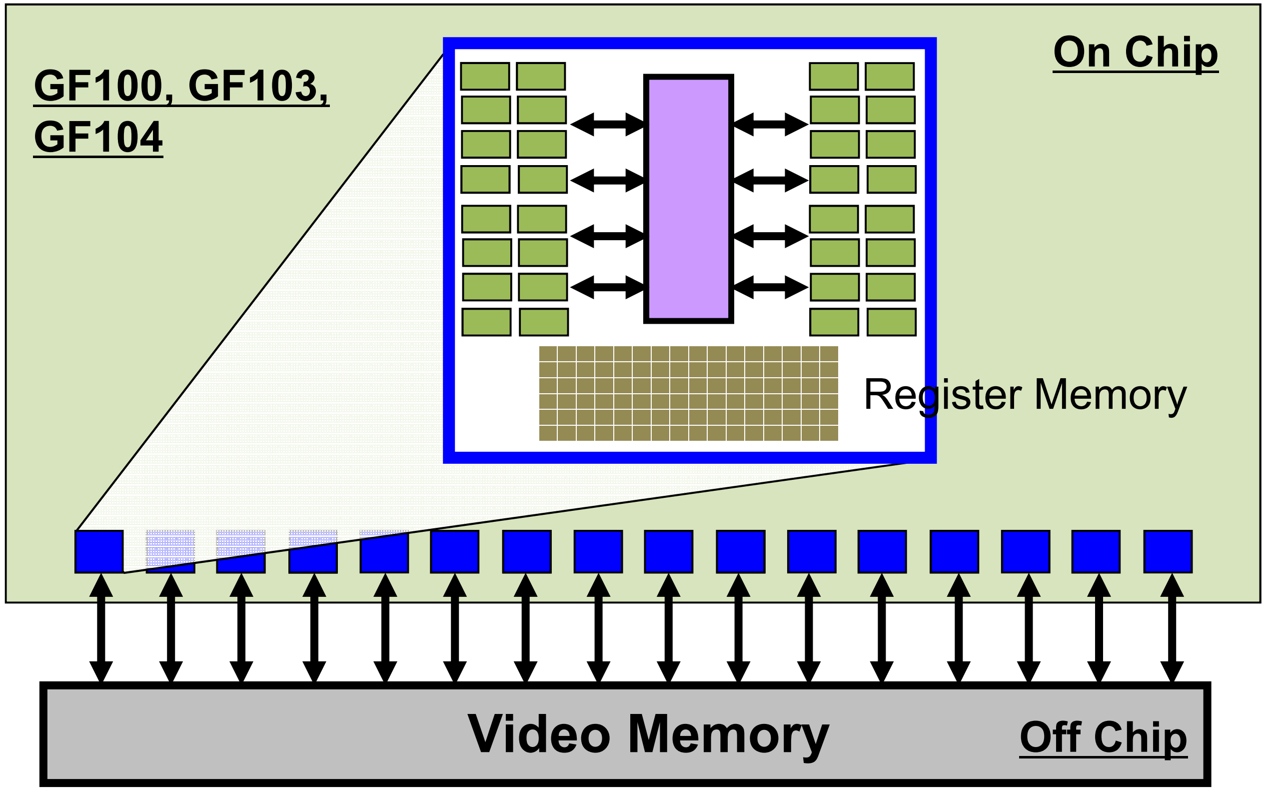


Tesla M2050
Peak Power : 225W

Peak Power : 244W

GPU Architecture

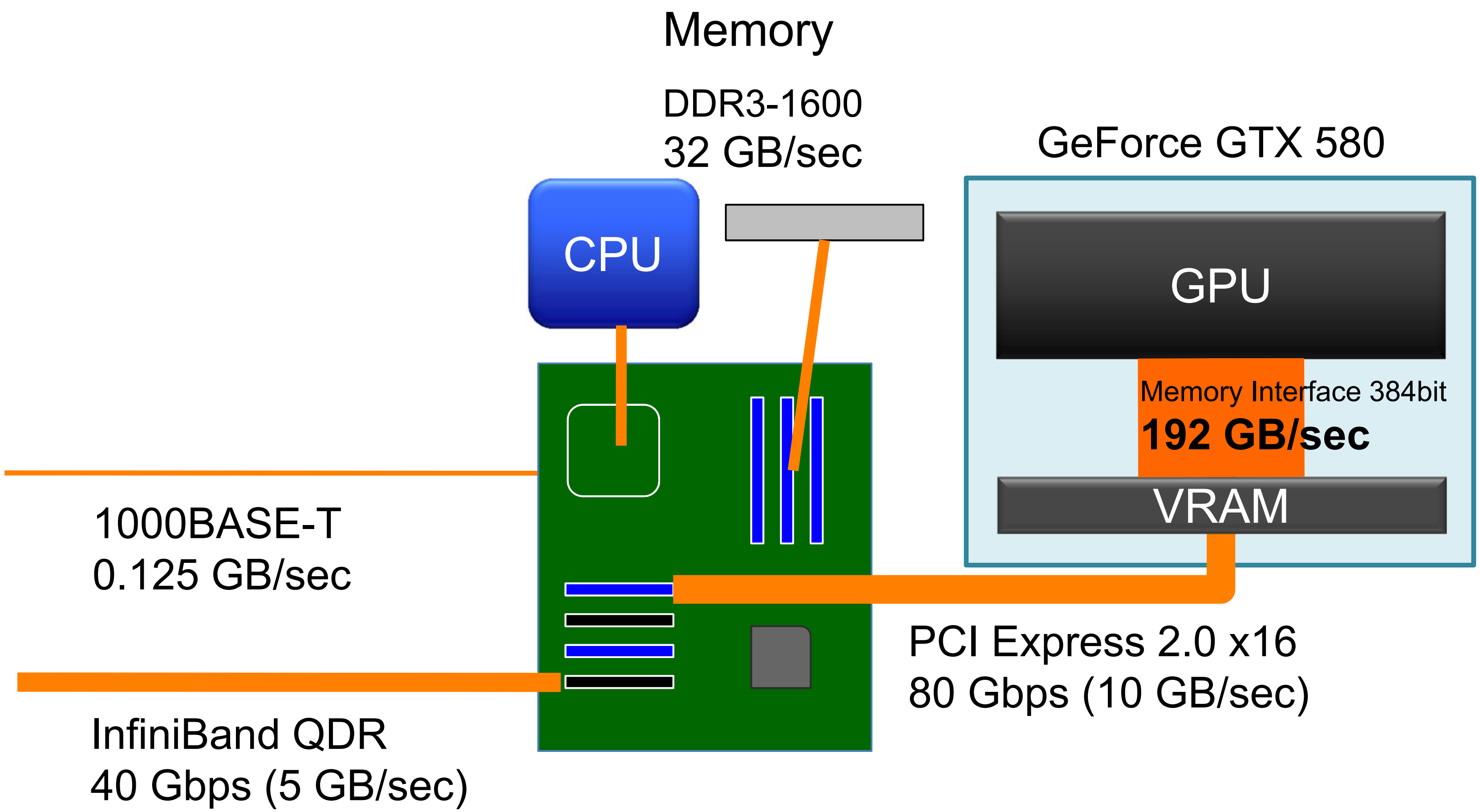
GP GPU



Global memory	~6GB (VRAM
Streaming Multiprocessor	~16 (C2050 (GF100): 14)
Shared memory + L1 Cache	64 Kbyte
Streaming Processor (CUDA core)	8～48 per SM, total 512

Heterogeneous Computer

■ Several Bandwidth Bottle Necks



CFD Performances

in GPU Computing

GP GPU

Partial GPU Implementation **30% up 〜 ×3**

※ Only Hot spot (Intensive part) : small cost

※ Overhead of host (CPU) memory
device (GPU) memory communication

FULL GPU Implementation **×10 〜 ×100**

※ Limitation of device (GPU) on board memory size

Real-time TSUNAMI Simulation

GP GPU

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Assuming

hydrostatic balance

in the vertical direction,

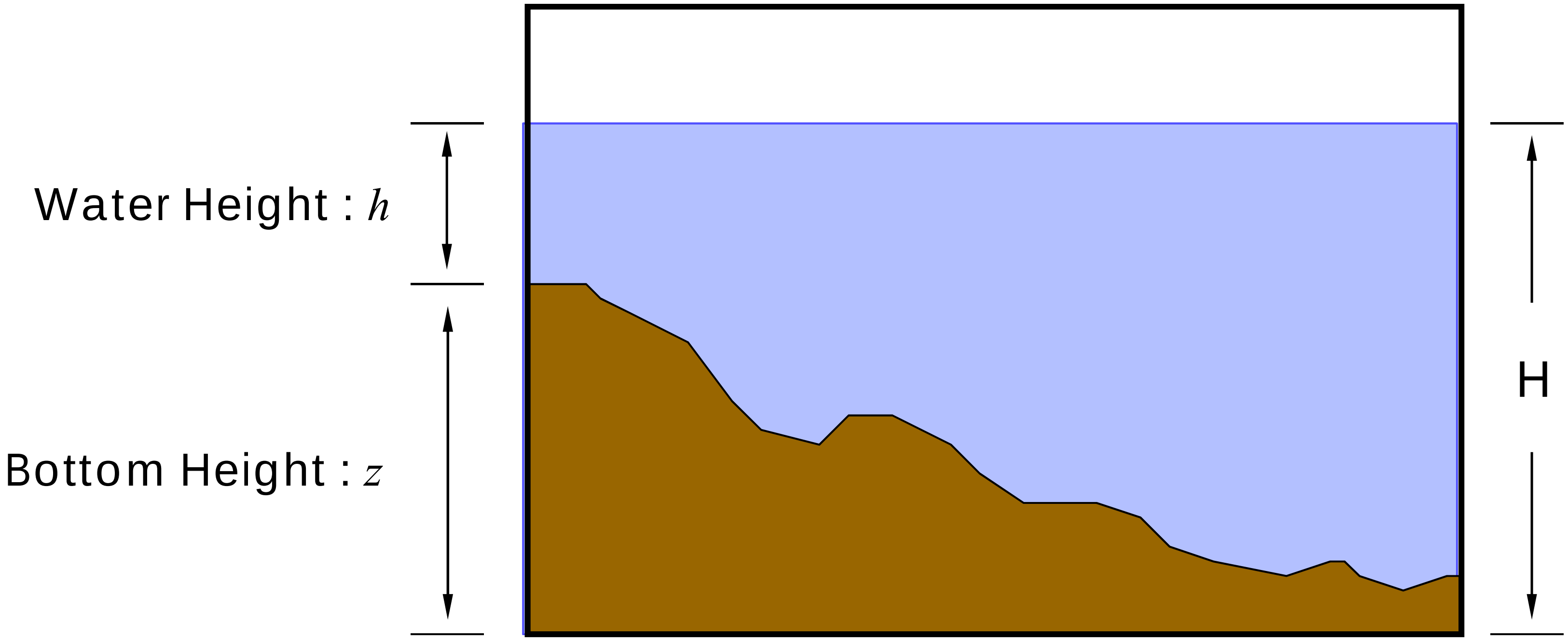
$$\frac{\partial hu}{\partial t} + \frac{\partial}{\partial x}\left(hu^2 + \frac{1}{2}gh^2\right) + \frac{\partial huv}{\partial y} = -gh\frac{\partial z}{\partial x}$$

$$\frac{\partial hv}{\partial t} + \frac{\partial huv}{\partial x} + \frac{\partial}{\partial y}\left(hv^2 + \frac{1}{2}gh^2\right) = -gh\frac{\partial z}{\partial y}$$

3D → **2D equation**

Tsunami Modeling

free surface flow



Directional-Splitting Method

GP GPU

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

First Step: x-directional computation

$$\frac{\partial h}{\partial t}+\frac{\partial hu}{\partial x}=0 \qquad \frac{\partial hv}{\partial t}+\frac{\partial uhv}{\partial x}=0 \qquad \frac{\partial hu}{\partial t}+\frac{\partial}{\partial x}\left(hu^2+\frac{1}{2}gh^2\right)=-gh\frac{\partial z}{\partial x}$$

Second Step: y-directional computation

$$\frac{\partial h}{\partial t}+\frac{\partial hv}{\partial y}=0 \qquad \frac{\partial hu}{\partial t}+\frac{\partial vhu}{\partial y}=0 \qquad \frac{\partial hv}{\partial t}+\frac{\partial}{\partial y}\left(hv^2+\frac{1}{2}gh^2\right)=-gh\frac{\partial z}{\partial y}$$

For Characteristics-based Method
For Conservative Semi-Lagrangian Method

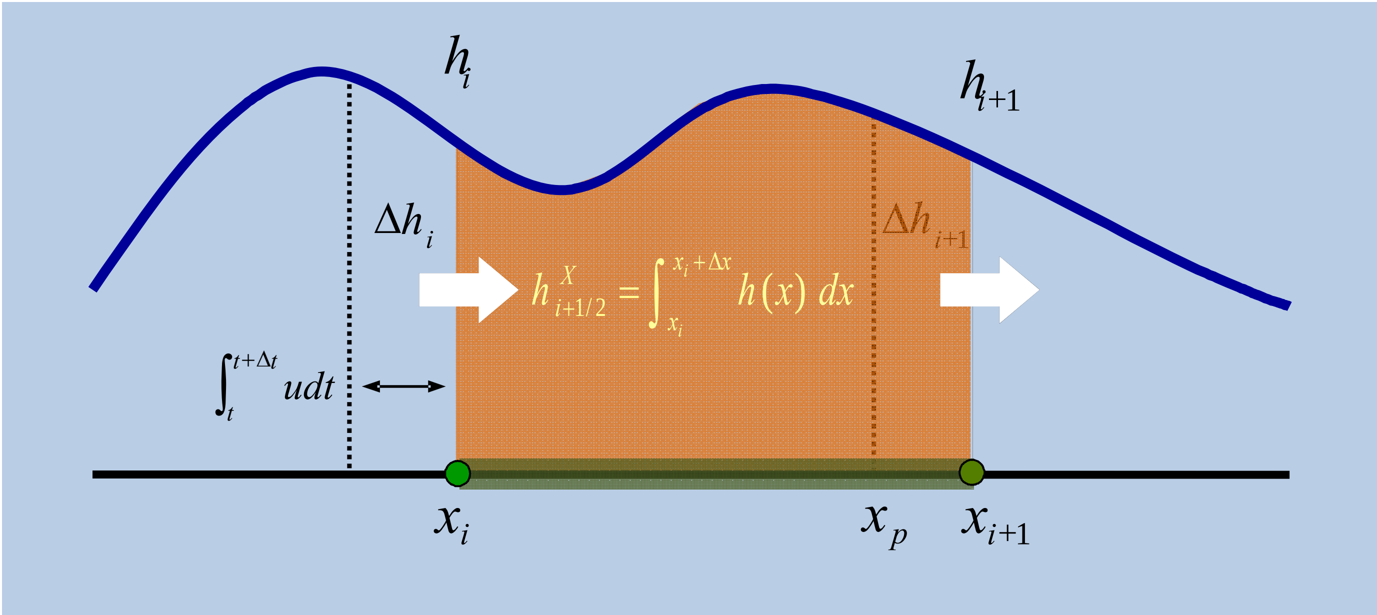
CIP-CSL2 (Conservative Semi-Lagrangian)

R. Tanaka, T. Nakamura, and T. Yabe, Comp. Phys. Comm., 126, 232-243 (2000).

GP GPU

Continuum Eq.

$$\frac{\partial h}{\partial t} + \frac{\partial hu}{\partial x} = 0$$



$$h_i(x) = a(x - x_i)^2 + b(x - x_i) + h_i \qquad a = \frac{3h_{i+1} + 3h_i}{\Delta x^2} - \frac{6h^X_{i+1/2}}{\Delta x^3}, \quad b = \frac{6h^X_{i+1/2}}{\Delta x^2} - \frac{2h_{i+1} + 4h_i}{\Delta x}$$

$$h_{x,i} = \frac{6h^X_{i+1/2}}{\Delta x^2} - \frac{2h_{i+1} + 4h_i}{\Delta x}$$

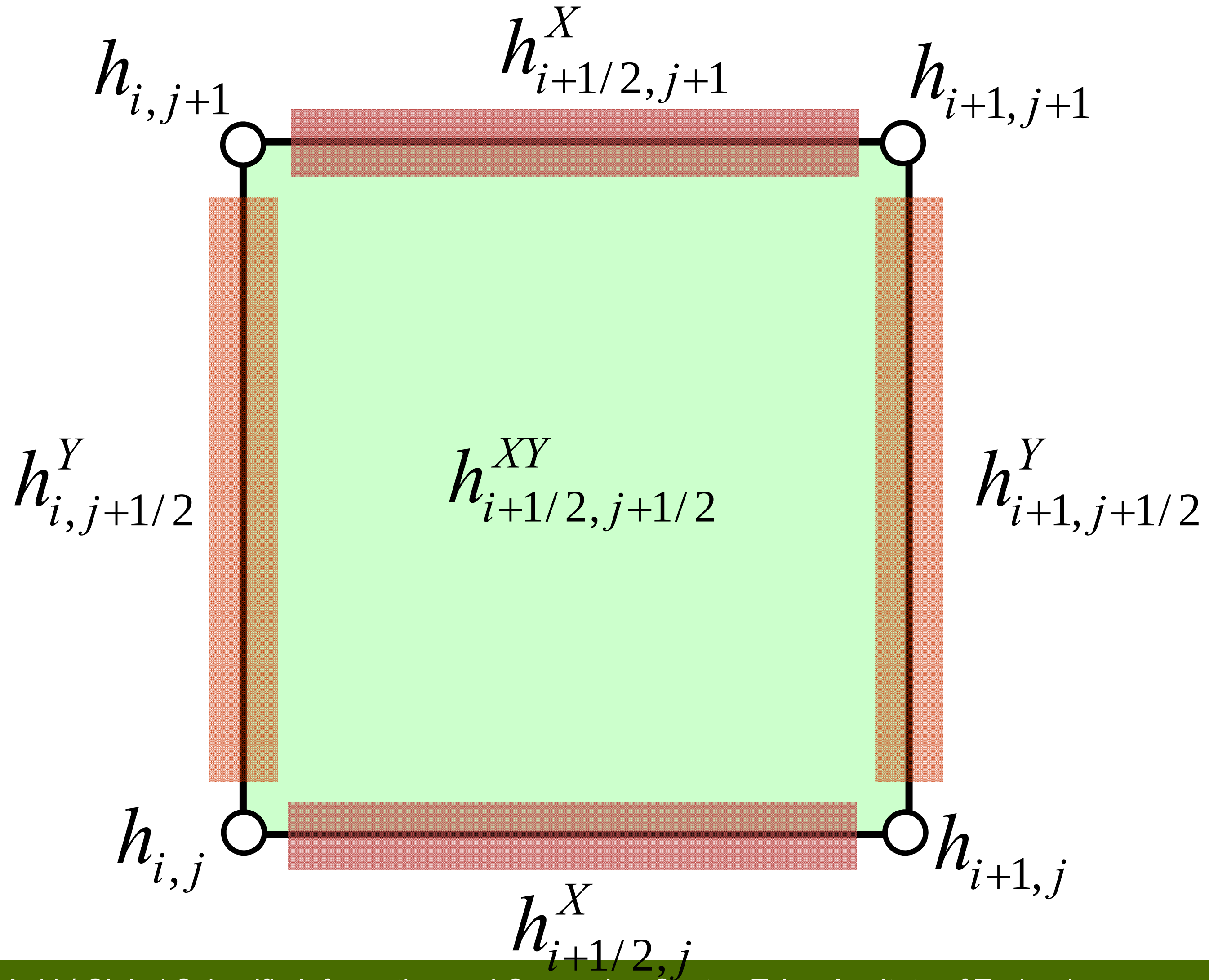
$$h_i(x_i) = h_i^n \qquad h_i(x_i + \Delta x) = h_{i+1}^n \qquad \int_{x_i}^{x_i+\Delta x} h_i(x)dx = h^X_{i+1/2}$$

$$\Delta h^X_{i+1} = \int_{x_p}^{x_{i+1}} h_i^n(x)dx$$

$$= -\left(\frac{a^n}{3}\xi^3 + \frac{b^n}{2}\xi^2 + h_i^n\xi\right)$$

$$h_i^{n+1} = h_j^n(x_i - u\Delta t) \qquad h^{X,n+1}_{i+1/2} = h^{X,n}_{i+1/2} - \Delta h^n_{i+1} + \Delta h^n_i$$

2-dimensional
Variable Configuration



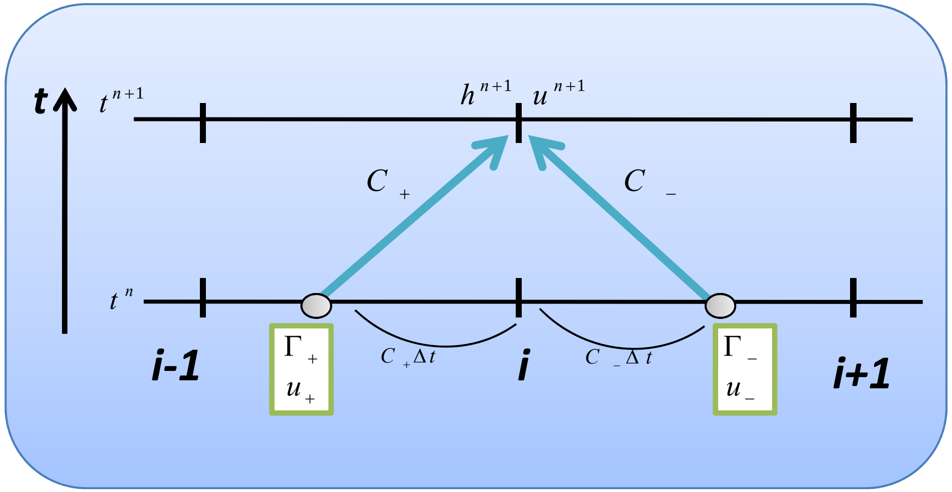
Characteristics-Based Method

$$\frac{\partial U}{\partial t}+\frac{\partial F}{\partial x}=0 \quad U=\begin{bmatrix} h \\ hu \end{bmatrix},\ F=\begin{bmatrix} hu \\ hu^2+\frac{1}{2}gh^2 \end{bmatrix}$$

Factorizing:

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

for $\Gamma=\sqrt{gh}$



Riemann invariants :

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

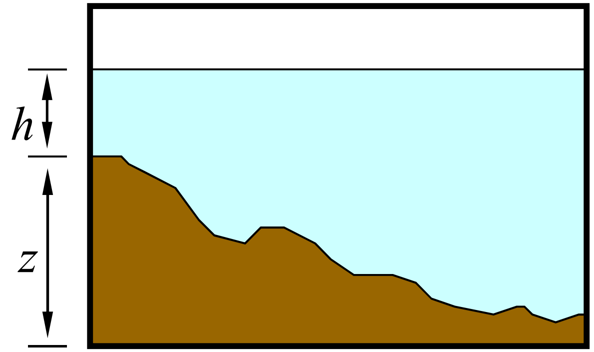
$$\Gamma^{\pm}=\Gamma\pm\frac{1}{2}u$$

$$\frac{\partial \Gamma^{\pm}}{\partial t}+\lambda^{\pm}\frac{\partial \Gamma^{\pm}}{\partial x}=0$$

$$\left.\begin{aligned} \Gamma^{n+1}&=\frac{1}{2}\left\{\Gamma^{+\,n+1}+\Gamma^{-\,n+1}+\frac{1}{2}\left(u^{+}-u^{-}\right)\right\} \\ u^{n+1}&=\frac{1}{2}\left\{u^{+}-u^{-}+2\left(\Gamma^{+}-\Gamma^{-}\right)\right\} \end{aligned}\right\} \Rightarrow \begin{matrix} h^{n+1} \\ (hu)^{n+1} \end{matrix}$$

Hydrostatic Balance (1/2)

$$H = h + z \quad \Rightarrow \quad h = H - z$$



$$\frac{\partial hu}{\partial t} + \frac{\partial}{\partial x}\left(hu^2 + \frac{1}{2} g h^2 \right) = -gh \frac{\partial z}{\partial x}$$

$$\frac{\partial hu}{\partial t} + \frac{\partial}{\partial x}\left(hu^2 + \frac{1}{2} g (H-z)^2 \right) = -g(H-z) \frac{\partial z}{\partial x}$$

$$\frac{\partial hu}{\partial t} + \frac{\partial}{\partial x}\left(hu^2 + \frac{1}{2} g H^2 - ghHz + \frac{1}{2} g z^2 \right) = -gH \frac{\partial z}{\partial x} + gz \frac{\partial z}{\partial x}$$

$$\frac{\partial hu}{\partial t} + \frac{\partial}{\partial x}\left(hu^2 + \frac{1}{2} g H^2 \right) = gH \frac{\partial z}{\partial x} + gz \frac{\partial H}{\partial x} - gH \frac{\partial z}{\partial x}$$

$$\frac{\partial hu}{\partial t} + \frac{\partial}{\partial x}\left(hu^2 + \frac{1}{2} g H^2 \right) = gz \frac{\partial H}{\partial x}$$

Hydrostatic Balance (2/2)

GP GPU

For characteristics-based method,

$$\frac{\partial h}{\partial t} + \frac{\partial hu}{\partial x} = 0 \qquad \frac{\partial hu}{\partial t} + \frac{\partial}{\partial x}\left(hu^2 + \frac{1}{2} gH^2 \right) = gz \frac{\partial H}{\partial x}$$

$h = H - z$

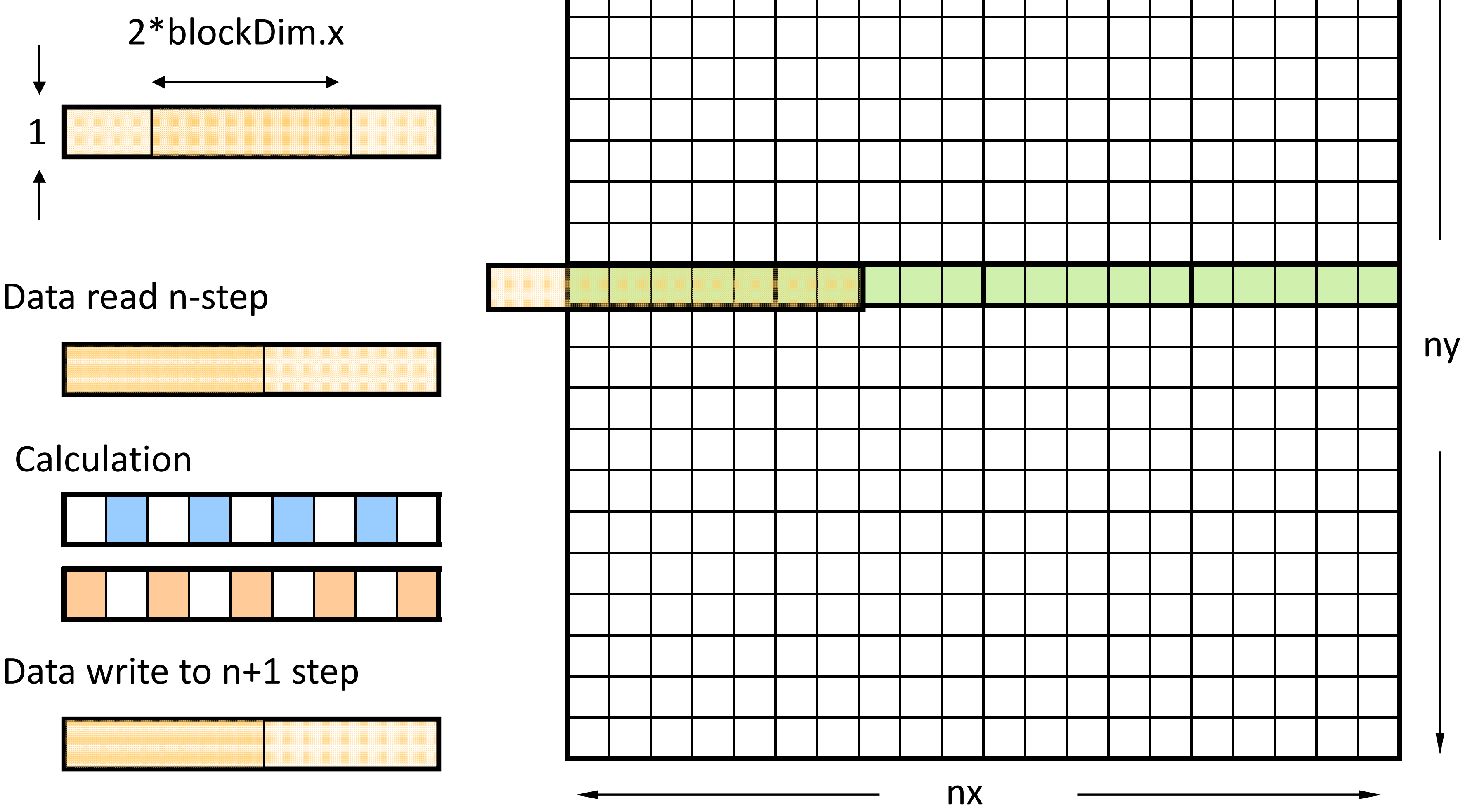
$$\frac{\partial H}{\partial t} + \frac{\partial Hu}{\partial x} = \frac{\partial zu}{\partial x} \qquad \frac{\partial Hu}{\partial t} + \frac{\partial}{\partial x}\left(Hu^2 + \frac{1}{2} gH^2 \right) = u \frac{\partial zu}{\partial x}$$

Characteristics-based Method for *H* and *Hu*

+ Fractional Step : $\frac{\partial H}{\partial t} = \frac{\partial zu}{\partial x} \qquad \frac{\partial Hu}{\partial t} = u \frac{\partial zu}{\partial x}$

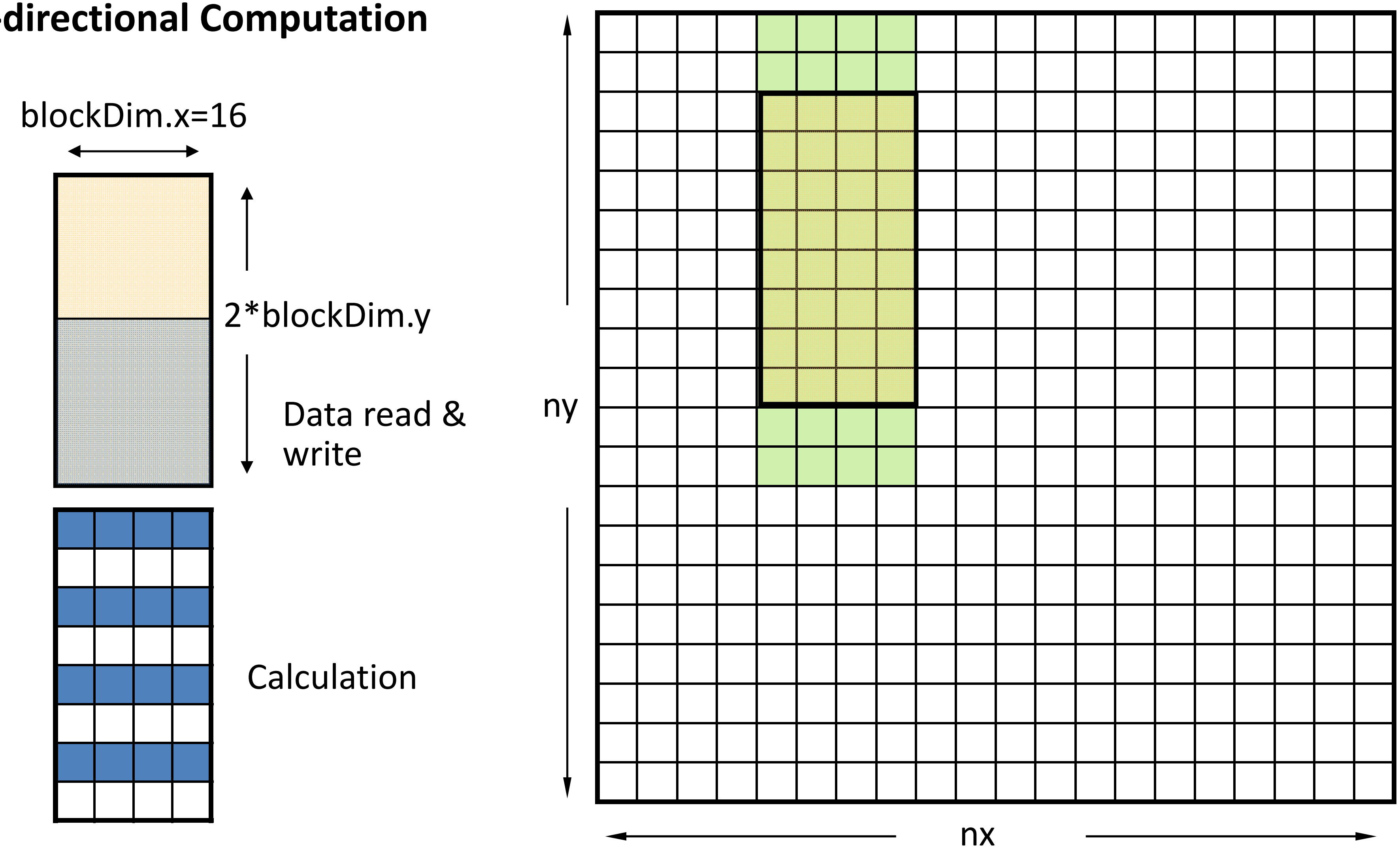
CUDA GPU Computing

x-directional Computation



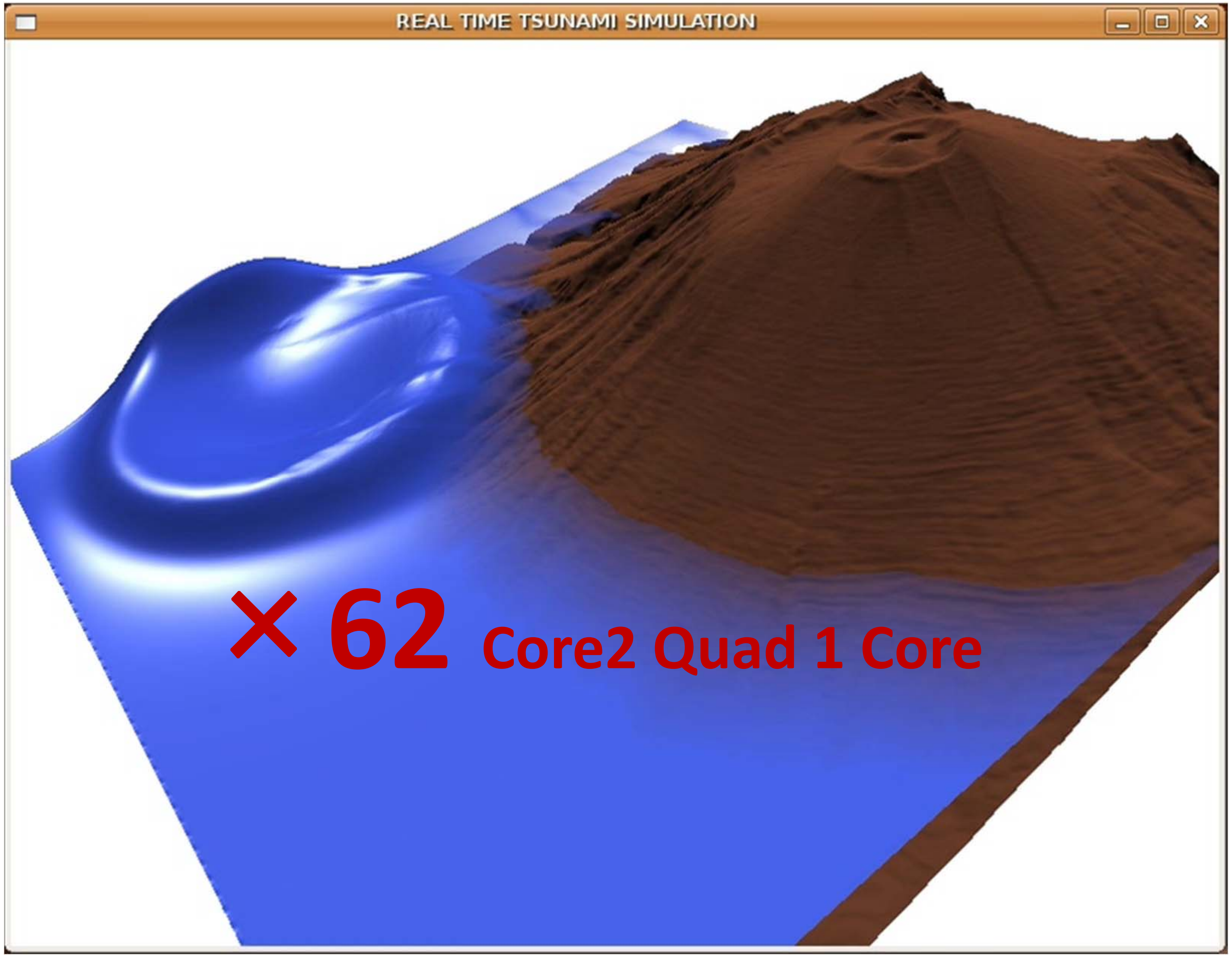
CUDA GPU Computing

y-directional Computation

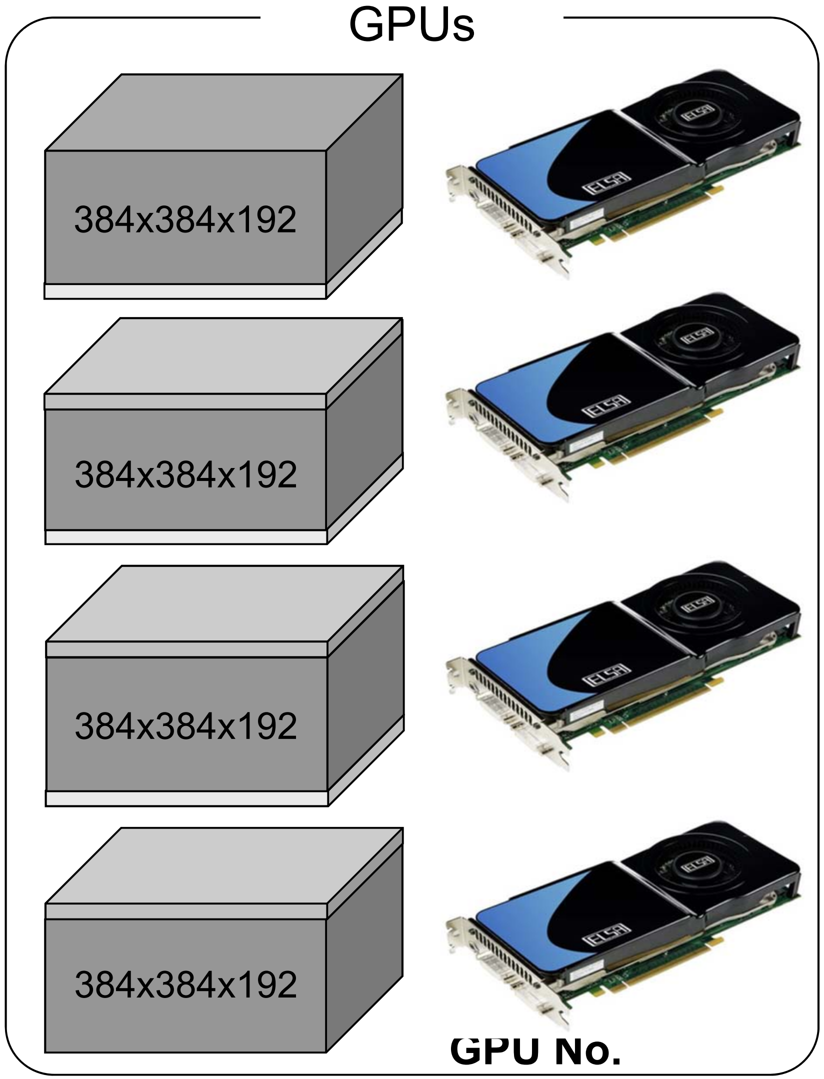


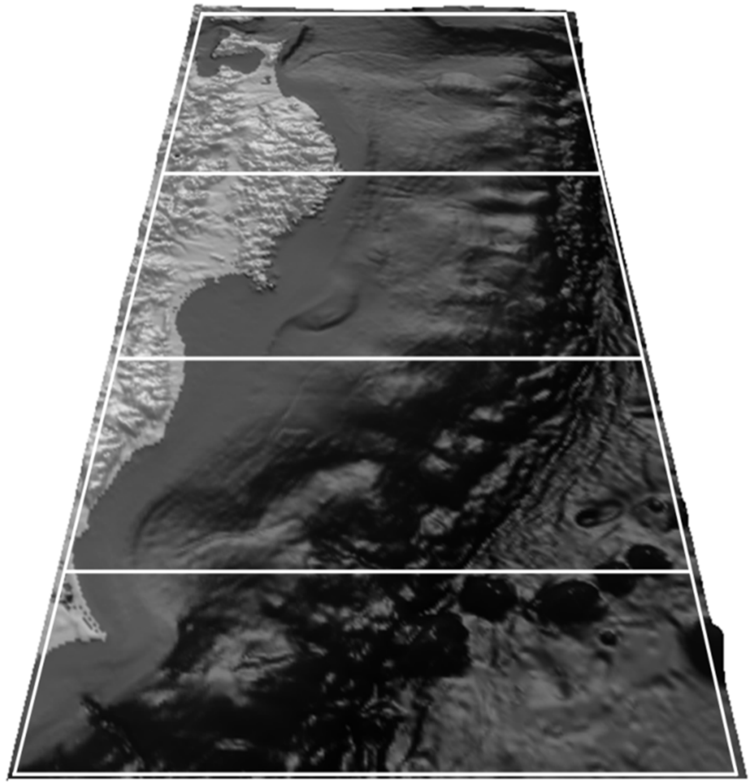
SCREEN Capture

GP GPU



Large-scale Real-time
Tsunami Simulator

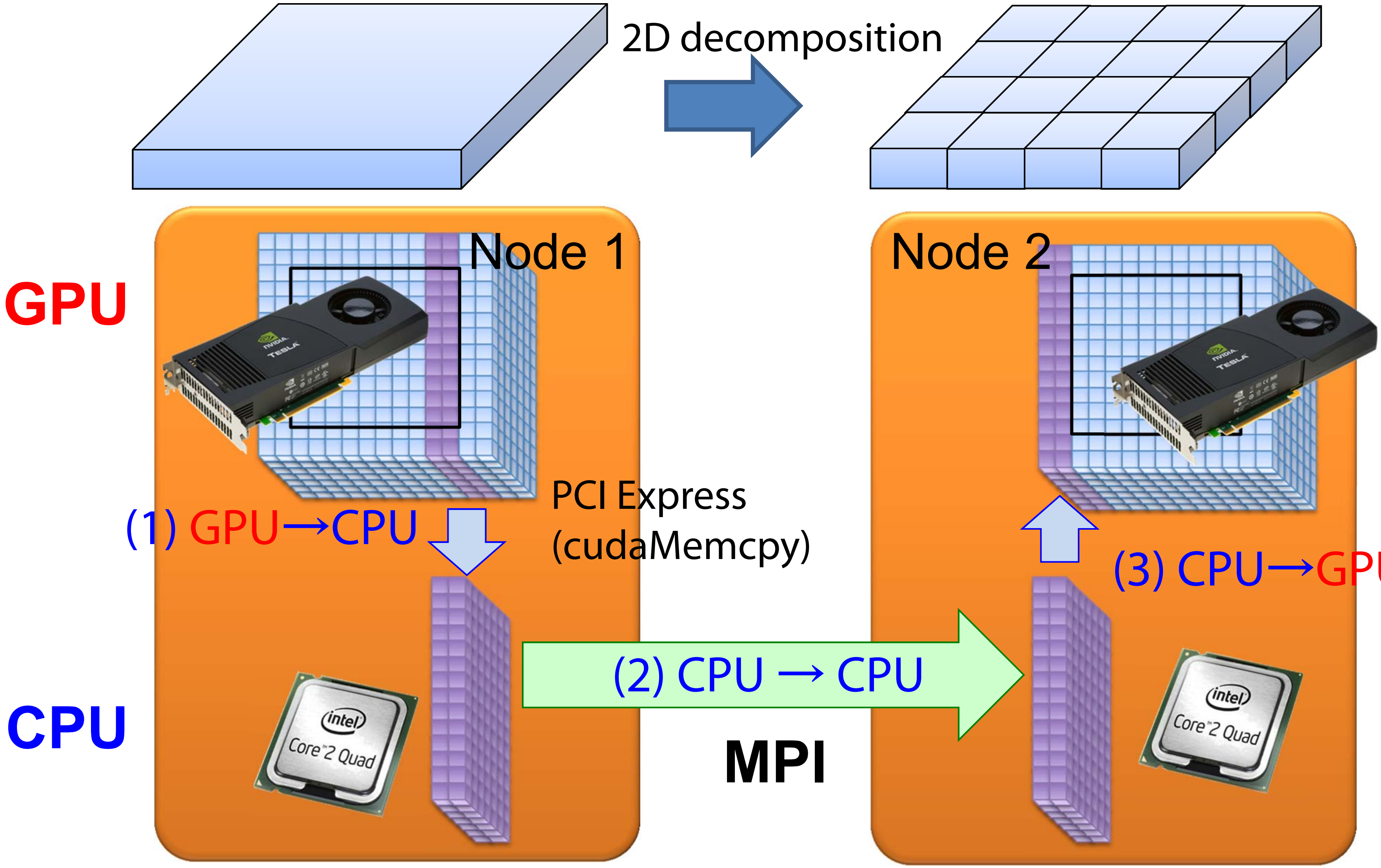




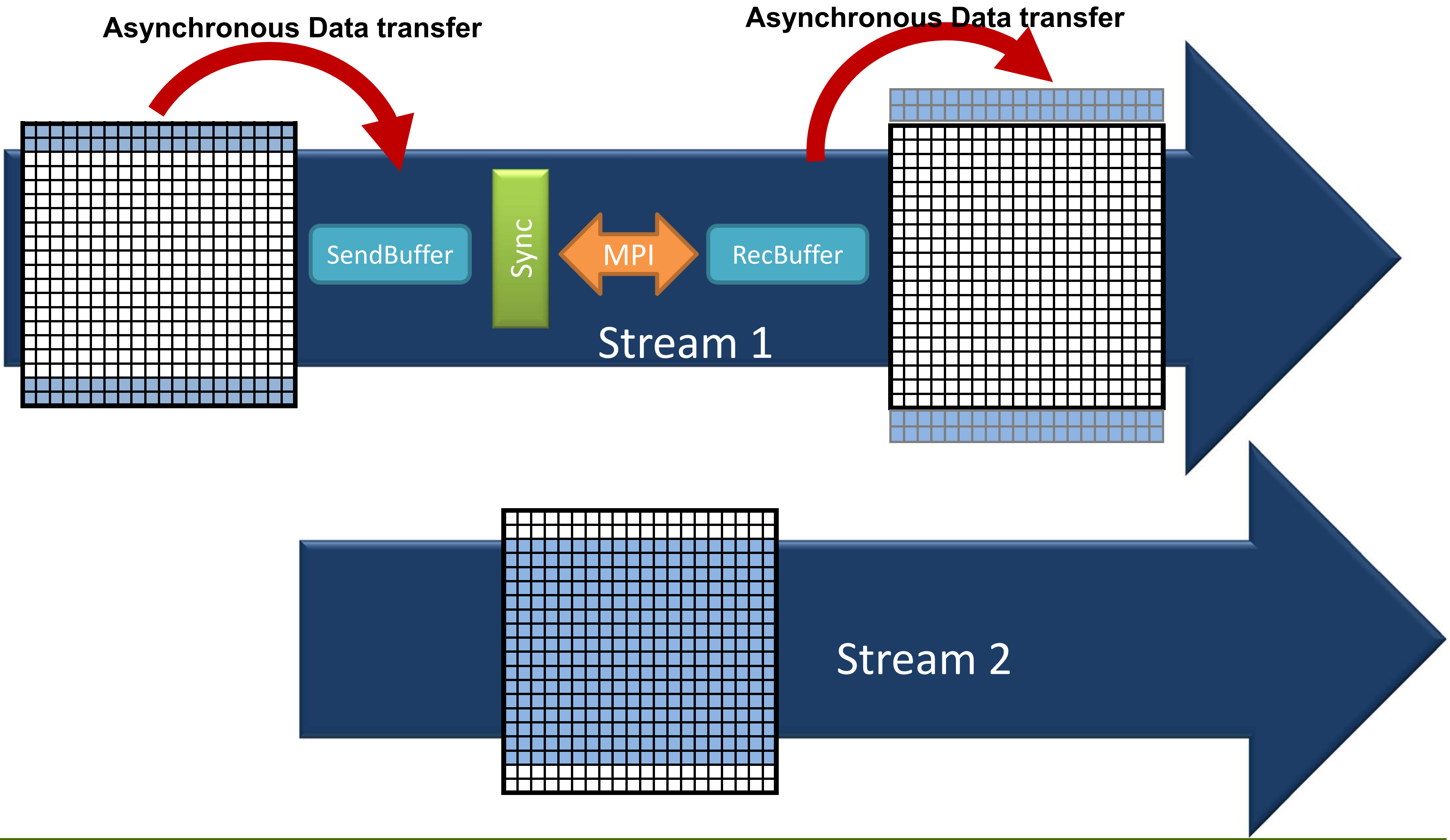
8 GPU 400km×800km
（100m mesh）

within 3 min

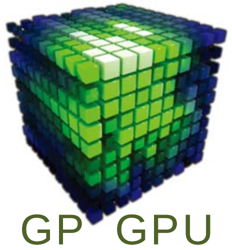
Multi-GPU : Domain decomposition

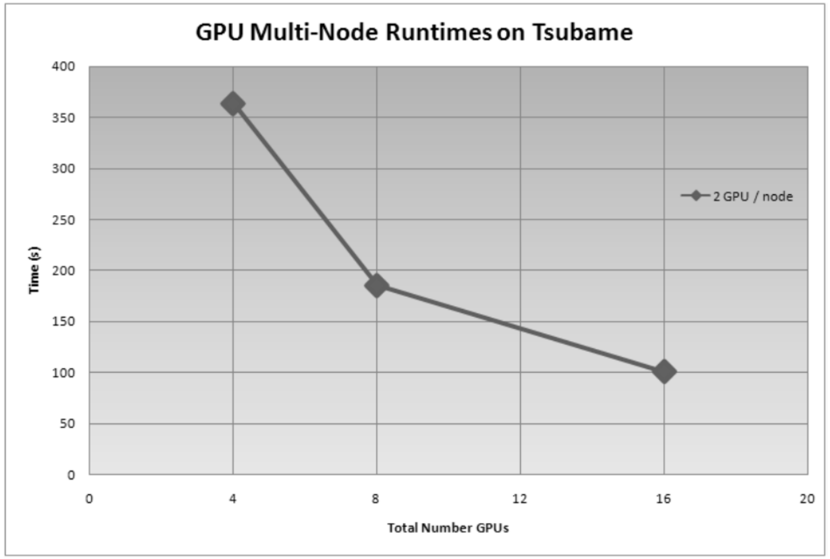


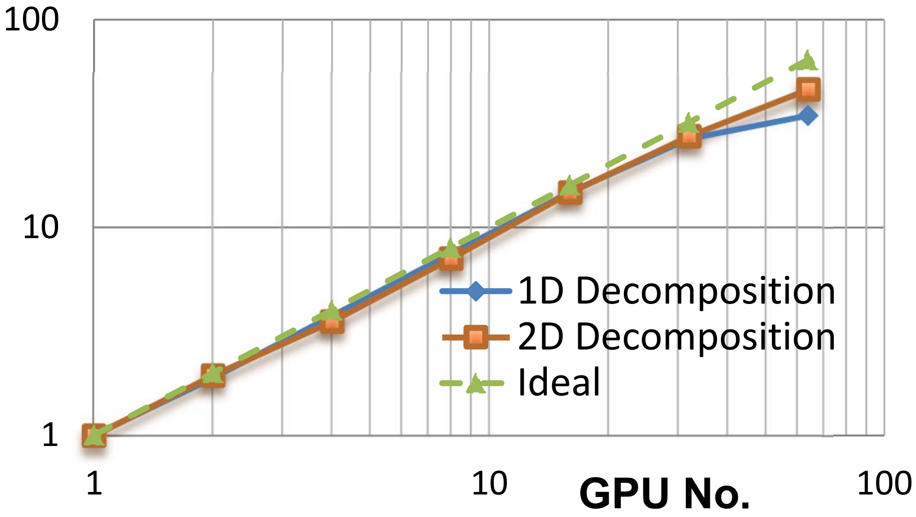
Overlapping between Computation and Communication

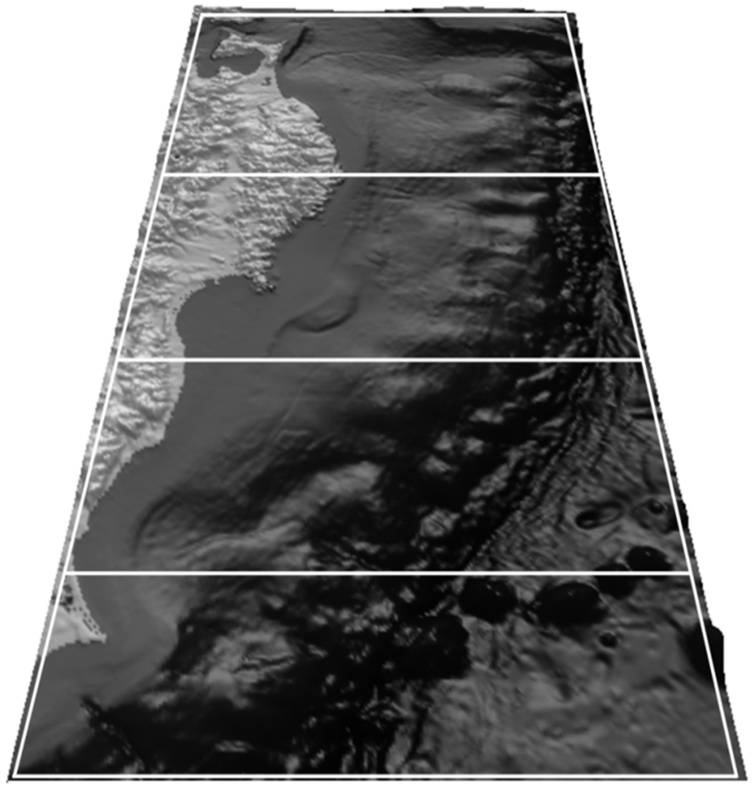


Large-scale Real-time Tsunami Simulator









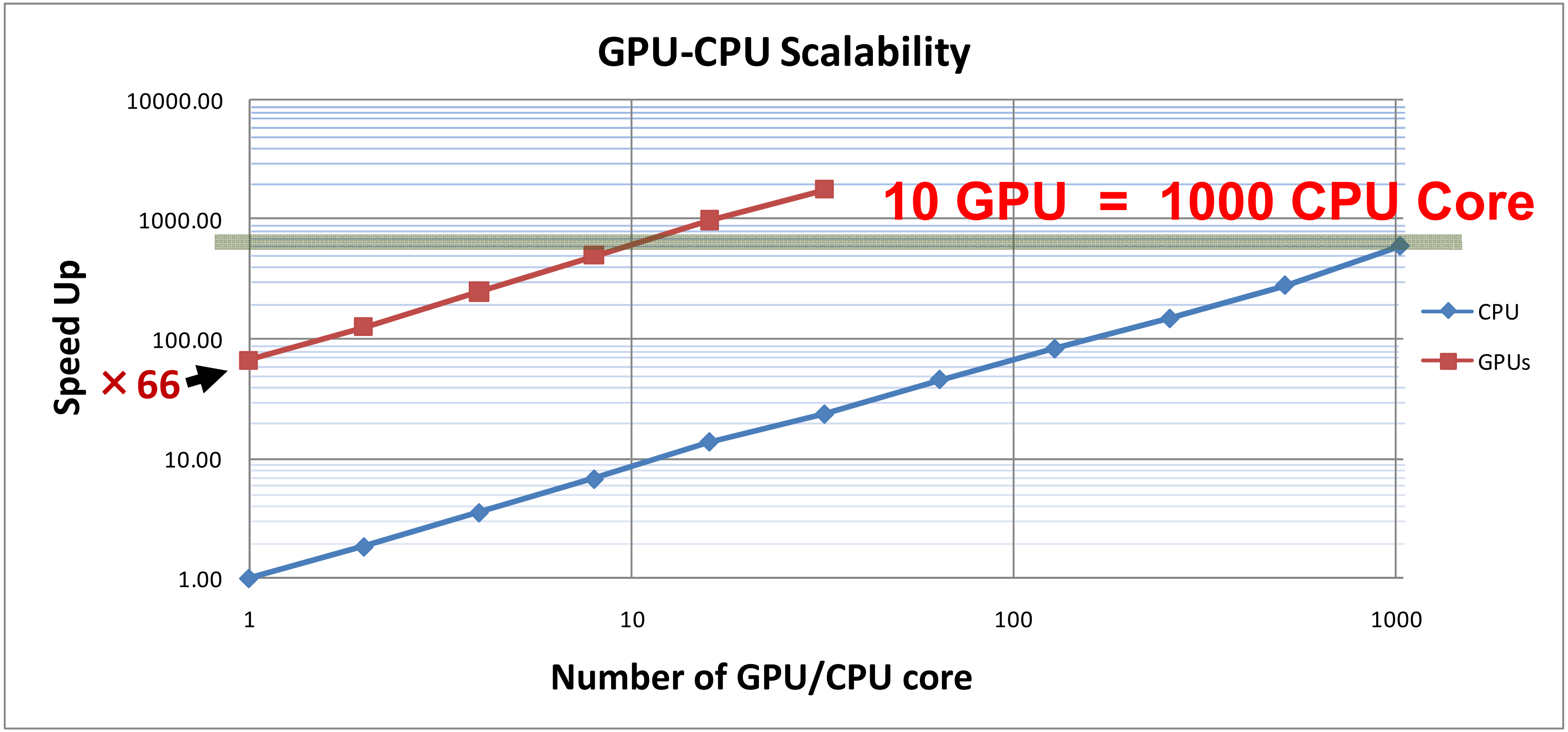
8 GPU 400km × 800km (100m mesh)

within 3 min

CPU-GPU
Performance Comparison

GP GPU

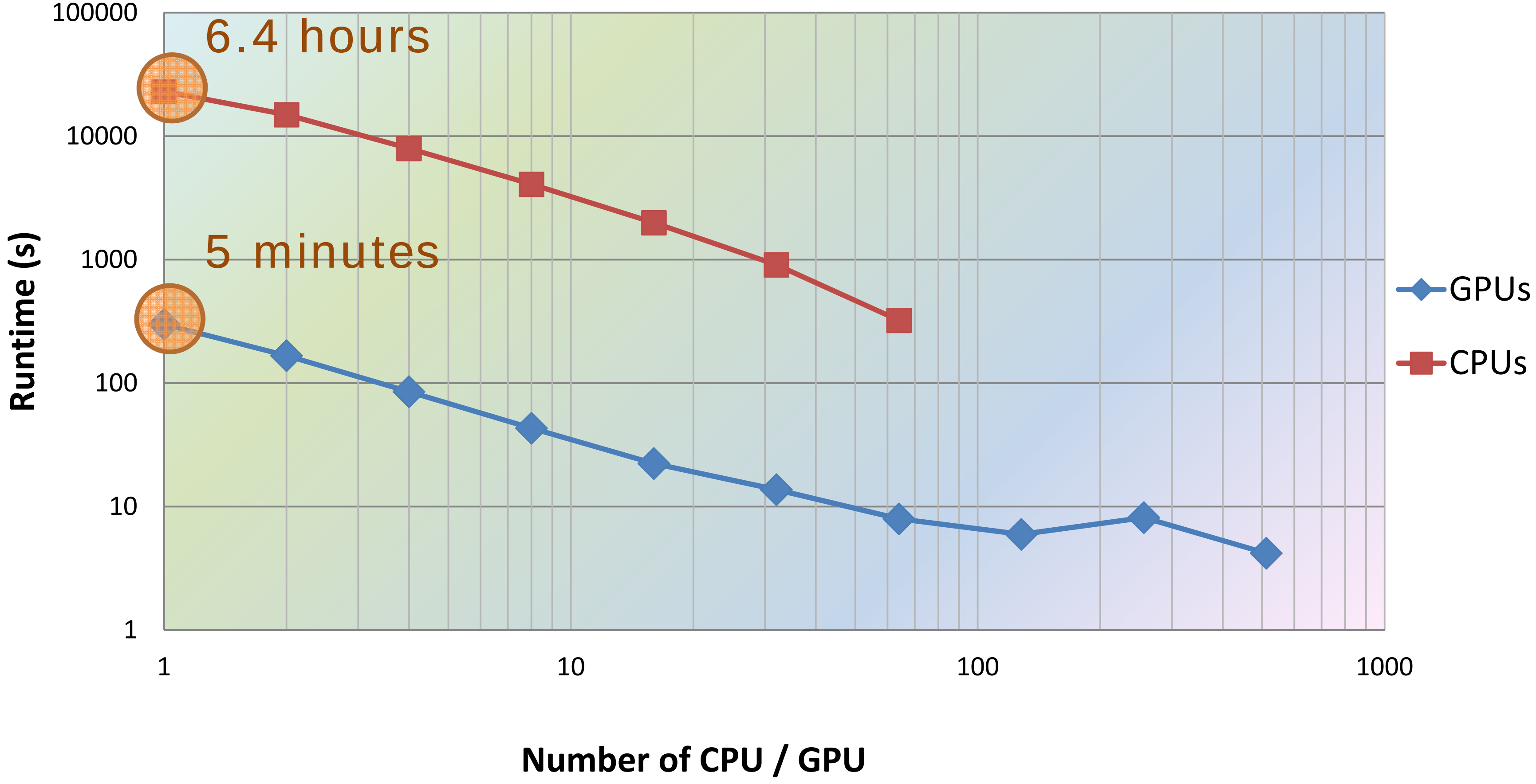
(1 CPU Core based)



Results on Multi-node Computing

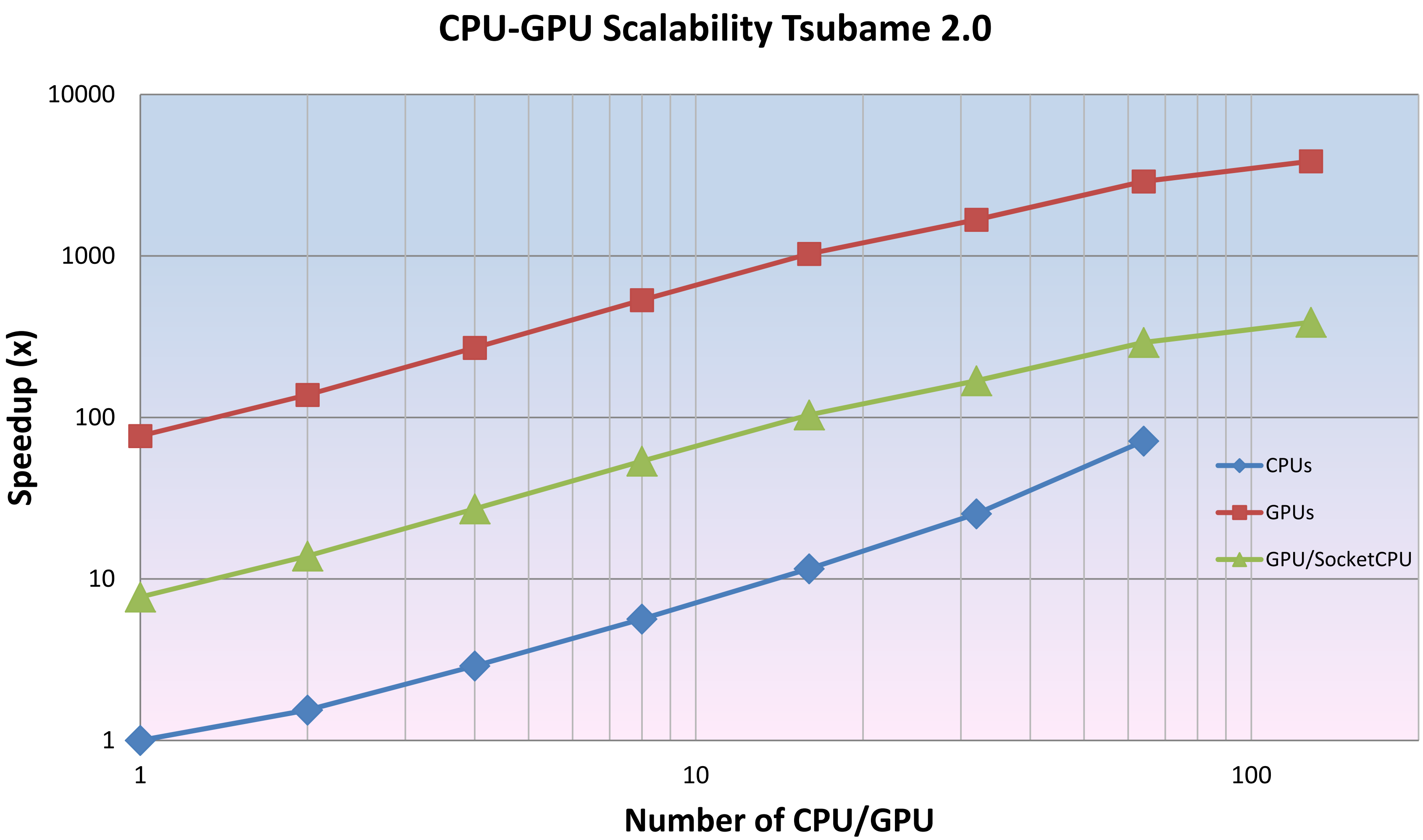
GP GPU

Tsubame 2.0



Multi-GPU Scalability

Tsubame 2.0



Two-Phase Flow Simulation

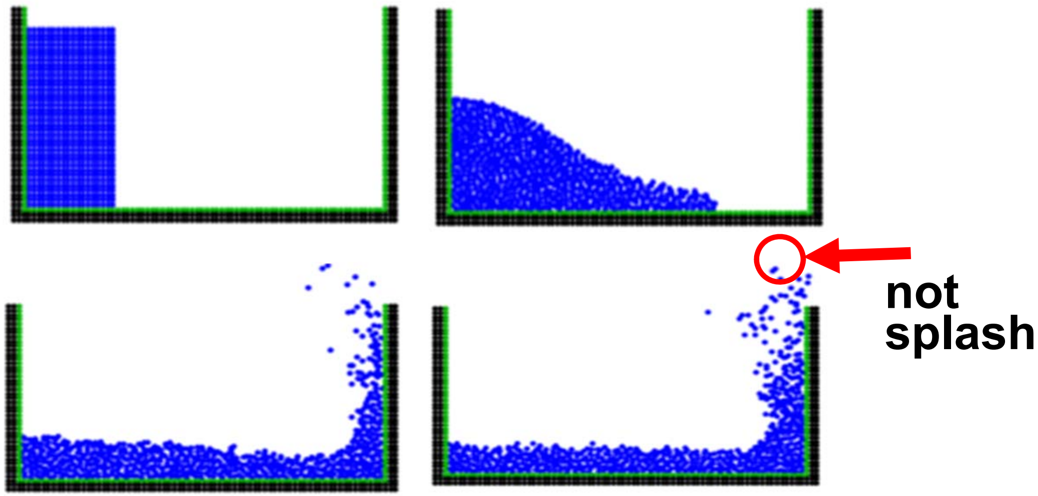
GP GPU

Particle Method
ex. SPH

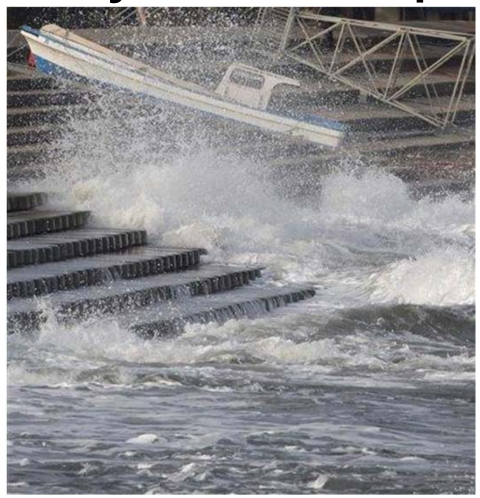
Low accuracy
< 10^6 particles

Mesh Method (Surface Capture)

- 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)



High accuracy > 10^8 mesh points



Numerical noise and unphysical oscillation

EQUATIONs for Two-Phase Flow

GP GPU

Time Integration : 3rd-order TVD Runge-Kutta

$$\nabla \cdot \mathbf{u} = 0$$

5th-upFD or 5th HJ-WENO

diffusion : 4th FD

Surface Tension CSF

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\,\mathbf{u} = -\frac{1}{\rho}\nabla p + \nu \nabla^2 \mathbf{u} + \frac{1}{\rho}\mathbf{F}$$

5th HJ-WENO →

$$\frac{\partial \phi}{\partial t} + (\mathbf{u} \cdot \nabla)\,\phi = 0$$

Re-initialization 5th HJ-WENO

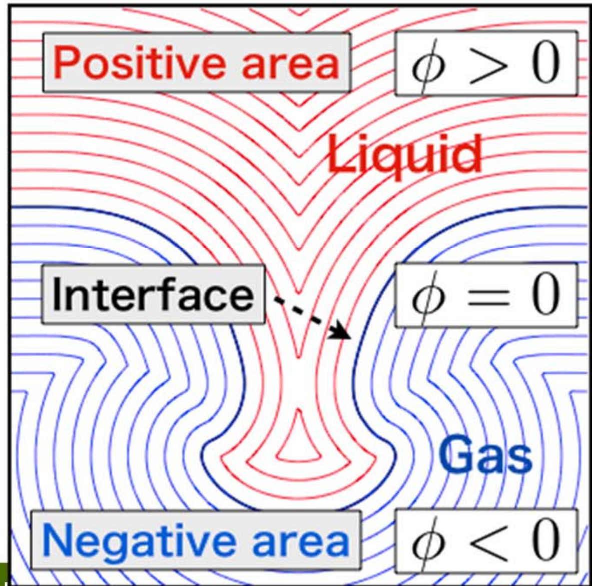
$$\frac{\partial \phi}{\partial \tau} = sgn(\phi)\,(1 - |\nabla \phi|)$$

Advection VOF THINC/WLIC →

$$\frac{\partial \psi}{\partial t} + \nabla \cdot (\mathbf{u}\psi) = 0$$

$$\rho = \rho_g + (\rho_l - \rho_g)\; H(\phi)$$

$$\nu = \nu_g + (\nu_l - \nu_g)\; H(\phi)$$

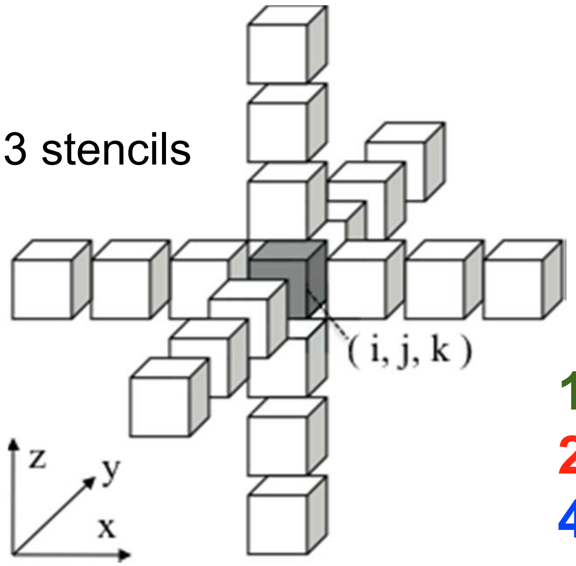


3D Advection Computation

Advection equation

$$\frac{\partial f}{\partial t} + (\boldsymbol{u} \cdot \nabla) f = 0$$

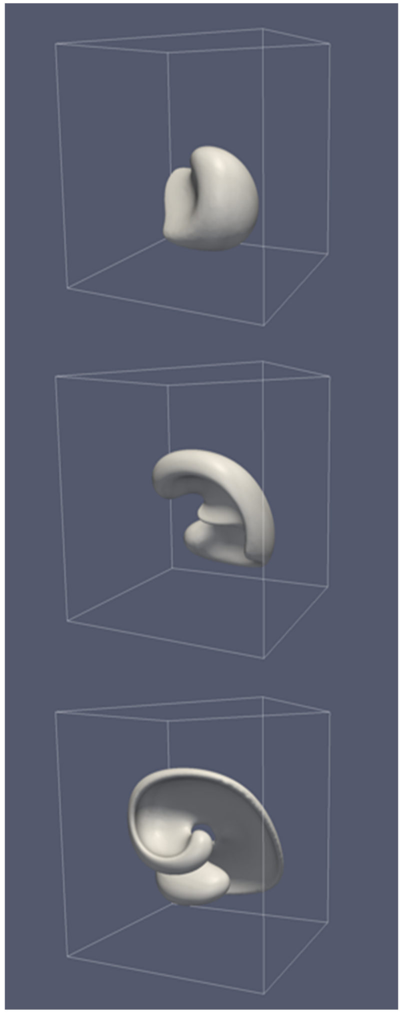
3 stencils



19 input values/cell
259 flop/cell (5th-WENO)
49 flop/cell (5th-up FD)

Discretization: Space : 5th-WENO
Time : 3rd TVD Runge-Kutta

312 GFlops (1GPU:GTX285)



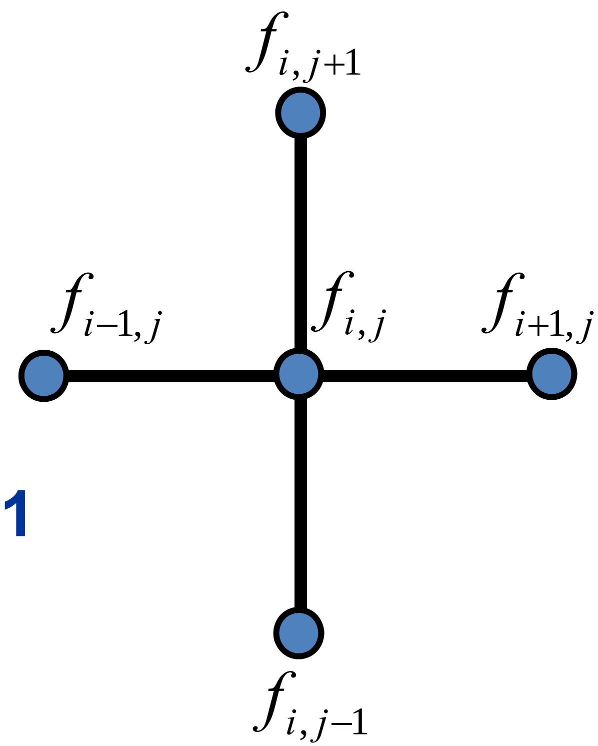
Stencil Computation

GP GPU

■ **Example: 2-dimensional diffusion Equation by FDM**

$$\frac{f_{i,j}^{n+1} - f_{i,j}^{n}}{\Delta t} = \kappa \left(\frac{f_{i+1,j}^{n} - 2f_{i,j}^{n} + f_{i-1,j}^{n}}{\Delta x^2} + \frac{f_{i,j+1}^{n} - 2f_{i,j}^{n} + f_{i,j-1}^{n}}{\Delta y^2} \right)$$

$$f_{i,j}^{n+1} = c_0 f_{i,j}^{n} + c_1 f_{i+1,j}^{n} + c_2 f_{i-1,j}^{n} + c_3 f_{i,j+1}^{n} + c_4 f_{i,j-1}^{n}$$



FLOP = 9

Byte = 4*6 = 24 byte : read 5, write 1

FLOP/Byte = 9/24 = 0.375

Arithmetic INTENSITY: FLOP/Byte

GP GPU

FLOP = number of FP operation for applications
Byte = Byte number of memory access for applications

F = Peak Performance of floating point operation
B = Peak Memory Bandwidth

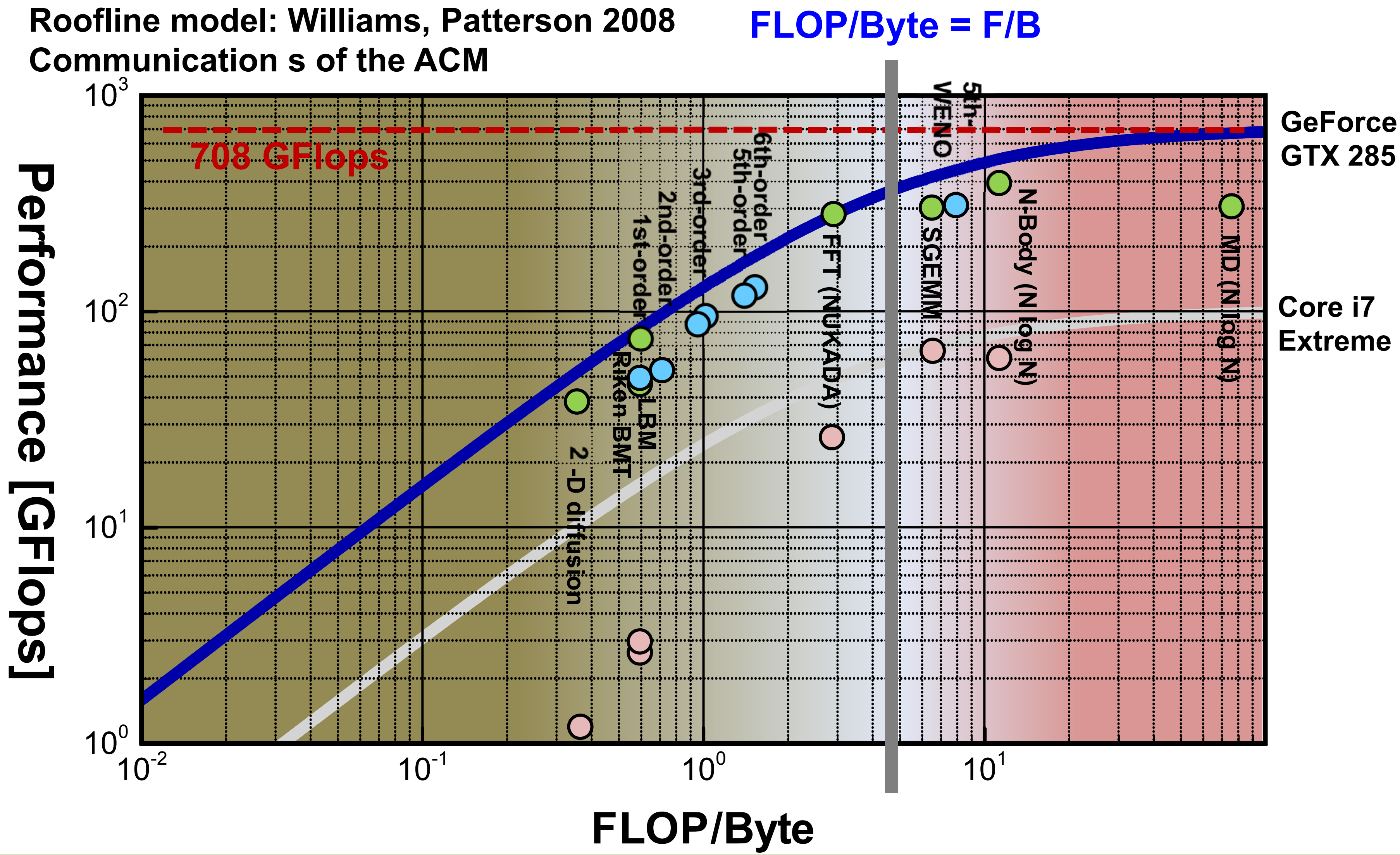
$$\text{Performance} = \frac{\text{FLOP}}{\text{FLOP/F} + \text{Byte/B} + \alpha}$$

$$= \frac{\text{FLOP/Byte}}{\text{FLOP/Byte} + \text{F/B} + \alpha} \text{F}$$

Application Performances

GP GPU

Roofline model: Williams, Patterson 2008
Communication s of the ACM

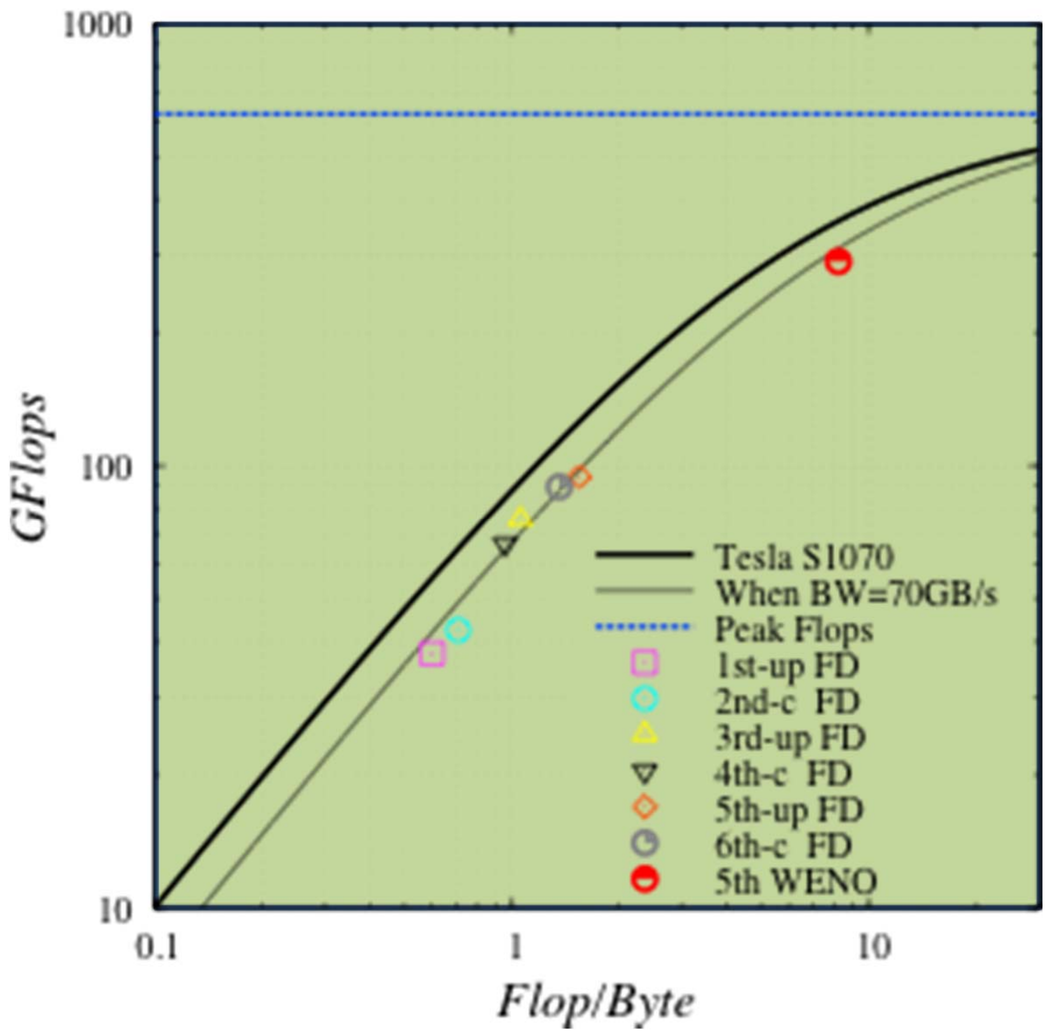


Performance of Advection Computation

GP GPU

	flop/byte		GFlops
Scheme	no-SMem	SMem	Tesla S1070
1st-up FD	0.29	0.60	37.61
2nd-c FD	0.34	0.71	42.46
3rd-up FD	0.38	1.06	75.49
4th-c FD	0.34	0.96	66.64
5th-up FD	0.45	1.55	94.58
6th-c FD	0.4	1.36	89.62
5th-WENO	2.40	8.22	289.66

3D advection 416x416x416 cells
Time integration: 3rd-order TVD Runge-Kutta



Level-Set method (LSM)

The Level-Set methods (LSM) use the signed distance function to capture the interface. The interface is represented by the zero-level set (zero-contour).

ϕ **: Level-Set function(distance function)**

H : Heaviside function

$$
\begin{cases}
H(\phi) = \frac{1}{2} & \phi > \varepsilon \\
H(\phi) = \frac{1}{2}\left(\frac{\phi}{\varepsilon} + \frac{1}{\pi}\sin\left(\frac{\pi\phi}{\varepsilon}\right)\right) & |\phi| \le \varepsilon \\
H(\phi) = -\frac{1}{2} & \phi < -\varepsilon
\end{cases}
$$

Re-initialization for Level-Set function

$$
\frac{\partial\phi}{\partial\tau} = sgn(\phi)\left(1 - |\nabla\phi|\right)
$$

Advantage : Curvature calculation, Interface boundary

Drawback : Volume conservation

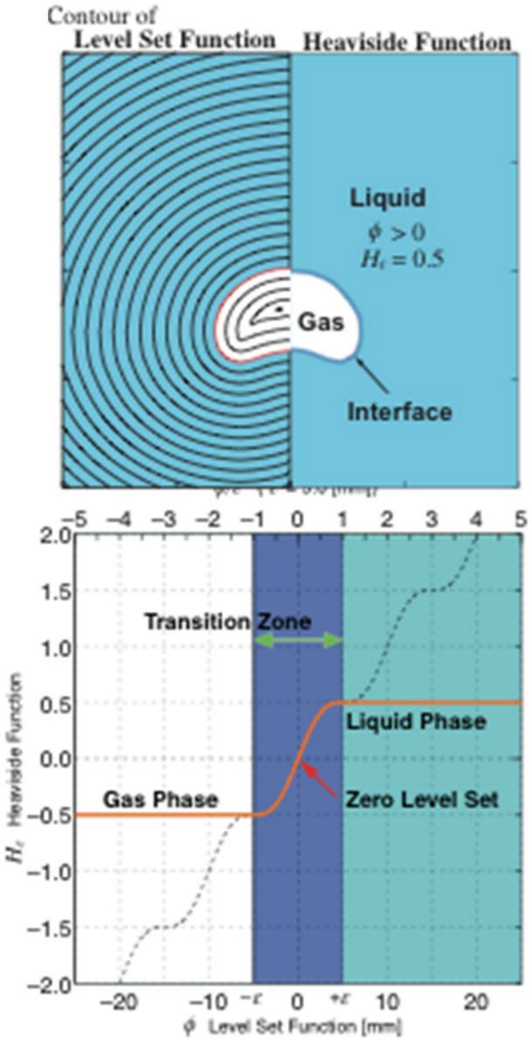


Fig. Takehiro Himeno, et. Al., JSME, 65-635,B(1999),pp2333-2340

Continuous Surface Force (CSF) model by Brackbill, Kothe and Zemach (1991)

The interfacial surface force is transformed to a volume force in the region near the interface via a delta function

Curvature

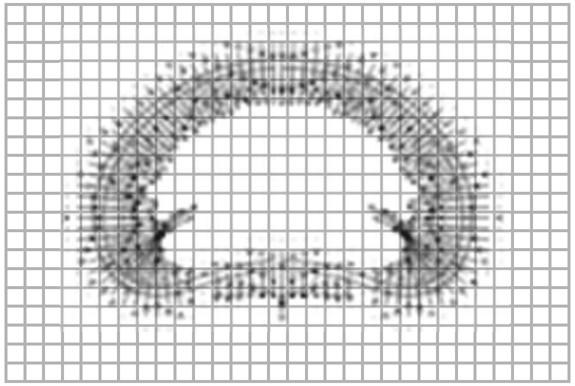
Surface tension force

$$\mathbf{F}_S = \sigma \ \kappa \ \mathbf{n}$$

Normal vector

$$\kappa = -\nabla \cdot \mathbf{n} = -\nabla \cdot \frac{\nabla \phi}{|\nabla \phi|}$$

$$\mathbf{F}_S = \sigma \ \kappa \ \delta(\phi) \ \nabla \phi$$

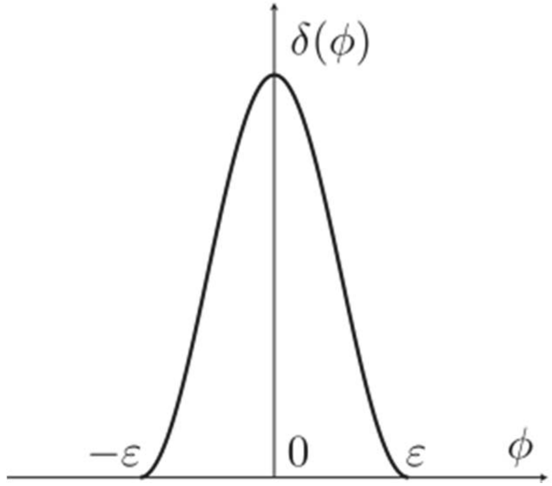


Surface tension represented by volume force

Approximate delta function

$$\delta(\phi) = \frac{\partial H(\phi)}{\partial \phi} = \frac{1}{2}\left(\frac{1}{\varepsilon} + \frac{1}{\varepsilon}\cos\left(\frac{\pi \phi}{\varepsilon}\right)\right)$$

$$\int_{-\varepsilon}^{\varepsilon} \delta(\phi) \ d\phi = 1$$



Anti-diffusive Interface Capture

GP GPU

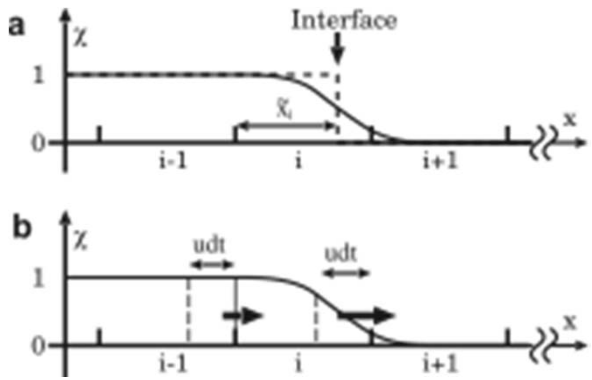
THINC (tangent of hyperbola for interface capturing) Scheme

[Xiao, etal, Int. J. Numer. Meth. Fluid. 48(2005)1023]

- VOF(volume of fluid) type interface capturing method
- Flux from tangent of hyperbola function
- Semi-Lagrangian time integration

$$F_i(x) = \frac{1}{2}\left(1 + \alpha \tanh\left(\beta\left(\frac{x - x_{i-1/2}}{\Delta x} - \tilde{x}_i\right)\right)\right)$$

$$\alpha = \begin{cases} 1 & (\text{if} \quad n_x > 0) \\ -1 & (\text{if} \quad n_x \leq 0) \end{cases}$$



- 1D implementation can be applied to 2D & 3D → Simple

$$Fl_{x,i+1/2} = -\int_{x_{i+1/2}}^{x_{i+1/2} - u_{i+1/2}\Delta t} F_{up}(x)\ dx \qquad up = \begin{cases} i & (\text{if} \quad u_{i+1/2} > 0) \\ i+1 & (\text{if} \quad u_{i+1/2} \leq 0) \end{cases}$$

- Finite Volume like usage
  * THINC is the method how to compute flux

→ 3 krenel (x, y, z) can be fused to 1 kernel. Merit in memory R/W

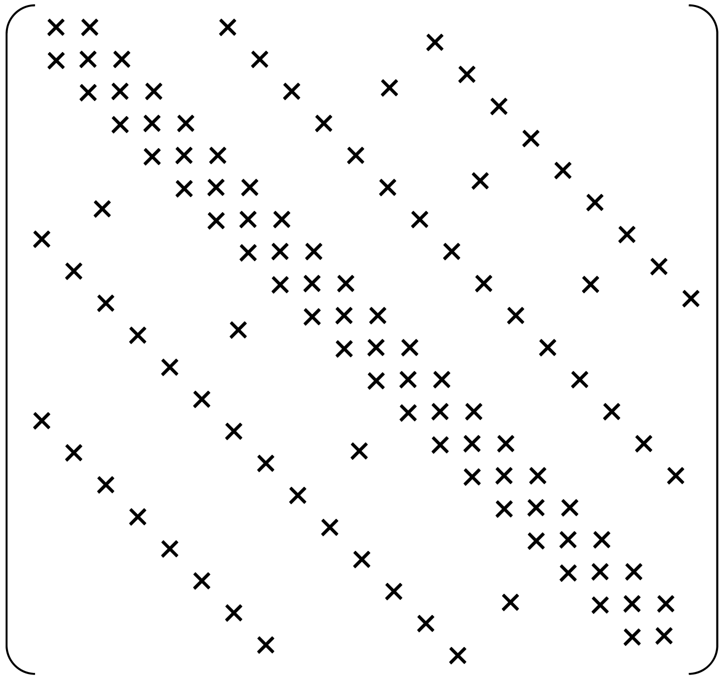
Sparse Matrix Solver

$$\mathbf{A}x = b \quad \textit{for} \quad \nabla \cdot \left(\frac{1}{\rho} \nabla p \right) = \frac{\nabla \cdot \boldsymbol{u}}{\Delta t}$$

Krylov sub-space methods:
CG, BiCGStab, GMRes, , ,

Pre-conditioner:
Incomplete Cholesky,
ILU, MG, AMG,
Block Diagonal Jacobi

Non-zero Packing:
CRS → ELL, JDL



BiCGStab + MG

GP GPU

Collaboration with
Mizuho Information & Research Institute

Set $k = 0 \quad \boldsymbol{r}_0 = \boldsymbol{p}_0 = \boldsymbol{M}^{-1}(\boldsymbol{b} - \boldsymbol{A}\boldsymbol{x}_0)$

for $\boldsymbol{k} = 0;\ \boldsymbol{k} < N;\ \boldsymbol{k}{+}{+};$

$$\alpha_k = \frac{(\boldsymbol{r}_0, \boldsymbol{r}_k)}{(\boldsymbol{r}_0, \boldsymbol{M}^{-1}\boldsymbol{A}\boldsymbol{p}_k)} \qquad \boldsymbol{q}_k = \boldsymbol{r}_k - \alpha_k \boldsymbol{M}^{-1}\boldsymbol{A}\boldsymbol{p}_k \qquad \omega_k = \frac{(\boldsymbol{q}_k, \boldsymbol{M}^{-1}\boldsymbol{A}\boldsymbol{q}_k)}{(\boldsymbol{M}^{-1}\boldsymbol{A}\boldsymbol{q}_k, \boldsymbol{M}^{-1}\boldsymbol{A}\boldsymbol{q}_k)}$$

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \alpha_k \boldsymbol{p}_k + \omega_k \boldsymbol{q}_k$$

$$\boldsymbol{r}_{k+1} = \boldsymbol{q}_k - \omega_k \boldsymbol{M}^{-1}\boldsymbol{A}\boldsymbol{q}_k$$

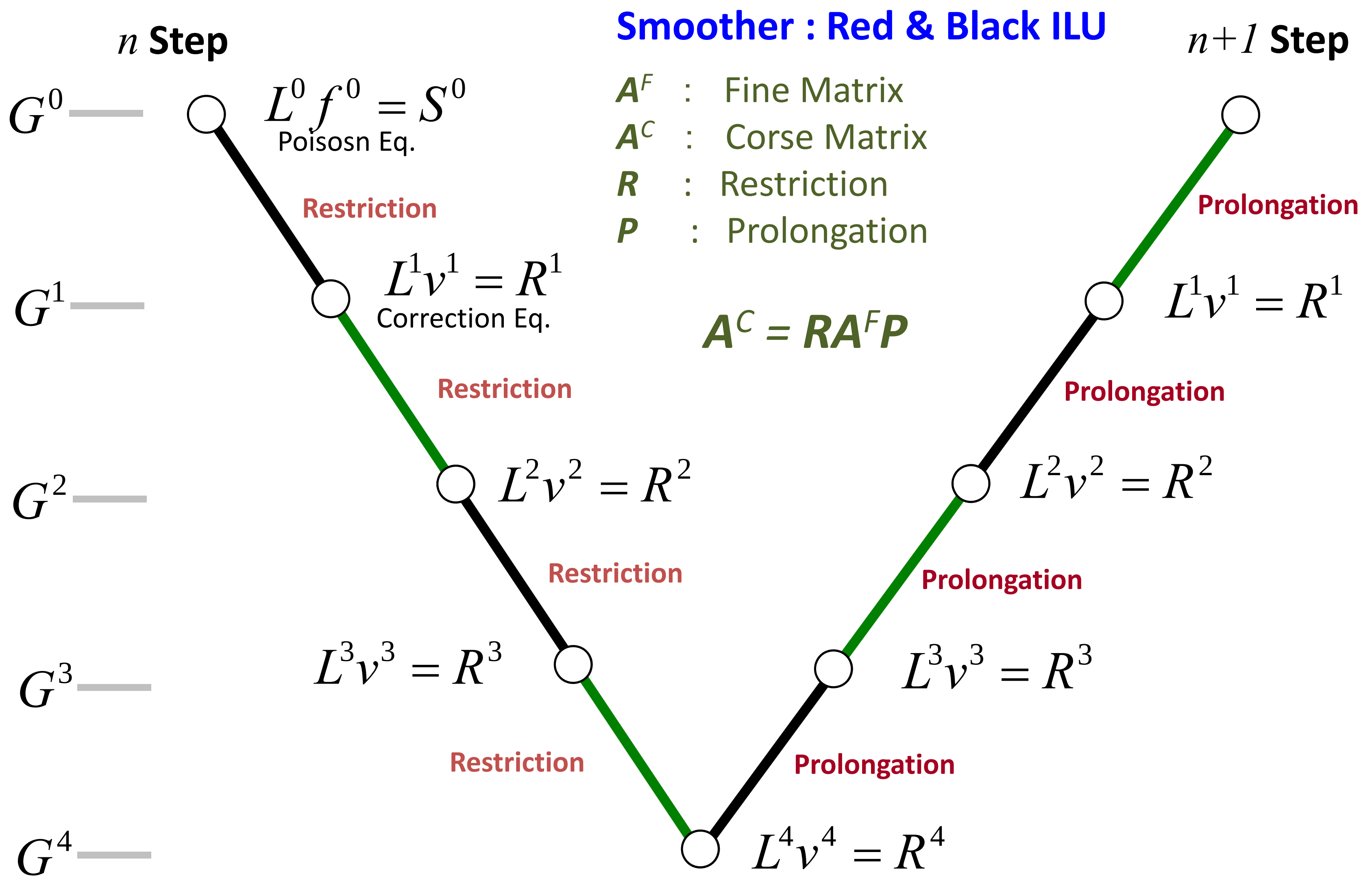
if $(\boldsymbol{r}_{k+1}, \boldsymbol{r}_{k+1}) < \varepsilon^2 (\boldsymbol{b}, \boldsymbol{b})$ **exit;**

$$\beta_k = \frac{(\boldsymbol{r}_0, \boldsymbol{r}_{k+1})}{\omega_k (\boldsymbol{r}_0, \boldsymbol{M}^{-1}\boldsymbol{A}\boldsymbol{p}_k)}$$

$$\boldsymbol{p}_{k+1} = \boldsymbol{r}_{k+1} + \beta_k (\boldsymbol{p}_k - \omega_k \boldsymbol{M}^{-1}\boldsymbol{A}\boldsymbol{p}_k)$$

loop end

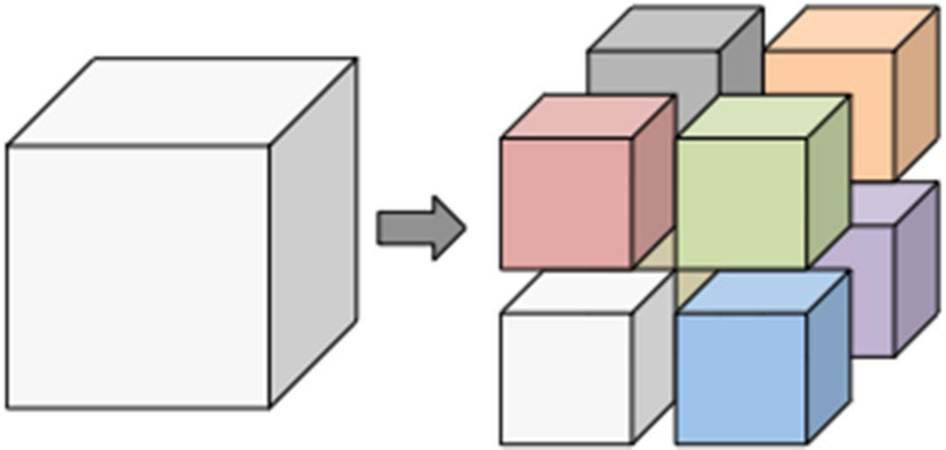
MG V-Cycle



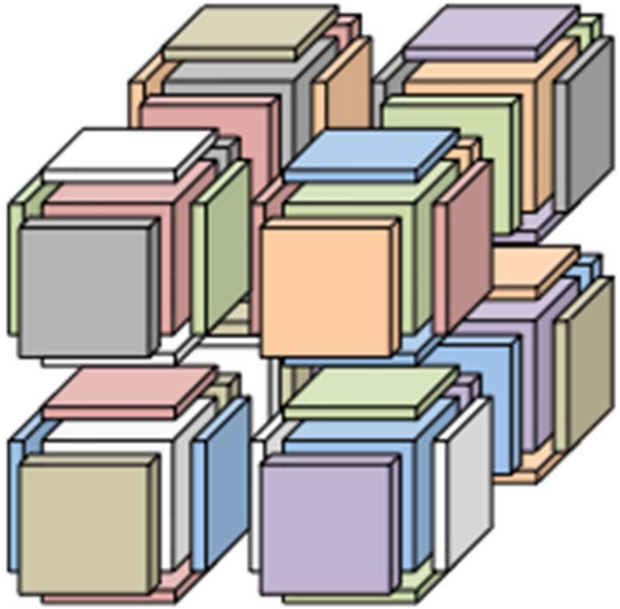
n Step
Smoother : Red & Black ILU
$n+1$ Step
A^F : Fine Matrix
A^C : Corse Matrix
R : Restriction
P : Prolongation
$A^C = RA^FP$
G^0
G^1
G^2
G^3
G^4
$L^0 f^0 = S^0$
Poisosn Eq.
Restriction
$L^1 v^1 = R^1$
Correction Eq.
Restriction
$L^2 v^2 = R^2$
Restriction
$L^3 v^3 = R^3$
Restriction
$L^4 v^4 = R^4$
Prolongation
$L^3 v^3 = R^3$
Prolongation
$L^2 v^2 = R^2$
Prolongation
$L^1 v^1 = R^1$
Prolongation

Multi-Dimensional
Domain Decomposition

GP GPU



- 3D domain decomposition
- 1 GPU is assigned to each domain

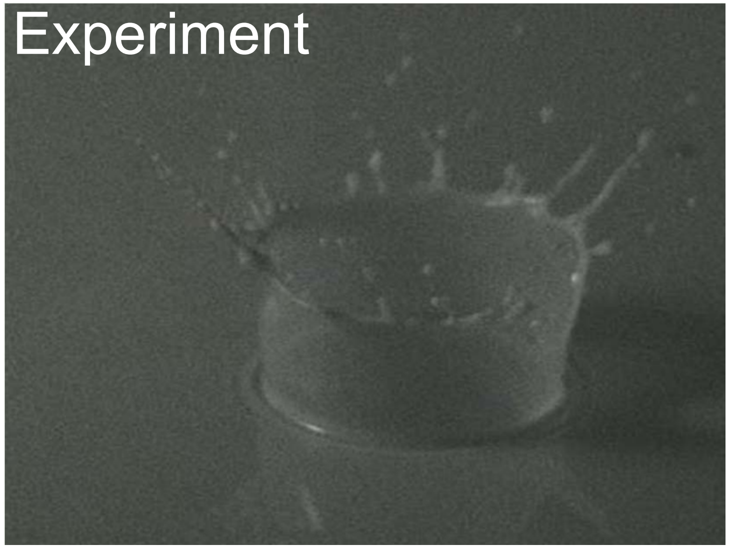


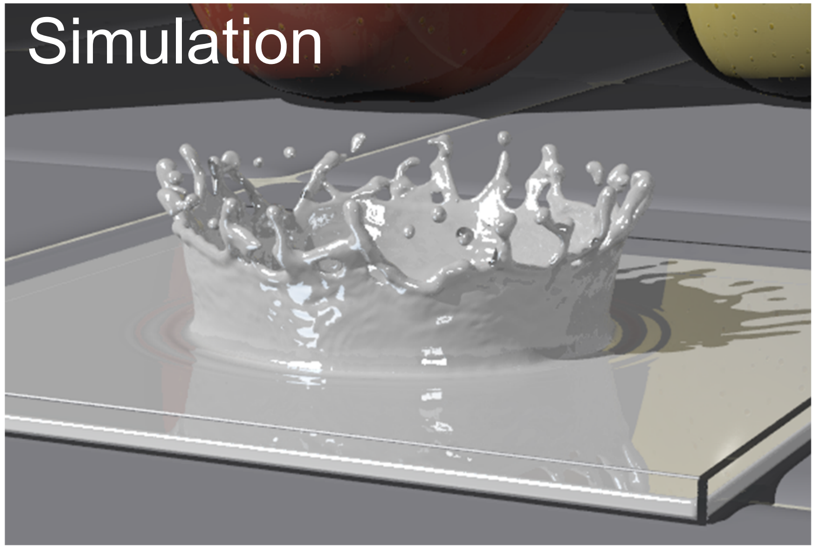
- Communication buffer for each face
- Host buffer & Device buffer

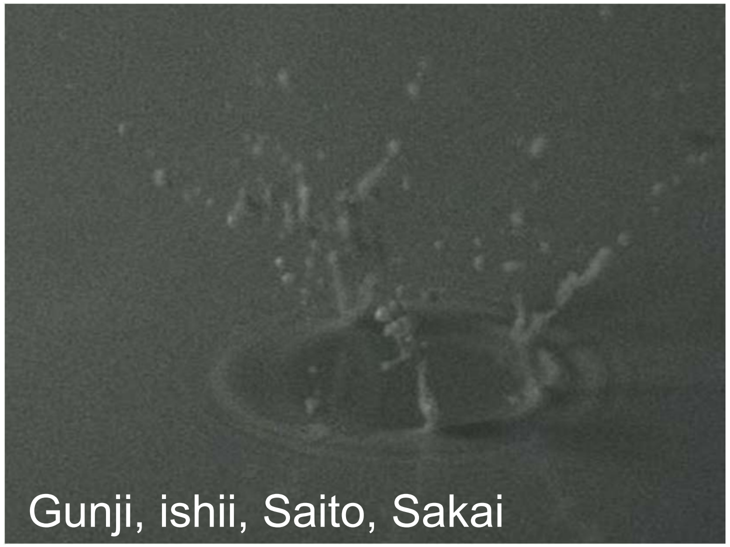
Milk Crown Formation

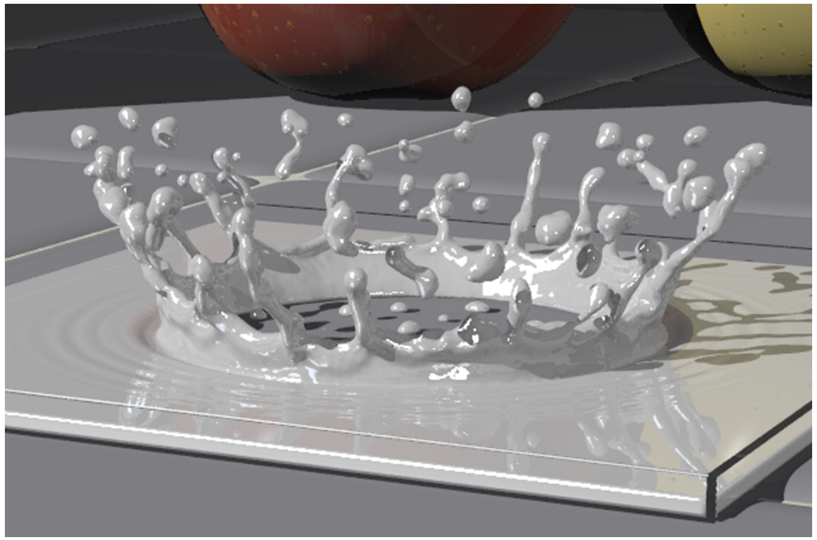
GP GPU

4.0 m/sec impact speed









Rayleigh-Taylor Instability

with Surface Tension Force

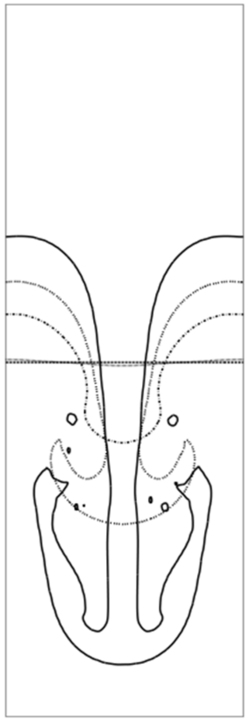
GP GPU

When a heavy fluid is supported against gravity by a light fluid, a Rayleigh-Taylor instability develops in which perturbations of the interface grow exponentially in time as exp(nt) for small amplitudes.

$$n^2 = Kg\left[A - \frac{K^2\sigma}{g(\rho_h - \rho_l)}\right]$$

$$A = \frac{\rho_h - \rho_l}{\rho_h + \rho_l}$$

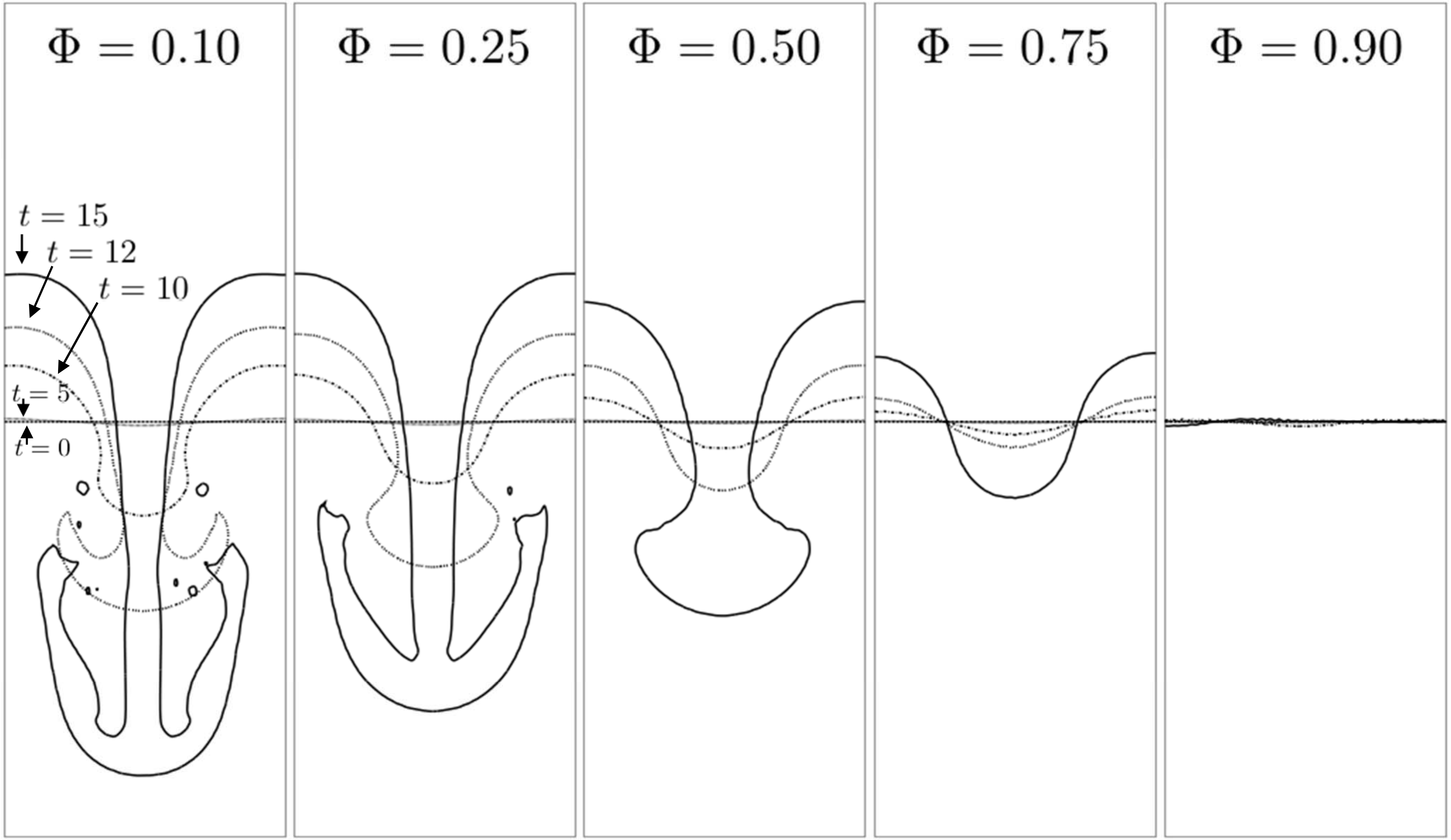
$$\Phi = \frac{\sigma}{\sigma_c} = \frac{\sigma K^3}{g(\rho_h - \rho_l)}$$



$\rho_l = 0.25$
$\rho_h = 1.0$
$K = 1$
$g = 1$
$\mu = 0$
$L_x = 2\pi$
$L_y = 6\pi$

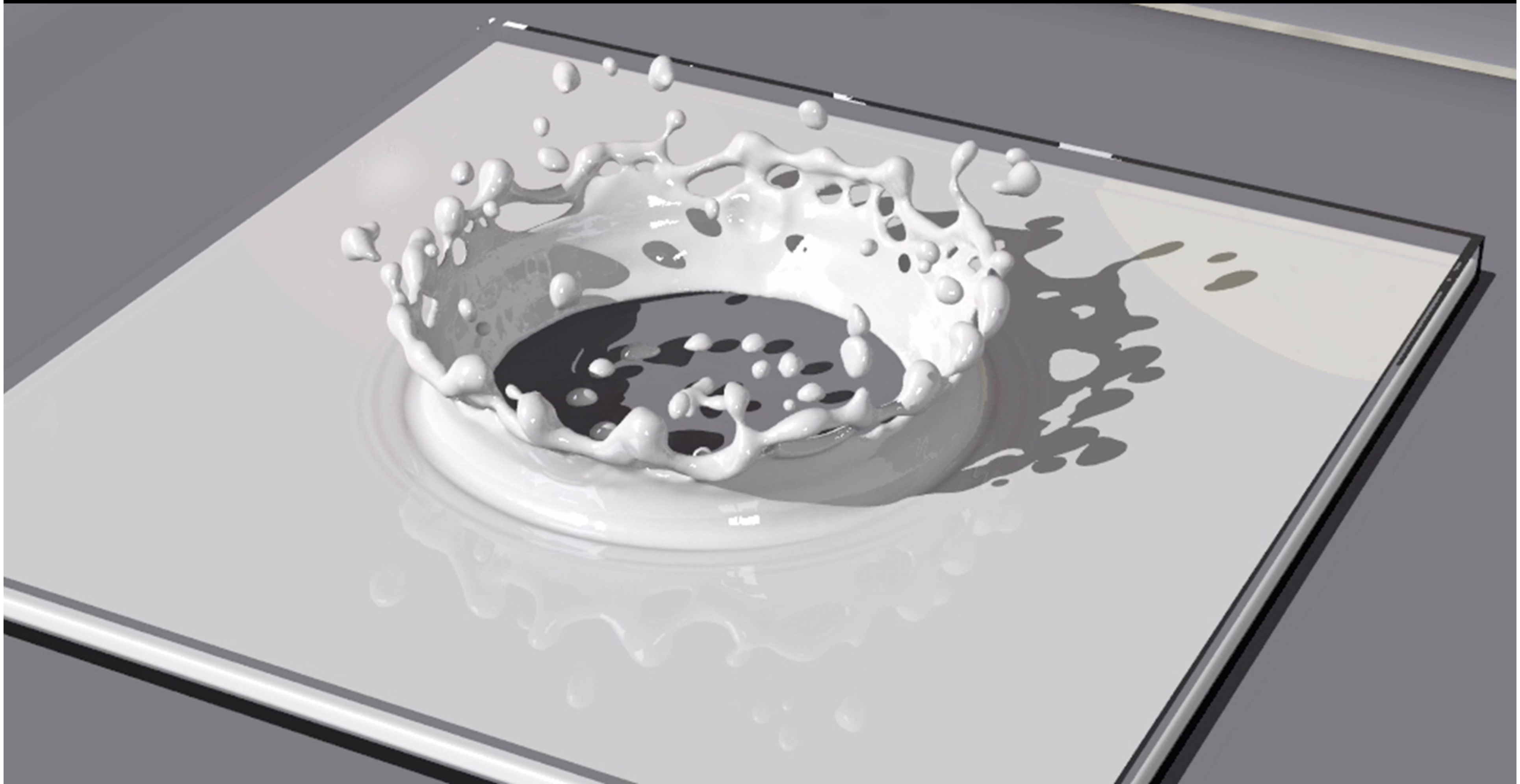
Bellman, R., Pennington, R.H.: Effect of surface tension and viscosity on Taylor instability. Q. Appl. Methods **12**, 12, 151 (1954)
Drazin, P.G., Reid, W.H.: Hydrodynamic Stability. Cambridge University Press, Cambridge (1967)
Daly, B.J.: Numerical study of the effect of surface tension on interface instability. Phys. Fluids **12**, 1340 (1969)

Snapshots of the R-T Instability

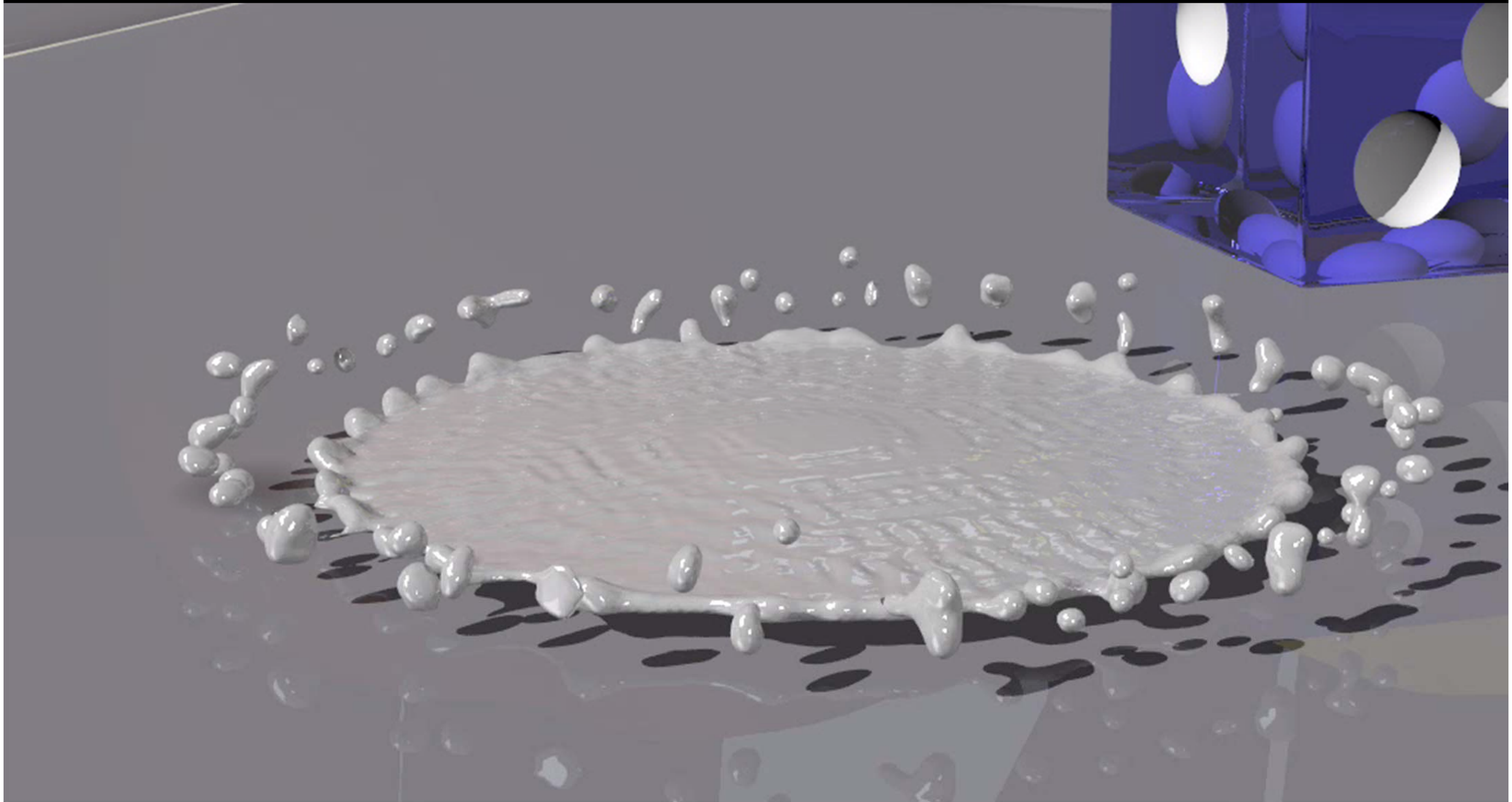


1024x192 cells

Milk Crown



Drop on dry floor



Broken dam Problem

J.C.Martin and W.J. Moyce (1952)

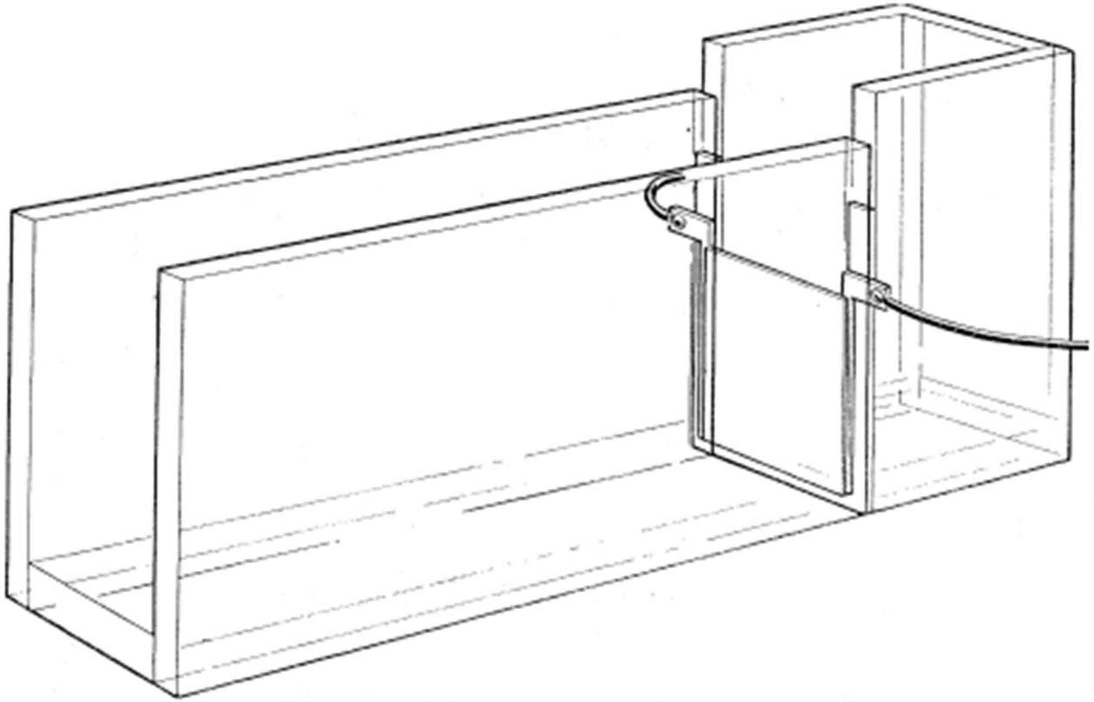


FIGURE 1. Diagram of typical apparatus.

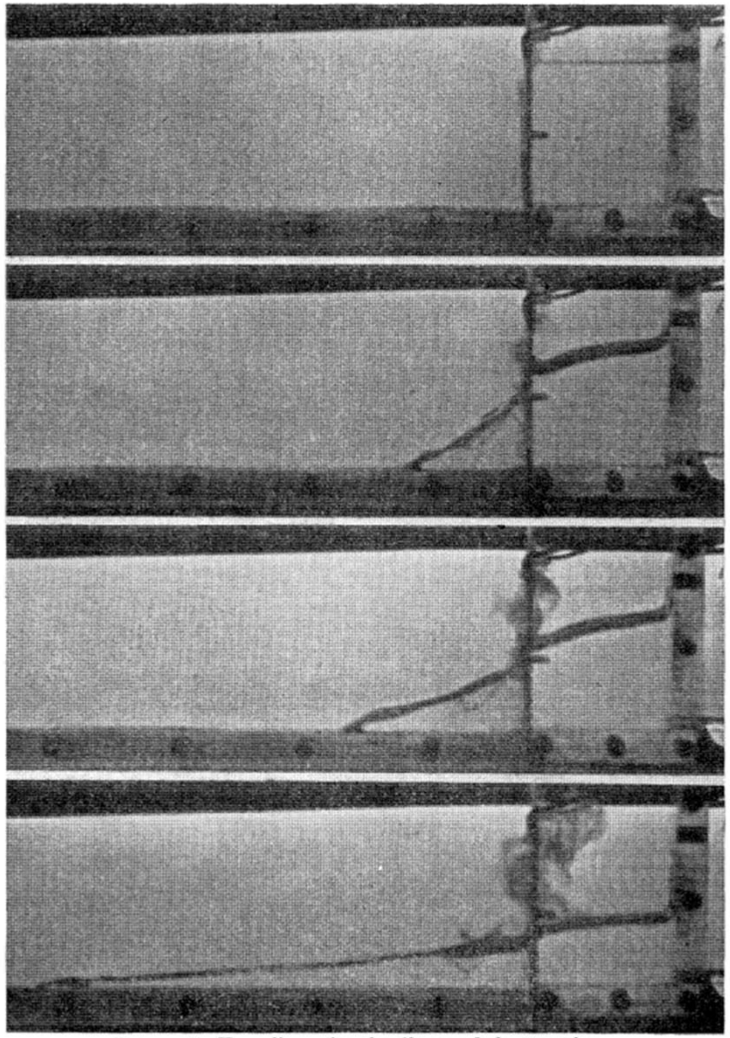
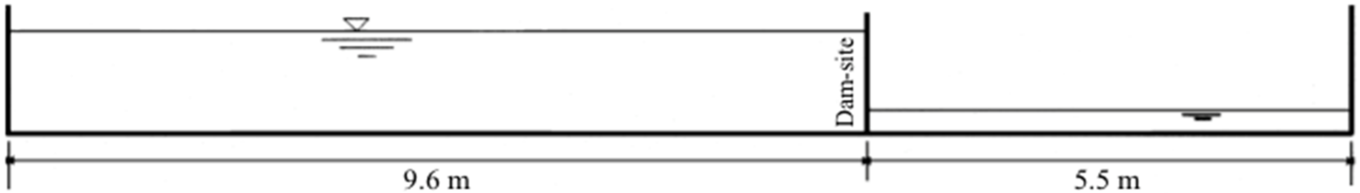


FIGURE 2. Two dimensional collapse of $n^2 = 1$ section.

Initial stages of dam-break flow

P.K.Stanby, A.Chegini and T.C.D.Barnes (1998)

(*a*)



(*b*)

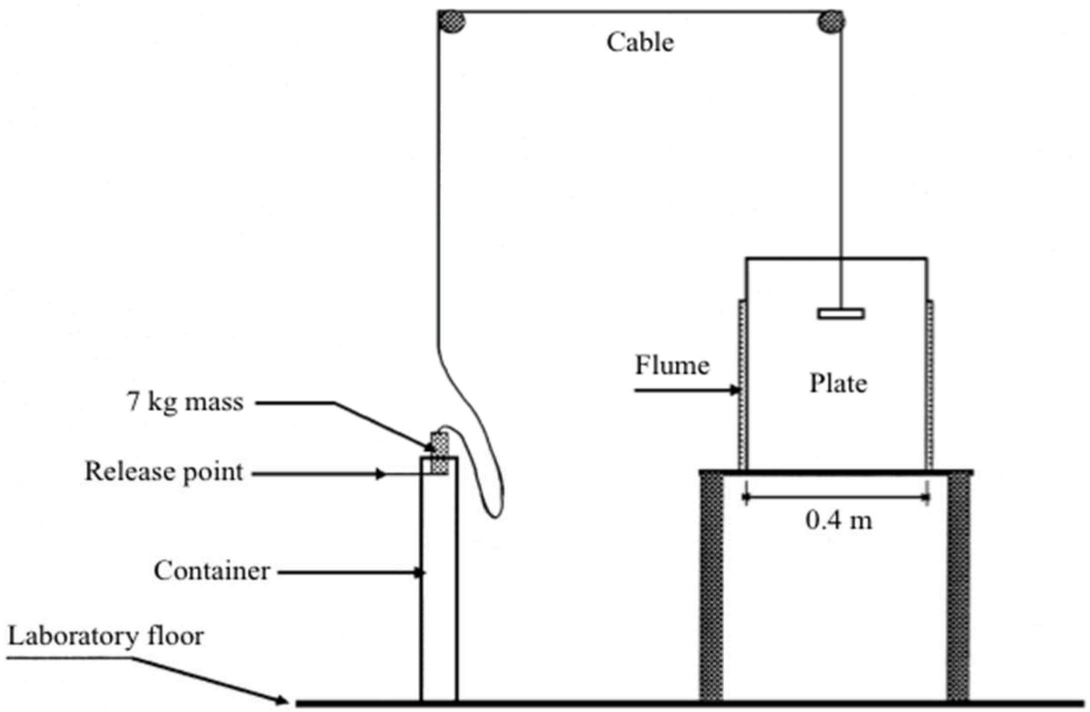
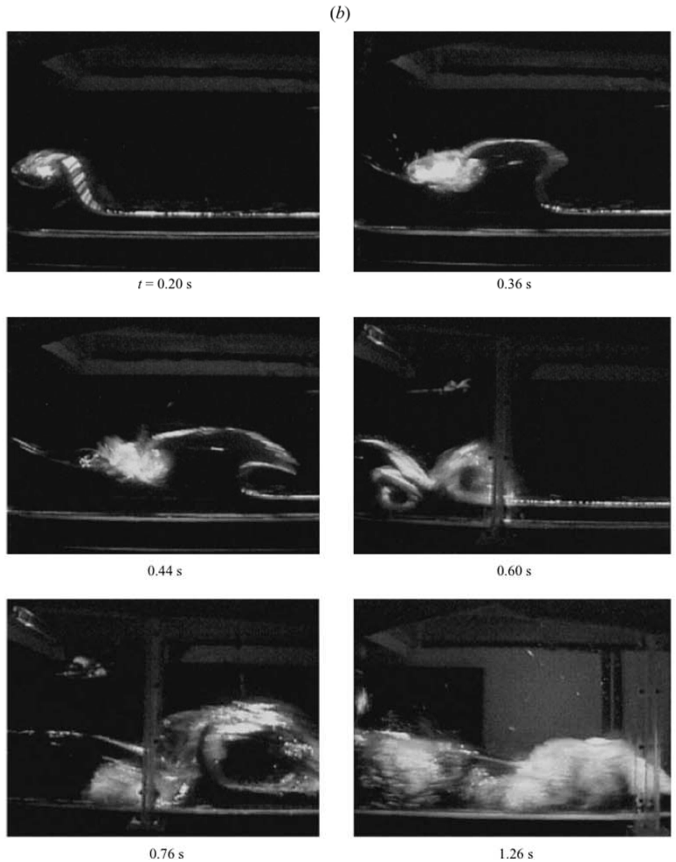
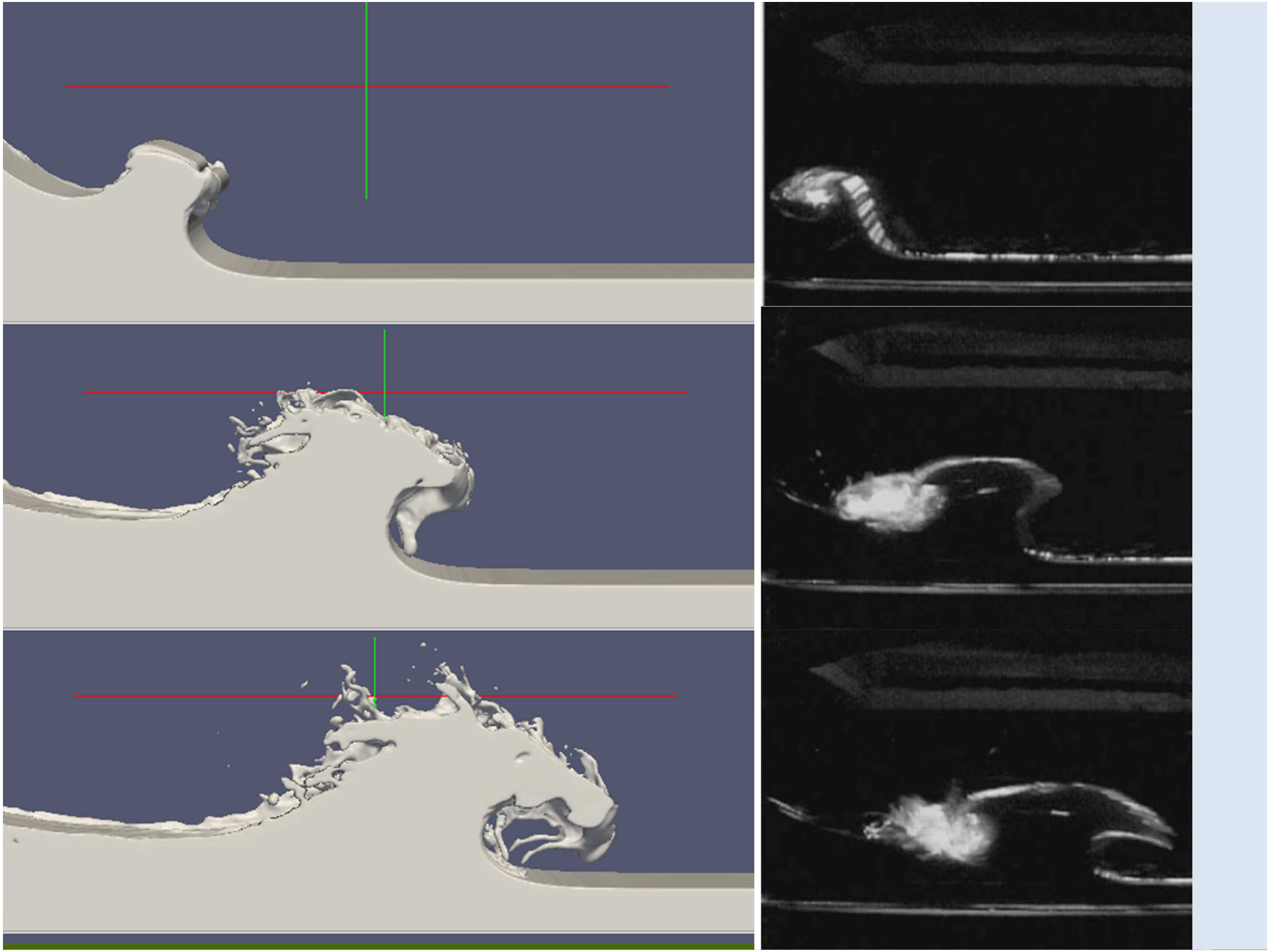
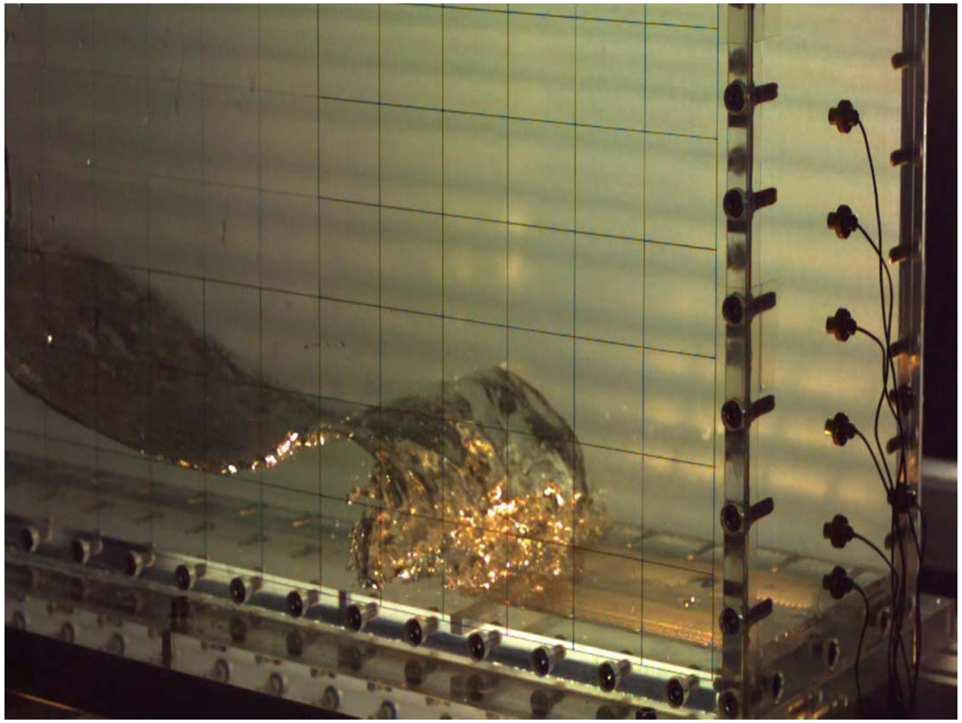


FIGURE 1. Sketch of experimental arrangment: (*a*) side view; (*b*) section showing pulley/weight system.





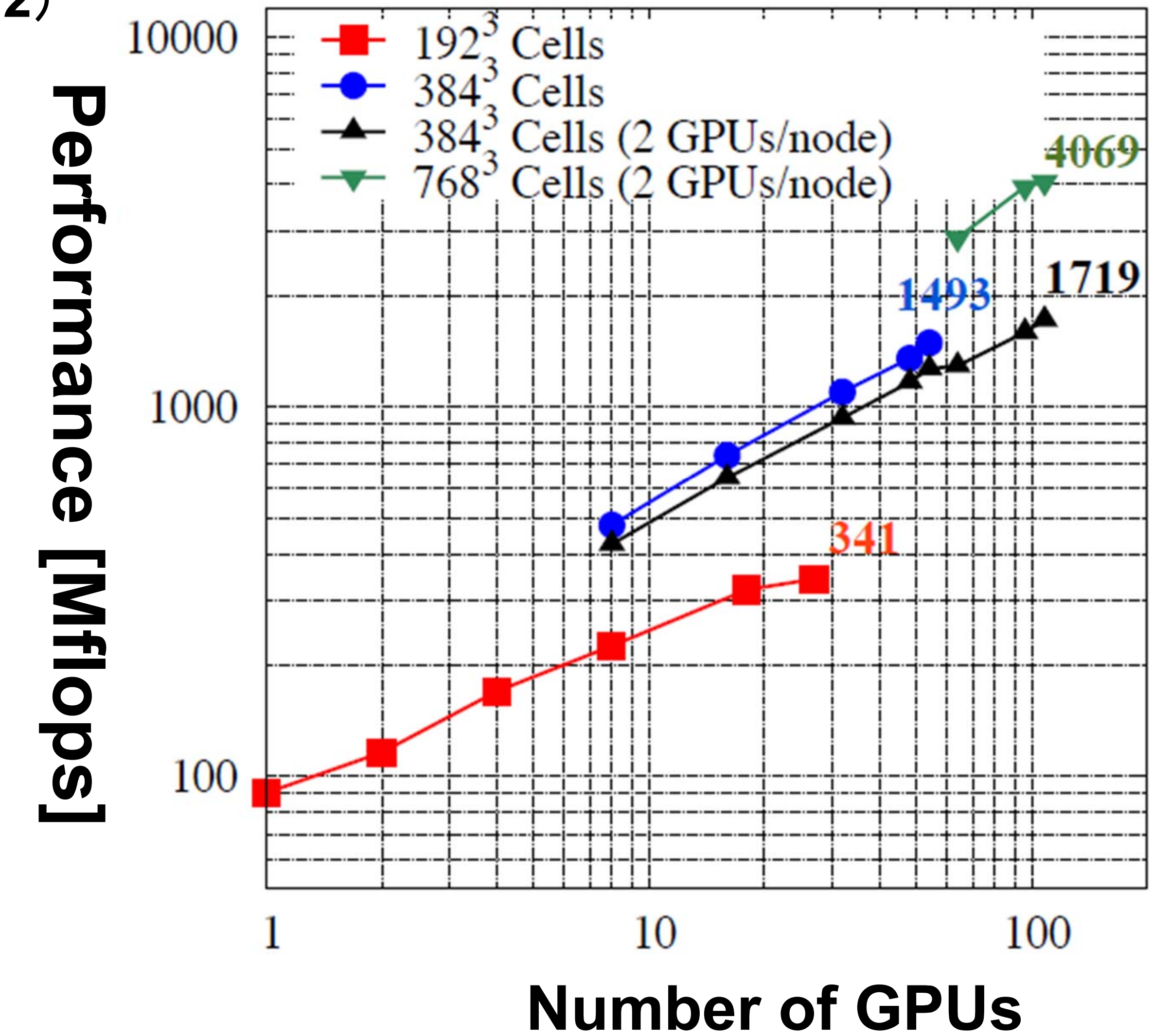
Experiment



Simulation


MULTI-GPU Performance

（TSUBAME 1.2）



Next Generation

Weather Prediction

GP GPU

Collaboration: Japan Meteorological Agency

Meso-scale Atmosphere Model:

Cloud Resolving Non-hydrostatic model

Compressible equation taking consideration of sound waves.

Meso-scale

2000 km ↔ **a few km**

Typhoon

Tornado, Down burst
Heavy Rain

Atmosphere Model

GP GPU

Dynamical Process:

Full 3-D Navior-Stokes Equation

$$\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} = -\frac{1}{\rho} \nabla P - 2\Omega \times \boldsymbol{u} - \Omega \times (\Omega \times \boldsymbol{r}) + \boldsymbol{g} + \boldsymbol{F}$$

Physical Process:

Cloud Physics, Moist, Solar Radiation, Condensation,
Latent heat release, Chemical Process, Boundary Layer

So called “Parameterization” including many empirical rules.

WRF GPU Computing

WRF (Weather Research and Forecast)

Community Code developed by NCAR, NCEP, OU, NOAA/FSL, AFWA

WSM5 (WRF Single Moment 5-tracer) Microphysics*

Represents condensation, precipitation and thermodynamic effects of latent heat release

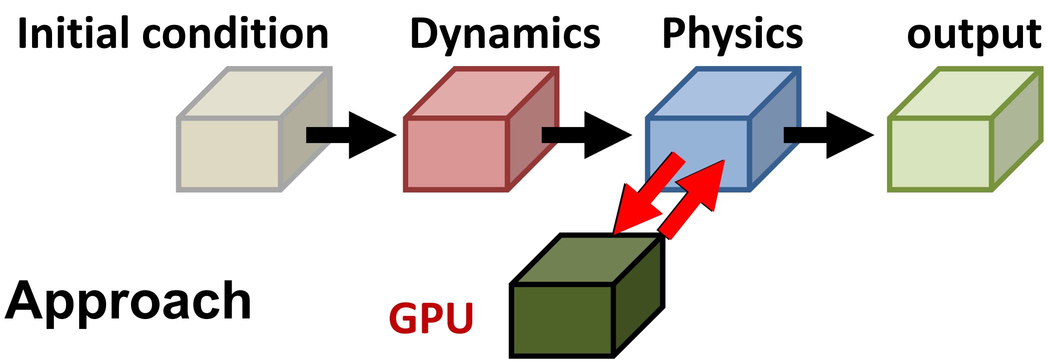
1 % of lines of code, 25 % of elapsed time

⇒ 20 x boost in microphysics (1.2 - 1.3 x overall improvement)

WRF-Chem**

provides the capability to simulate chemistry and aerosols from cloud scales to regional

⇒ x 8.5 increase



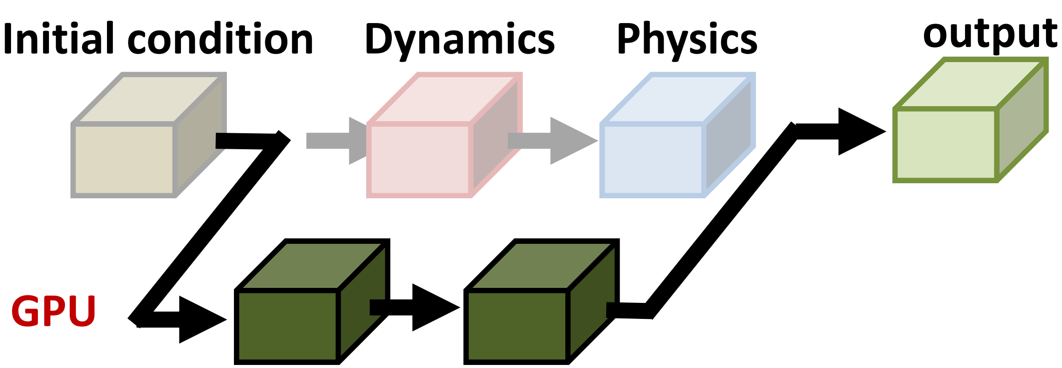
Accelerator Approach

Full GPU Implementation

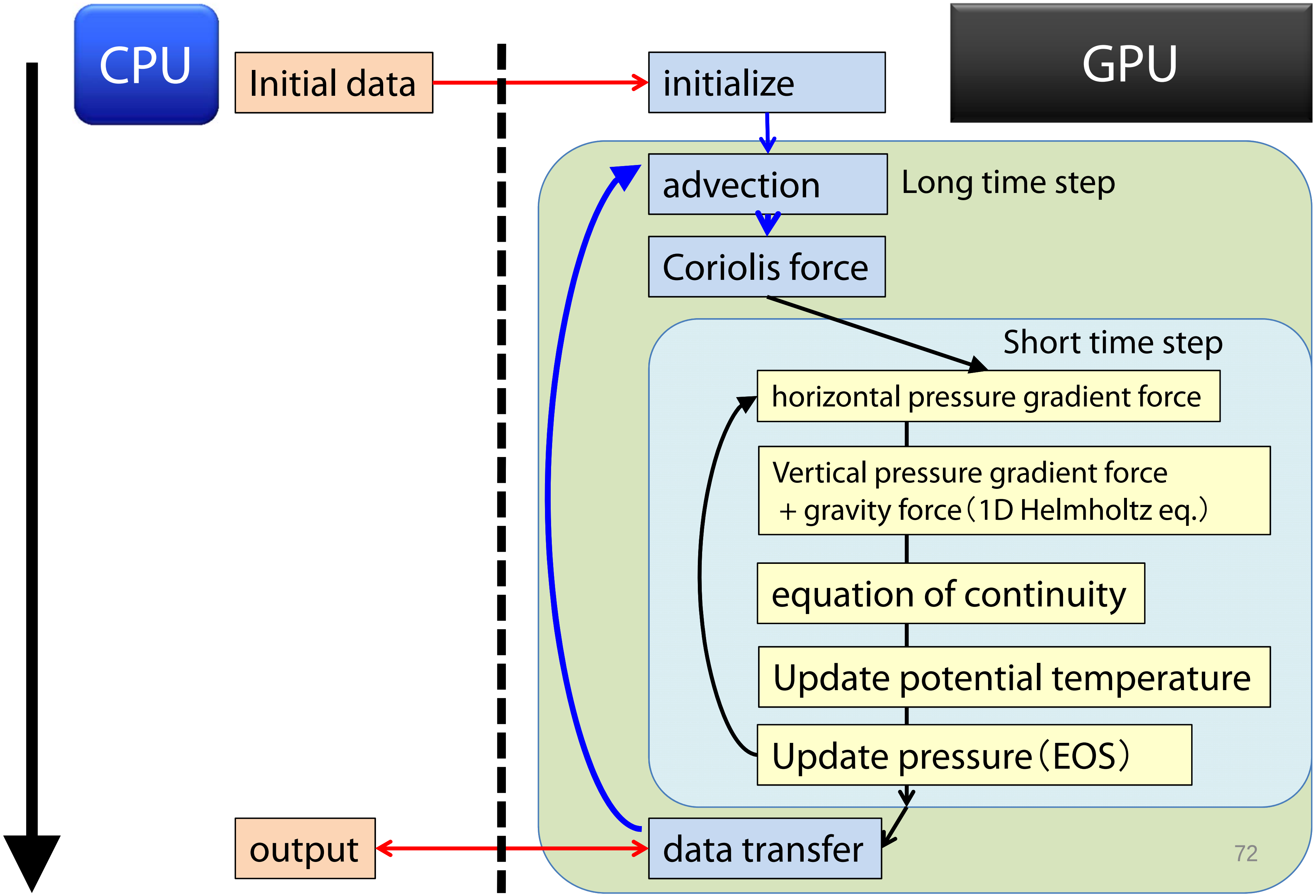
- **ASUCA Production Code**
  - ✓ *A next-generation high resolution weather simulation code that is being developed by Japan Meteorological Agency (JMA)*
  - ✓ *ASUCA succeeds the JMA-NHM as an operational non-hydrostatic regional model at JMA*

- **Similar Structure as WRF**
  - ✓ *HEVI (Horizontally explicit Vertical implicit) scheme*
  - ✓ *Dynamical Core uses a numerical scheme with 3rd-order accuracy in time and space*
    - *Flux-form non-hydrostatic compressible equation*
    - *Generalized coordinate*

Full GPU Approach

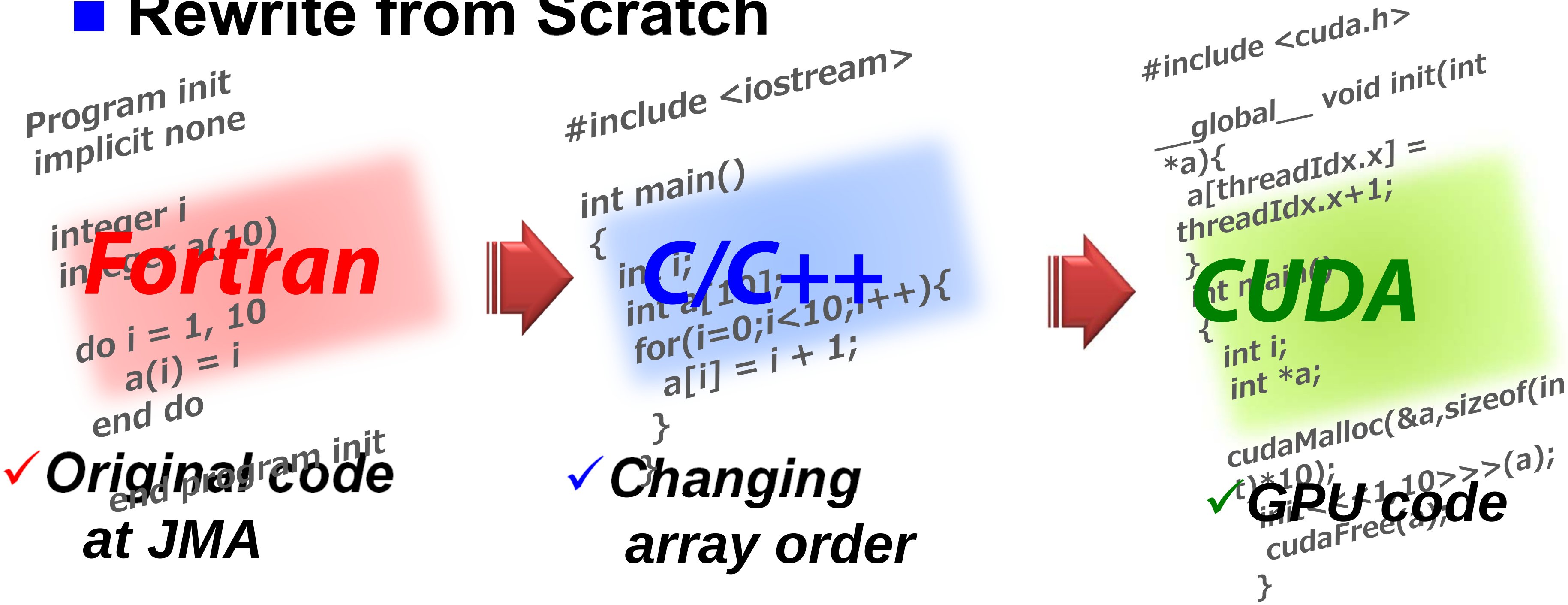


Computatinal Flow of ASUCA



Entire Porting Fortran to CUDA

- **Rewrite from Scratch**

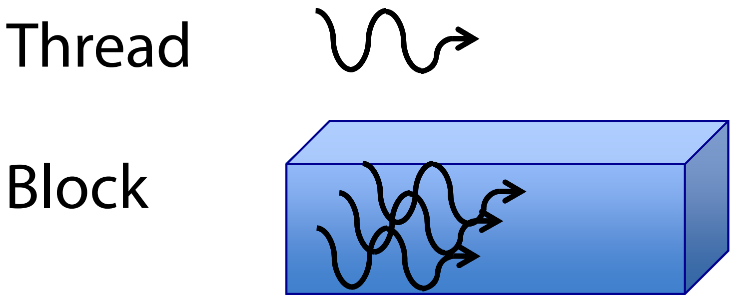


z,x,y (k,i,j)-ordering	x,z,y (i,k,j)-ordering	x,z,y (i,k,j)-ordering

- **1 Year**

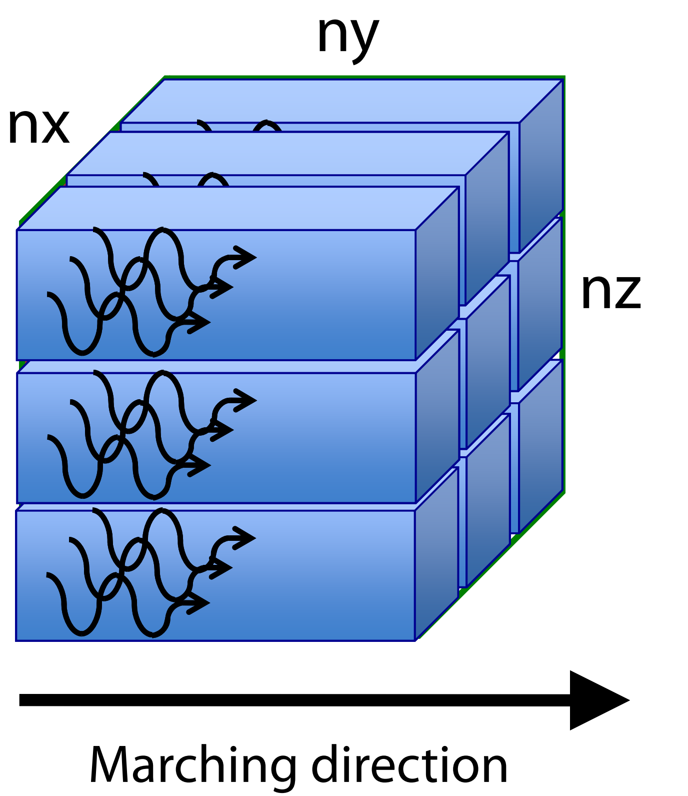
  Introducing many optimizations, overlapping the computation with the communication, kernel fuse, reordering kernel execution

Implementation : Advection



64 x 4 threads (2D) in a block

- Each thread specifies a (x, z) point、marching in y
  - ✓ Improve data transfer performance using domain decomposition



Using Shared Memory

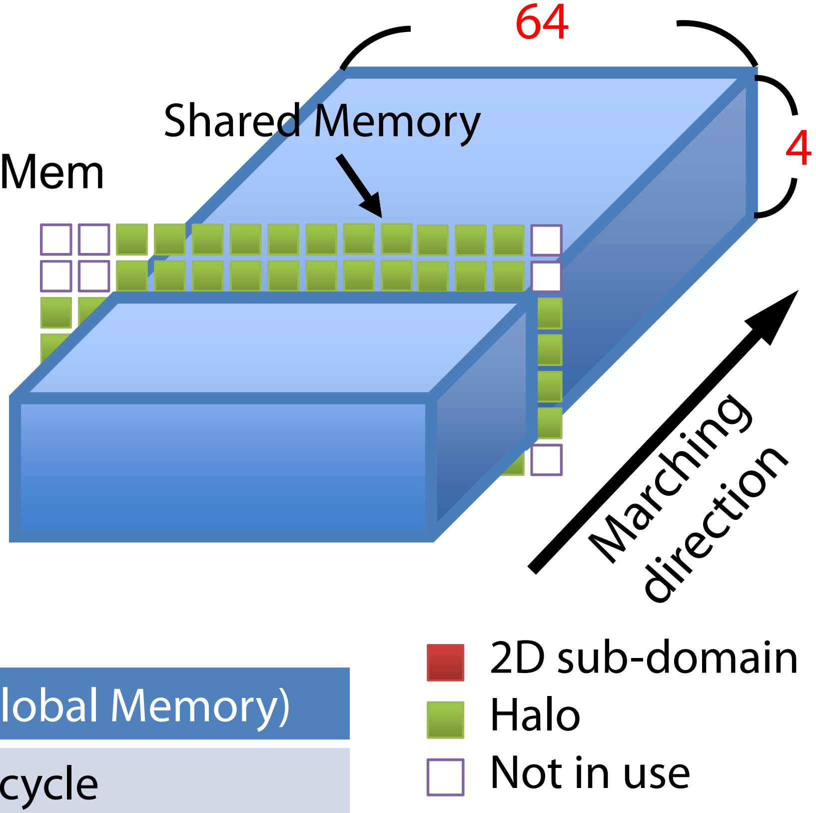
- Shared Memory (SMem) = Software Managed Cache
- Read a 2D sub-domain from VRAM into SMem

1 Block
= 64 x 4 threads

- Advection : 12-point stencil
  - ✓ Store the xz-slice in (64 + 3) x (4 + 3) SMem

Access GMem directly : 4 + 4 read, 1write

Using SMem : ~1 read, 1write

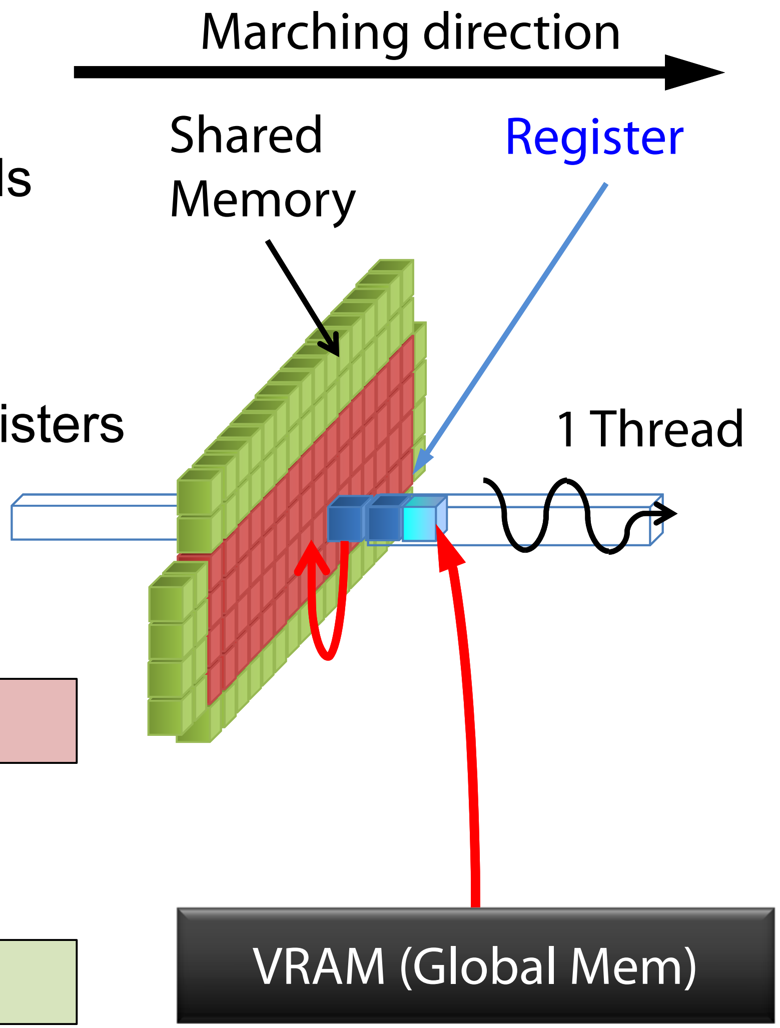


	Shared Memory	VRAM (Global Memory)
Access speed	~ 2 cycle	400-600 cycle
Capacity	16 kByte/Block	2 GByte (Total)

Using Registers in marching direction

- Register
  - ✓ Access speed : 1 cycle
  - ✓ used for data not shared among threads

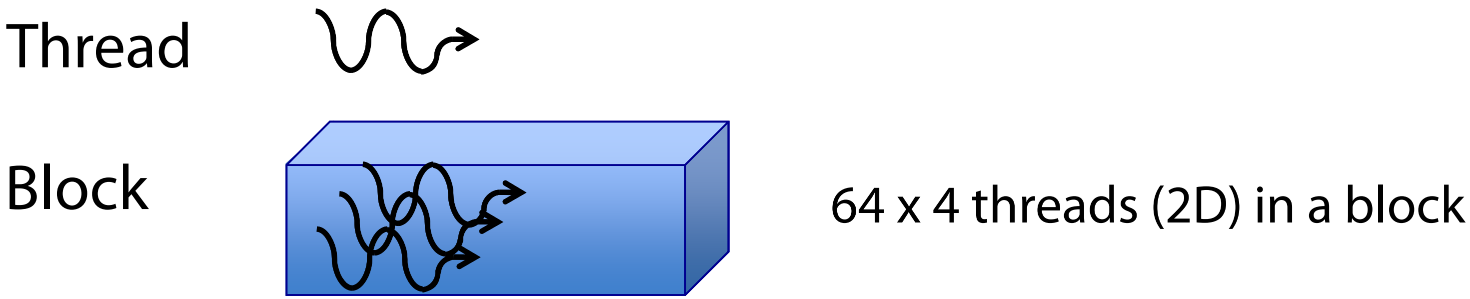
- Advection : 12-point stencil
  - ✓ Each thread keeps 4 y-elements in registers
  - ✓ Elements are reuse



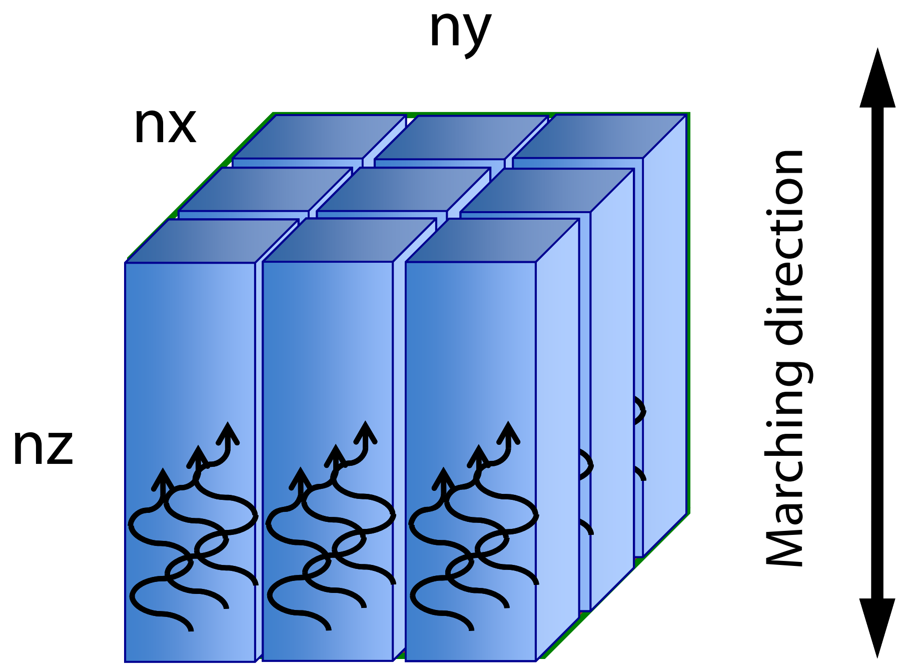
Access GMem directly : 4 + 4 + 4 read, 1write

Using SMem and Registers : ~1 read, 1write

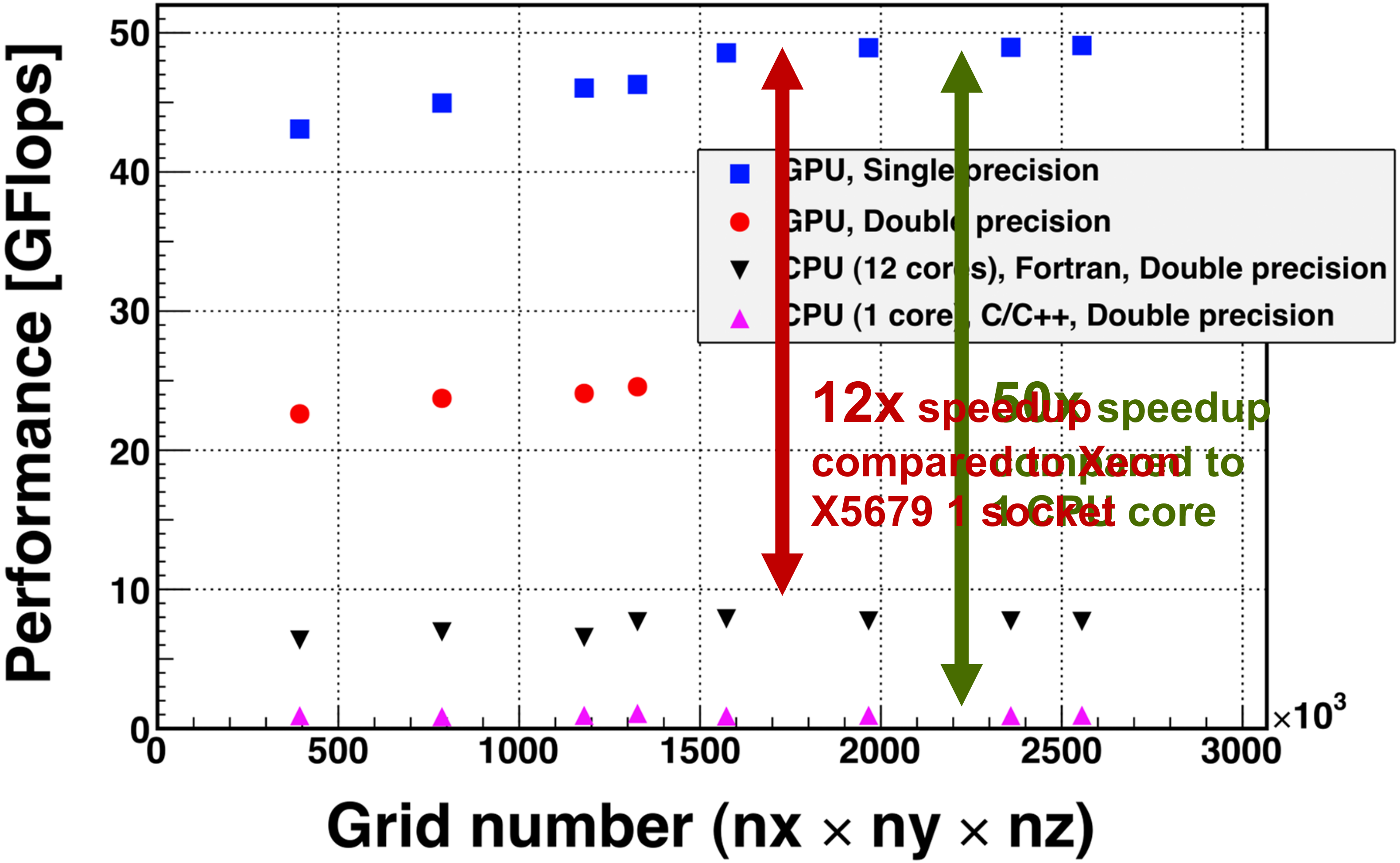
Implementation : 1D Helmholtz equation



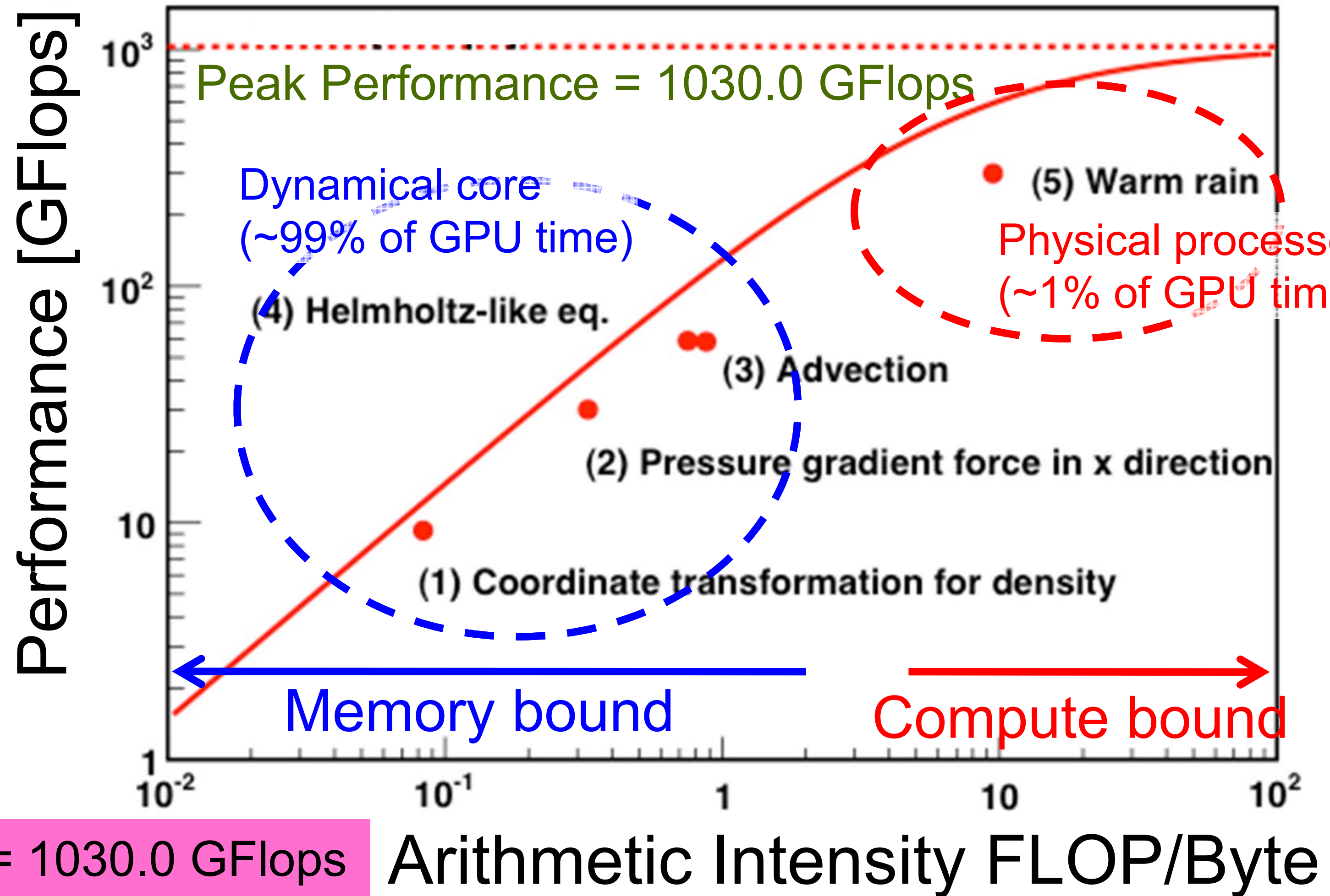
- 1D Helmholtz equation
  - ✓ Element in k depends on elements in k+/- 1
  - ⇒ marching in z direction



TSUBAME 2.0 (1 GPU)

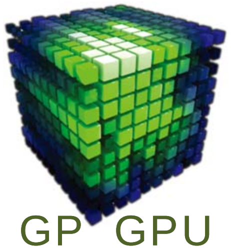


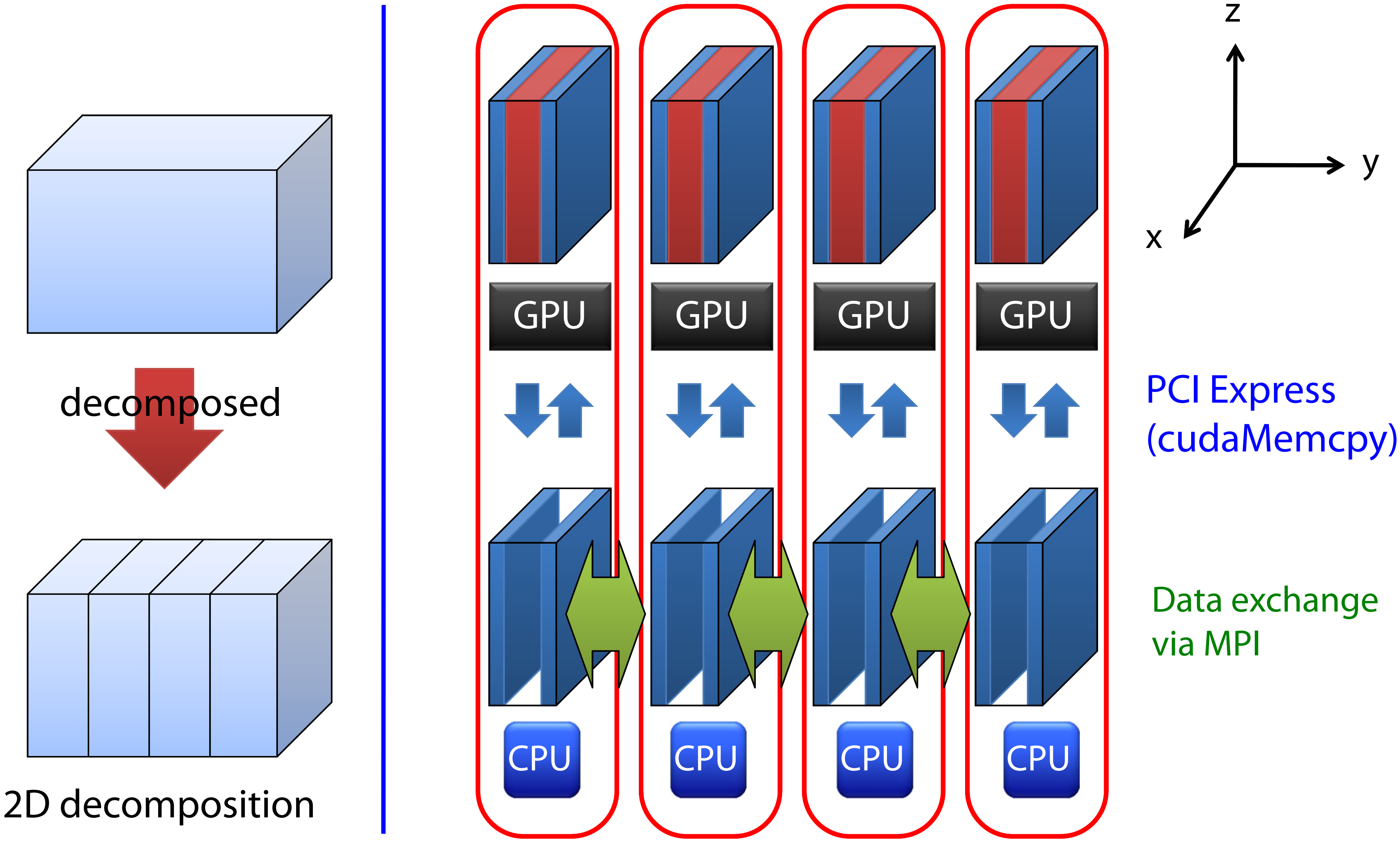
Performance of 5 kernels

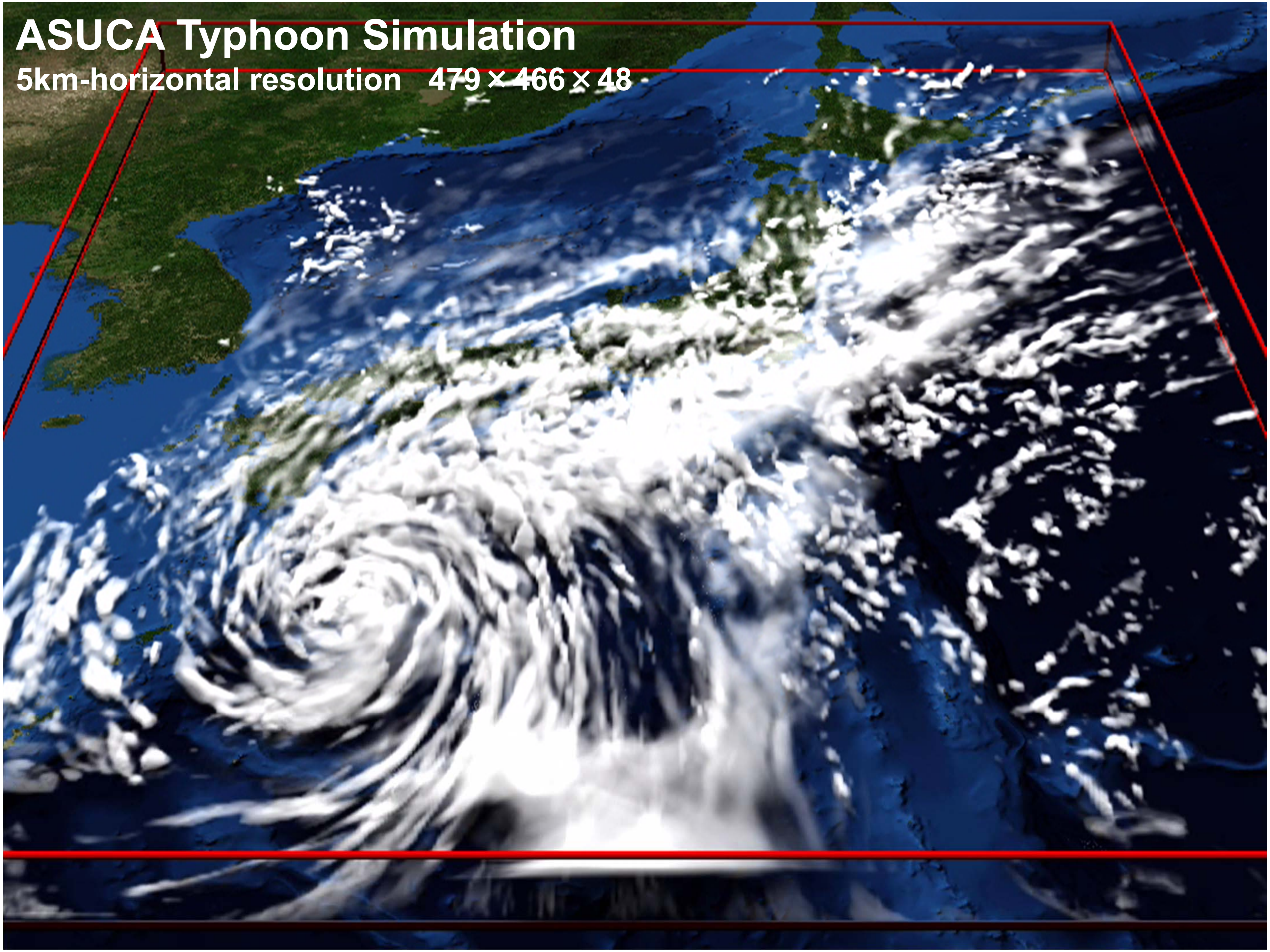


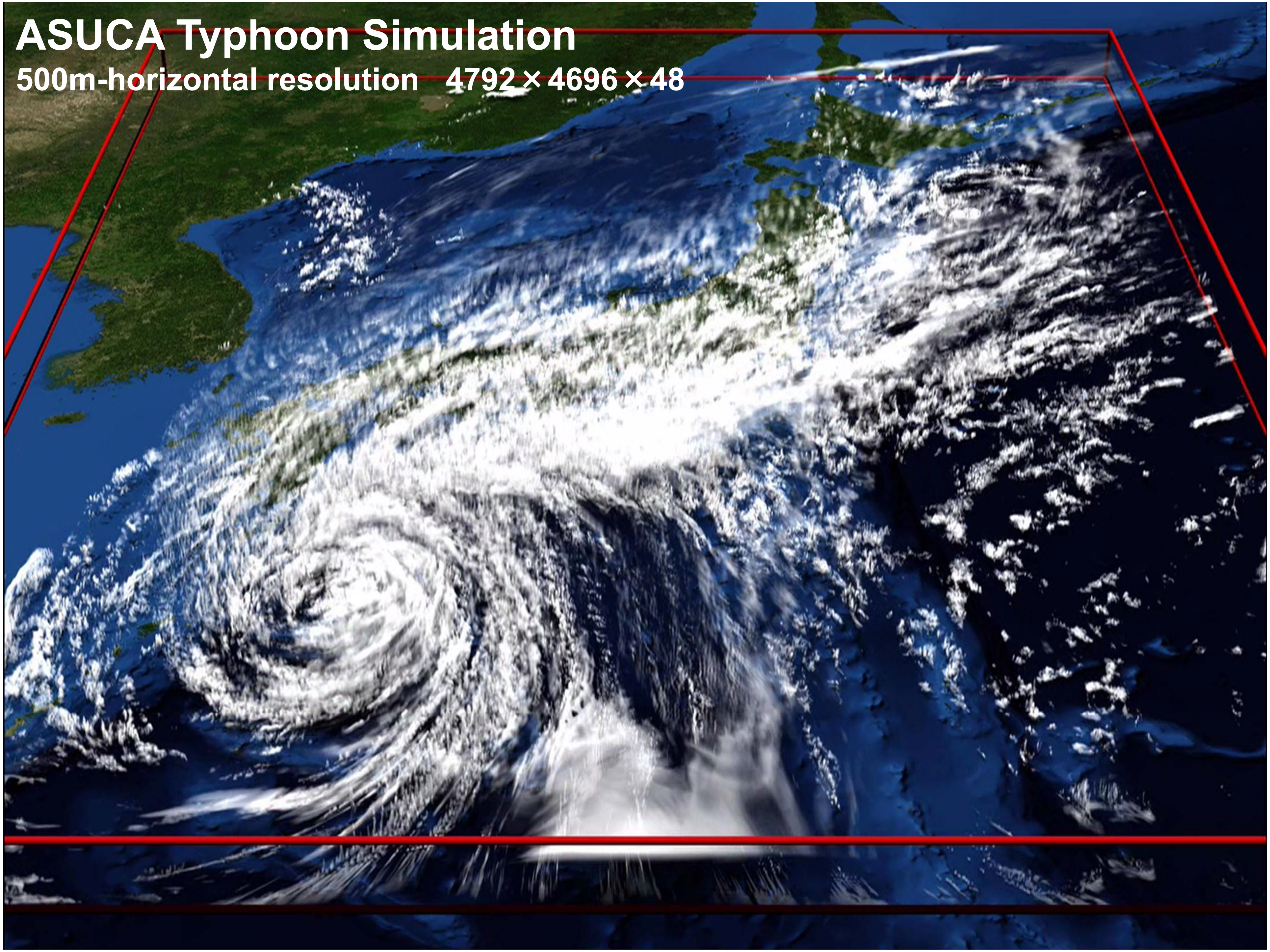
F_{peak} = 1030.0 GFlops
B_{peak} = 148.0 GByte/s

Multi-GPU : Domain decomposition

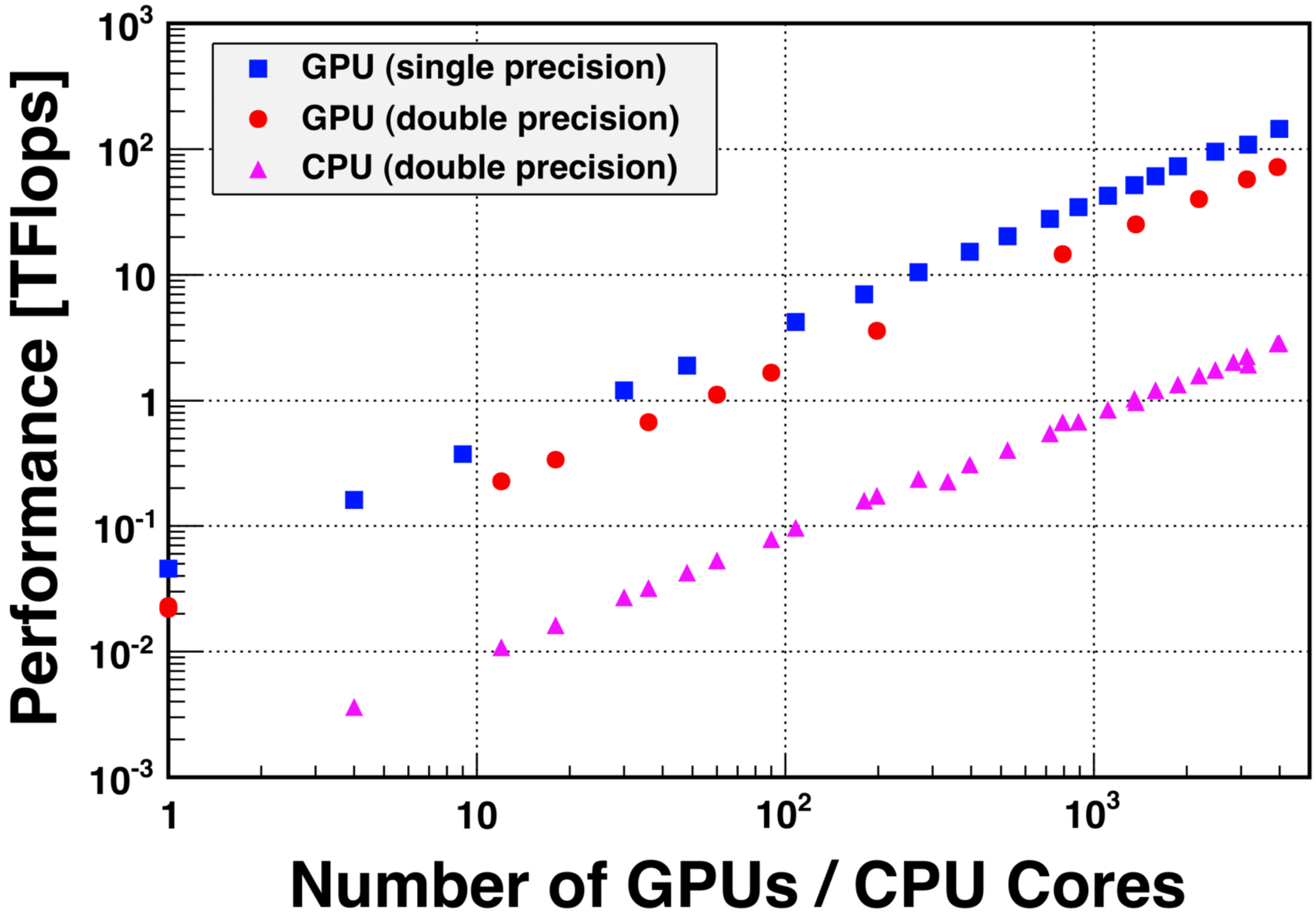





ASUCA Typhoon Simulation
5km-horizontal resolution 479×466×48


ASUCA Typhoon Simulation
500m-horizontal resolution 4792×4696×48

TSUBAME 2.0 Weak Scaling



145.0 Tflops
Single precision

76.1 Tflops
Doublele precision

Fermi core Tesla M2050

3990 GPU

SUMMARY

GP GPU

FEATURES of GPU

High Performance and Low Power

- **Major differences from Previous Accelerators**

  ClearSpeed, Grape, , ,

High Memory Bandwidth

suitable for wide variety of applications

Consumer Product

inexpensive

Software Development Environment

CUDA, Open CL