2011 Gordon Bell Awarded Peta-scale Applications

Peta-scale Phase-field Simulation for Dendritic Solidification

1 Phase-field Model

The mechanical properties of metal materials largely depend on their intrinsic internal microstructures. The phase-field simulation is the most powerful method known to simulate the micro-scale dendritic growth during solidification in a binary alloy. The phase-field model introduces a continuous order parameter (a phase-field variable) to describe whether the material is solid or liquid.

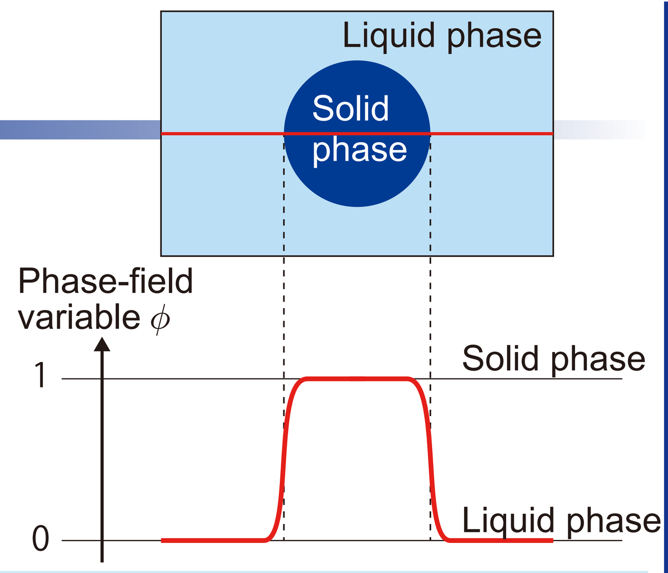


Figure 1: Phase-field variable ϕ

Governing equations

- Time integration of phase field (Allen-Cahn equation)

$$\frac{\partial \phi}{\partial t} = M_\phi \left[\nabla \cdot (a^2 \nabla \phi) + \frac{\partial}{\partial x}\left(a \frac{\partial a}{\partial \phi_x} |\nabla \phi|^2 \right) + \frac{\partial}{\partial y}\left(a \frac{\partial a}{\partial \phi_y} |\nabla \phi|^2 \right) + \frac{\partial}{\partial z}\left(a \frac{\partial a}{\partial \phi_z} |\nabla \phi|^2 \right) - \Delta S \Delta T \frac{dp(\phi)}{d\phi} - W \frac{dq(\phi)}{d\phi} \right]$$

M_ϕ: Mobility
a: Anisotropy
ΔS: Entropy of fusion
ΔT: Undercooling

$$p(\phi) = \phi^3(10 - 15\phi + 6\phi^2)$$
$$q(\phi) = \phi^2(1-\phi)^2$$

- Time integration of solute concentration

$$\frac{\partial c}{\partial t} = \nabla \cdot [D_S \phi \nabla c_S + D_L (1-\phi) \nabla c_L]$$

$$c_S = \frac{kc}{1-\phi+k\phi}, \quad c_L = \frac{c}{1-\phi+k\phi}, \quad k = c_S/c_L$$

D_S: Diffusion coefficient in solid phase
D_L: Diffusion coefficient in liquid phase

Implementation

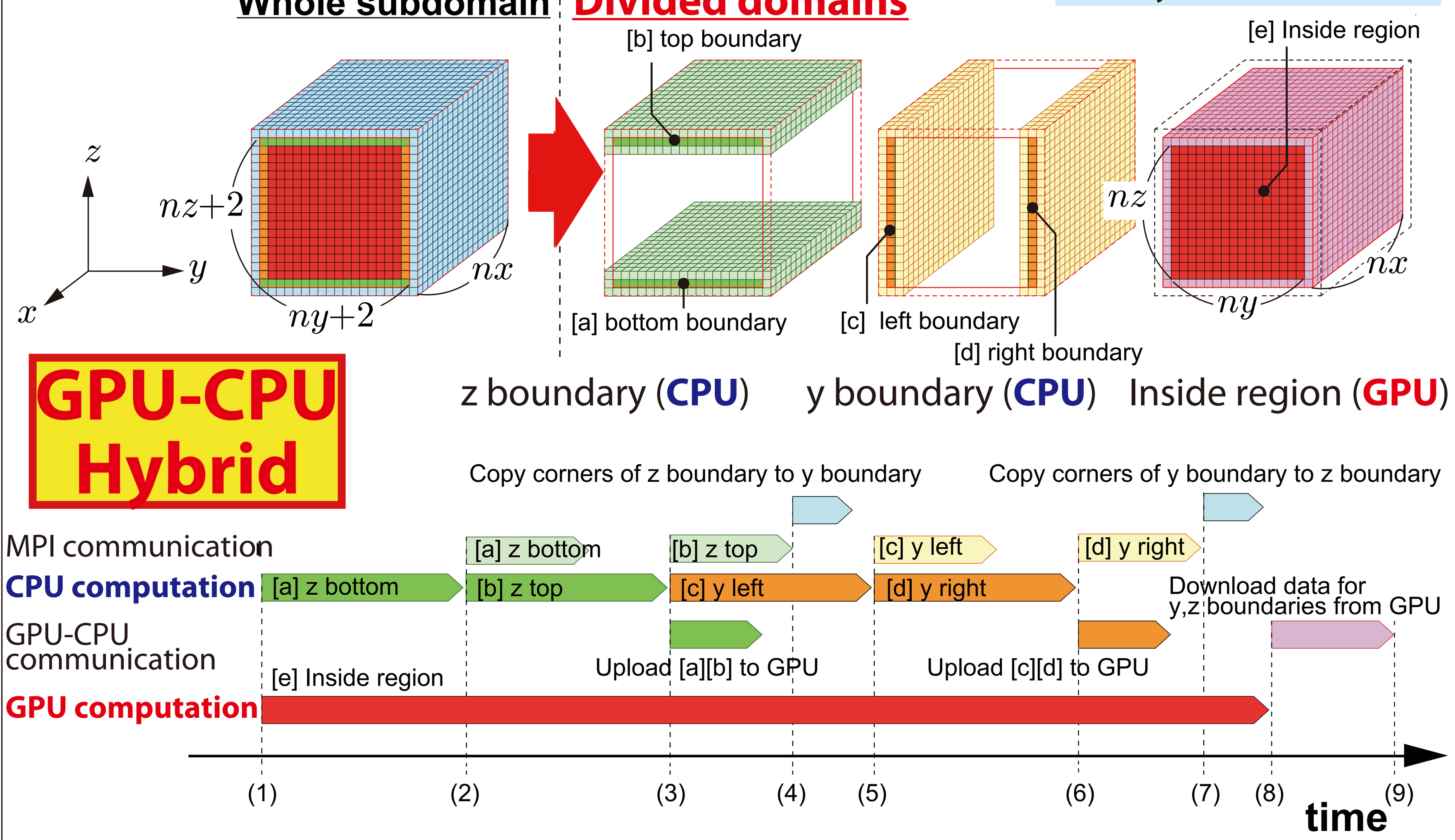


Figure 2: Scheme of the Hybrid-YZ method

ACM Gordon Bell Prize
Special Achievements in Scalability and Time-to-Solution
& SC'11 Technical Paper
"Peta-scale Phase-Field Simulation for Dendritic Solidification on the TSUBAME 2.0 Supercomputer"
T. Shimokawabe, T. Aoki, T. Takaki, A. Yamanaka, A. Nukada, T. Endo, N. Maruyama, and S. Matsuoka,

2 Simulation using TSUBAME 2.0

2.000 PFlops!!! on 4000 GPUs with 16000 CPU cores

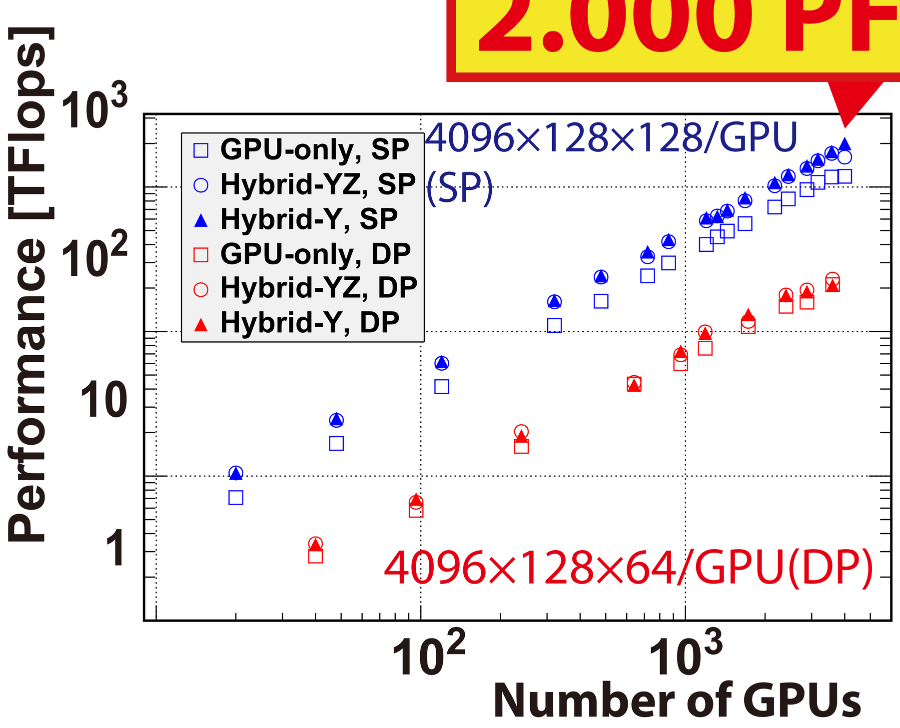


Figure 3: Weak scaling results

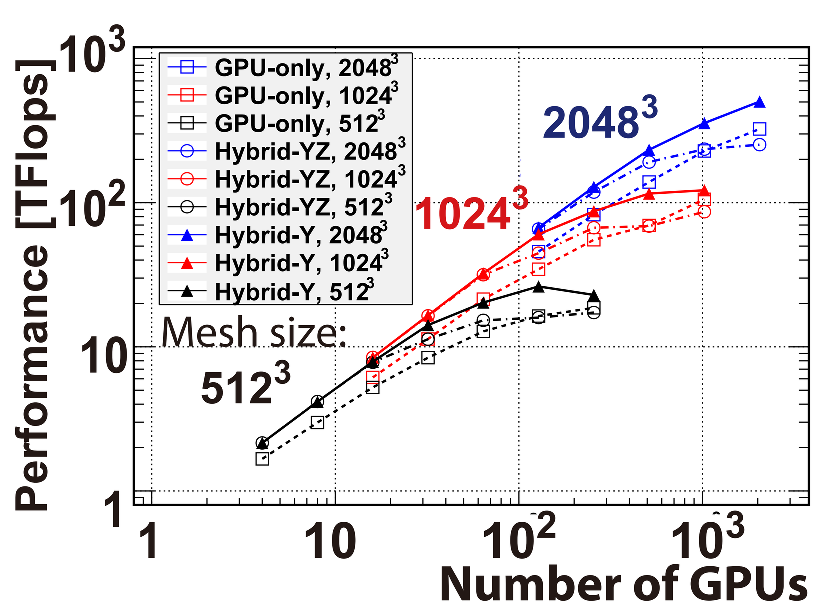
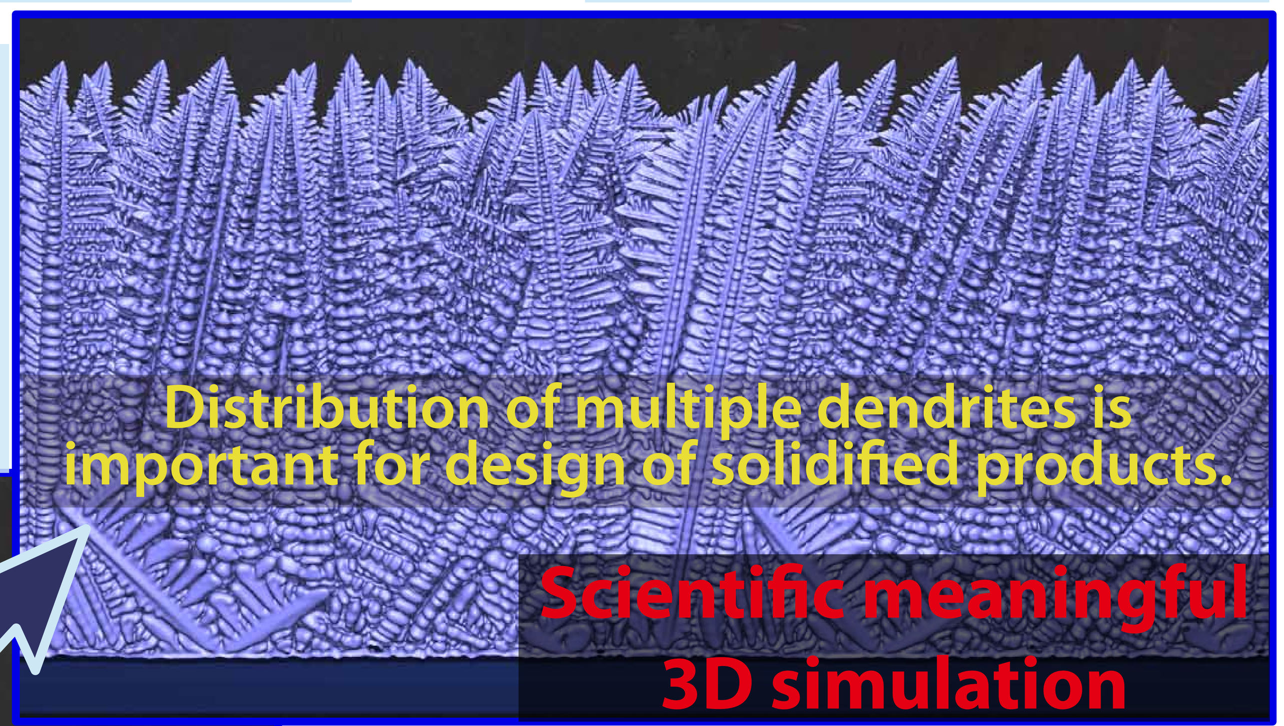
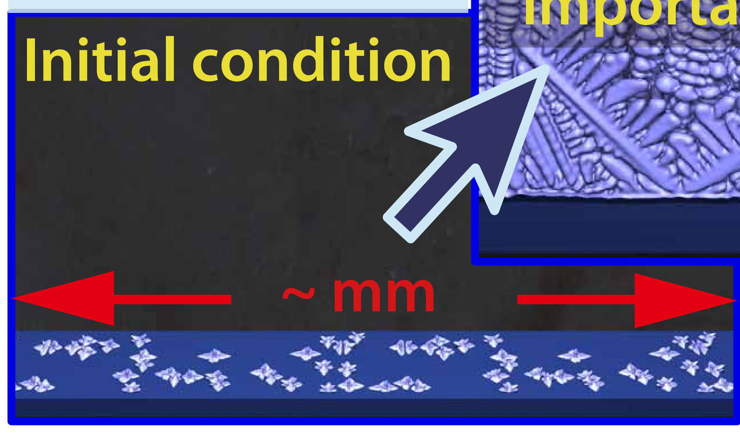


Figure 4: Strong scaling results

Figure 5: Dendritic growth in the binary alloy solidification with $4096 \times 1024 \times 4096$ mesh with 768 GPUs of TSUBAME2.0

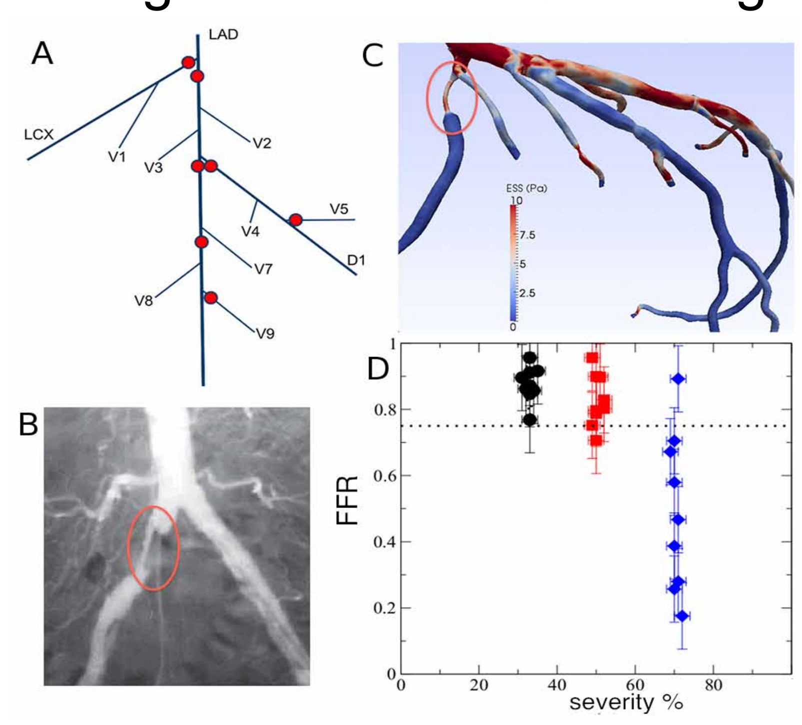




Petaflop Biofluidics Simulations on a Two-Million Core System

Multiscale Computational Hemodynamics

Clinical guidance for determining dangerous plaques

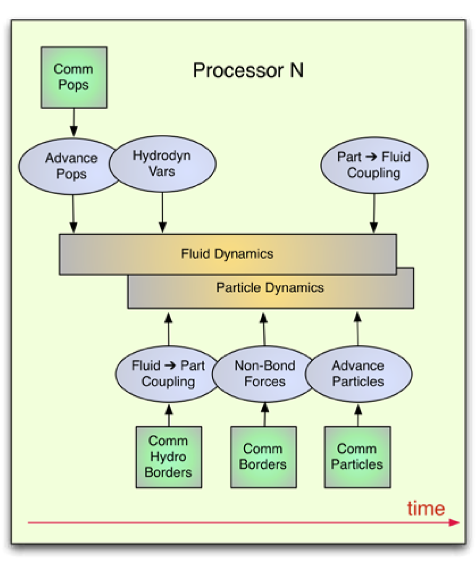


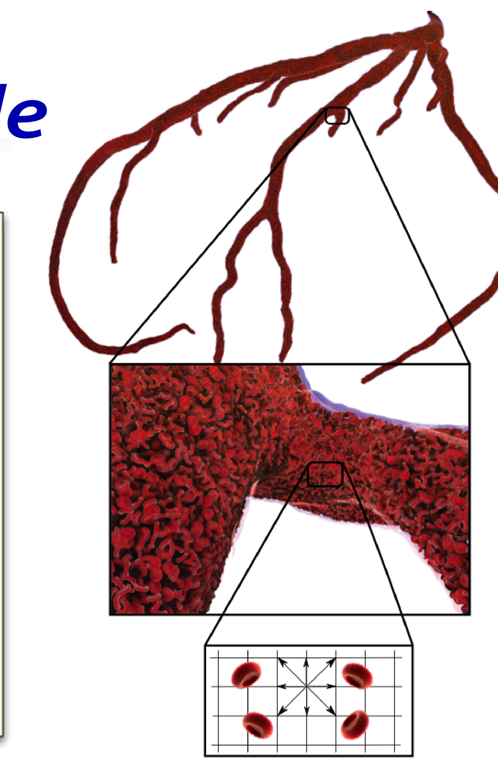
Time to completion is crucial for clinical intervention

HPC is mandatory

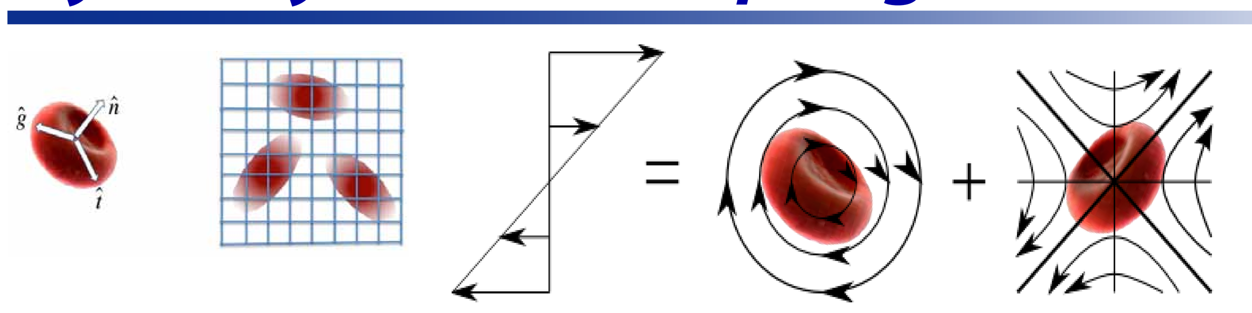
The MUPHY code for Multiscale Hemodynamics

Blood Plasma:
Lattice Boltzmann Method
coupled
Red Blood Cells:
Molecular Dynamics





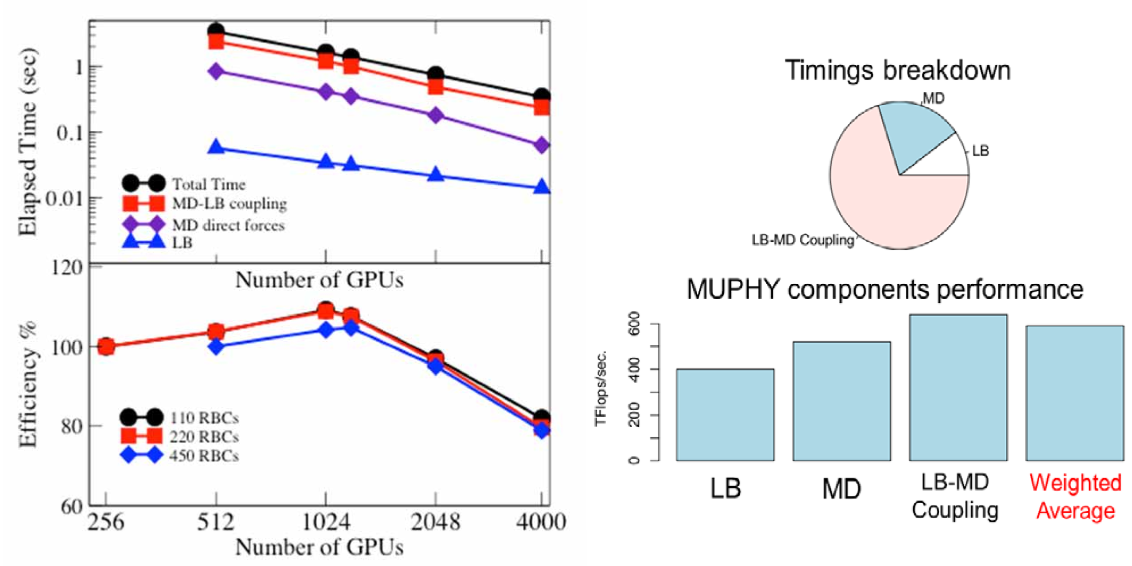
Hydrodynamic Coupling



Tensorial drag
Tank Treading
Complex Rheology

- **Strip off degrees of freedom: O(10) per Red Blood Cell**
- **Complex boundaries via local collisions (no Green's function)**

Performance on 4000GPUs of TSUBAME 2.0



0.6PFlops aggregate performance

Time to sompletion: 3hours

2011 ACM Gordon Bell Prize Honorable Mention
"Petaflop Biofluidics Simulations On A Two Million-Core System"
Massimo Bernaschi, Mauro Bisson, Toshio Endo, Massimiliano Fatica, Satoshi Matsuoka, Simone Melchionna, Sauro Succi

Collaborative work with IAC-CNR, Italy, NVIDIA and Harvard University

http://www.gsic.titech.ac.jp/sc12