Wrap-up Meeting Group C

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Software Defined Systems on HPC using Containers

- Complexity of HPC systems and diversity of software stacks i.e. libraries and tools have been increased although exa-scale computing becomes essential to solve most problems in genomics, environmental sciences, energy and manufacturing.
- Software-defined systems (SDS) will address these challenging issues by building a computing environment on HPC equivalent to other platforms using Linux containers. All dependencies and configurations needed to run applications are included in a software stack as a container image and HPC container tools such as Singularity from Lawrence Berkeley National Lab and Shifter from National Energy Research Scientific Computing Center along with multi-kernel (McKernel/mOS) development from RIKEN AICS might be used for post-K computer that solves science problems i.e. atmospheric science and plasma simulation with better performance and easier software management than the current systems.

Kenta Sueki

- Back ground
 - Scientist of meteorology
- What I want to do?
 - To investigate unrevealed structure of atmosphere and mechanism of various kinds of atmospheric phenomena
- Why I should use HPC
 - For realistic simulation of atmosphere
 - For high-resolution idealized numerical experiment of atmospheric phenomena
- Contribution to our society
 - Accurate weather forecasting for disaster reduction
 - Prediction of climate change

Brief introduction of my research

• Analysis of high-resolution simulation of clouds





83.5F 84F 84.5F

85.5F



5×101

- 5×10°

- 5×10⁻¹

- 5×10⁻²

Regional simulation (Not global)



- Fine scale structure of clouds can be simulated
- Statistical characteristics of convective clouds is now investigated

Future perspective

- Higher resolution
 - More realistic structure can be simulated
- Wider domain size and longer integration time
 - More reliable statistical analysis



Miyamoto et al. (2013)

Global clouds simulation with horizontal resolution of 870m

- Many variables to be solved (wind, temperature, density, water...)
- Other physical processes (cloud processes, radiation, ocean, land...)

> If we perform global **200-m** simulation, we need **exa-scale**!

University of Tsukuba barotropic general circulation model

(Tanaka 1991,1998)

$$\frac{dw_i}{d\tau} + i\sigma_i w_i = -i\sum_{j=1}^K \sum_{k=1}^K r_{ijk} w_j w_k + f_i (i = 1, 2, 3, ..., K)$$

- Evaluated by decomposing the primitive equations with 3D normal mode function.
- Calculating only vertical average (barotropic) component of atmosphere
- Energetic interaction coefficient *r* is essentially three dimensional matrix. but because of limited computer resources, we have calculated only east-west symmetry components of *r*.
- We want to calculate all three dimensional components.

Study about effects on LETKF's Transform matrix



In 15 km resolution, vertical wind is not clearly observed. We need more high-resolution experiments.

(Saito et al. 2017)

High Performance Computing in Numerical Weather Prediction

- HPC is essential in NWP both running forecasts of atmospheric conditions and in data assimilation (DA)
- Global NWP require as much computational resources for DA (integrating simulations with observations) as 10 day forecast (Miyoshi et al, 2016)
- LETKF (Localized Ensemble Transform Kalman Filter) DA system – performs analysis (updating) independently for each grid with subset of local observations – good DA system for parallel computing
- Run ensemble of forecasts (50-100) suitable for parallel computing





Update grid (red dot) with subset of local observations (purple diamonds)

Future of NWP will come from using ultra-high resolution numerical models (sub km) ("Big Simulations") and assimilation of large quantities of observations ("Big Data")

Require the power of K computer and Post K computer!

"Big Simulations"

SCALE-RM [Sub 1km resolution in DA domain, require large number of simulations, ensembles]

"Big Data"

Phased Array Weather Radar [Provides Obs up 60km, 100m resolution, every 30 secs]



We need to combine high-resolution simulations with high volumes of observational data to bring revolution to NWP

Challenge of Big Data Assimilation at RIKEN (Miyoshi et al 2016)

- Provide accurate high resolution (~100m) 30 min forecasts of severe weather systems though the assimilation of PAWR data every 30 secs
- 30 sec cycling currently not yet possible takes too long!



Target Model Configuration and timings

- Work alongside designers of SCALE model optimize model set up 2D domain decomposition by MPI communication
- How to improve design SCALE-LETKF to run 30 sec cycling at high resolution (100m)?
 - Identify which processes take too much time to complete
 - How can we optimize parallelization to allow for 30 sec cycling
- Post K can help us achieve goals of Big Data Assimilation

Plasma

- ≻One of the four fundamental states of matter
- >An ionized state of matter similar to gas
- ➢ It is estimated that more than 99 percent of matter in the universe exists as plasma; examples include stars, sun, nebulae, and interstellar particles.



Langmuir Probe

- Key plasma diagnostic used by scientists interested in plasma characterization to measure the internal parameters of the plasma.
- Electron/Ion temperature
- Electron/Ion density
- Plasma potential
- Energy Distribution Function (EEDF)
- Have been installed on satellites and sounding rockets to observe the general characteristics of thermal plasma in the ionosphere for more than five decades.
- Used in laboratory Plasma diagnostic too. i.e. Tokamak, Fusion reactors

Probe Type and Dimensions

➤The geometry will be chosen depending on the purpose of the measurements and the platform configuration.



Plasma Applications

≻Low pressure discharge

Plasma created in reactors at low pressure are used in the manufacture of microchips and the application of coatings.

≻Lighting

Fluorescent tubes and CFL are both plasma technology.

>Atmospheric pressure

Plasma are very good to destroy the bacteria and have been used in water treatment.

≻Use in medicine

Sterilization and surgery

≻Space research

Understanding the Ionosphere, Magnetosphere environment

>Energy propose

Tokamak. Fusion reactors

The real problems with fusion Energy and Plasma Simulation

Small Sized Tokamak Fusion Reactor

For solve this we need to better understand what's going on between the fusion plasma and the reactor wall.

≻Plasma Confinement

Turbulence and instabilities in the plasma were a serious problem.

≻Understanding Turbulence in Plasma

Turbulence plays an important role in all plasmas. Small fluctuations in tokamak plasmas lead to turbulence, and turbulent eddies can very effectively transport heat from the hot core across confining magnetic field lines out to the cooler plasma edge, degrading the plasma performance. Predicting this phenomenon of turbulent-transport is essential for the understanding and development of fusion reactors. ➢Researchers use supercomputers to study plasma turbulence via direct numerical simulation. In order to simulate the turbulence in the fusion plasmas, powerful computers are needed.

Some simulations use more than 20 Million CPU hours running on the some of the world's fastest supercomputers.



A schematic view of the DIII-D tokamak shows magnetic islands, alongside computer simulations of a magnetic island and turbulence.

➤ The knowledge gained from computational studies will enable us to better design magnetic confinement reactors and helps characterize the plasma parameters easily in the hopes of leading to reactors that confine plasmas for long enough and solve the future energy crisis.

➢ We can not treat plasma as a fluid, we have to treat plasma as a particle. Calculating one billion plasma particles is a challenging job.

Video simulation will puts a new twist on fusion plasma research and plasma characterization.

➢Hope our upcoming Post K Supercomputer will address this mysterious job; physics behind the plasma turbulences and instabilities.