RIKEN AICS HPC Youth WS -group work-

Group C

2016/11/30

Group C member

- Swann Perarnau (ANL, CS)
- Francios Simon Tessier (ANL, CS)
- Tetsuya Odajima (RIKEN, CS)
- William Dawson (RIKEN, App.)
- Thomas Schilden (RWTH Aachen Uni., App.)
- Manabu Yagi (RIKEN, App.)

Mentors
- Yoshifumi Nakamura (RIKEN, App)
- Balazs Gerofi (RIKEN, CS)

Group work

- Presentations
  - Argo, OS for resource managements on exa-scale (by Swann)
  - Data aggregation for intensive I/O (by Francios)
  - GPU-GPU communications (by Tetsuya)
  - Quantum chemistry : matrix functions, SPDgemm (by William)
  - Turbulence (Supersonic blunt body) flow by CFD, FVM, Runge-Kutta, unstructured grid, random access (by Thomas)
  - Megnetosphere By Magnetohydrodynamics(MHD), rational constrained interpolated pseudo-particle(difference method), 4th Runge –Kutta, stencil calculation (by Manabu)
- Discussion
  - ………
  - ………

Example

- How to organize International collaboration for exa-scale computing

- Technological requirements to achieve exa-scale computing

- Technologies and apps to integrate exa-scale computing and big data

- Collaborations on computational science and computer science

We chose

- How to organize International collaboration for exa-scale computing

- Technological requirements to achieve exa-scale computing

- Technologies and apps to integrate exa-scale computing and big data

- Collaborations on computational science and computer science

Group work

- Presentations
  - Argo, OS for resource managements on exa-scale
  - Data aggregation for intensive I/O
  - GPU-GPU communications
  - Quantum chemistry : matrix functions, SPDgemm
  - Turbulence (Supersonic blunt body) flow by CFD, FVM, Runge-Kutta, unstructured grid, random access
  - Megnetosphere By Magnetohydrodynamics(MHD), rational constrained interpolated pseudo-particle(difference method), 4th Runge –Kutta, stencil calculation
- Discussion
  - Collaborations on computational science and computer science

Discussion on how to collaborate computer and computational scientist

- **We need to understand each other**
    - Communication problem: We are using different languages in different fields
- We need to know algorithm and problem each other
    - How much memory do you need?
    - How do you access memory?
    - How do you parallelize?
    - What is communication pattern?
    - Categorizing computation is important
    - Talking about all level : Science problem, mathematical model, method, implementation, architecture

Conclusion:
Towards possible collaborations

- starting from basic things, information exchange is necessary

1. (app): Setting target problems (sizes) on exa-scale computers
   - What do you need : memory, time to solve, amount of computing, algorithmic specification
   - App1, turbulence flow : ….
   - App2, Quantum chemistry : ….
   - App3, Magnetosphere : ….
2. (app): Picking up computing intensive kernel
3. (CS): code analysis
4. Applying CS's techniques, optimizing code

My impression

(random thoughts)

- Group member : nice balance
  - Fields : 3 CS + 3 App
  - From : 3 RIKEN + 2 ANL + 1 Aachen
  - Geometric: 2 JP + 2 FR + 1 DE + 1 US
- We went to British PUB. Useful to know each other
- We had a fruitful time with many kinds of opinions
- We need more time to discuss
- Practically, we need regular meeting every 2nd week or so with TV conference system. We need time for it
- Topic choice
  - Easier to start new term rather than existing term
- time ~ money & topic choice : financial and political issues
- So we some scheme to start new collaboration easily.