Large-scale CFD Applications (Weather Prediction) on TSUBAME 2

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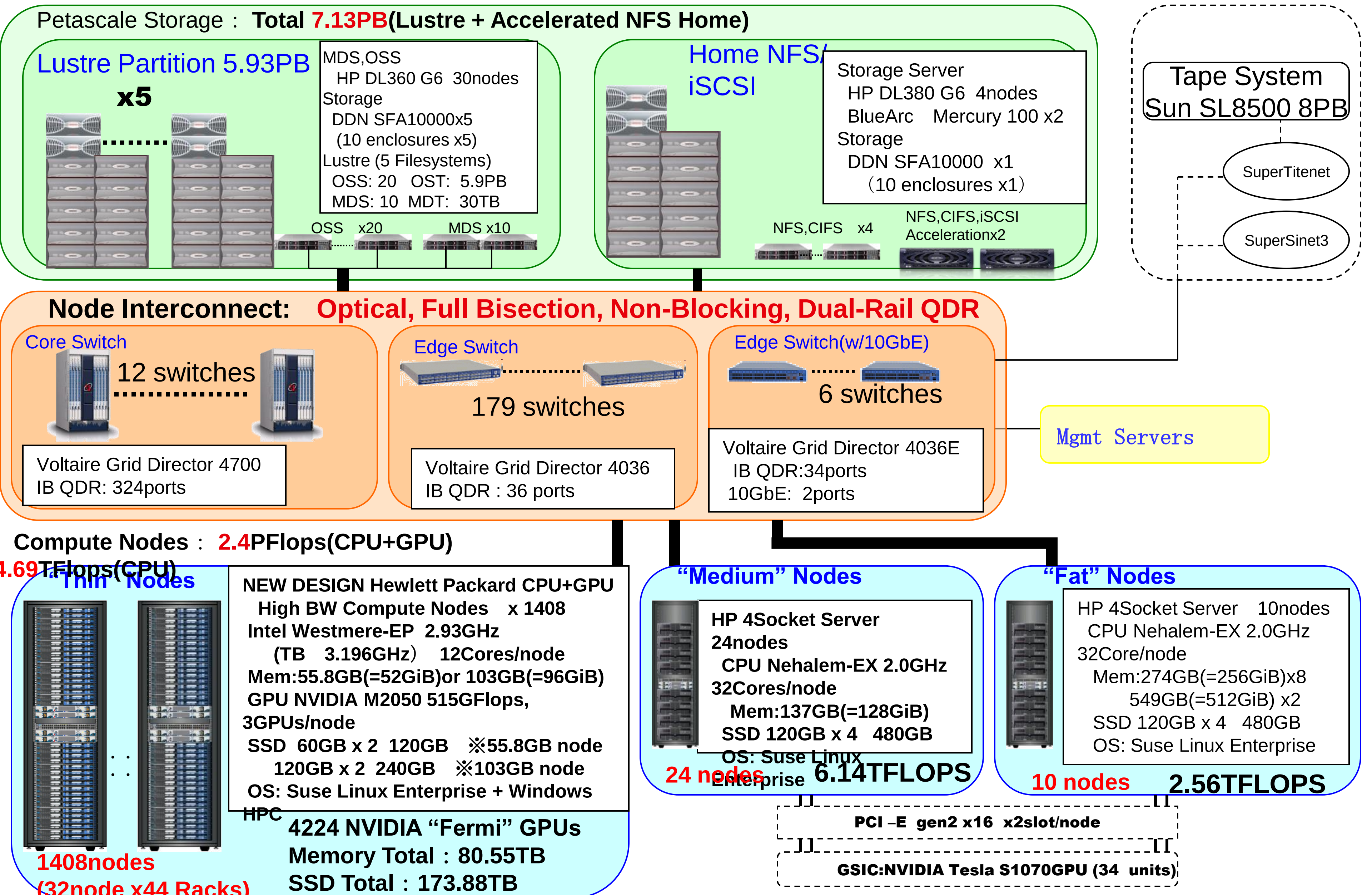
Tokyo Institute of Technology

Supercomputer in the world

2010 November

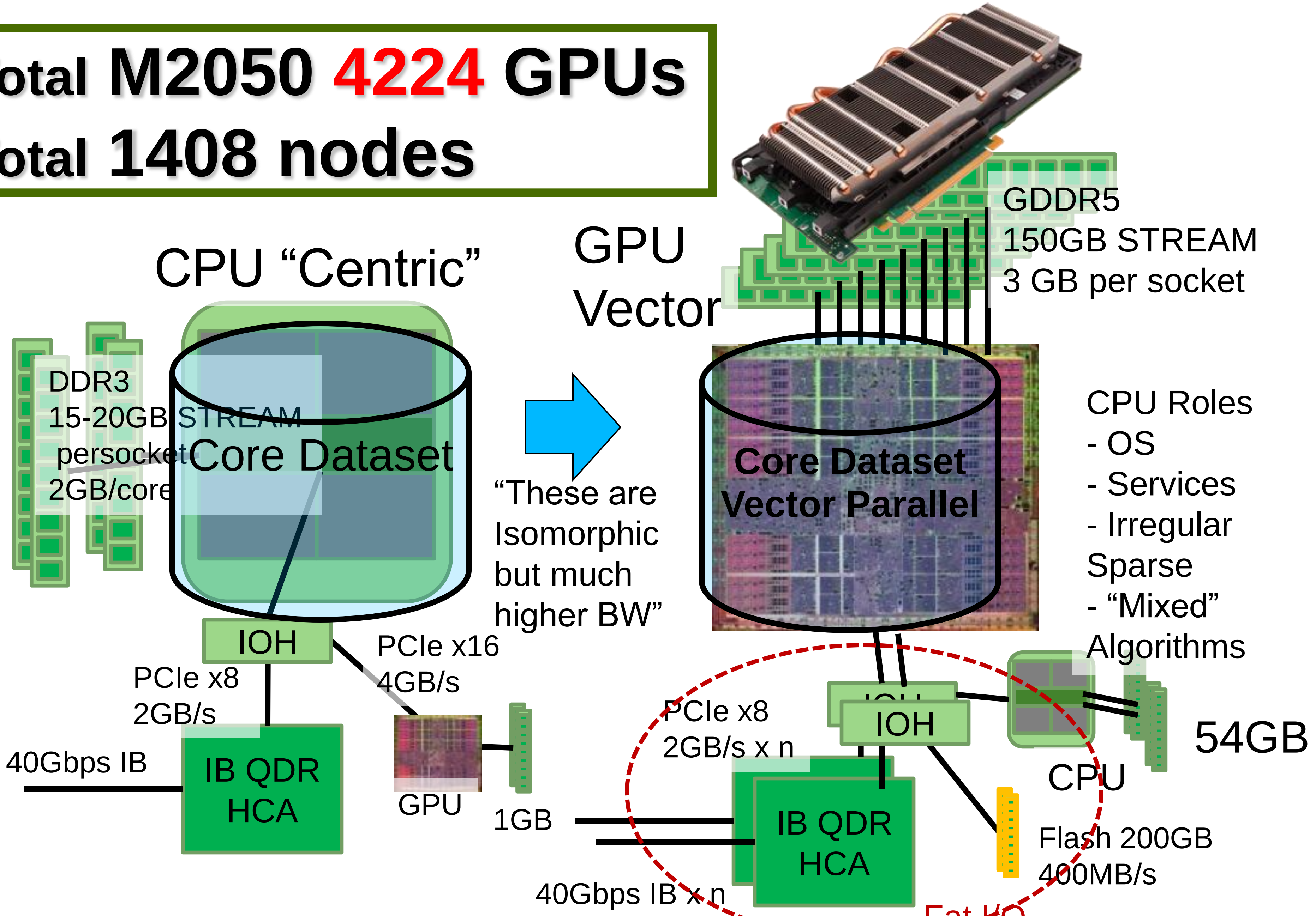
Rank	Site	Computer/Year Vendor	Cores	R_{max}	R_{peak}	Power
1	National Supercomputing Center in Tianjin China	Tianhe-1A - NUDT YH Cluster, X5670 2.93Ghz 6C, NVIDIA GPU, FT-1000 8C / 2010 NUDT	186368	2566.00	4701.00	4040.00
2	DOE/SC/Oak Ridge National Laboratory United States	Jaguar - Cray XT5-HE Opteron 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

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



TSUBAME 2.0: GPU Centric Nodes

Total M2050 4224 GPUs
Total 1408 nodes



GPU Applications
of our group

- Higher-order Compressible Flow
- Lattice Boltzmann for Pulmonary Airflow
- FDTD for Electromagnetic wave Propagation
- Large-Eddy Simulation for Turbulence Flow
- Real-time TSUNAMI Simulation
- Dendrite Solidification based on Phase Field Model
- Numerical Weather Prediction
- Two-Phase Flow Simulations

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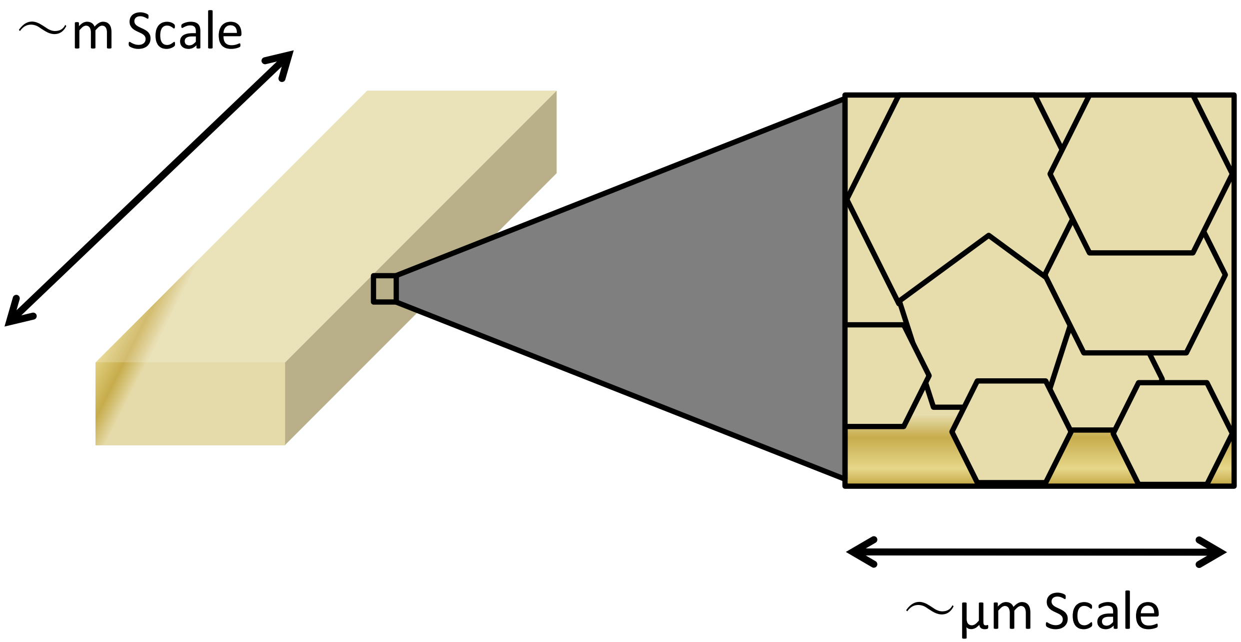
Material Compound



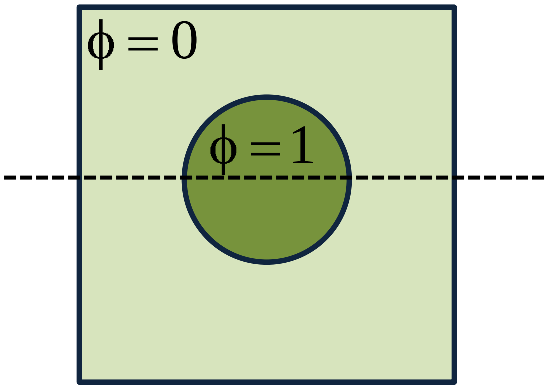
Meso-scale Analysis for Solidification Process

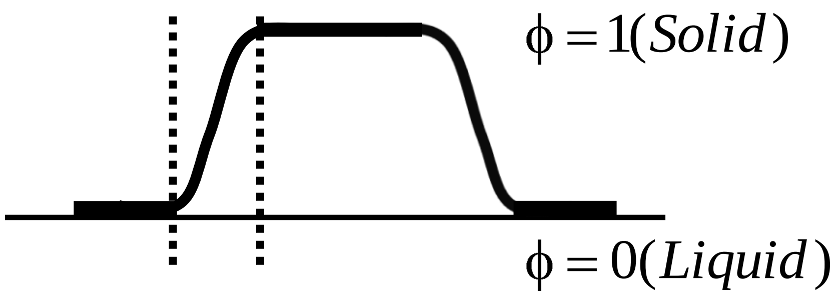
Phase Field Model

- Non-equilibrium Statistical Physics
- Phase Field Model ϕ
  - Introduction of index function

$\phi = 0$	$\phi = 1$
liquid	solid

  - diffusive surface
  - stabilization of surface energy





- High computational cost of non-linear term

Phase Field Equation

Allen-Cahn Equation

$$\frac{\partial \phi}{\partial t} = M\left[\frac{\partial}{\partial x}\left(\varepsilon^2\frac{\partial \phi}{\partial x} + \varepsilon\frac{\partial \varepsilon}{\partial \phi_x}|\nabla\phi|^2\right) + \frac{\partial}{\partial y}\left(\varepsilon^2\frac{\partial \phi}{\partial y} + \varepsilon\frac{\partial \varepsilon}{\partial \phi_y}|\nabla\phi|^2\right) + \frac{\partial}{\partial z}\left(\varepsilon^2\frac{\partial \phi}{\partial z} + \varepsilon\frac{\partial \varepsilon}{\partial \phi_z}|\nabla\phi|^2\right) + 4W\phi(1-\phi)\left\{\phi - \frac{1}{2} + \beta + a\chi\right\}\right]$$

$$\beta = -\frac{15L}{2W}\frac{T-T_m}{T_m}\phi(1-\phi) \qquad \varepsilon = \bar{\varepsilon}\left(1 - 3\gamma + 4\gamma\frac{\phi_x{}^4 + \phi_y{}^4 + \phi_z{}^4}{|\nabla\phi|^4}\right)$$

↑ Introduction of non-isotropic surface energy

Thermal Conduction

$$\frac{\partial T}{\partial t} = k\nabla^2 T + \frac{L}{C}30\phi^2(1-\phi)^2\frac{\partial \phi}{\partial t}$$

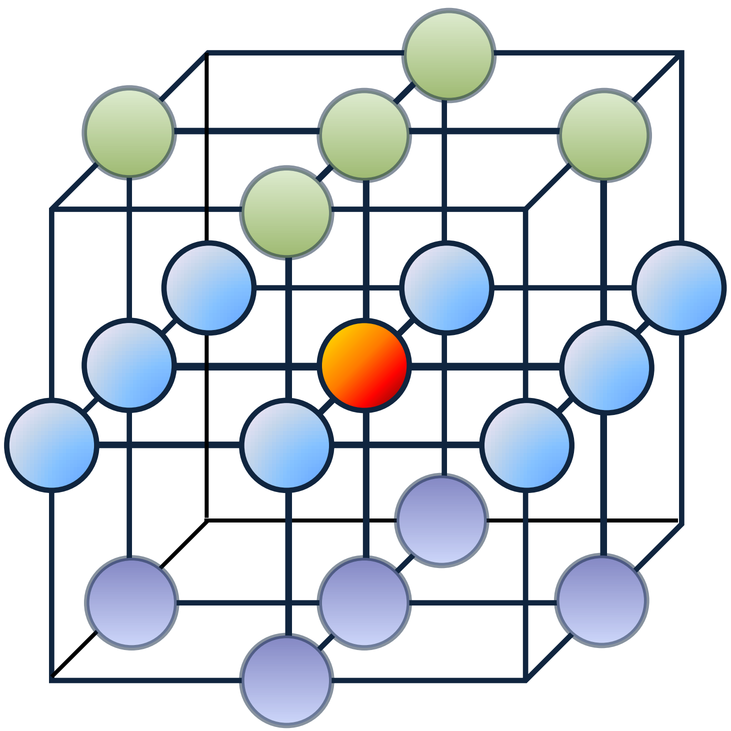
Phase Field $0 < \phi < 1$
Liquid $\phi = 0$
Solid $\phi = 1$

Second-order Finite Difference Method and 1st-order Euler Time Integration

Numerical Stencil Access

Phase Field ϕ

19 points to solve $\phi_{i,j,k}$



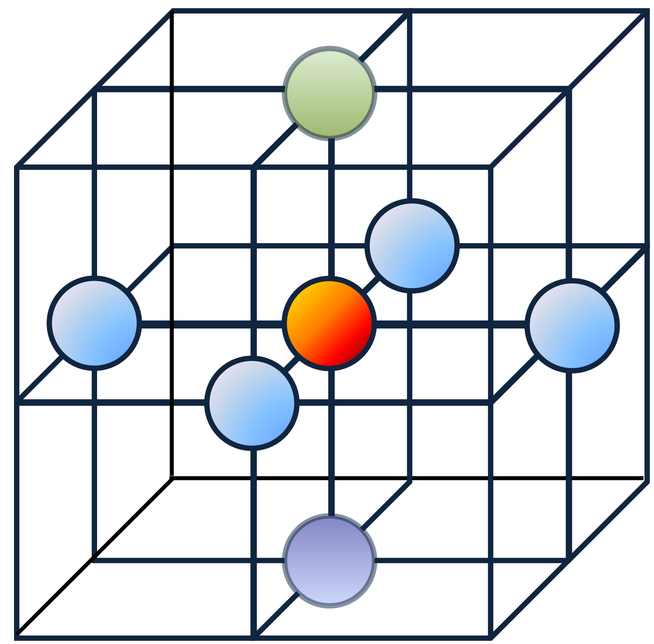
$z = k - 1$

$z = k$

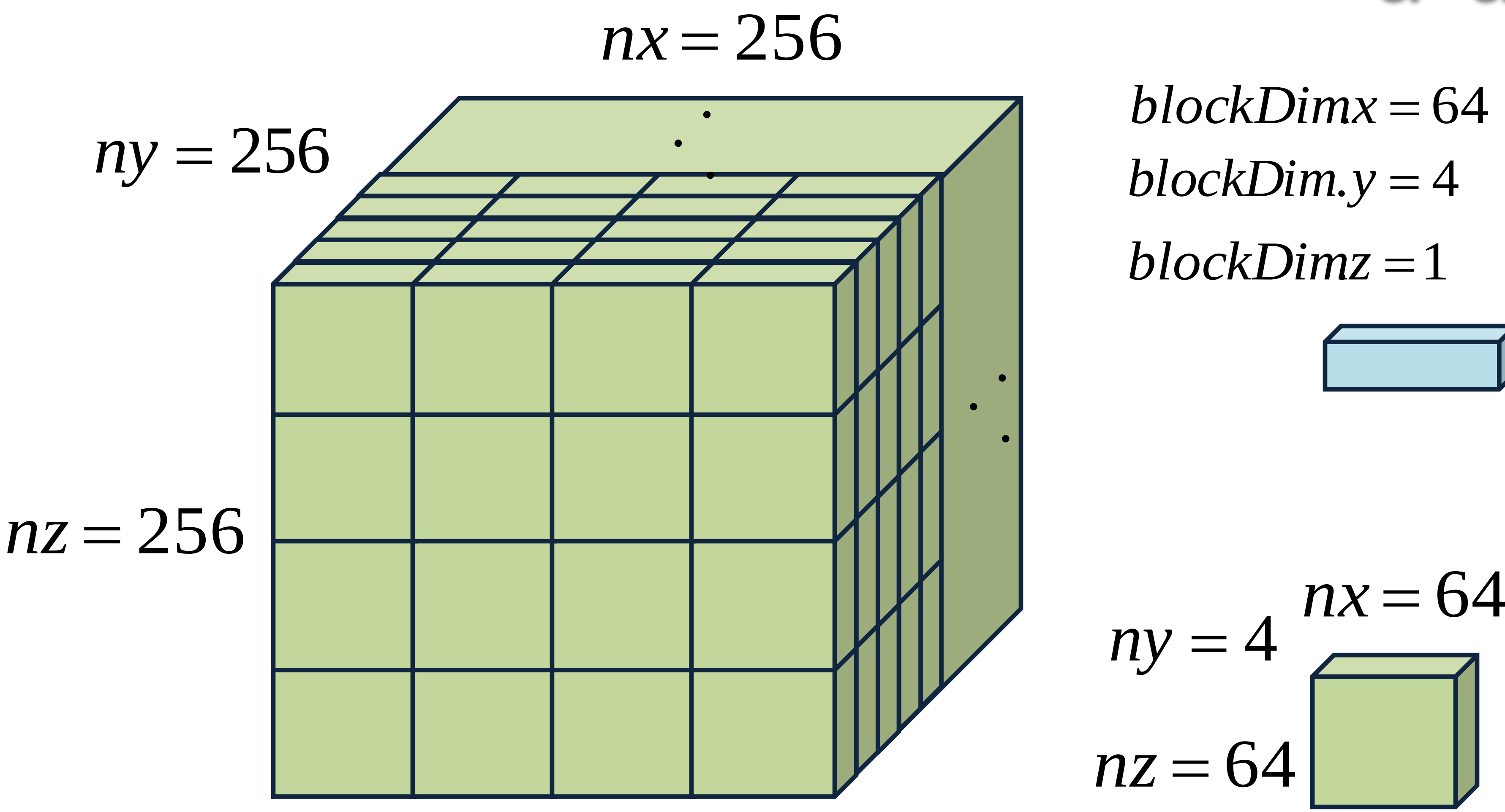
$z = k - 1$

Temperature T

7 points to solve $T_{i,j,k}$

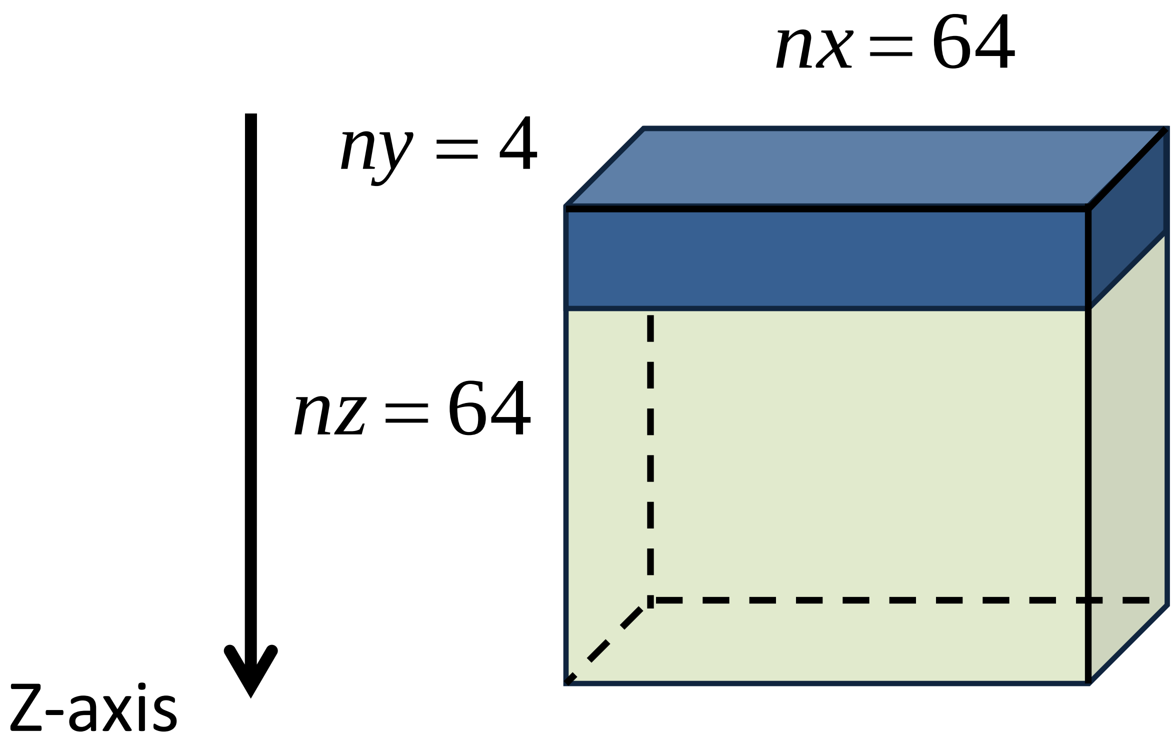


Thread Assignment



64 threads in the x-direction for Coalaesed memory access

Sweep of 1 thread in a block



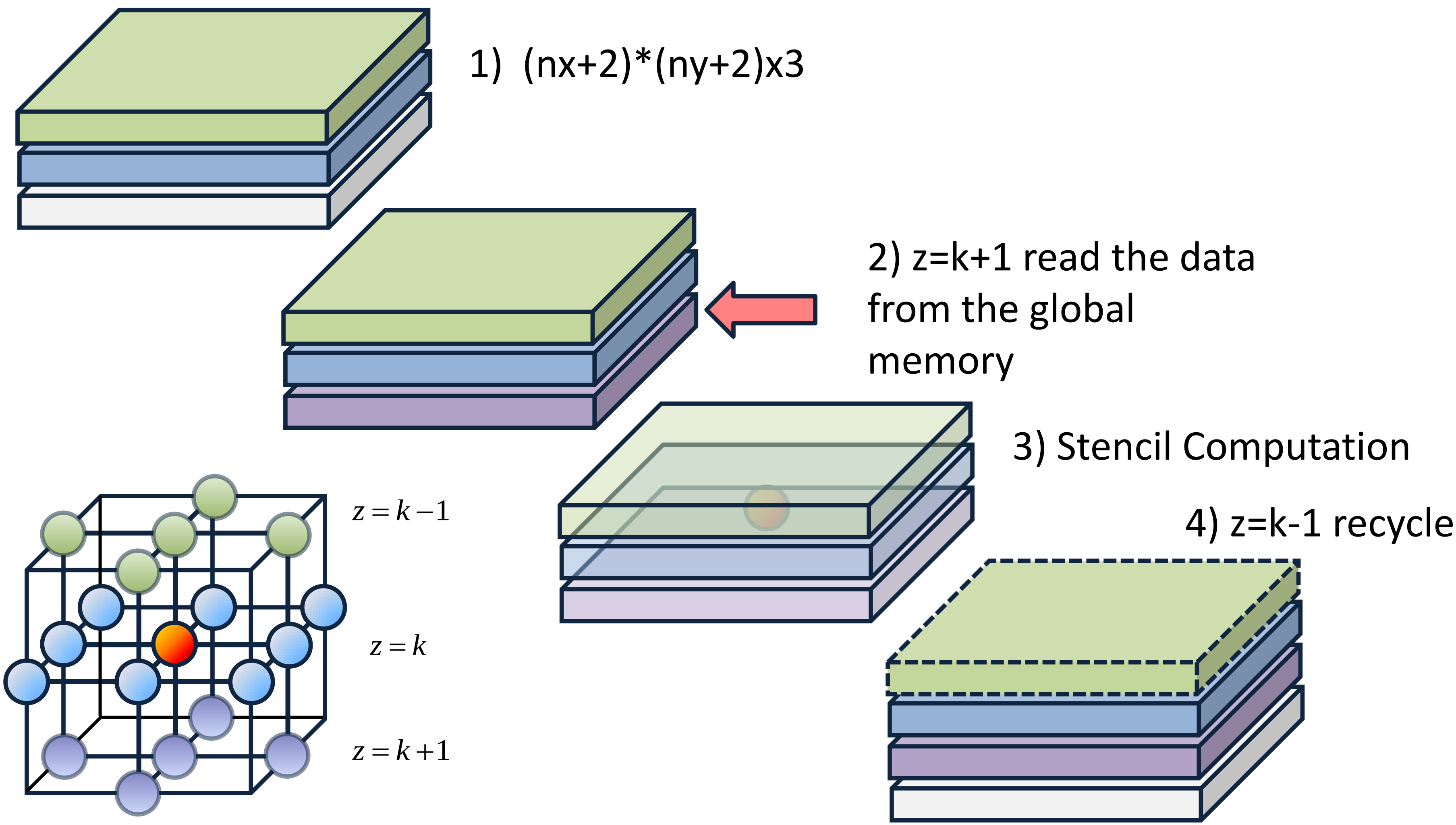
$$threadDim.x = 64$$

$$threadDim.y = 4$$

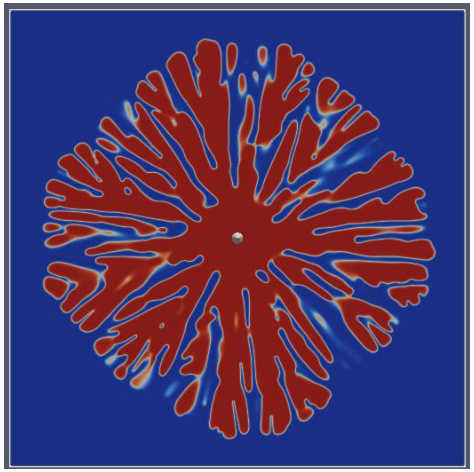
$$threadDim.z = 1$$

Marching in the z-directional direction

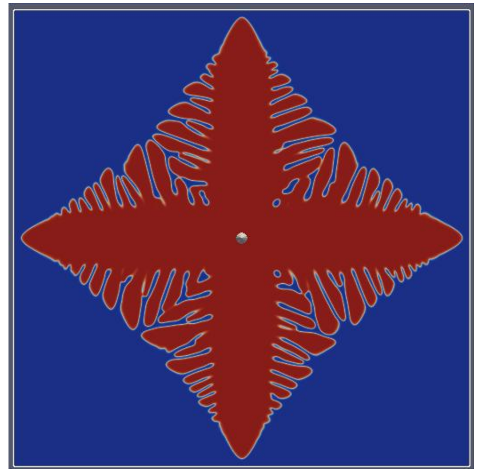
Recycle of Shared Memory



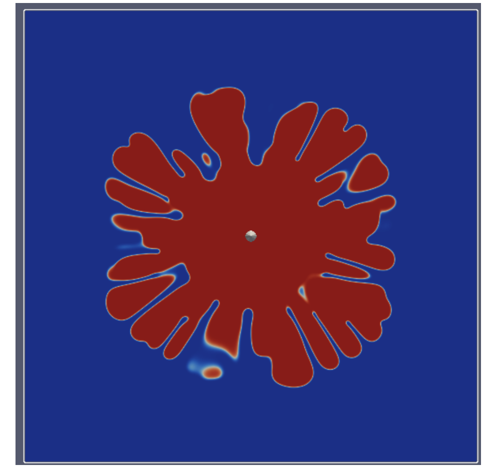
Dependence on Parameters



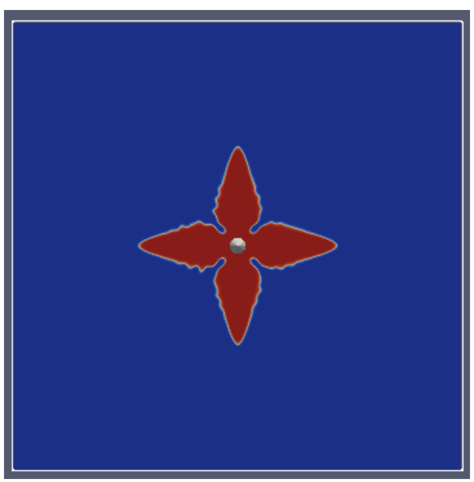
γ = 0.015, A=0.01



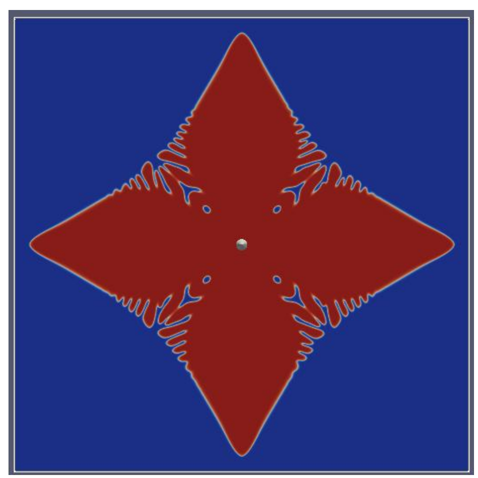
γ = 0.075, A=0.01



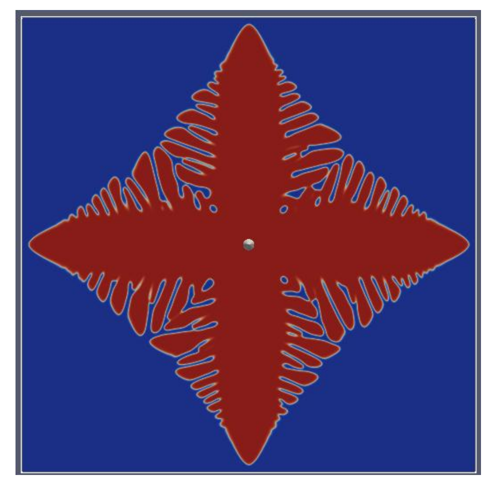
γ = 0.015, A=0.01, Δt=half



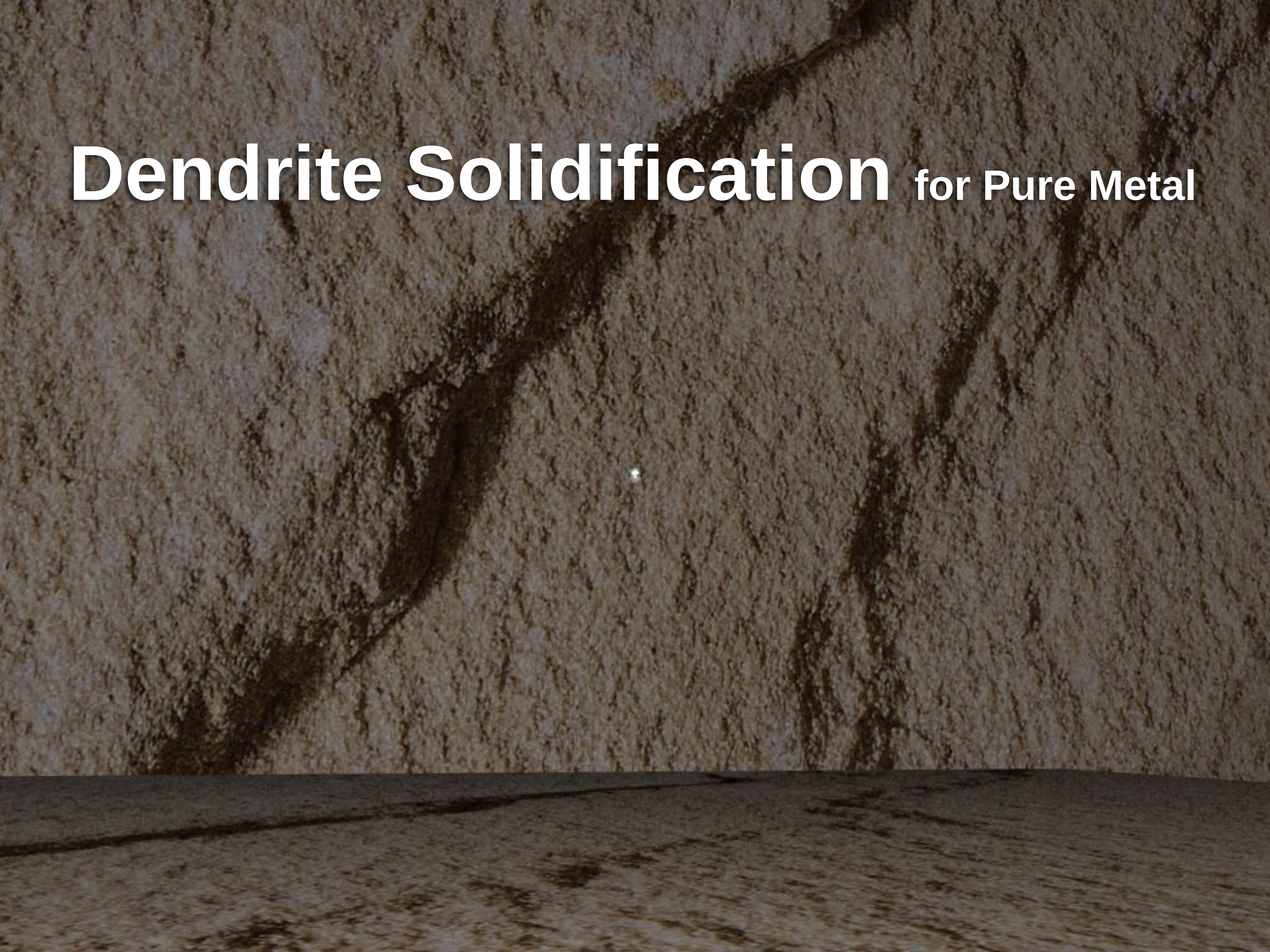
γ = 0.1, A=0.01



γ = 0.075, A=0.01

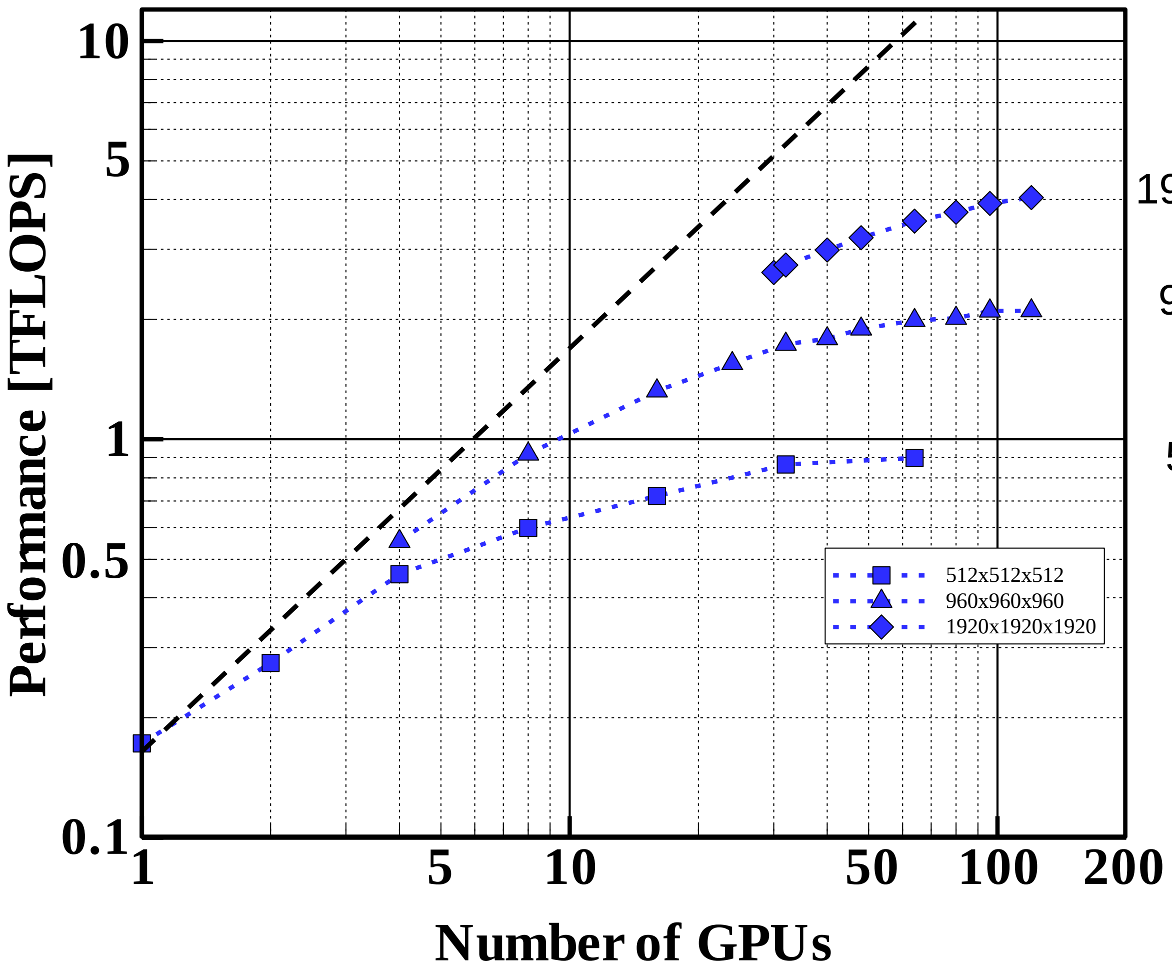


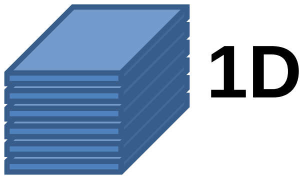
γ = 0.075, A=0.005


Dendrite Solidification for Pure Metal

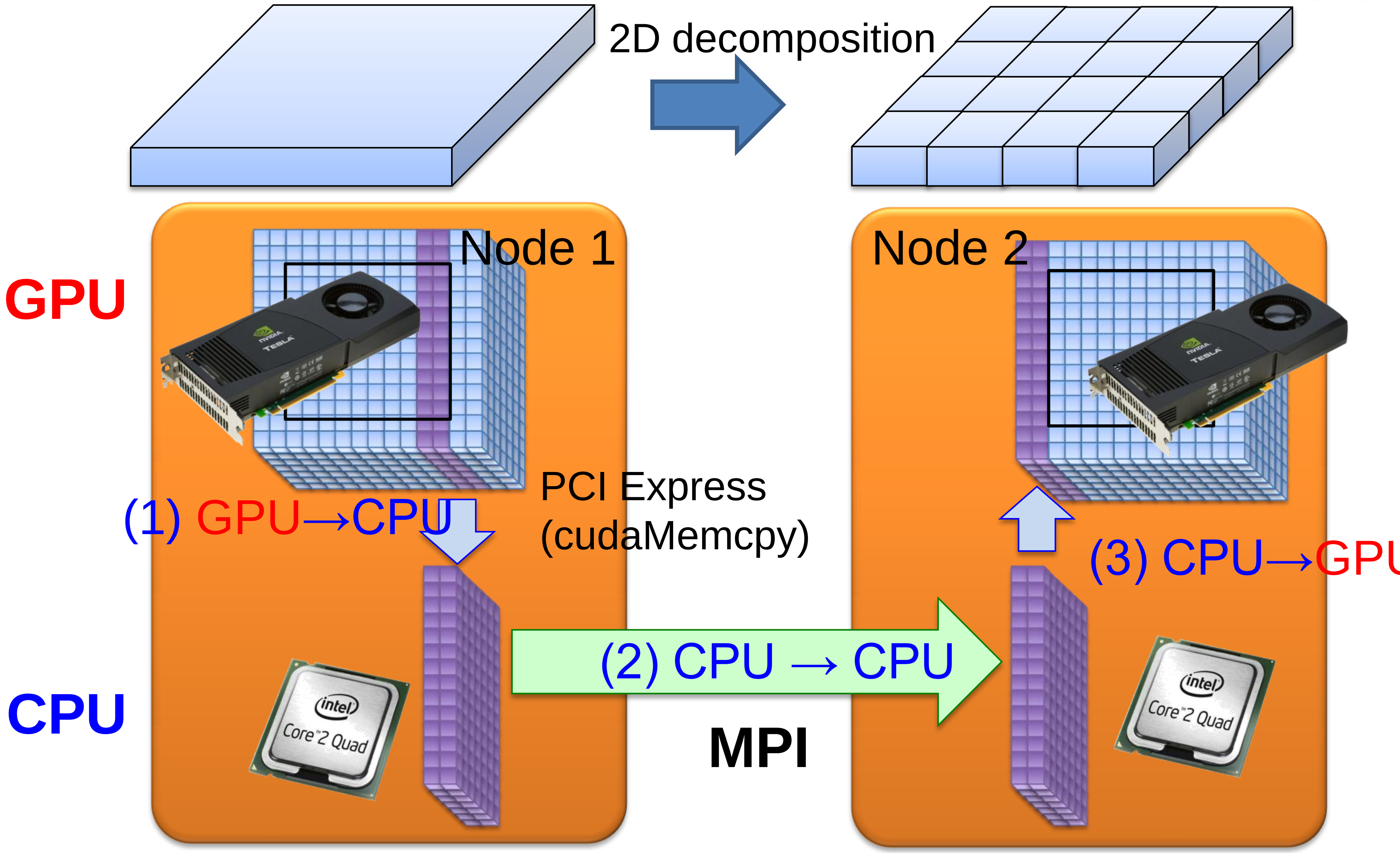
Multi-GPU Peformance

w/o overlapping

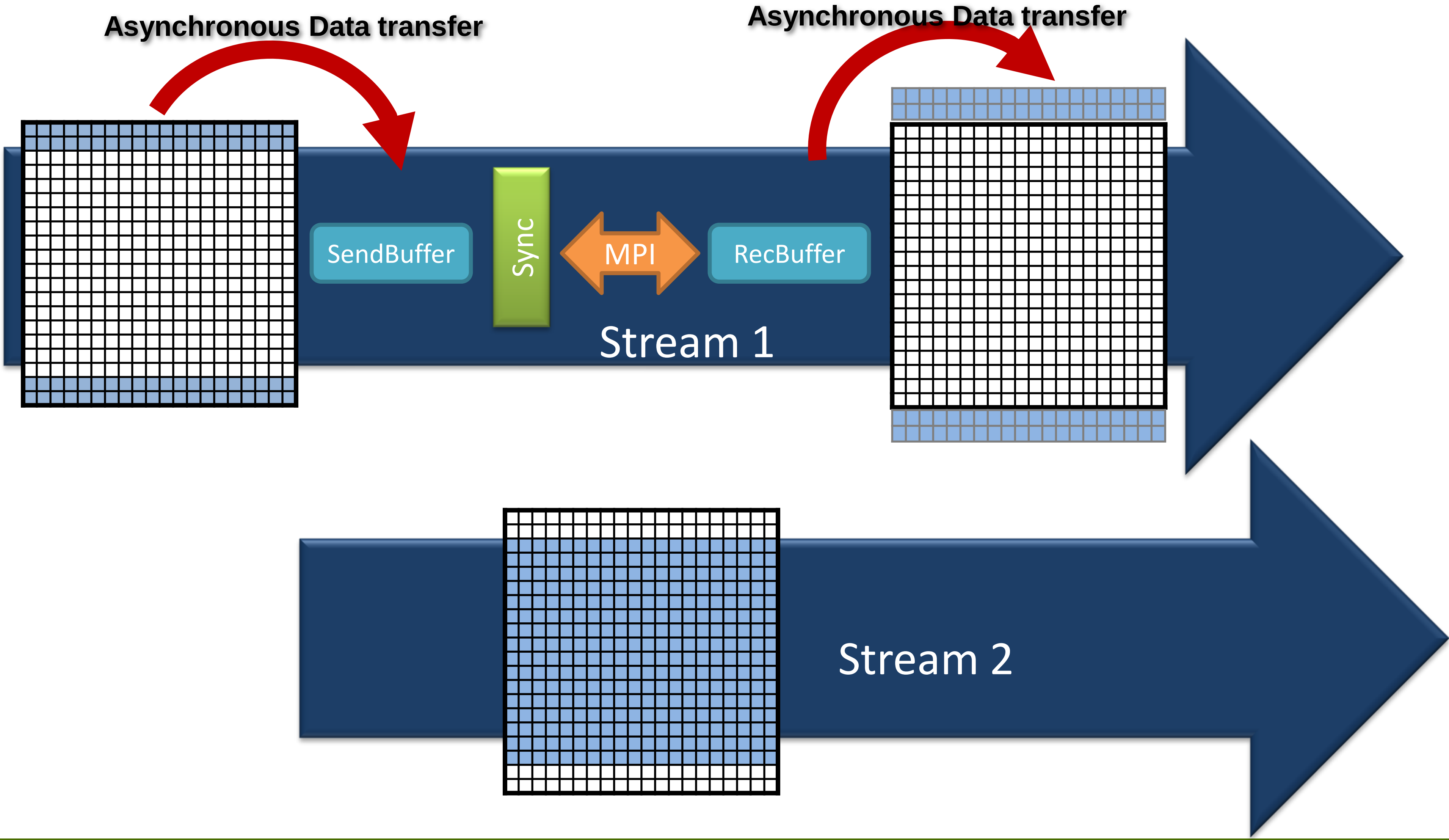




Multi-GPU : Domain decomposition



Overlapping between Computation and Communication

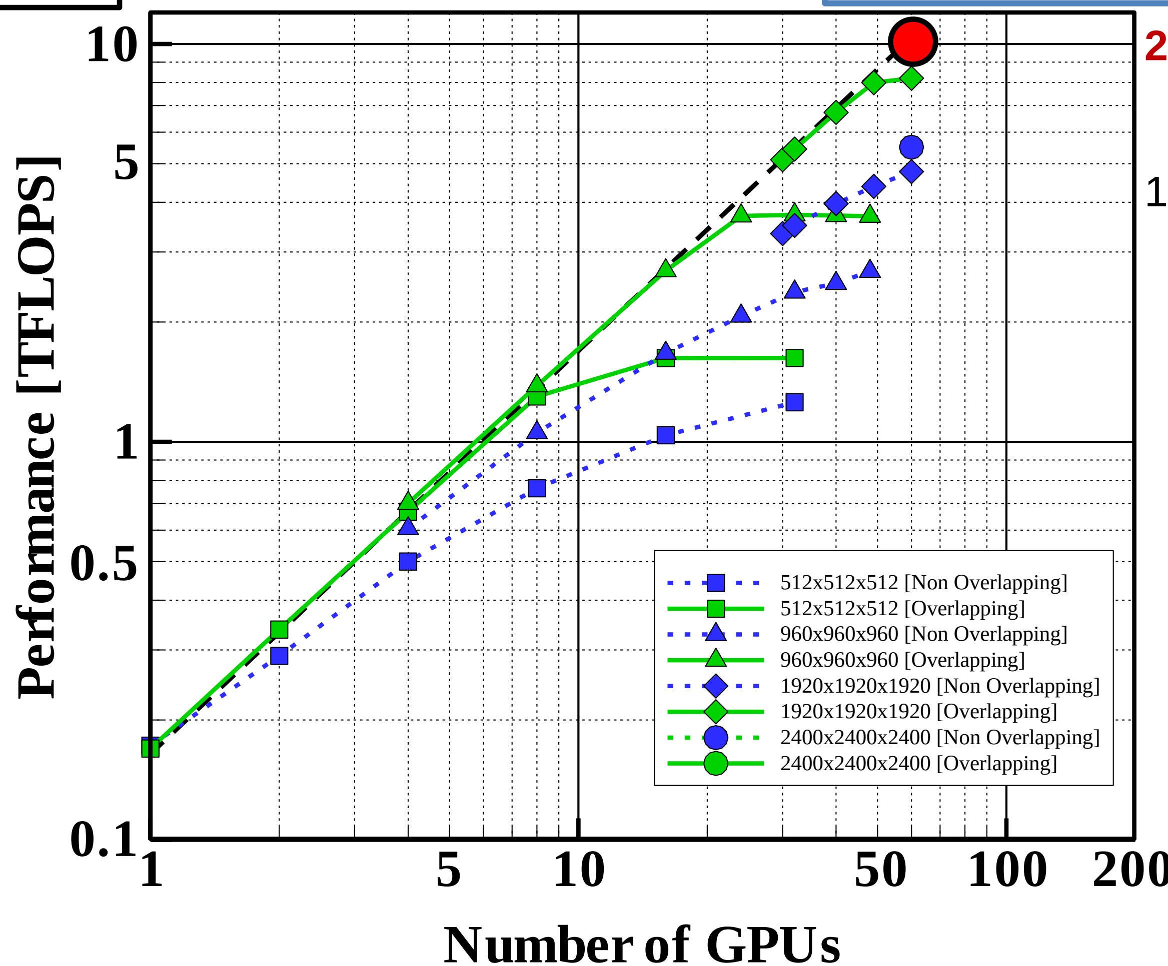


Multi-GPU Peformance

w/o overlapping

1 GPU/node

10TFLOPS : 60GPU

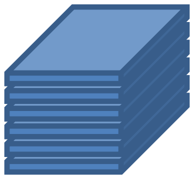


2400×2400×2400

1920×1920×1920

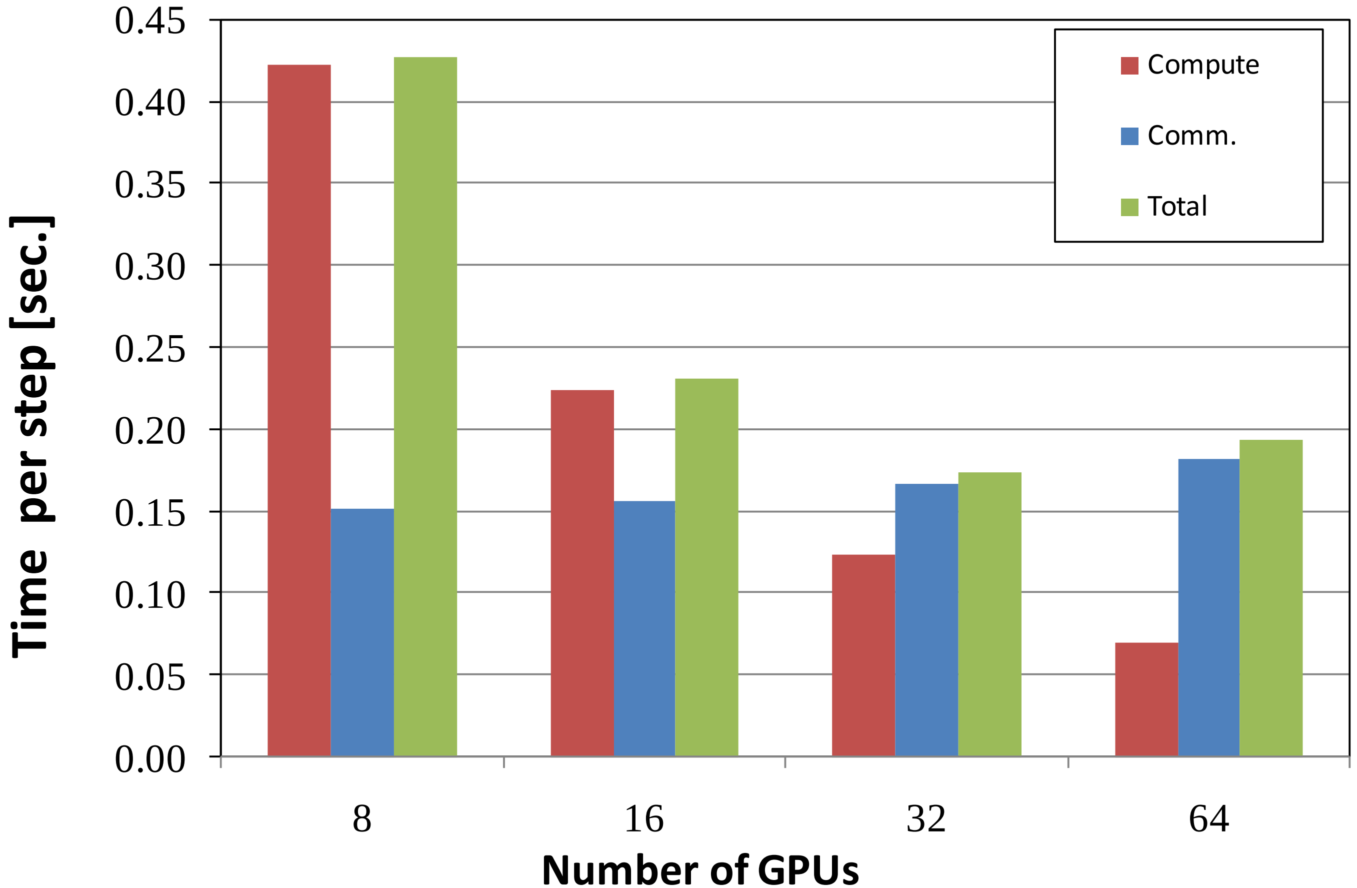
960×960×960

512×512×512



1D

Breakdown of Overlapping Case

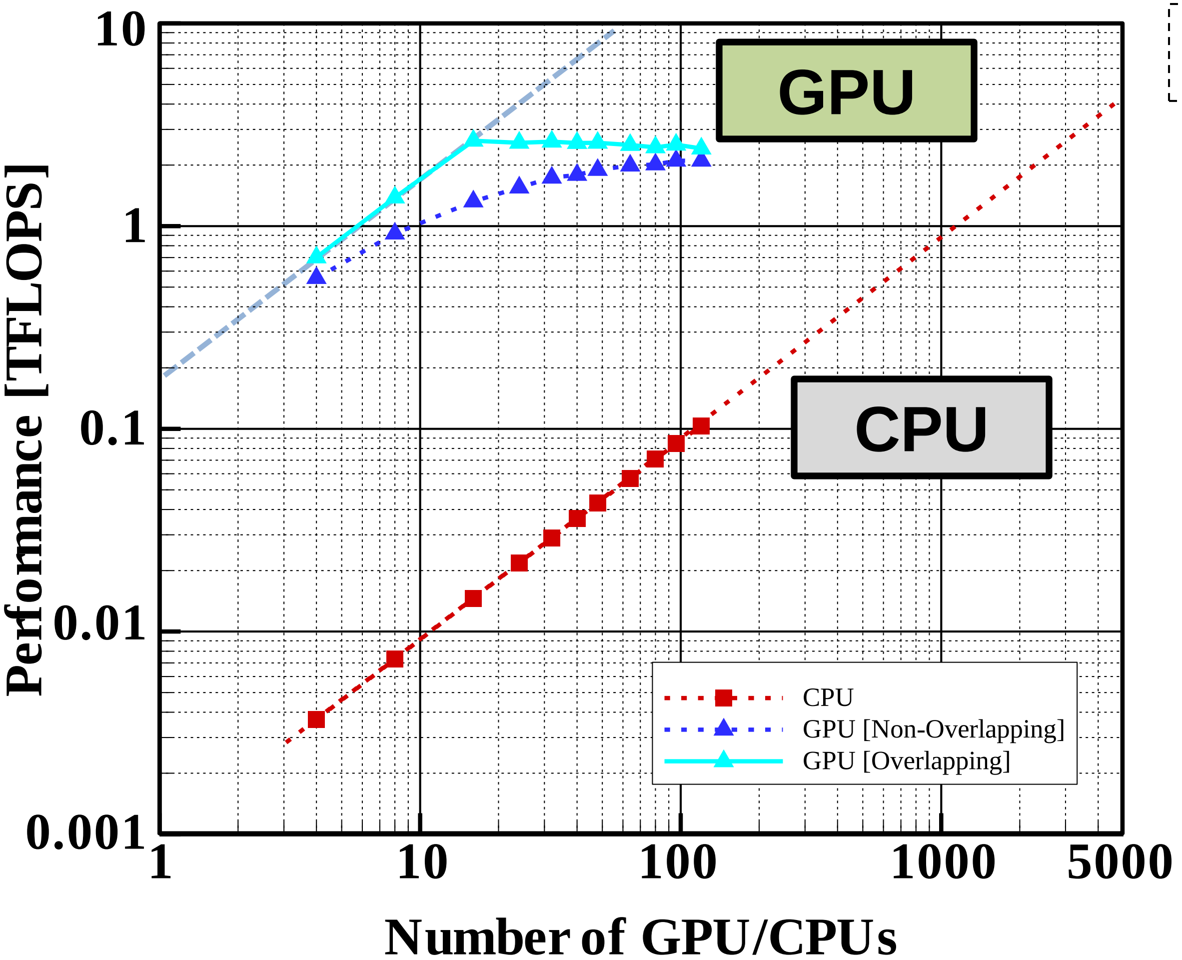


Grid Number:
1024x1024x1024

Machine:
TSUBAME
Tesla S1070
Infiniband
(hpc1tes2 Queue)

- Computational time becomes short for more GPU numbers
- Communication time is almost same
- The communication time can not be hidden for more than 32 GPUs

Direct Comparison : CPU/GPU



960^3 mesh

Tesla S1070

60 GPU

10000 CPU core

TSUBAME 1.0

Next Generation

Weather Prediction

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

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

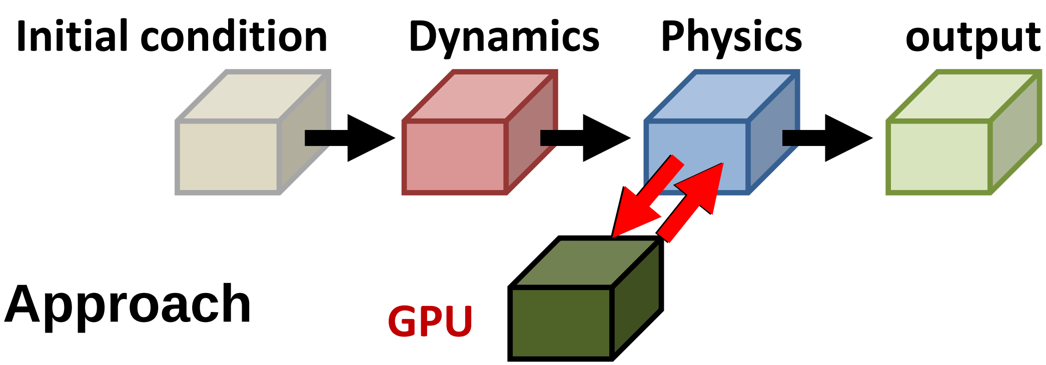
1 % of lines of code, 25 % of elapsed time

⇒ 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

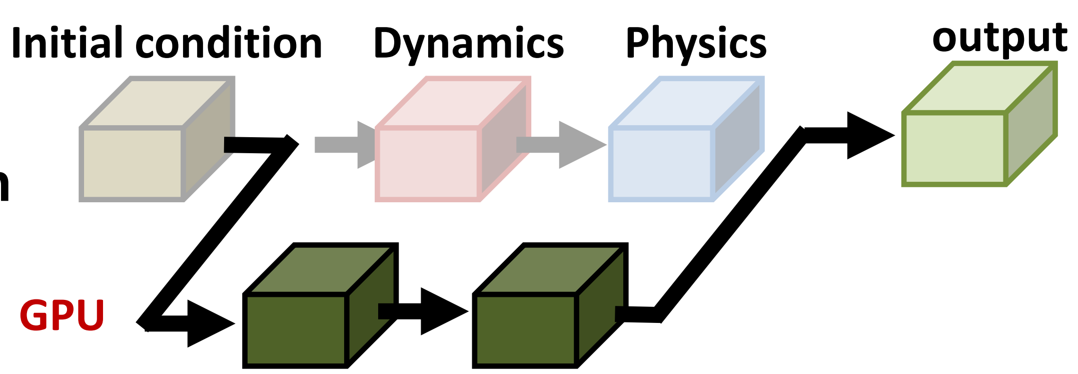
■ASUCA Production Code

- ✓ 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

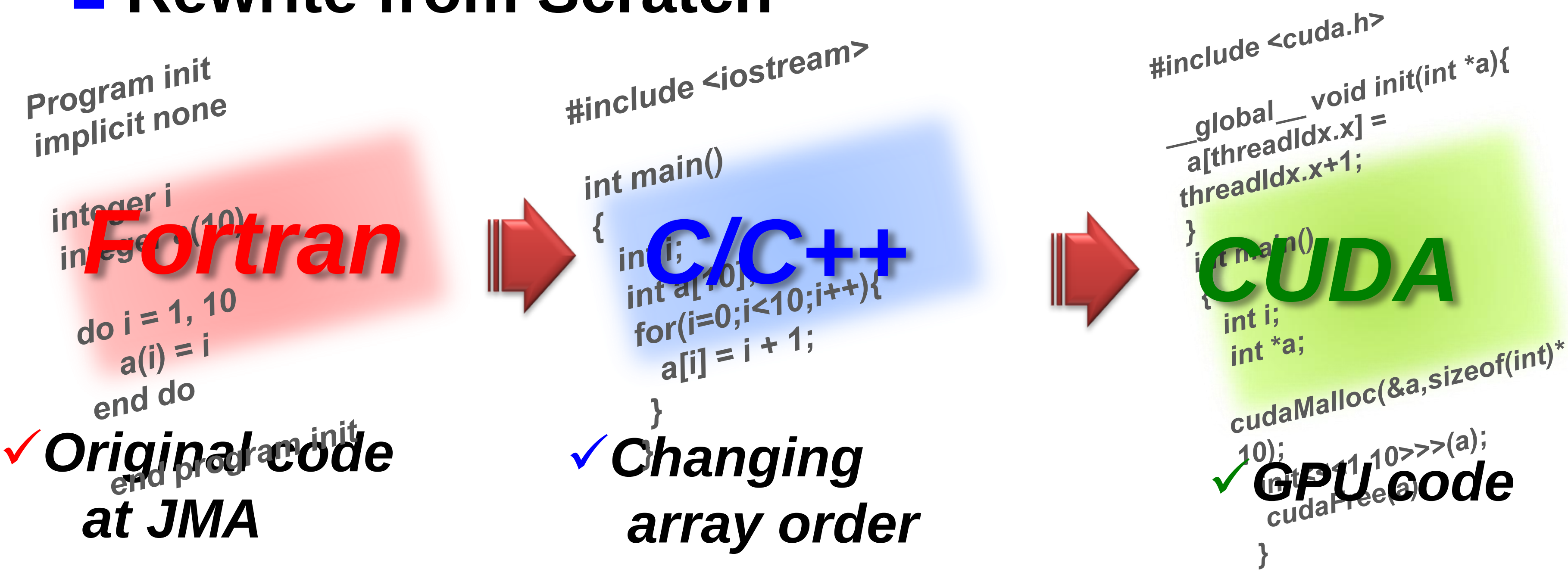
- ✓ HEVI (Horizontally explicit Vertical implicit) scheme
- ✓ Dynamical Core uses a numerical scheme with 3rd-order accuracy in time and space
    - Flux-form non-hydrostatic compressible equation
    - Generalized coordinate

Full GPU Approach



Entire Porting Fortran to CUDA

- Rewrite from Scratch



✓ *Original code at JMA*

✓ *Changing array order*

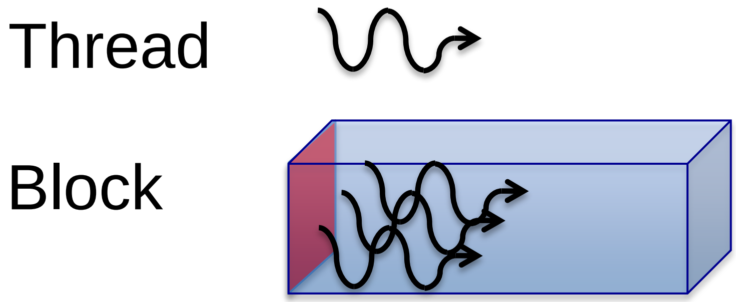
✓ *GPU code*

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

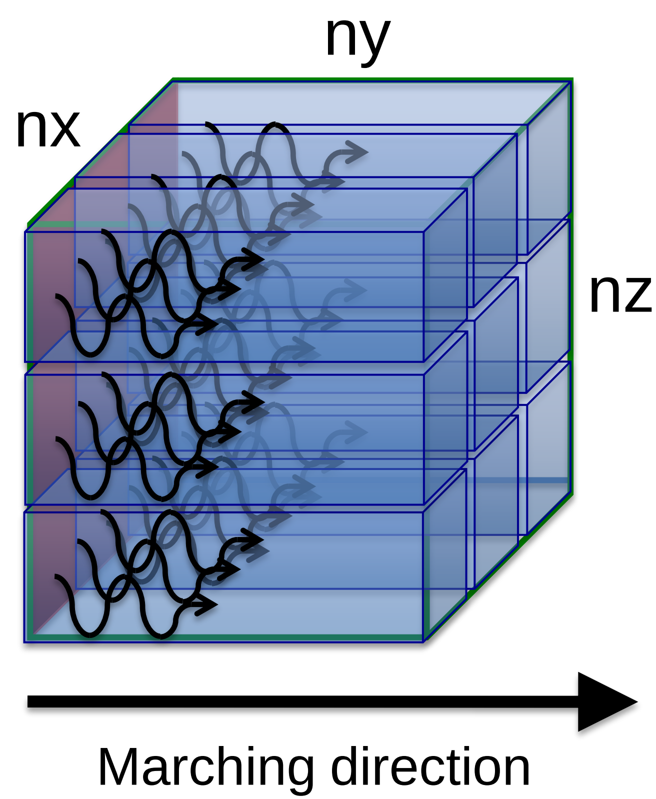
- 1 Year by a Ph.D student

  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

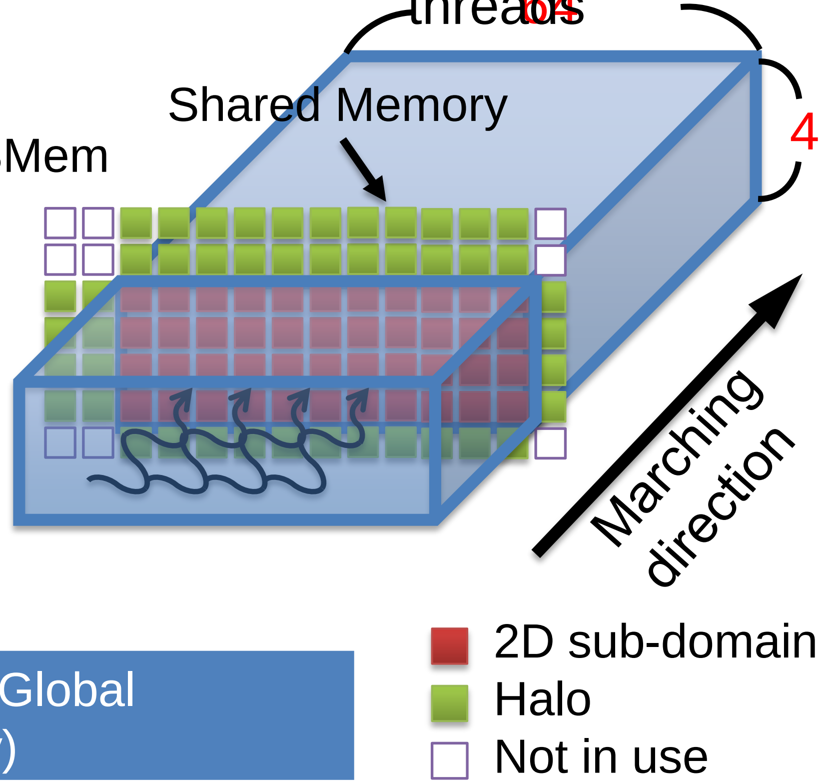
- Shared Memory (SMem) = Software Managed Cache
- Read a 2D sub-domain from VRAM into SMem

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



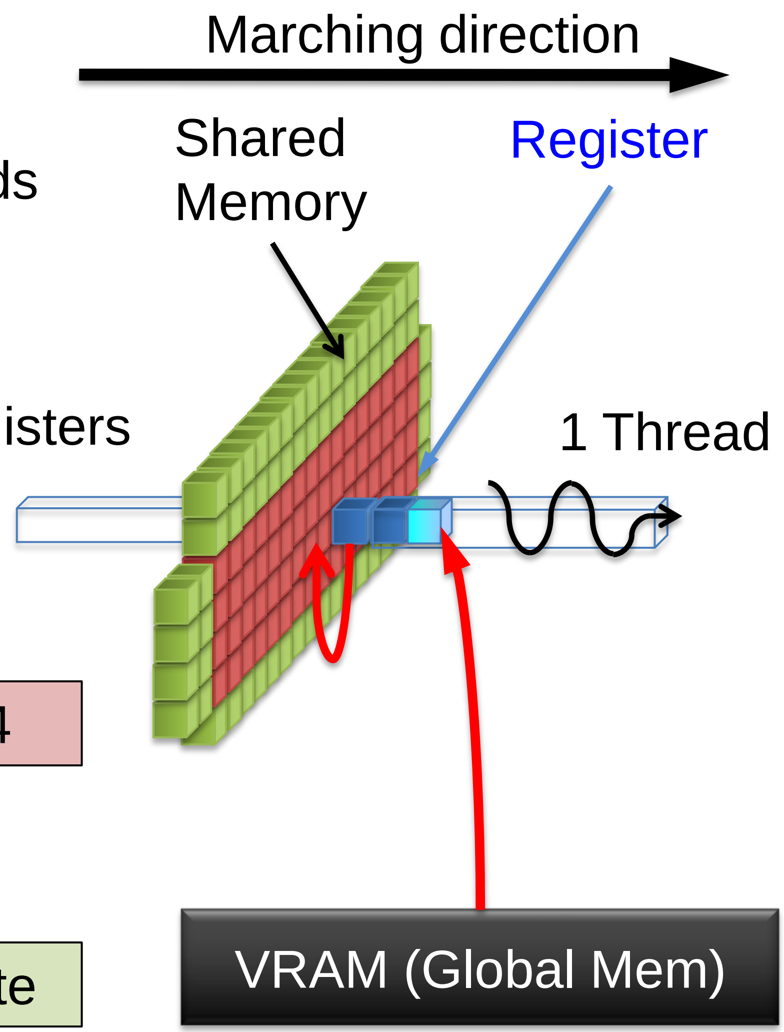
	Shared Memory	VRAM (Global Memory)
Access speed	~ 2 cycle	400-600 cycle
Capacity	16 kByte/Block	2 GByte (Total)

Using Registers in marching direction

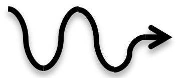
- Register
  - ✓ Access speed : 1 cycle
  - ✓ used for data not shared among threads
- Advection : 12-point stencil
  - ✓ Each thread keeps 4 y-elements in registers
  - ✓ Elements are reuse

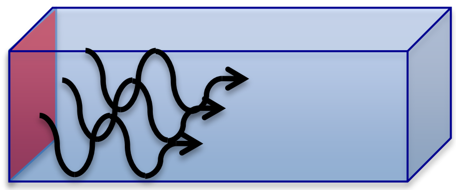
Access GMem directly : 4 + 4 + 4 read, 1write

Using SMem and Registers : ~1 read, 1write



Implementation : 1D Helmholtz equation

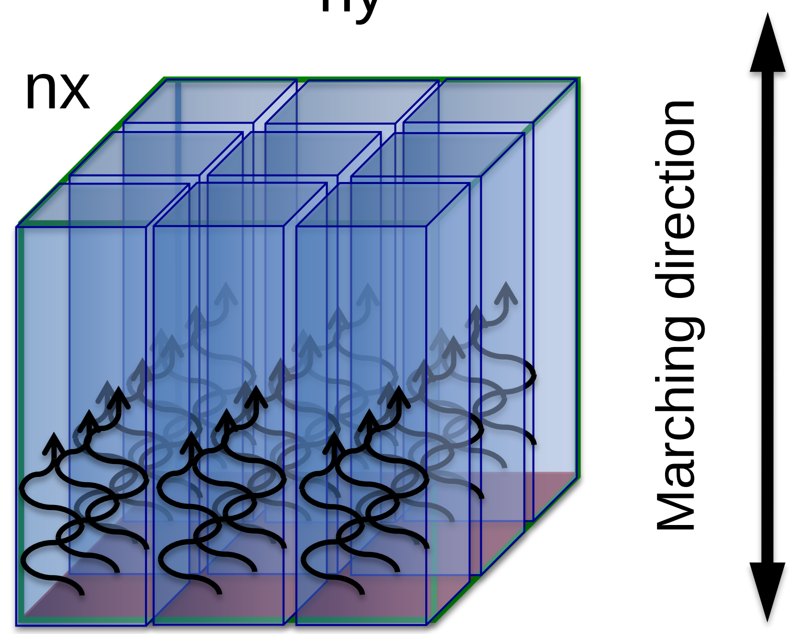
Thread 

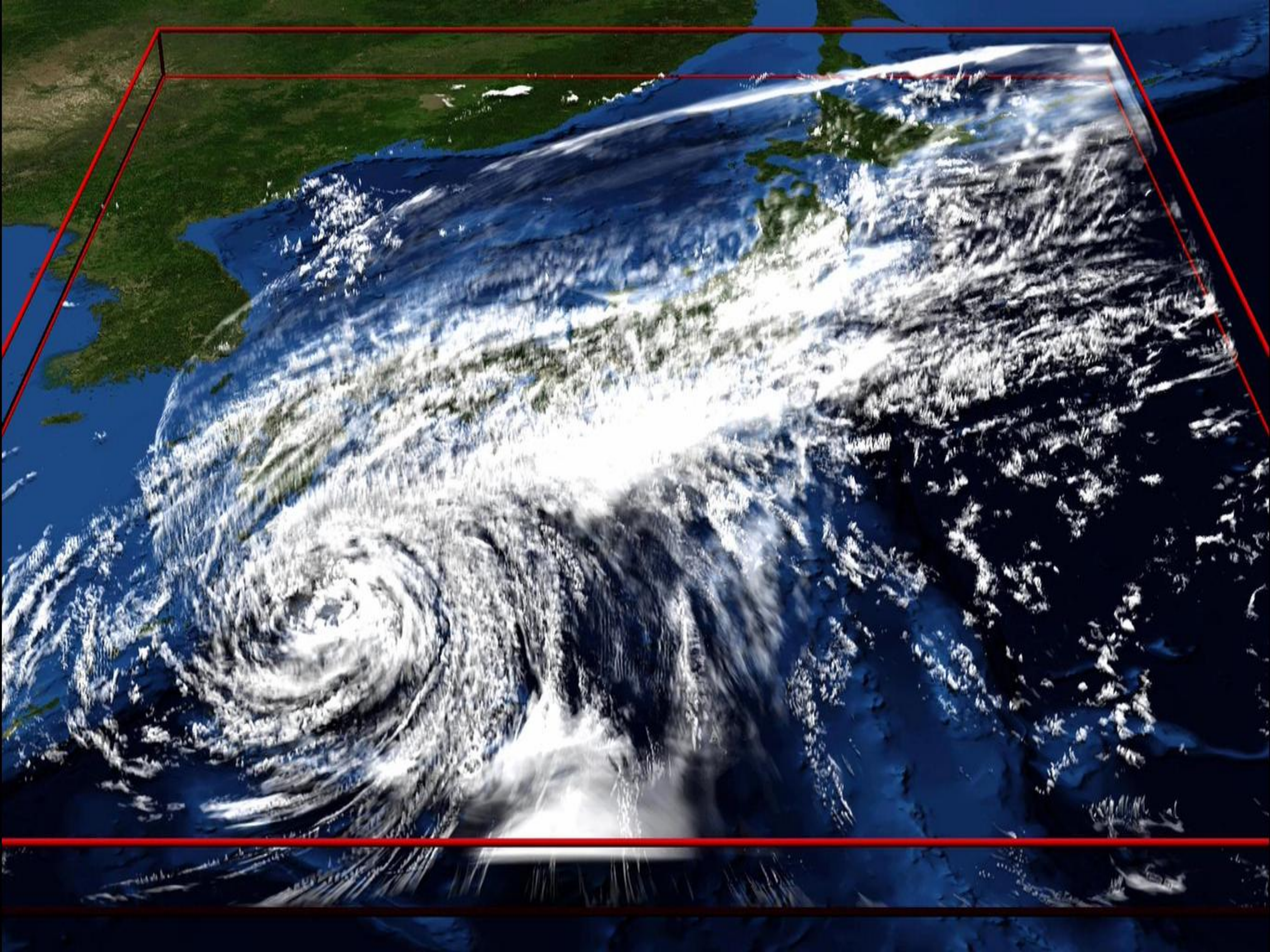
Block 

64 x 4 threads (2D) in a block

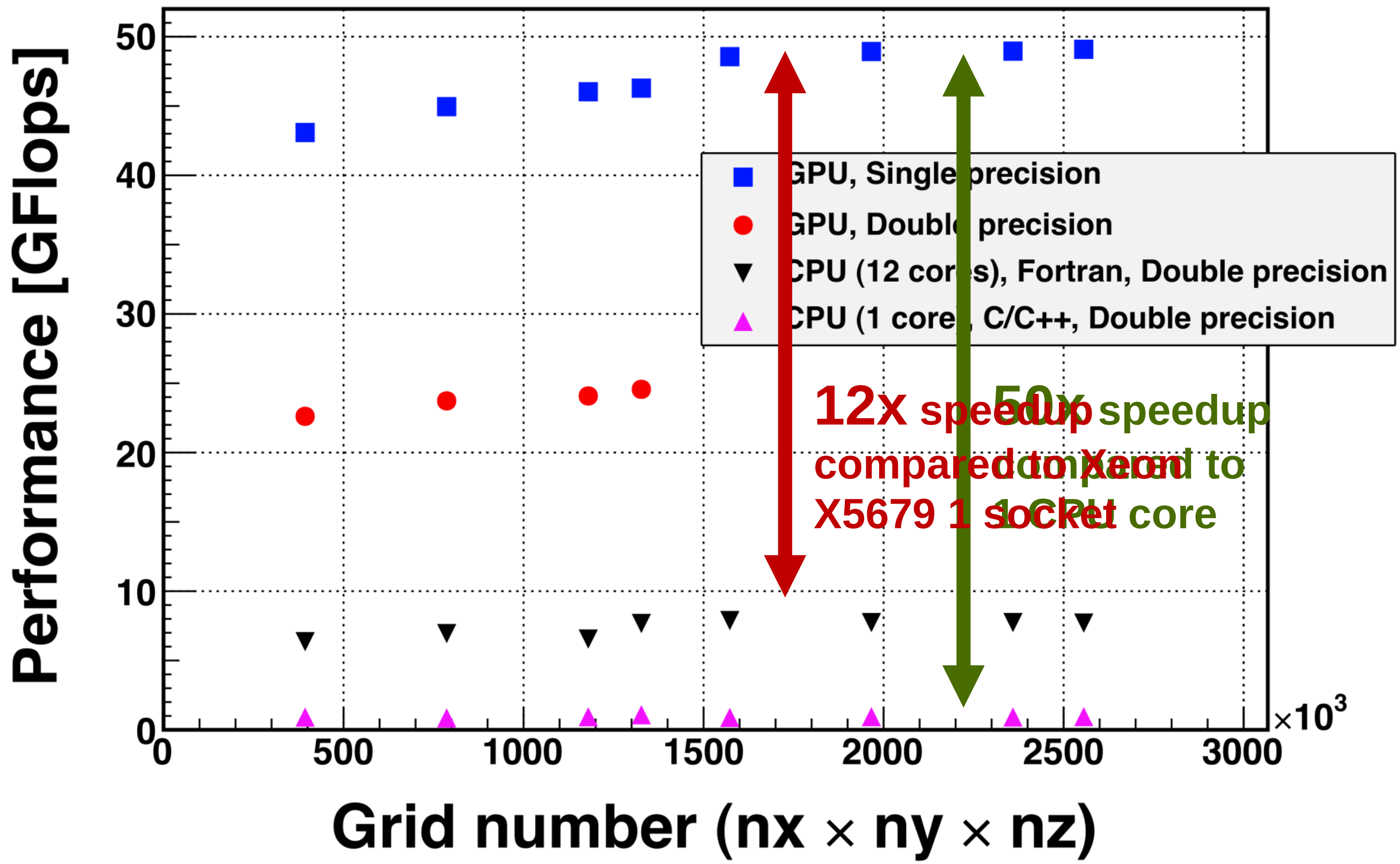
- 1D Helmholtz equation
  - ✓ Element in k depends on elements in k+/- 1

⇒ marching in z direction

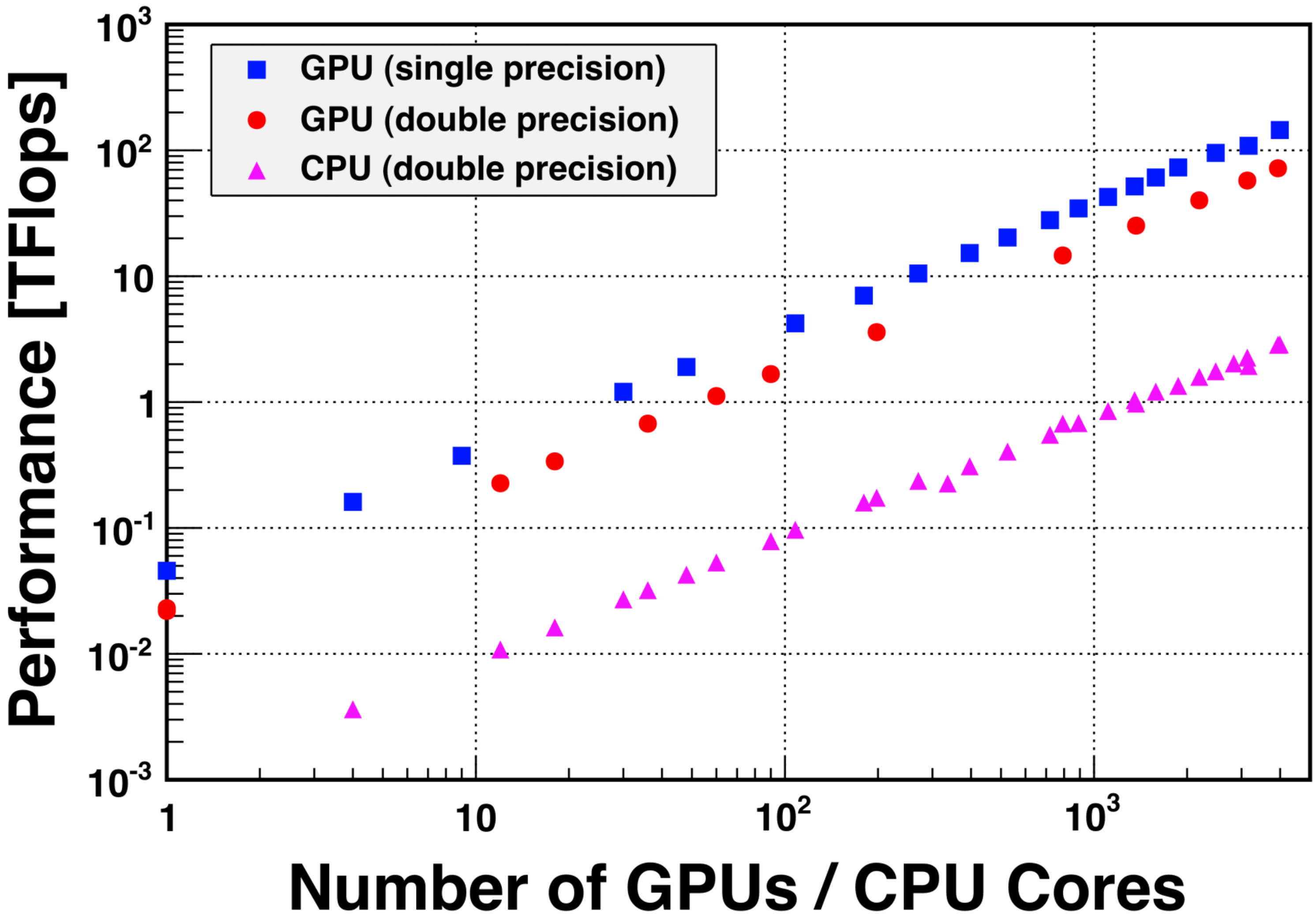




TSUBAME 2.0 (1 GPU)



TSUBAME 2.0 Weak Scaling



145.0 Tflops
Single precision

76.1 Tflops
Doublele precision

Fermi core Tesla M2050

3990

Two-Phase Flows

GP GPU

Mesh Method different from SPH

High accuracy

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

Continuum eq.

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

Momentum eq.

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

Level-Set advection

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

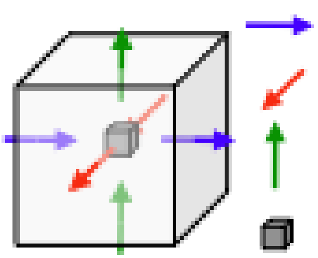
VOF continuum eq.

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

Level-Set re-initialization

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

Staggered variable position



u : velocity on x-direction

v : velocity on y-direction

w : velocity on z-direction

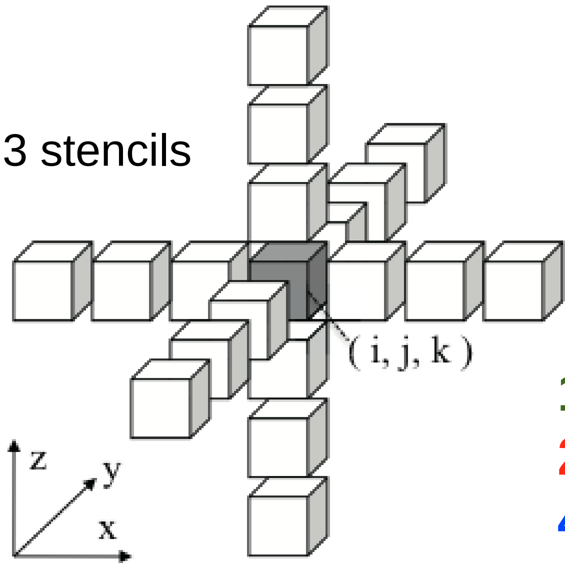
p,φ,ψρ : scalar variables

3D Advection Equation

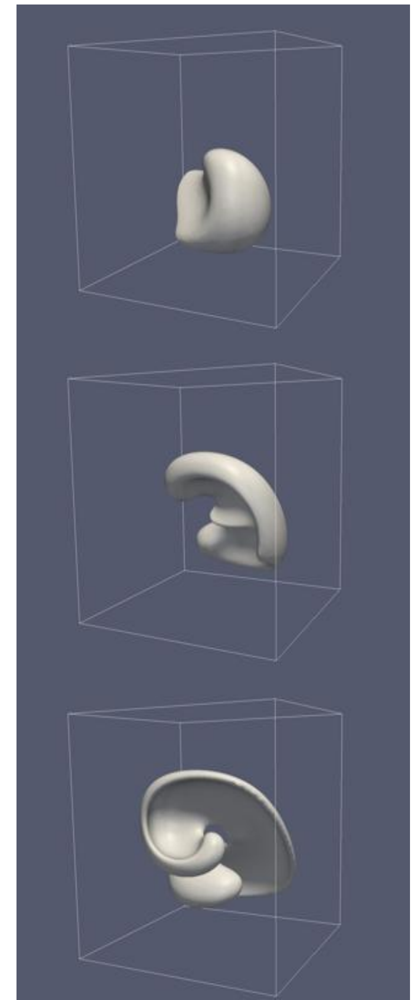
Advection equation

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

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)

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

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

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

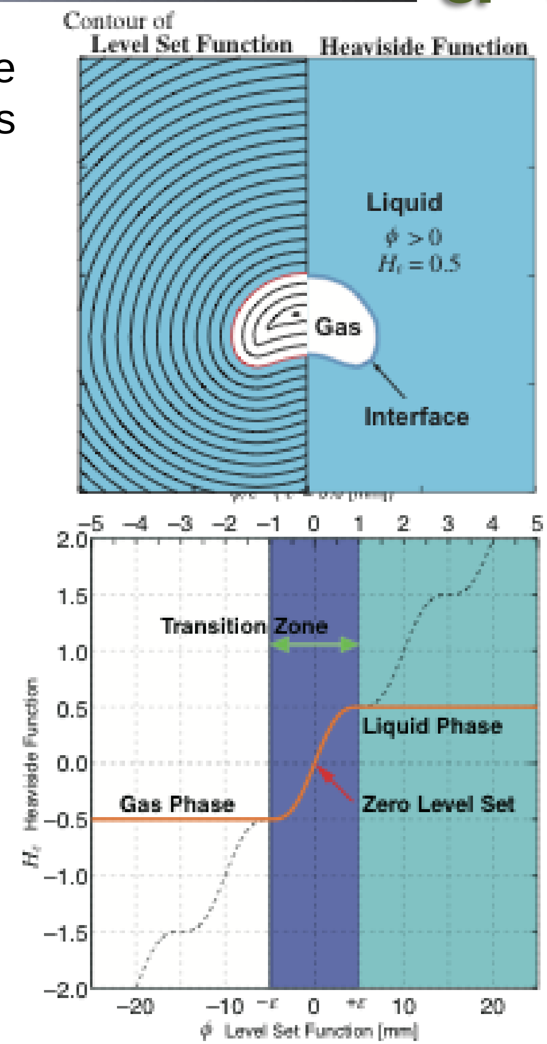
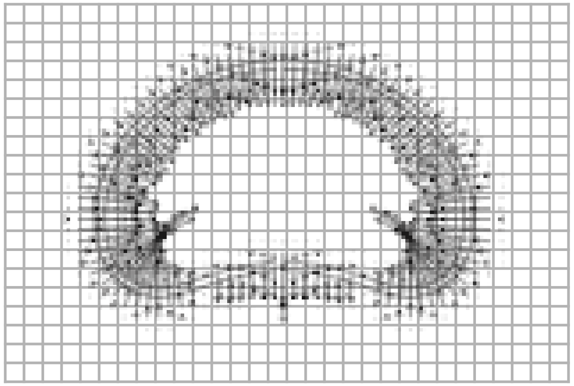


Fig. Takehiro Himeno, et. Al., JSME, 65-635,B(1999),pp2333-2340

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



Surface tension represented by volume force

Surface tension force — Curvature — Normal vector

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

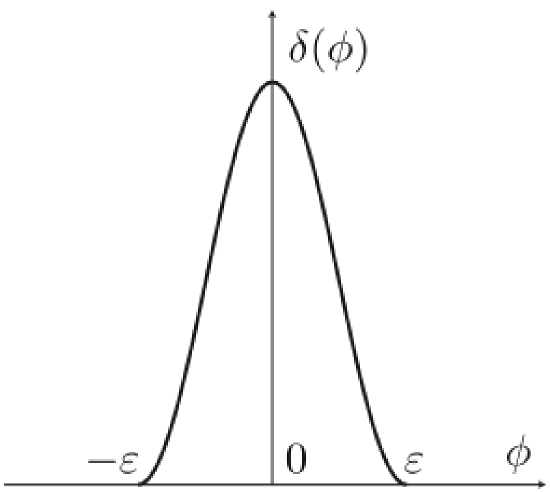
$$\kappa = -\nabla \cdot \mathbf{n} = -\nabla \cdot \frac{\nabla \phi}{|\nabla \phi|}$$

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

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

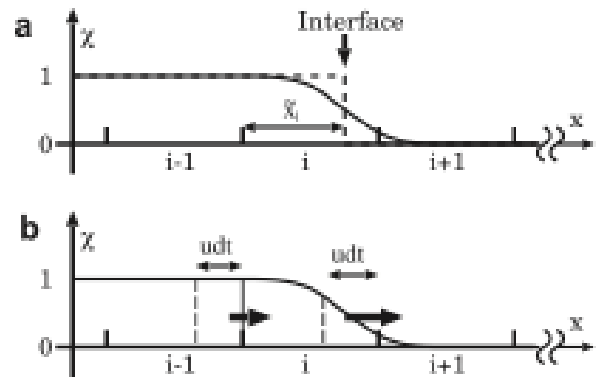
THINC (tangent of hyperbola for interface capturing) Scheme

[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

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

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



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

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

- 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

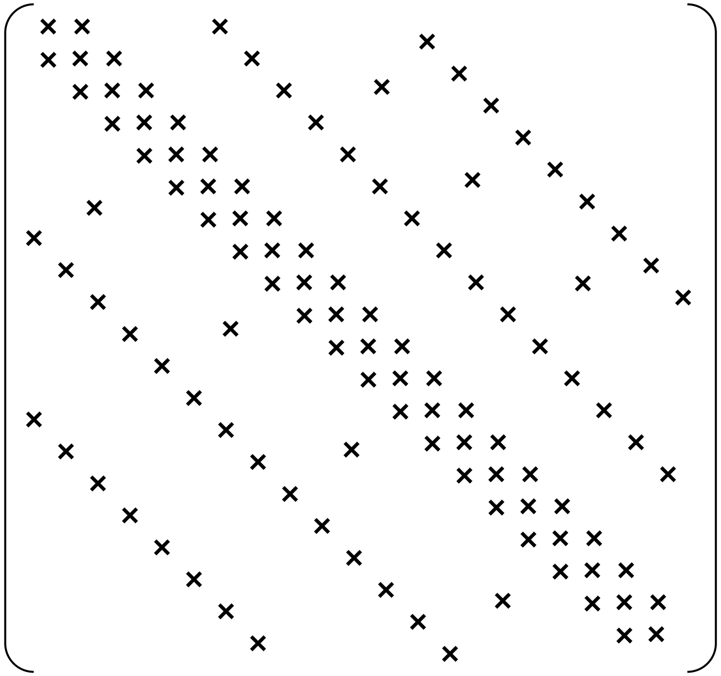
Sparse Matrix Solver

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

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

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

Non-zero Packing:
CRS → ELL, JDL



BiCGStab + AMG

Collaboration with Mizuho Information & Research Institute

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

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

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

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

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

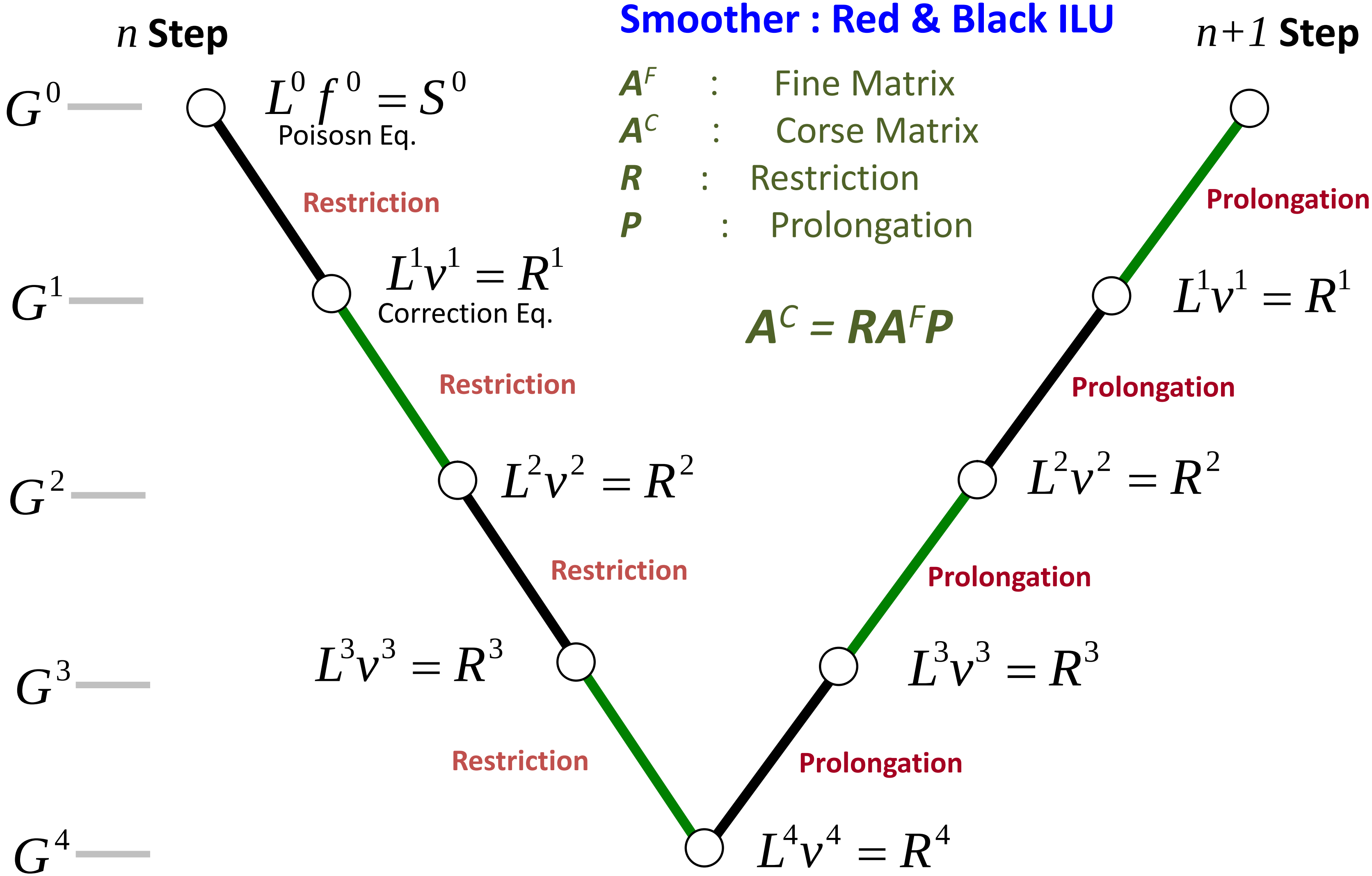
if $(\boldsymbol{r}_{k+1}, \boldsymbol{r}_{k+1}) < \varepsilon^2 (\boldsymbol{b}, \boldsymbol{b})$ **exit;**

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

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

loop end

AMG V-Cycle



Smoother : Red & Black ILU

A^F : Fine Matrix

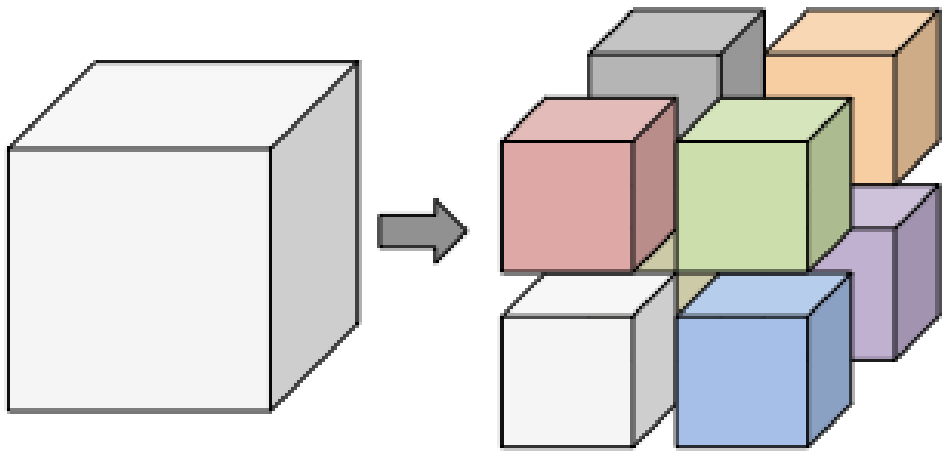
A^C : Corse Matrix

R : Restriction

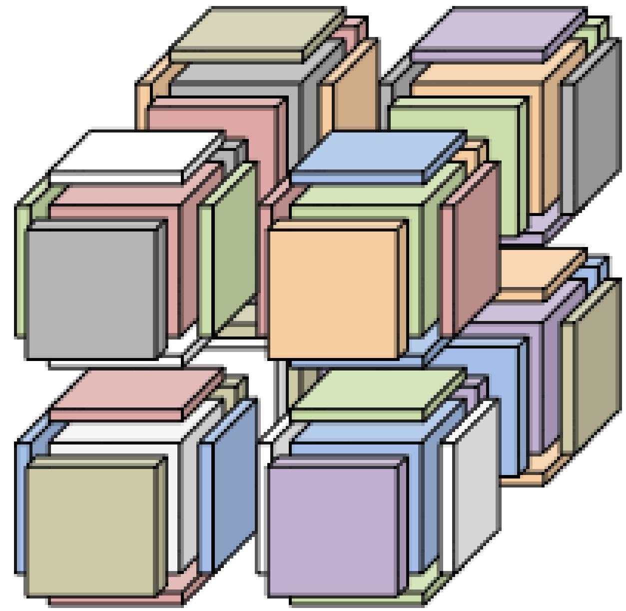
P : Prolongation

$$A^C = RA^F P$$

Multi-Dimensional
Domain Decomposition

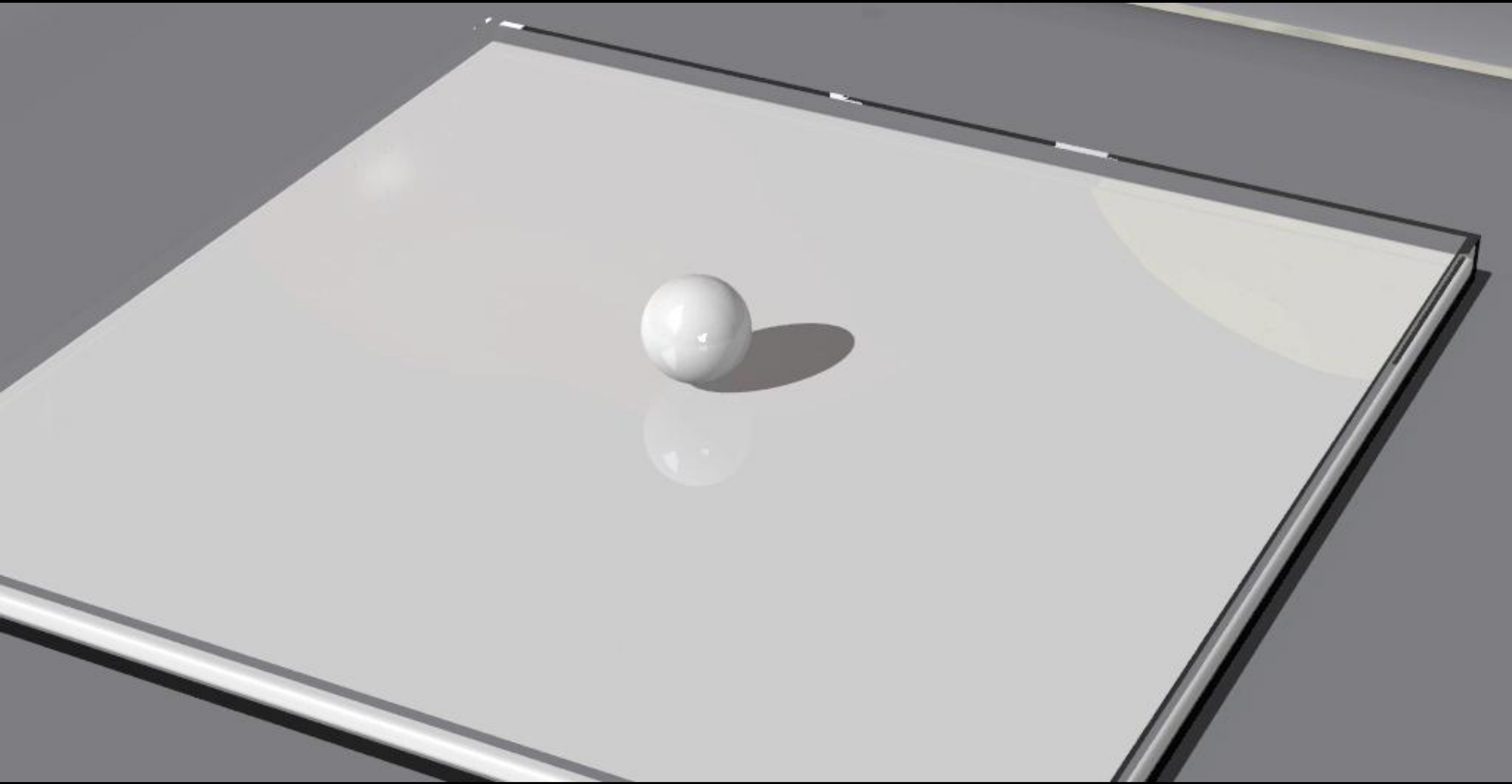


- 3D domain decomposition
- 1 GPU is assigned to each domain

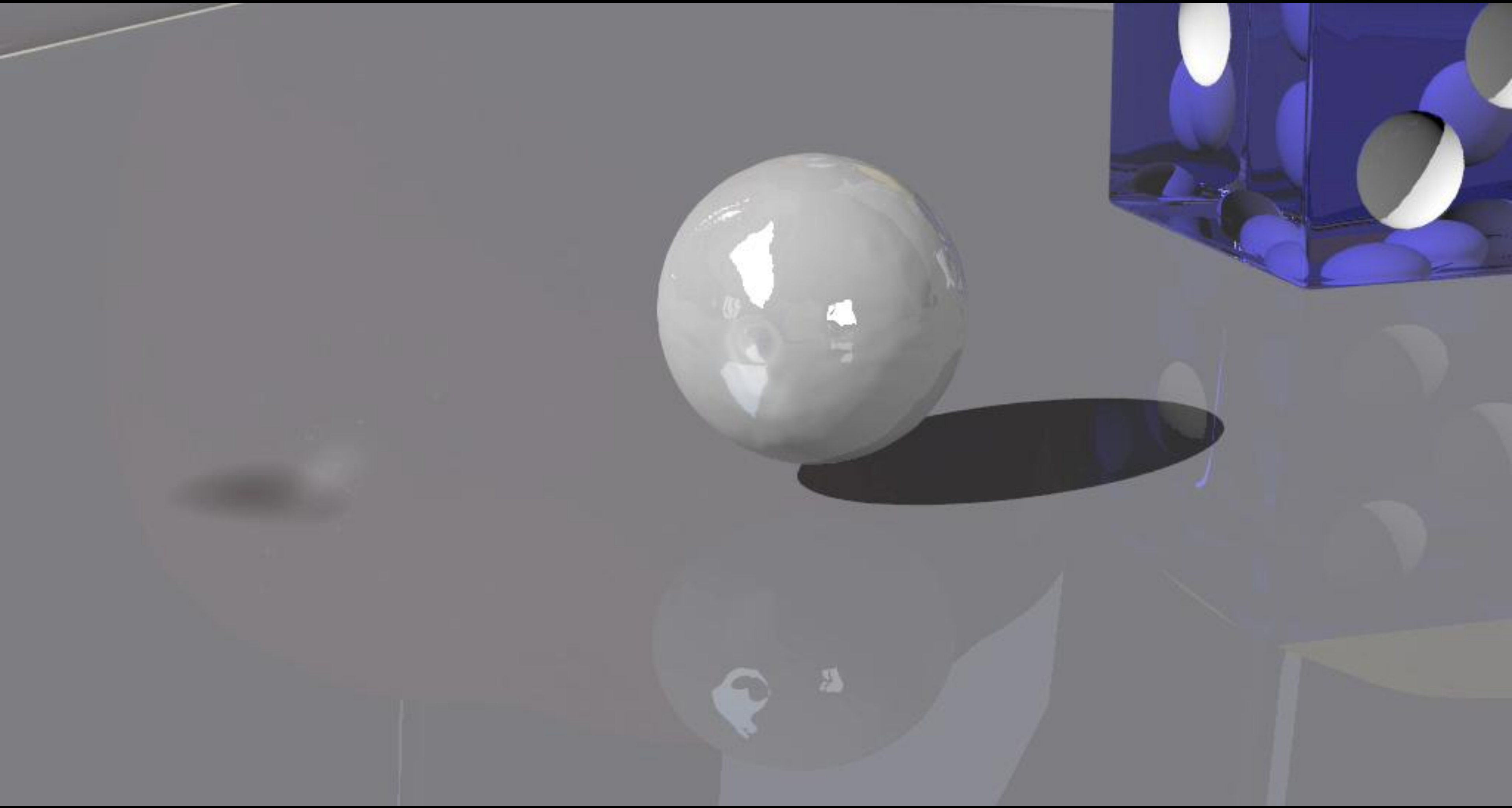


- Communication buffer for each face
- Host buffer & Device buffer

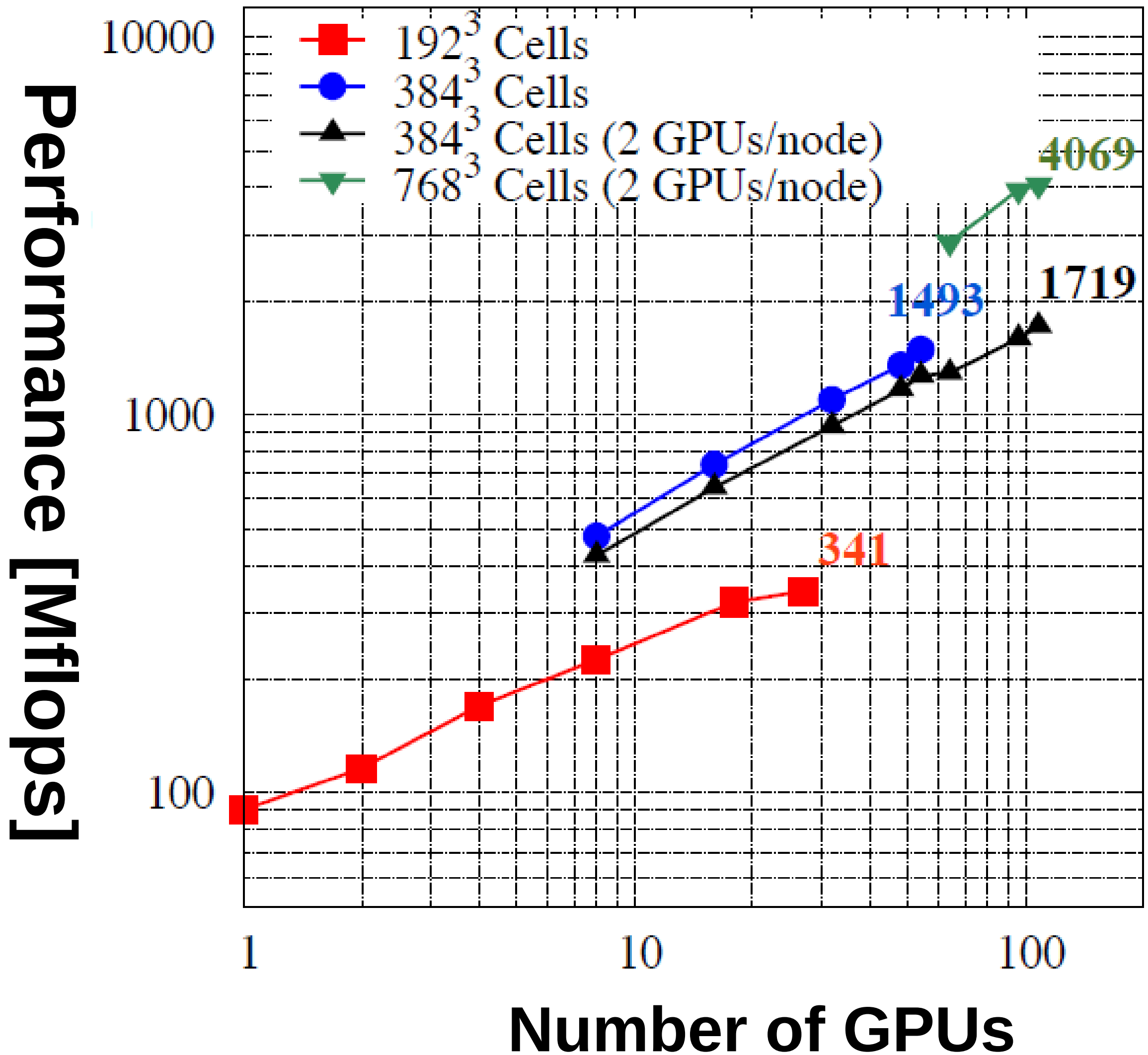
Milk Crown



Drop on dry floor



Multi-GPU Performance on TSUBAME 1.2



Multi-GPU Summary

Some CFD applications show good strong scalability up to 32 GPUs in the case of TSUBAME.

The balance between computation and communication performance becomes bad because of the high GPU performance.

In order to achieve high performance for multi-GPU application, the overlapping technique between computation and communication is very important.

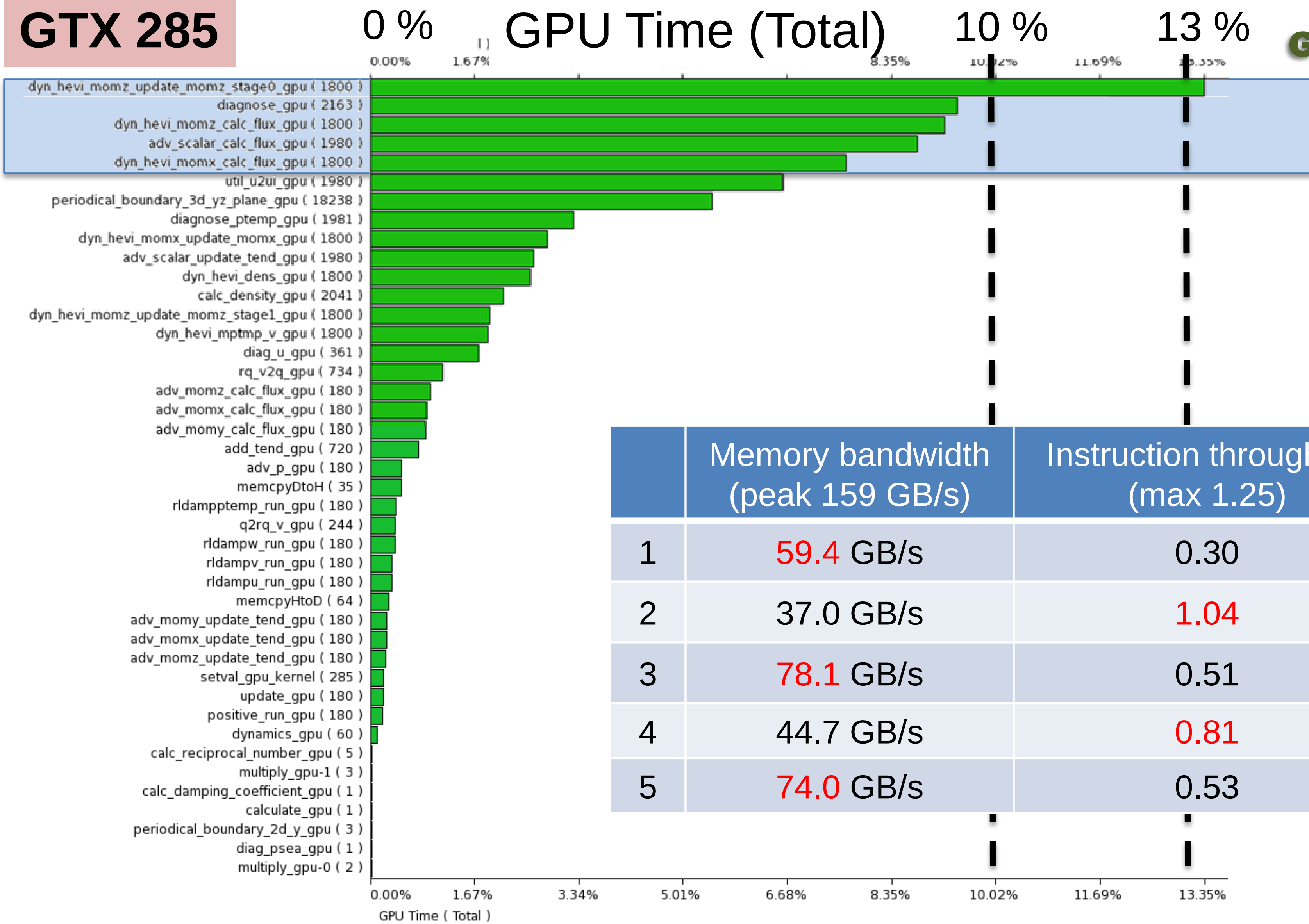
Be careful for GPU-to-CPU data transfer (cudaMemcpy) and CPU-to-CPU data transfer (MPI library).

Thank you

for your kind attention

Profile of functions in ASUCA

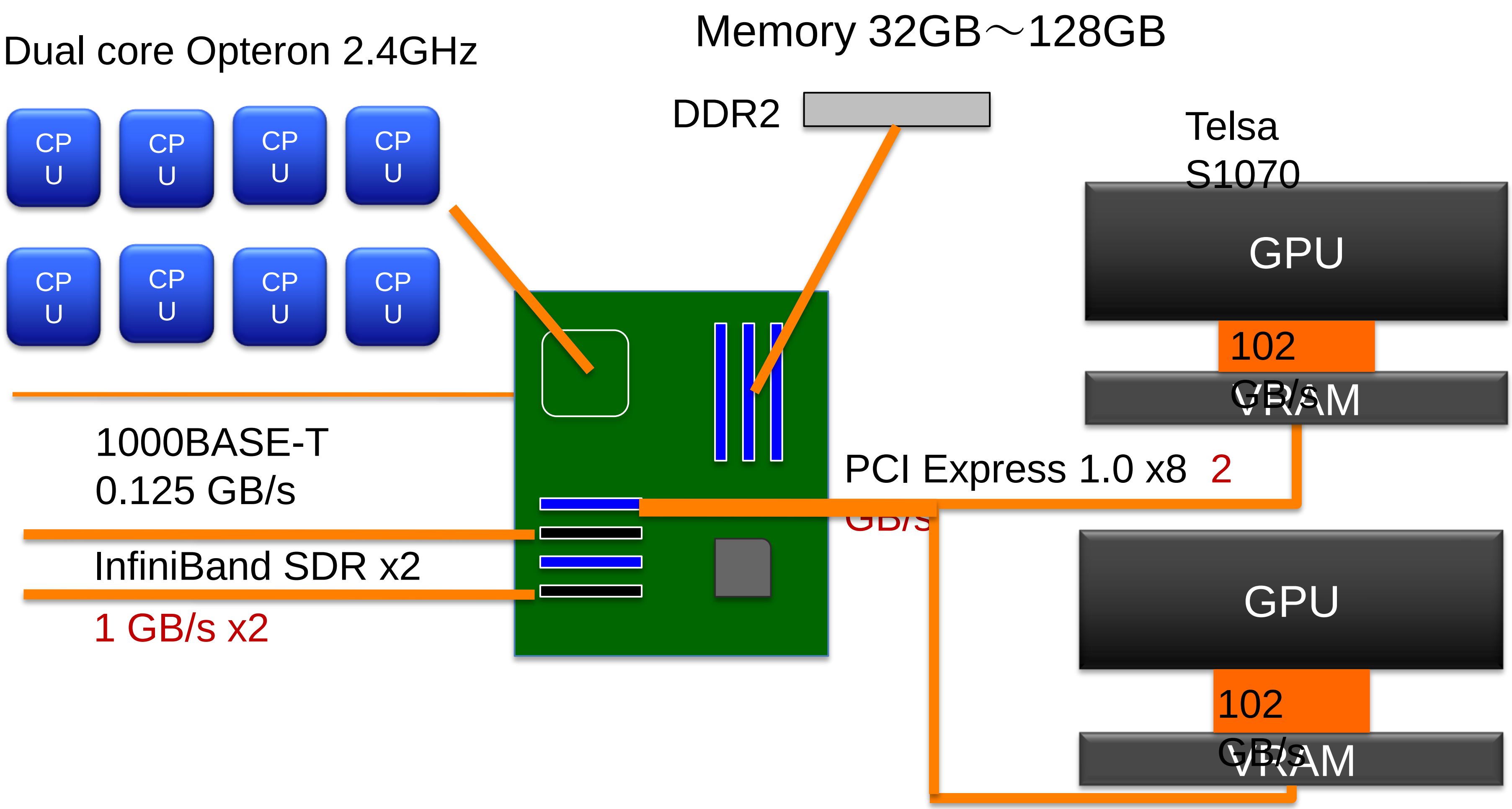
GTX 285



	Memory bandwidth (peak 159 GB/s)	Instruction throughput (max 1.25)
1	59.4 GB/s	0.30
2	37.0 GB/s	1.04
3	78.1 GB/s	0.51
4	44.7 GB/s	0.81
5	74.0 GB/s	0.53

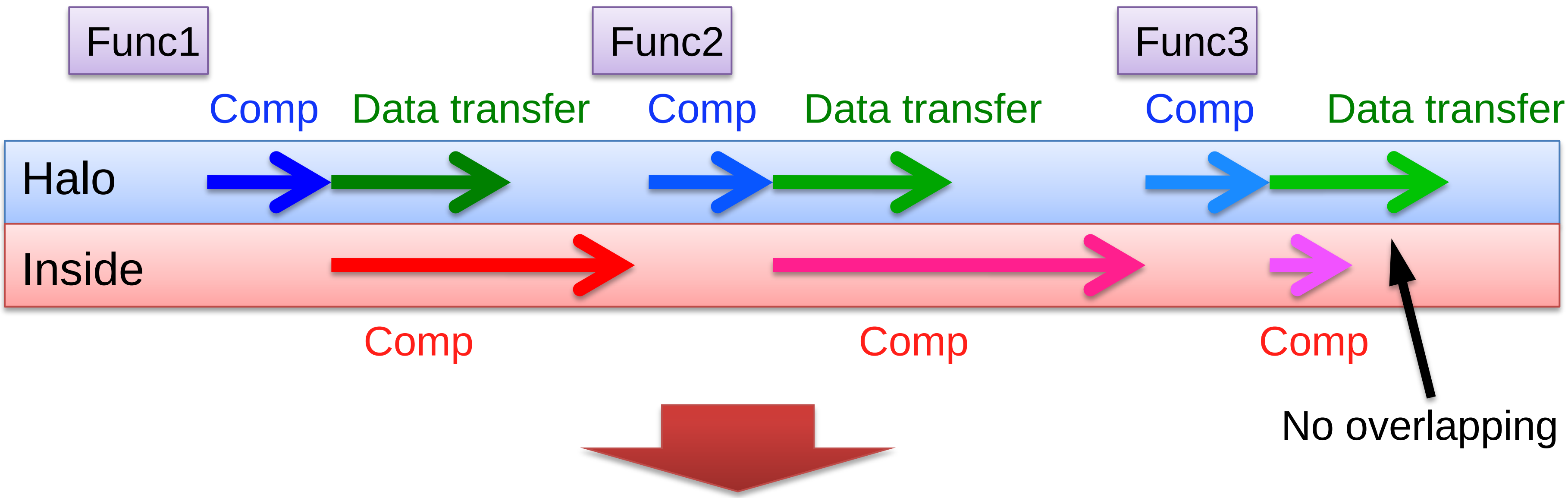
TSUBAME 1.2 node detail

SunFire X4600

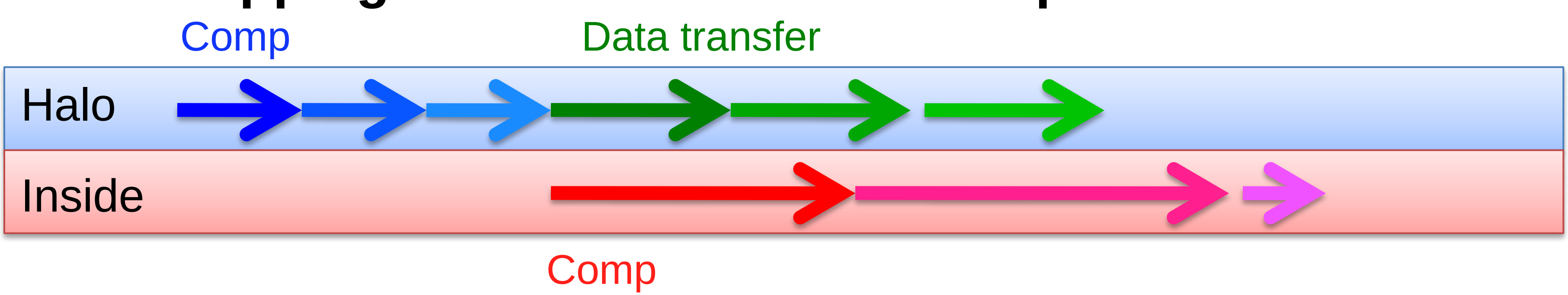


Re-ordering the communication and computation

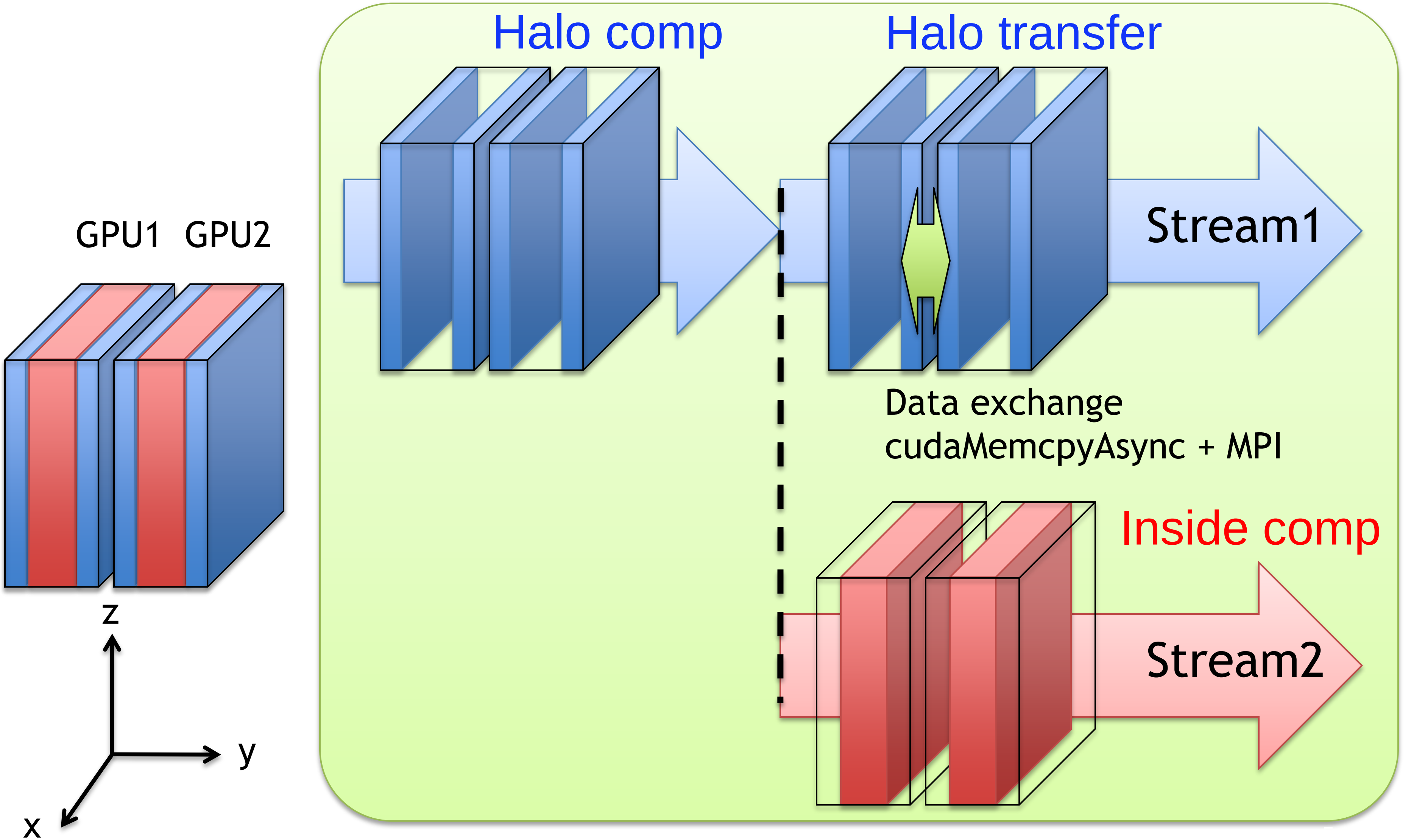
- **Overlapping comm and comp in each function**



- **Overlapping overall comms and comps in functions**



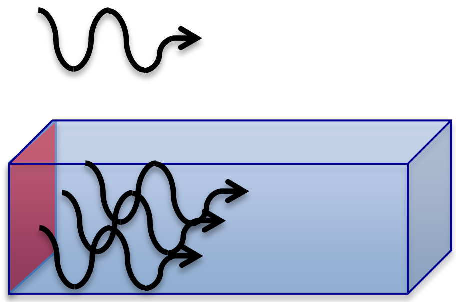
Overlapping communication with computation



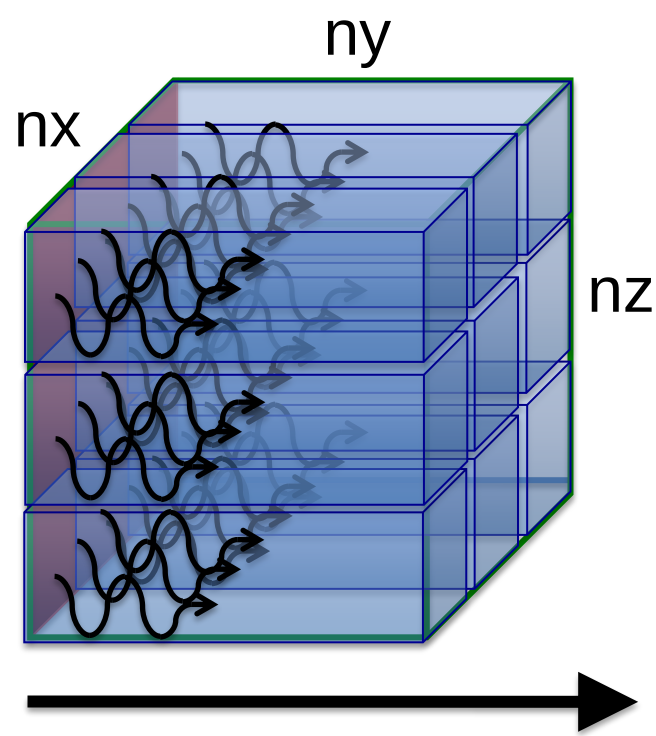
Implementation : Advection

Thread

Block



64 x 4 threads (2D) in a block



Marching direction

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

Using Shared Memory

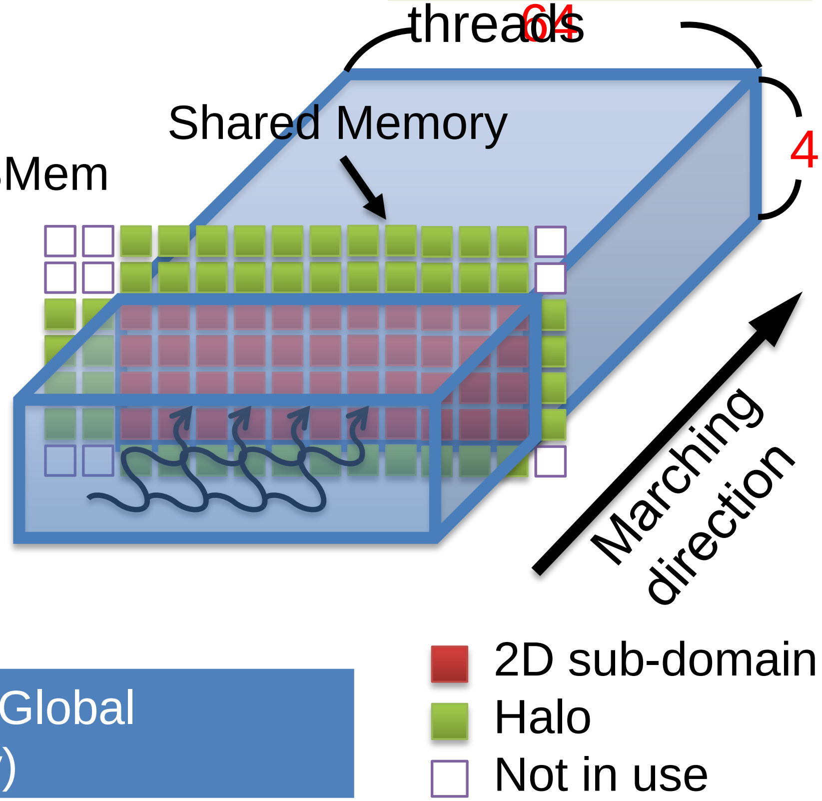
- Shared Memory (SMem) = Software Managed Cache
- Read a 2D sub-domain from VRAM into SMem

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

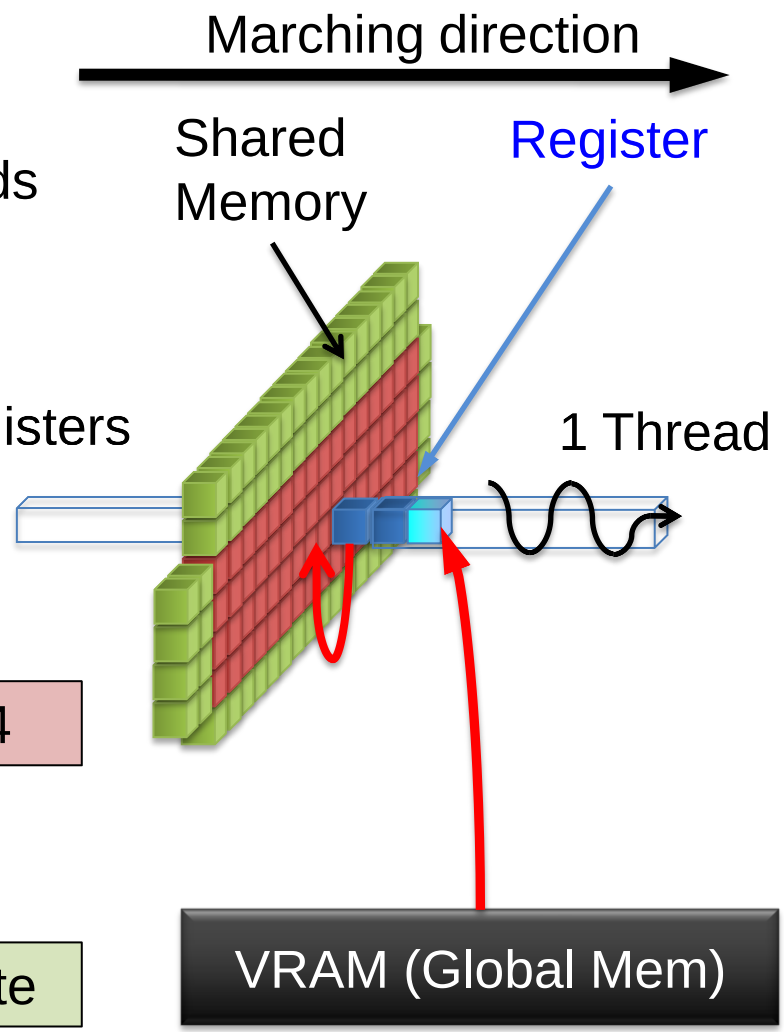
Using SMem : ~1 read, 1write



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

Using Registers in marching direction

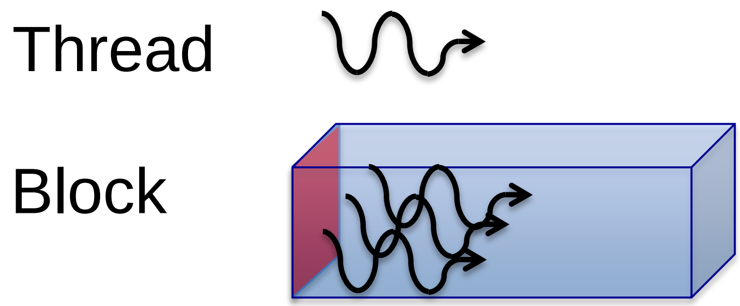
- Register
  - ✓ Access speed : 1 cycle
  - ✓ used for data not shared among threads
- Advection : 12-point stencil
  - ✓ Each thread keeps 4 y-elements in registers
  - ✓ Elements are reuse



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

Using SMem and Registers : ~1 read, 1write

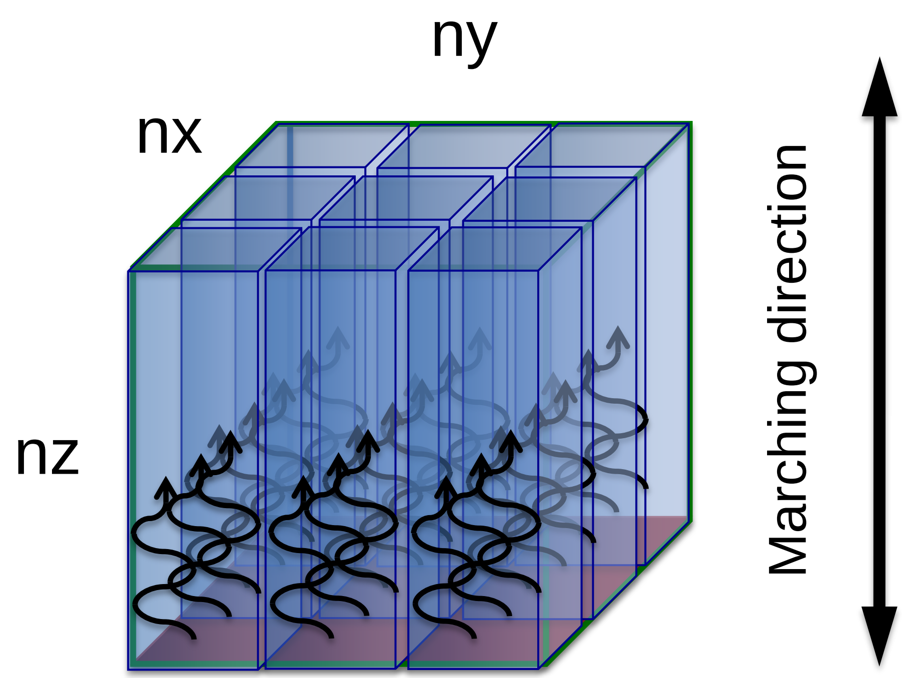
Implementation : 1D Helmholtz equation



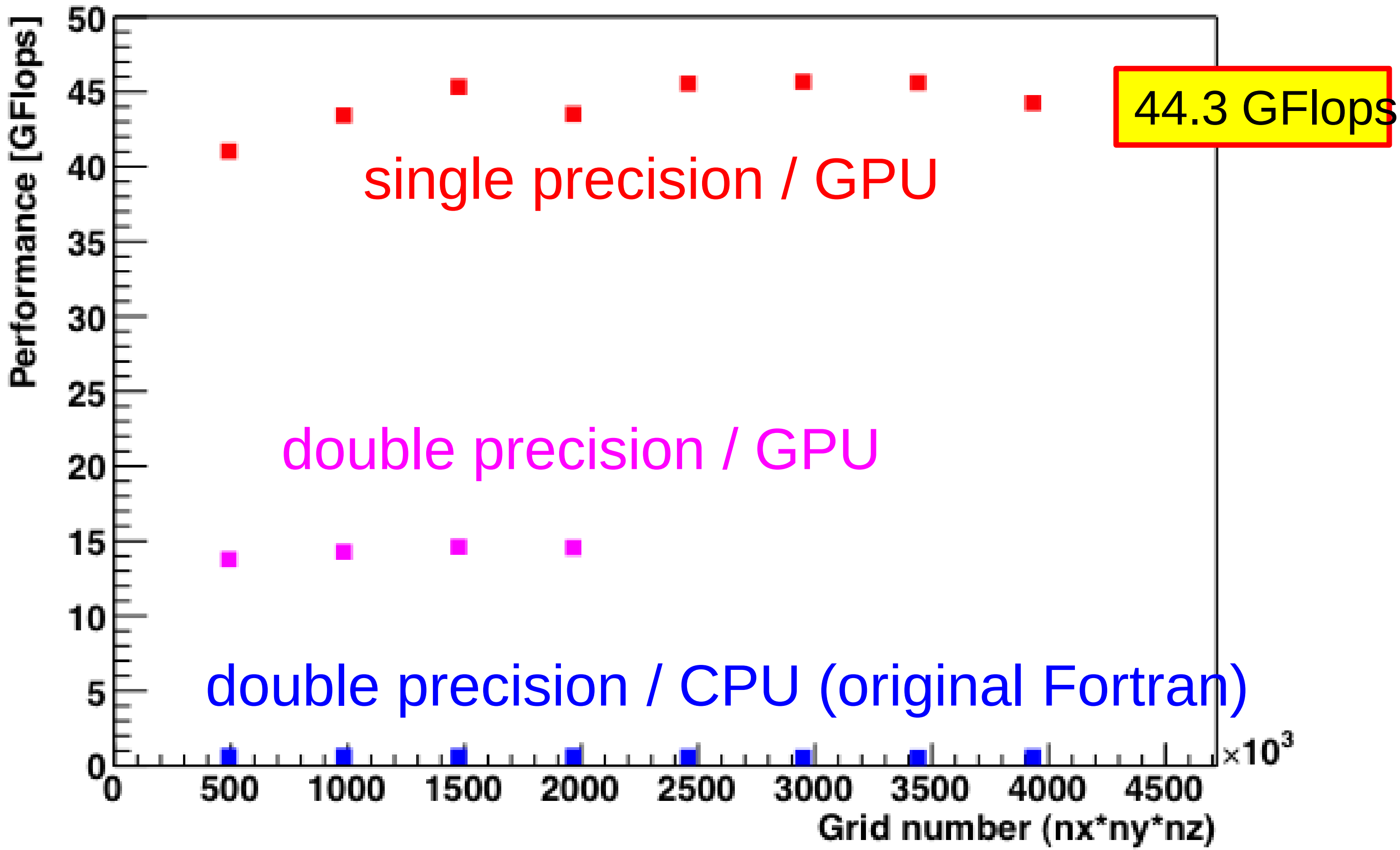
64 x 4 threads (2D) in a block

- 1D Helmholtz equation
  - ✓ Element in k depends on elements in k+/- 1

⇒ marching in z direction



Single GPU Performance

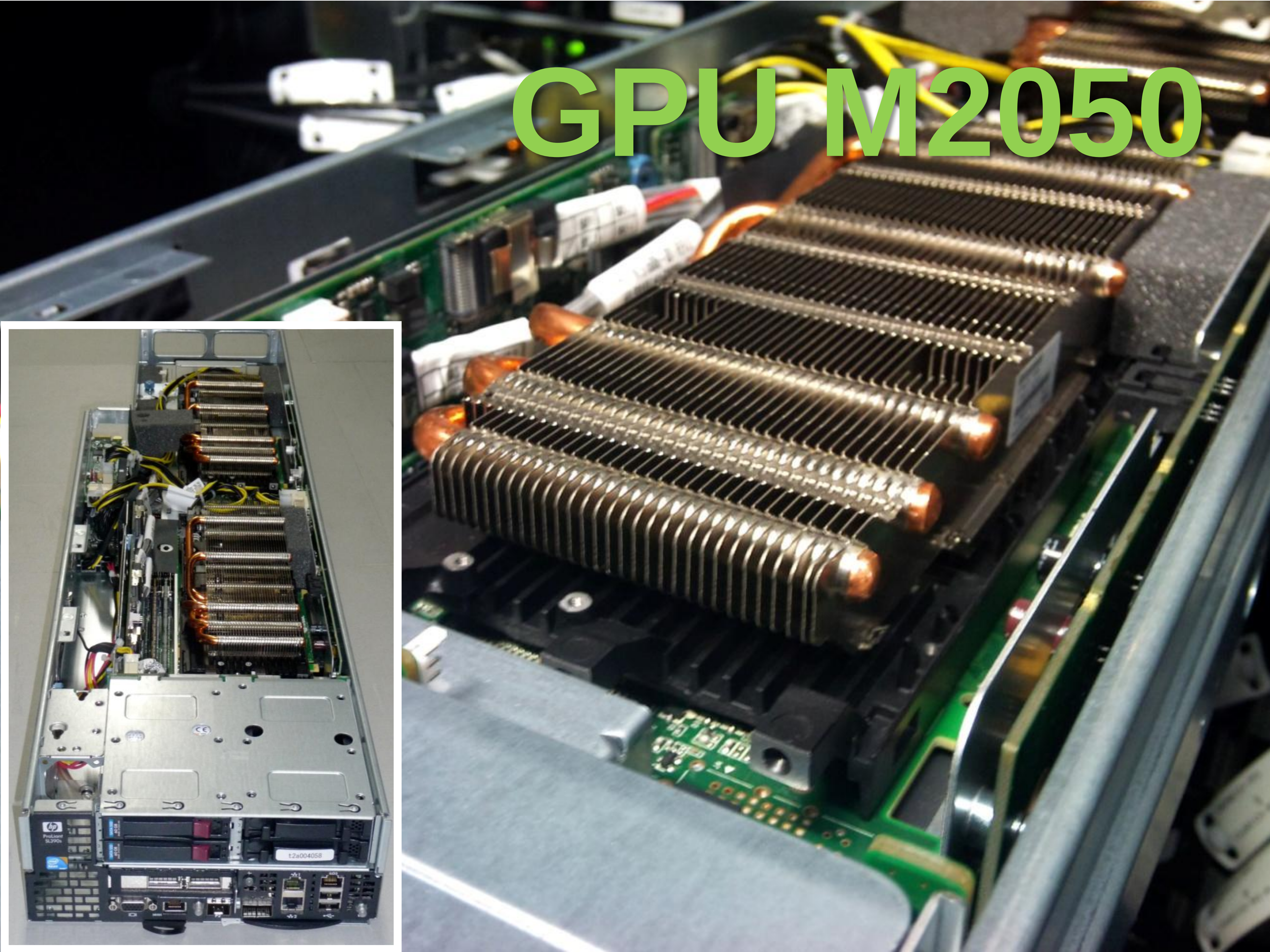


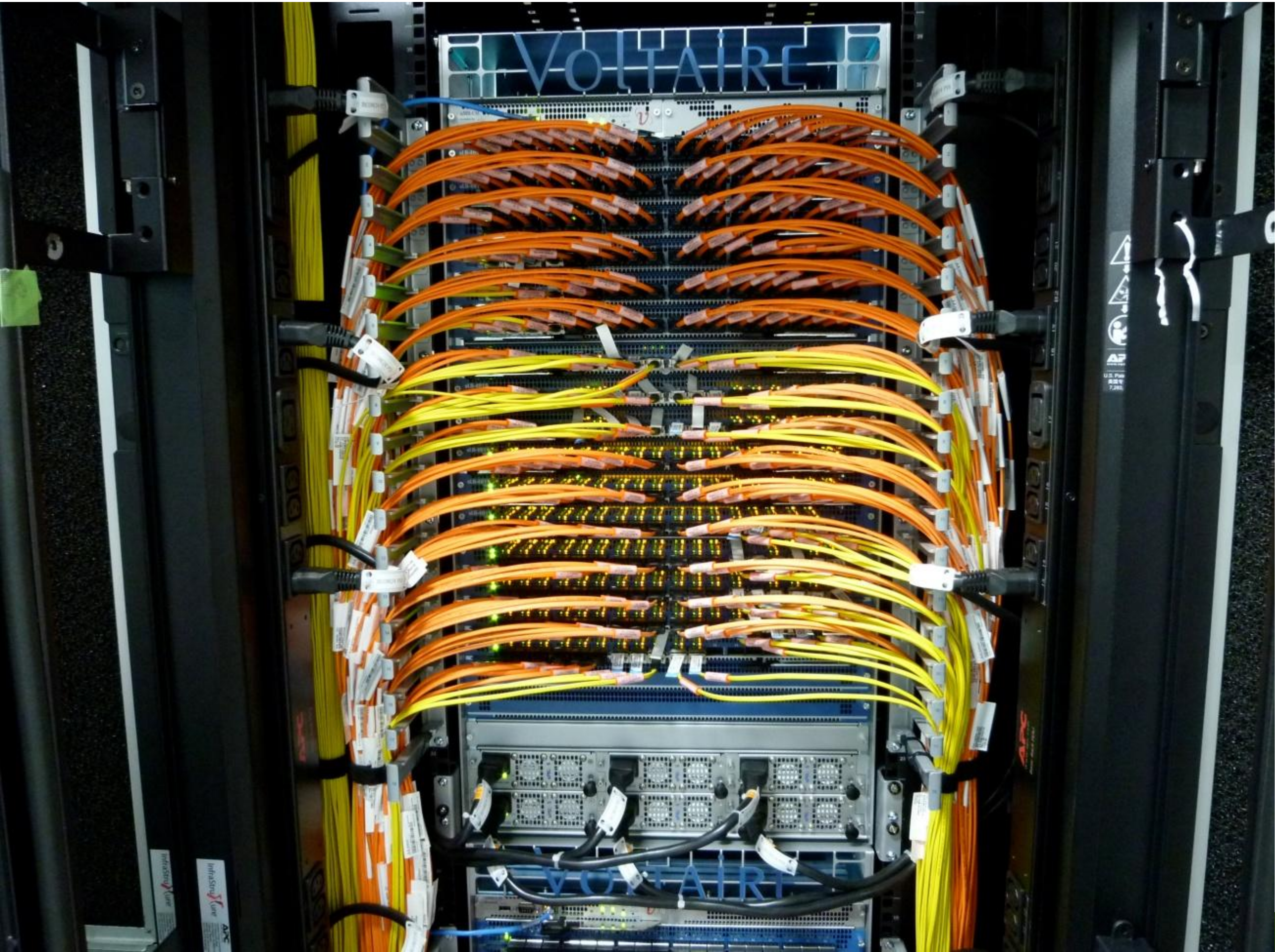
320 x 256 x 64

Mountain Wave Test
NVIDIA Tesla S1070 card

TSUBAME 2.0

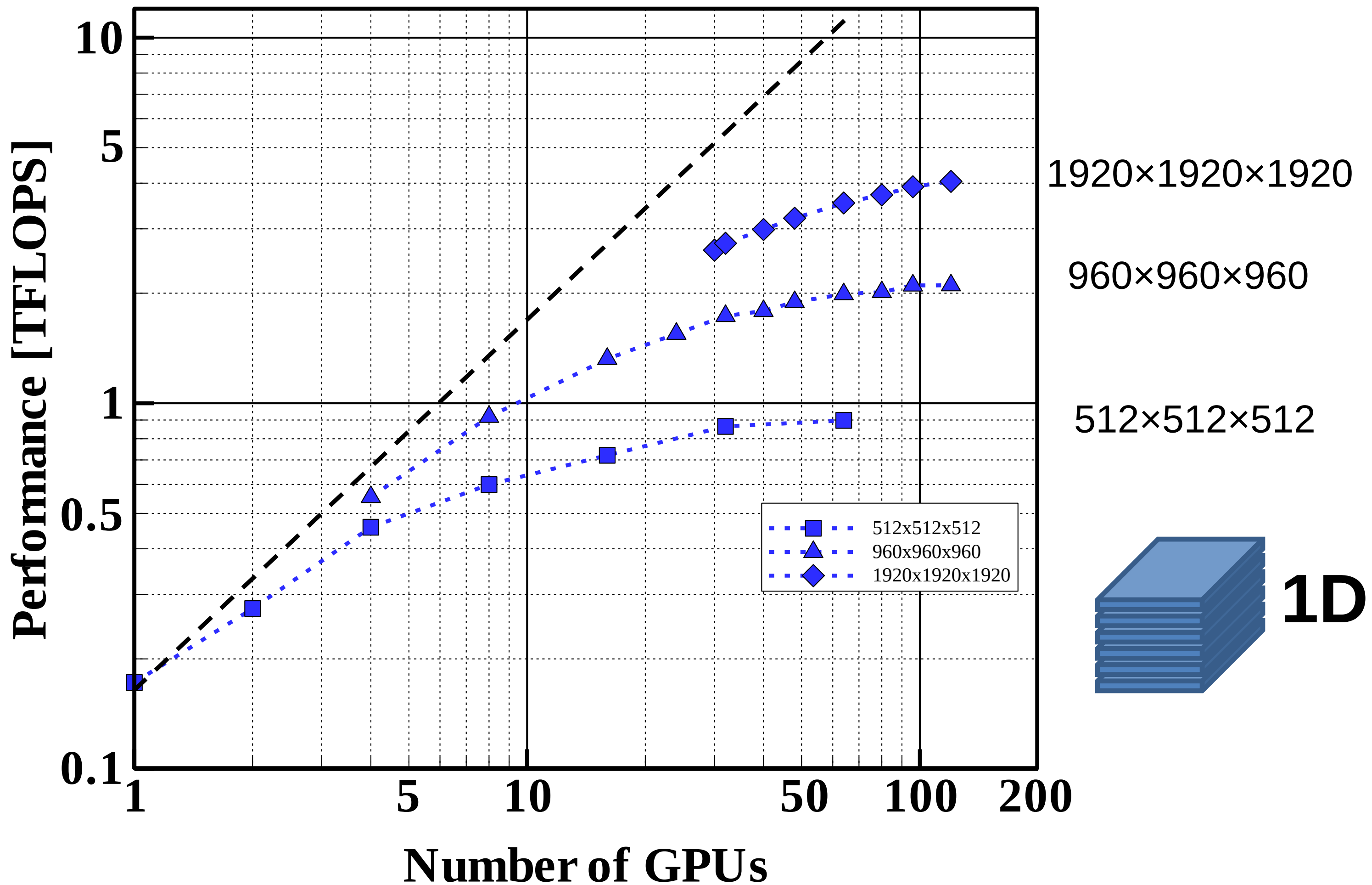
GPU M2050




VOLTAIRE

Multi-GPU Peformance

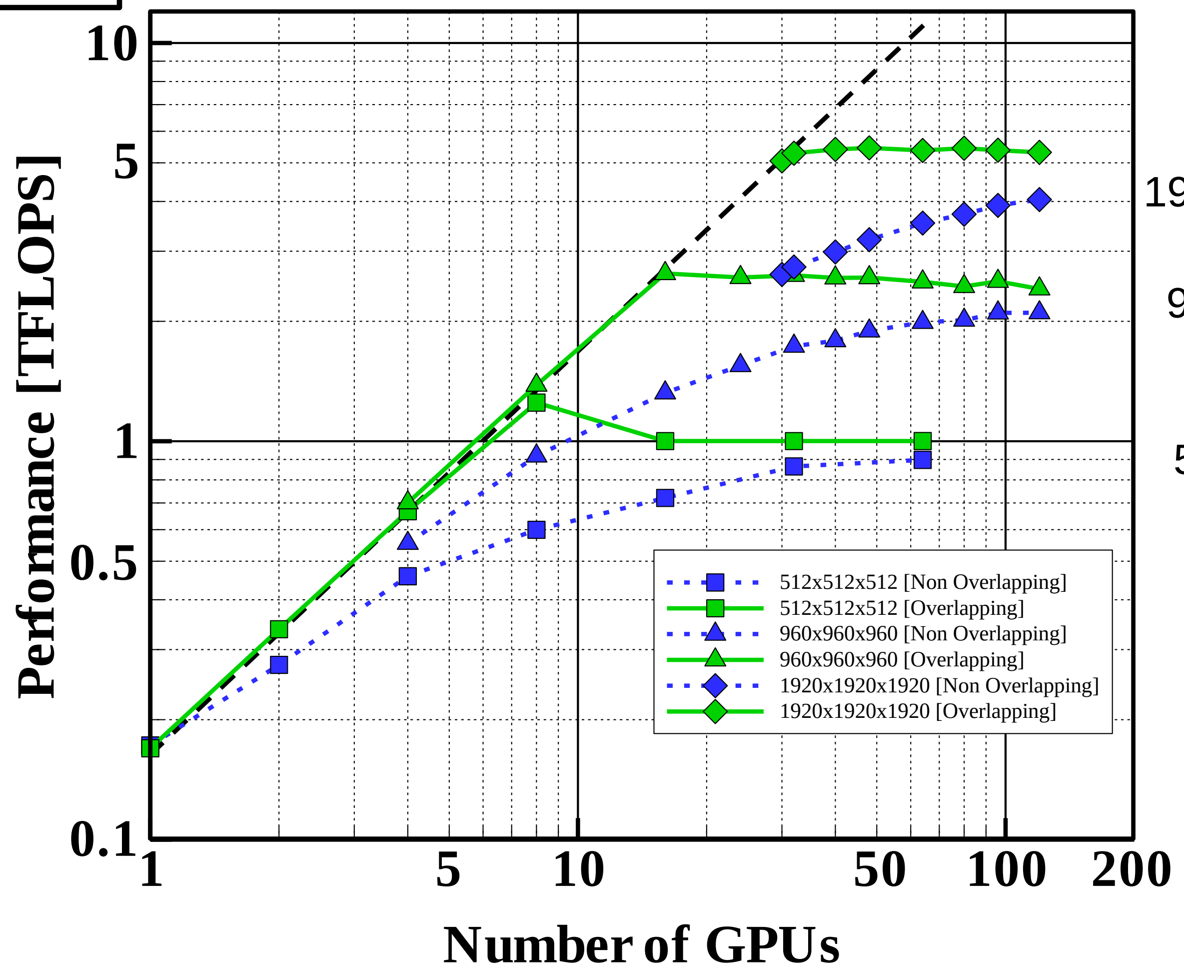
w/o overlapping

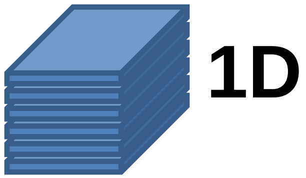


Multi-GPU Peformance

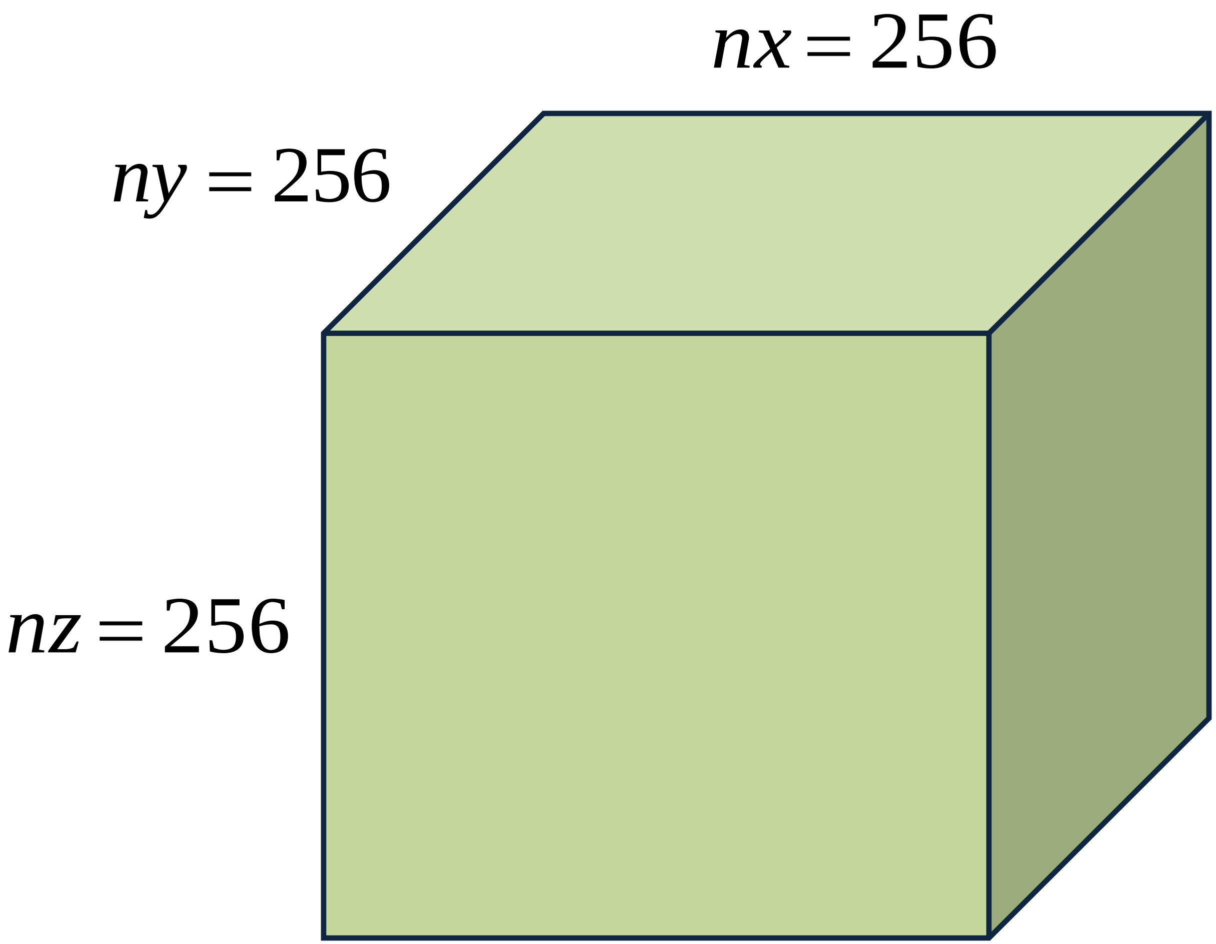
w/o overlapping

2 GPU/node





Thread Assignment



Mesh number
256x256x256

Thread Assignment