Contribution of Supercomputer “Fugaku” for the Fight against COVID-19
~ Droplet/Airborne Simulation as an Example~

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“Research Infrastructures Mobilization in Response to COVID-19: Lessons Learned”
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RIKEN Center for Computational Science (R-CCS)

- RIKEN is Japan’s largest comprehensive research institution under the jurisdiction of the Ministry of Education, Culture, Sports, Science and Technology (MEXT).
- Developing and operating Japan’s Flagship supercomputer since 2011.
  - K computer (10 PFLOSP): 2012~2019
  - Supercomputer Fugaku (488 PFLOPS): 2021~
- Implementing the newest research that integrates “simulation”, “big data analysis”, and “AI” through high performance computing to solve scientific and social issues and to bring about revolutionary development of our society.
HPC Infrastructures and “Fugaku”

- High-Performance Computing Infrastructures supporting various scientific fields.
  - 158,976 nodes with peak performance of 488PFLOPS
- “Fugaku” means Mt. Fuji, representing the very high peak performance and very wide area of its applications.
- During the development of Fugaku, priority area selected for the software development:
  - Health and longevity
  - Disaster prevention and climate problems
  - Energy
  - Industrial competitiveness
  - Basic science
Fugaku’s Response to COVID-19

- **Top-down and rapid reaction to COVID-19 crisis.**
  - In April 7th, 2020, MEXT and RIKEN R-CCS decided to utilize its resources for COVID-19 research, and projects were adopted by open call.
    - Still in test run at that time (only 70% access and full installation was in May 13th.)
    - Two more projects accepted accordingly (droplet simulation and genetic analysis)
    - Shared use started from March 9th, 2021.

- **Access to “Fugaku” is fully on-line!**
  - Social lock-down is not critical for scientists utilizing IT infrastructures.
  - Physical access to R-CCS has been strictly restricted.

- **Research results promptly open to public through the media.**
  - Lectures to the press held once for one to two months supported by Public Relations Department of R-CCS.
Fugaku’s Fight against COVID-19
– Prompt response to social demands in the Society 5.0 era –

Exploring new drug candidates for COVID-19

Molecular dynamics calculations to identify therapeutic drug candidates for the target proteins of COVID-19 from approximately 2,000 existing drugs.

(Yasushi Okuno, RIKEN / Kyoto University)

Prediction of conformational dynamics of proteins on the surface of SARS-CoV-2

Atomistic molecular dynamics simulations of the spike protein in solution to predict experimentally undetectable dynamic structures on the surface of COVID-19.

(Yuji Sugita, RIKEN)

Fragment molecular orbital calculations for COVID-19 proteins

Fragment molecular orbital calculations on COVID-19 proteins for the detailed interaction analyses.

(Yuji Mochizuki, Rikkyo Univ.)

Prediction and Countermeasure for Virus Droplet Infection under the Indoor Environment

Coupling simulation of virus droplet scattering with airflow and heat transfer under the indoor environment of such as a commuter train, offices, classrooms and hospital rooms, for the infection risk evaluation and its countermeasure.

(Makoto Tsubokura, RIKEN / Kobe University)

Simulation analysis of pandemic phenomena

Simulations of disease propagation and economic activities for the estimations of possible future of our social and economic activities, and policy options to control and resolve the situation.

(Nobuyasu Ito, RIKEN)

Host genetic analysis for severe COVID-19 cases

Performing whole-genome sequencing of severe cases of COVID-19 and mild or asymptomatic infections, and identifying risk-associated genetic variants for severe disease.

(Satoru Miyano, Tokyo Medical and Dental University)
Droplet/Airborne Simulation

Unscientific fear and unfounded contempt against infection

Lack of scientific data for new diseases

High-precision simulation and visualization of droplet dispersion utilizing overwhelming computer resources to handle a large number of infection situations

Enlightening society with a correct understanding of droplet/airborne infections and prevention

Contributing to the formulation and revision of guidelines by providing scientific data, in collaboration with government agencies
Complex Unified Simulation Framework: CUBE

- Simulation software developed at R-CCS since 2012.
- Developed through tight collaboration with industry for complicated fluid/structure/thermal interaction problems.
- Internal combustion engine simulation module utilized for the droplet/aerosol simulation.

IC engine simulation on the K-computer and fuel droplet dispersion

Viral droplet/aerosol simulation on Fugaku
High-precision, -speed, multi-case analysis handled by “Fugaku”

- Concert hall
- Chorus activity
- Taxi
- Face masks for sports activity
- Karaoke box room
- Social distance while walking
- Double face masks
- School room ventilation
- On-dining risk
- Airplane cabin
- Small pub restaurant
- Commuter bus
- Commuter train
- Partitions in the office
- Taxi
- Conductor hall
- Chorus activity
- Face masks for sports activity
- Karaoke box room
- Social distance while walking
- Double face masks
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- Commuter bus
- Commuter train
- Partitions in the office
Academia-Industry-Government Collaboration

Steering members

National Univ. of Singapore

Cooperative members

Administrative organizations

Kobe
Concluding Remarks

- Fugaku’s fight against COVID-19.
- IT research infrastructures are quite powerful for COVID-19, because physical access is not necessary and lock-down is not critical.
- Top-down and rapid reaction to COVID-19 crisis.
- Research results promptly open to public through the media.
  - Droplet/aerosol simulation reported through more than 300 TV/radio, 250 newspapers, and 1150 web news.
- Currently tight collaboration with government agencies like cabinet office and some ministries to establish or modify the guidelines for starting or restricting social activities.
- Fugaku’s current resource distribution plan.

<table>
<thead>
<tr>
<th>Academic use (40%)</th>
<th>Priority issues (40%)</th>
<th>Industrial use (10%)</th>
<th>R-CCS (10%)</th>
<th>Political priority (add.)</th>
</tr>
</thead>
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100%
Eulerian Air and Lagrangean Spray Coupling

**Flow Solver**

**Eulerian Mesh**

**Conservation Equations**

**Navier-Stokes**

\[
\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F} = S,
\]

\[
S_{\rho_{f,k}} = -\frac{1}{\Delta V} \sum_n \frac{d m_{d,k}}{d t}
\]

**Species transport**

\[
\frac{d x_d}{d t} = u_d, \quad \frac{d u_d}{d t} = \frac{6 \rho_g}{8 d_d \rho_d} |\mathbf{u} - \mathbf{u}_d|
\]

\[
C_d = \begin{cases} 
0.424 & \text{Re}_p > 1000 \\
24 \left( 1 + \frac{1}{6} \text{Re}_p^{2/3} \right) & \text{Re}_p \leq 1000 
\end{cases}
\]

\[
\text{Re}_p = \frac{\rho_g |\mathbf{u} - \mathbf{u}_d| d_d}{\mu}
\]

**time stepping**

**Lagrangian Particles**

**Spray equations**

**Particle tracking**

**Drag Model**

\[
\frac{d T_d}{d t} = \frac{Nu}{3 Pr} \left( \frac{c_p}{c_l} \right) \frac{f_2}{f_d} (T - T_d) \frac{1}{m_d} \left( \frac{d m_d}{d t} \right) \frac{L_V}{c_{p,d}}
\]

**Evaporation Model**

\[
\dot{m}_d = \frac{m_d}{\tau_d} \left( \frac{Sh}{3 Sc} \right) \ln (1 + B_M)
\]

\[
B_M = \frac{Y_{V,S} - Y_V}{1 - Y_{V,S}}
\]

\[
\tau_d = \frac{\rho_d a_d^2}{18 \mu}
\]

Wall Reflection Model

<table>
<thead>
<tr>
<th>Regime transition state</th>
<th>Critical Weber number</th>
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<tbody>
<tr>
<td>Adhesion (stick/spread) → splash</td>
<td>( \text{We}_c = 2630 \cdot \text{La}^{-0.183} )</td>
</tr>
</tbody>
</table>

(a) STICK

(b) BOUNCE

\[
\text{We} = \rho V_{d}^2 d_l / \sigma \quad \text{La} = \rho \sigma d_l / \mu^2
\]