Application of HPC-CFD for Industrial Problems on the K Computer and toward Fugaku

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Backgrounds and Motivations
How HPC can change the industrial CFD?

- **High-resolution turbulence simulation**
  - Higher time resolution realizing the unsteady simulation, capturing the transient phenomena.
  - Higher spatial resolution realizing the highly accurate simulation, independent on turbulence modeling.

- **Coupled analysis realizing real-world simulation**
  - Application of CFD to what conventional experiments are difficult to treat.
  - Coupling simulation of fluid motion with other physics such as structure deformation/vibration, heat and mass transfer, or aero-acoustics.

- **Big data analysis**
  - Optimization, Machine/Deep learning based on AI technique.
Backgrounds and Motivations

FrontFlow/red-HPC on the K computer

- **Unstructured** Finite Volume Method.
  - Most popular and conventional data structure in industry.

- **Hybrid OpenMP/MPI** for HPC.

- **Single node performance.**
  - Thread parallelization by OpenMP.
  - 9.5%/7.4% for hexa/tetra-hedral elements.

- **Parallel efficiency.**
  - Domain decomposition by application “METIS”.
  - MPI among nodes.
  - 96.5% parallelization efficiency (weak scaling).

- Up to 10 billion unstructured meshes on 10,000 nodes (80,000 cores) on the K-computer.

- Various moving boundary methods including ALE.
Success of the Unstructured CFD on the K Computer

- Precise prediction of aerodynamic forces comparable to wind-tunnel measurements.
  - The key is the surface resolution of less than 1mm.

- Real-World Aerodynamics Simulation.
  - Coupled with 6DoF vehicle motion and driver’s reaction.

- Successful from the view point of academic research, but…
Backgrounds and Motivations
Surface Clean-up for Mesh Generation

- Industrial CAD is always very dirty...
- Higher resolution requires very long time for CAD clean-up.
- Resolution of less than 1mm surface is not realistic in industries.

- Red: gap
- Cyan: overlap

Surface repair by 5mm resolution using conventional wrapping technique (ANSA(R))

Surface repair by 1mm resolution
Conventional wrapping technique does not work...

Original CAD data
Numerical Methods

CUBE: Building Cube Method for Unified Simulation

- **Hierarchically structured** Finite Volume Method
  - A solver for coupled phenomena: fluid/structure/acoustics/chemical reaction...
  - **Building Cube Method** for the unified data structure (Nakahashi et al., 2003)
    - Easy tune for both single node and parallel performance
  - **Immersed Boundary Method** (Fadlun et al., 2002)
    1. Dirty CAD treatment (Onishi et al., 2013)
    2. Moving Boundary Method (Bale et al., 2016)
    3. Unified Compressible/Incompressible analysis (Li)
    4. Unified Fluid/Structure analysis (Nishiguchi)

Domain decomposition by different size of cubes

Allocation of meshes for each cube
Numerical Methods
Performance on the K computer

- Single node performance.
  - $16 \times 16 \times 16$ cells per cube.
  - 23.7% on the K computer (8 threads).

- Parallel efficiency.
  - 16 cubes per node.
  - Effective parallelization ratio: 99.99954%.
  - 75.324899% parallel efficiency (weak scaling).
    - Total nodes on the K computer

- Expected to be **25 times** faster on Fugaku

<table>
<thead>
<tr>
<th></th>
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<tbody>
<tr>
<td>$4 \times 4 \times 4$</td>
<td>64</td>
<td>262,144</td>
</tr>
<tr>
<td>$8 \times 8 \times 8$</td>
<td>512</td>
<td>2,097,152</td>
</tr>
<tr>
<td>$16 \times 16 \times 16$</td>
<td>4,096</td>
<td>16,777,216</td>
</tr>
<tr>
<td>$32 \times 32 \times 32$</td>
<td>32,768</td>
<td>134,217,728</td>
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<tr>
<td>$64 \times 64 \times 64$</td>
<td>262,144</td>
<td>1,073,741,824</td>
</tr>
<tr>
<td>$128 \times 128 \times 128$</td>
<td>2,097,152</td>
<td>8,589,934,592</td>
</tr>
</tbody>
</table>
Numerical Methods

Full-scale vehicle aerodynamics simulation

- World-largest full-scale vehicle simulation (27 billion meshes).

- Maximum of 27 billion meshes with 0.7 mm resolution within 1 hour from the dirty CAD data.

<table>
<thead>
<tr>
<th>Condition</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Finest grid size</td>
<td>0.763 [mm]</td>
</tr>
<tr>
<td>Num. of cells</td>
<td>26,893,365,248</td>
</tr>
<tr>
<td>Grid generation time</td>
<td>About 20 min.</td>
</tr>
<tr>
<td>Pre-flow computational time (immersed boundary preparation)</td>
<td>About 30 min.</td>
</tr>
<tr>
<td>Delta t</td>
<td>$1.0 \times 10^{-6}$ [s]</td>
</tr>
<tr>
<td>Solution time</td>
<td>0.010 [s]</td>
</tr>
<tr>
<td>Parallel num.</td>
<td>273,576 cores (37,197 nodes)</td>
</tr>
<tr>
<td>Flow computation time</td>
<td>Several days</td>
</tr>
</tbody>
</table>
Capacity Computing for Shape Optimization

Multi-Objective Shape Optimization

- **4 objectives** (0° and -3° yaws)
  - Drag and Lift at 0 yaw
  - Delta Drag (difference bet. 0 and -3)
  - Delta Lift (difference bet. 0 and -3)
  - Smaller is better for all four variables

- **8 design parameters**

- Multi-objective Genetic Algorithm
  - 18 models for each generation

Geometry

STL format

Aerodynamic characteristics (Objective function)

Shape parameters (Design variables)
Capacity Computing for Shape Optimization

Results of multi-objective shape optimization

- Genetic Optimization until 12\textsuperscript{th} generations.
- Tradeoff between some objective functions such as $C_d$ and $\Delta C_d$. 

\begin{align*}
C_d & \quad \Delta C_d \\
\Delta C_d & \quad C_L
\end{align*}
Real-World Simulation
Narrow band noise from a full-scale vehicle

- Acoustic feedback noise generated at a small gap.
- Very peaky and uncomfortable...
- For the prediction, full coupling simulation of flow and acoustics is needed.

<table>
<thead>
<tr>
<th>Grid size</th>
<th>0.2 mm/1.6mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cube num.</td>
<td>471,059</td>
</tr>
<tr>
<td>Cell num.</td>
<td>1,929,457,664</td>
</tr>
<tr>
<td>Core num.</td>
<td>13086x8 / 50 hrs</td>
</tr>
</tbody>
</table>
Real-World Simulation Coupled Aerodynamics, Vehicle Motion and Driver’s Reaction Simulation

- HPC-CFD for flow around a vehicle (Aerodynamics)
- Multi-Body vehicle motion analysis (6DoF body motion with suspension and steering)
- Autonomous Vehicle Motion by a Driver’s steering wheel, accelerator/braking actions
- Lane changing motion at 100km/h
Toward FUGAKU
Coupling Data Science and HPC-CFD for Innovative CAE

- Innovative Industrial CAE Solution by a Fusion of Data Science and High-Performance Computing Simulation

- Machine/Deep Learning, Data Assimilation, Multi-Objective Optimization...
  - **Surrogate Model**: Realizing real time evaluation of aerodynamic performance such as drag and lift force.
  - **Reduction Model**: Realizing complicated real world simulation and reproducing flow field at lower cost.

![Image showing Surrogate Model, Neural Network, Reduction Model by Proper-Orthogonal Decomposition, Real Time Performance Prediction, Digital Twin, Physical Space, Cyber Space, Co-operation design, Multi-objective optimization, Virtual on-road test, Training AI for automatic driving]
Toward FUGAKU
Shape Optimization based on a Surrogate Model

- Development of a Surrogate Model based on Neural Network.
  - Hundreds of HPC-CFD results as teaching data.
  - Prediction of Drag less than 5% error against the HPC simulation results.

- Coupling the Surrogate Model with Multi-Objective Genetic Algorithm.
  - AI proposes high-performance vehicle shape.

Low emission car (Lowest CD)

High crosswind stability car (Lowest ΔCd)
**Toward FUGAKU**

**Reduction Model of the Navier-Stokes Simulation**

- Reduced order model by Proper-Orthogonal Decomposition.
  - Full flow simulation results are projected on the reduced base functions.

\[
u(x, t) = \sum_{j=0}^{r} a_j(t) \varphi_j(x)
\]

\[
\frac{da_i}{dt} = \sum_{j=0}^{r} \sum_{k=0}^{r} F_{ijk} a_j a_k + \sum_{j=0}^{r} G_{ij} a_j,
\]

\[
F_{ijk} = - \langle \varphi_i, \varphi_j \cdot \nabla \varphi_k \rangle,
\]

\[
G_{ij} = \frac{1}{Re} \langle \varphi_i, \nabla^2 \varphi_j \rangle, \quad i = 1, \ldots, r.
\]

- The base functions are obtained by Neural Network (Murata).

**Inner product**

\[
\mathcal{F}_{\text{dec1}}[x] = \varphi_1 x
\]

**Scaling**

\[
\mathcal{F}_{\text{dec2}}[x] = \varphi_2 x
\]

**Summation**

\[
P x = \sum_{k=1}^{2} \varphi_k \varphi_k^T x
\]

**Full-NS simulation**

\[
\mathcal{F}_{\text{enc}}[x] = \begin{pmatrix} \varphi_1^T x \\ \varphi_2^T x \end{pmatrix}
\]

10,000 samples
2,000 epochs

\[a_0(t)\varphi_0(x)\]

\[a_1(t)\varphi_1(x)\]

\[a_2(t)\varphi_2(x)\]

\[a_3(t)\varphi_3(x)\]

\[a_5(t)\varphi_5(x)\]
Concluding Remarks

- CFD use in industries are conservative, which is just an alternative to conventional experiments, so far...
- HPC expands the possibility of CFD by exceeding their accuracy and applying to real-world problems, while data structure is the key to massively utilize HPC environment.
- Hierarchically structured data realized very fast and real-world aerodynamics simulation on the K computer.
- Coupling data science and HPC simulation will create next-generation Computer-Aided Engineering on FUGAKU.
  - Surrogate model for real time evaluation.
  - Reduction model for real world simulation.
Thanks to Industrial Partners

Consortium for next-generation Automotive CAE using HPC (Nov., 2017~)

Consortium for Combustion System CAE (April, 2018~)

Consortium for Construction CFD for Wind-Resistance