A Peta-scale LES (Large-Eddy Simulation) for Turbulent Flows Based on Lattice Boltzmann Method

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TSUBAME 2.0

Compute Node (3 Tesla M2050 GPUs)
Performance: 1.7 TFLOPS
Memory: 58.0GB(CPU) + 9.7GB(GPU)

Rack (30 nodes)
Performance: 51.0 TFLOPS
Memory: 2.03 TB

System (58 racks)
1442 nodes: 2952 CPU sockets, 4264 GPUs
Performance: 224.7 TFLOPS (CPU) ▲ Turbo Boost 2196 TFLOPS (GPU)
Total: 2420 TFLOPS
TSUBAME Supercomputer

2013 Q3 or Q4
All the GPU will be replaced by new accelerators

TSUBAME 2.5 will have 15-17 PFlops in single precision performance.
Drop on dry floor
Industrial Appl.
Steering Oil
Development of New Materials

Mechanical Structure

Low-carbon society

- Improvement of fuel efficiency by reducing the weight of transportation and mechanical structures
- Developing lightweight strengthening material by controlling microstructure
ACM Gordon Bell Prize
Special Achievements in Scalability and Time-to-Solution

Takashi Shimokawa, Takayuki Aoki, Tomohiro Takaki, Akinori Yamunaka, Akira Nakada, Toshio Endo, Naoya Maruyama, Satoshi Matsuoka

Peta-Scale Phase-Field Simulation for Dendritic Solidification on the TSUBAME 2.0 Supercomputer
Weather News
Full GPU Approach: ASUCA

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

J. Ishida, C. Muroi, K. Kawano, Y. Kitamura, Development of a new nonhydrostatic model “ASUCA” at JMA, CAS/JSC WGNE Reserch Activities in Atmospheric and Oceanic Modelling.
ASUCA Typhoon Simulation
500m-horizontal resolution 4792 x 4696 x 48
Using 437 GPUs
Lattice Boltzmann Method

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

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

Strongly Memory Bound Problem:

Collision step:  
Streaming step:

\( i \) is the value in the direction of \( ith \) discrete velocity  
\( \mathbf{e}_i \) is the discrete velocity set;  
\( w_i \) is the weighting factor  
\( c \) is the particle velocity  
\( \mathbf{u} \) is the macroscopic velocity
LES (Large-Eddy Simulation)

\[ f_i(x + c_i \Delta t, t + \Delta t) = f_i(x, t) - \frac{1}{\tau_*} (f_i(x, t) - f_i^{eq}(x, t)) + F_i \]

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

Energy spectrum

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LES modeling

- Simple
- \(\Delta\) inaccurate for the flow with wall boundary
- \(\Delta\) empirical tuning for the constant model coefficient

\[
\tau_{ij} = -2\nu_{SGS} S_{ij}
\]
\[
\nu_{SGS} = C\Delta^2 |S| \quad \text{\(C : \text{const}\)}
\]

- applicable to wall boundary
- \(\Delta\) complicated calculation
- \(\Delta\) average process over the wide area
- \(\rightarrow\) not available for complex shaped body
- \(\rightarrow\) not suitable for large-scale problem

\[

L_{ij} = \bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j
\]
\[
M_{ij} = 2\Delta^2 |\bar{S}| \bar{S}_{ij} - 2\Delta^2 |\bar{S}| \bar{\bar{S}}_{ij}
\]

\[
\nu_{SGS} = C\Delta^2 |S| \rightarrow \text{model coefficient determined by the second invariant of the velocity gradient tensor}
\]

- \(\Delta\) model coefficient
- \(\circ\) applicable to wall boundary
- \(\circ\) model coefficient is locally determined.

\[
C = C_1 |F_{CS}|^{3/2}
\]

\[
F_{CS} = \frac{Q}{E} = \frac{-1}{2} \frac{\partial \bar{u}_j}{\partial x_i} \frac{\partial \bar{u}_i}{\partial x_j} \quad E = \frac{1}{2} \left( \frac{\partial \bar{u}_j}{\partial x_i} \right)^2
\]

\((-1 < F_{CS} < 1)\)
LES modeling on LBM

Turbulence model:

\[ v_\ast = v_0 + v_t = \frac{1}{3} \left( \tau_\ast - \frac{1}{2} \right) c^2 \delta_t = \frac{1}{3} \left( \tau_0 + \tau_t - \frac{1}{2} \right) c^2 \delta_t, \quad v_t := \frac{1}{3} \tau_t c^2 \delta_t, \]

Molecular viscosity + eddy viscosity

\[ v_t = (C_S \Delta_x)^2 \bar{S} \]

Smagorinsky model subgrid closure

\[ C_S = 0.22 \]

\[ \bar{S}_{ij} = \frac{1}{2} \left( \partial_j \bar{u}_i + \partial_i \bar{u}_j \right) \quad \bar{S} = \sqrt{2 \sum_{i,j} \bar{S}_{ij} \bar{S}_{ij}} \]
Coherent-structure SGS model

Dynamic Smagorinsky model (DSM)
DSM requires to take an average operation for a wide area to determine the model parameter.

\[ \nu_{SGS} = C \Delta^2 |S| \]
\[ C = \frac{<L_{ij}L_{ij}>}{<M_{ij}M_{ij}>} \]
\[ L_{ij} = \tilde{u}_i \tilde{u}_j - \hat{u}_i \hat{u}_j \]
\[ M_{ij} = 2 \Delta^2 |\tilde{S}| \tilde{S}_{ij} - 2 \Delta^2 |\hat{S}| \hat{S}_{ij} \]
\[ < > : \text{average operation} \]

Coherent-structure Smagorinsky model
The model parameter is locally determined by the second invariant of the velocity gradient tensor.

\[ \nu_{SGS} = C \Delta^2 |S| \]
\[ C = C_1 |F_{CS}|^{3/2} \]
\[ F_{CS} = \frac{Q}{E} \]

- Automatically determine model coefficient
- Turbulent flow around a complex object
- Computational efficiency is poor

Second invariant of the velocity gradient tensor (Q) and Energy dissipation (ε)
Computational Area

Major part of Tokyo
Including Shinjuku-ku, Chiyoda-ku, Minato-ku, Meguro-ku, Chuou-ku,

10km ⎯ 10km

Building Data:
Pasco Co. Ltd.
TDM 3D

Map ©2012 Google, ZENRIN
Area Around Metropolitan Government Building

Flow profile at the 25m height on the ground

Wind

960 m

640 m

地图データ ©2012 Google, ZENRIN

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Performance of the GPU code

Performance estimation by using Improved Roofline Model

* CUDA Programming Tuning
  Using SFU (Special Function Unit) and single precision computation

Kernel fusion of the collision step and streaming step

Loop unrolling to save register usage

+ Reduction of the address calculation by use of a 32-bit compile option

32bit compile
198 GFlops (efficiency 92%)
310 MLUPS
(Mega Lattice site Updates /sec)

64bit compile
183 GFlops (efficiency 88%)
Performance (Strong Scalability)

- For the fixed problem size, the performances are shown with increasing the number of GPUs. By introducing the overlapping technique, the performance is improved up to 30%.

- It is found that the elapsed time is shortened by increasing GPUs.
Performance (Weak Scalability)

600 TFLOPS on 4000 GPUs

15% of the peak performance
Turbulent Flow behind football

Re = 100,000

Mesh:
2000x1000x1000
DriVar: BMW-Audi

3,000x1,500x1,500
Re = 1,000,000
SUMMARY

- Lattice Boltzmann LES turbulent simulation has been successfully conducted with 1-m resolution for 10km x 10km area by using the whole TSUBAME 2.0 resource.

- Coherent-Structure Smagorinsky model works well in association with LBM.

- The performance of 15% has been achieved on TSUBAME 2.0.
Thank you
for your kind attention