Collaborations between CEA and RIKEN

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The second French-Japanese-German Workshop on Programming and Computing for Exascale and Beyond, October 30-31, 2018

Overview

- An agreement to strengthen the partnership between **RIKEN** and **CEA** in the areas of high performance computing and computational science
  - as a part of an agreement between **the French Ministry of National Education, Higher Education and Research** and **the Ministry of Education, Culture, Sports and Science And Japanese Technologies (MEXT)**
- A broad range of areas including the development of open software libraries and applications as well as management issues
  - 9 tracks
- The Arm HPC Ecosystem
  - The European Processor Initiative (EPI) Arm processor
  - A64FX by Fujitsu: Arm based processor for the post-K supercomputer
- 50+ researchers have been contributing to the project

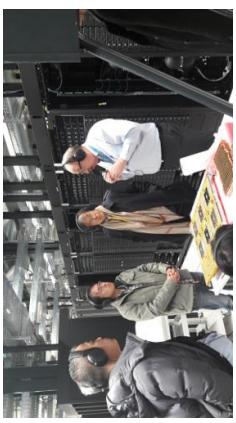
http://www.riken.jp/en/pr/topics/2017/20170118_1/

2018

October
Technical meeting @JP

July
2nd Joint Summer School @JP

June
Steering meeting @ISC18



March
Technical meeting @FR

November
Short steering meeting @SC17

2017

October
Technical meeting @JP

September
1st Joint Summer School @FR

February and March
Technical meeting @FR

January
Conclude an agreement @JP

2016

October
Kickoff technical meeting @JP

March
Preparation meeting @FR

2018

October
Technical meeting @JP

July
2nd Joint Summer School @JP

June
Steering meeting @ISC18

March
Technical meeting @FR

November
Short steering meeting @SC17

Spring Meeting in France
Autumn Meeting in Japan

2017

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Technical meeting @JP

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2016 2017 2018

March
Preparation meeting @FR

1st day: General technical background and collaboration options

1. Presentation of technical developments, interests in both
2. Discussion on possible collaboration

・・・・・・・ Discussions within each institute ・・・・・・・

2nd day: Possible framework and next steps,

1. Identify areas of our collaboration, Methods of collaboration
3. Next step and schedule

9 tracks

- 7 tracks had been identified at the preparation meeting in 2016
- 2 tracks have been added in 2018
  - Arm Performance Evaluation
  - AI & Big Data

Runtime Environment

- Collaborators
  - Jacques-Charles Lafoucriere , Gilles Wiber, Matthieu Hautreux, Aurélien Cedeyn
  - Yutaka Ishikawa, Masamichi Takagi, Balazs Gerofi, Takahiro Ogura
- Objective and Collaboration Topics
  - Improving (performance) portability of applications
  - Defining a standard of the runtime environment settings (including libraries, OS parameters and OS kernels)
  - Finding optimal settings in terms of application performance
  - Contributing to the OpenHPC community
- Background
  - CEA: SELFIE (profiling tool) and PCOCC (virtualization tool)
  - EasyBuild, a software build and installation framework, is used to manage open-source packages
  - RIKEN: Linux with IHK/McKernel (Light-weight OS Kernel)

OS: Linux
CPU: Intel Xeon, Intel Xeon Phi, Arm
Network: InfiniBand, Omni-Path, Fujitsu Tofu, Bull BXI

Runtime Environment

2017

- CEA tests McKernel on CEA's machines (KNL, BXI interconnect)
- RIKEN investigates EasyBuild
- CEA and RIKEN provide the current user demands

2018

- RIKEN implements missing McKernel features that CEA requested.

2019

- CEA evaluates McKernel on CEA's machine
- RIKEN will evaluate CEA's benchmark suite on McKernel
- RIKEN will investigate problems of the user-level portal4 on CEA's BXI

2020

- CEA and RIKEN will provide configuration standard, libraries, kernel parameters and kernels

Large DFT calculations and QM/MM (Quantum Mechanics/ Molecular Mechanics)

- Collaborators
  - Thierry Deutsch, Luigi Genovese
  - William Dawson, Takahito Nakajima
- Background
  - CEA's BigDFT, can be used as independent libraries, such as the FOE method (CHESS library) or the Poisson solver
  - RIKEN: NTChem and algorithms for linear-scaling DFT calculations, particularly, a sparse matrix multiplication library based on communication avoiding linear algebra algorithms
- Objective and Collaboration Topics
  - develop new computational approaches in materials science (e.g. for linear-scaling, electron correlation ...) that retain the advantages in each quantum chemistry, condensed-matter, and solid-state physics approach but reduce their own disadvantages
  - develop massively parallel libraries to calculate the properties of large scale systems in the theoretical frameworks of linear scaling DFT and QM/MM

Large DFT calculations and QM/MM

2017

- Porting of the BigDFT code to the K computer.
- Development and evaluation of two new libraries for DFT focused sparse matrix operations [1][2].

2018

- Common investigation on QM/MM based on the localization properties of the atomic systems.
- Development of two new metrics for partitioning QM/MM calculations
- The BigDFT has been used to compute the ground state electronic structure of the Laccase enzyme (7000+ atoms). 500-nodes, 9-hours on K computer

2019

- The Laccase enzyme for degrading Aflatoxins
- Goal is to perform QM/MM runs using these developed capabilities in collaboration with Dr. Marco Zaccaria of Boston College.

[1] Dawson, William, and Takahito Nakajima. "Massively parallel sparse matrix function calculations with NTPoly."Computer Physics Communications 225 (2018): 154-165.
[2] Mohr, Stephan, William Dawson, Michael Wagner, Damien Caliste, Takahito Nakajima, and Luigi Genovese. "Efficient Computation of Sparse Matrix Functions for Large-Scale Electronic Structure Calculations: The CheSS Library." Journal of chemical theory and computation 13, no. 10 (2017): 4684-4698.

Human Resource and Training

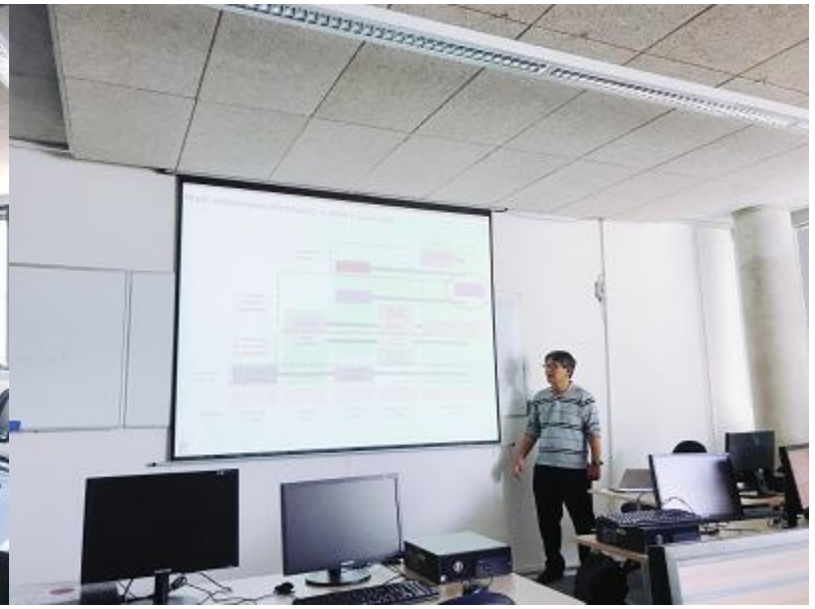
- Collaborators
  - Edouard Audit
  - Mitsuhisa Sato, Toshiyuki Imamura

- Host/Send Internship students, visiting researchers

- From CEA to RIKEN
  - Dominique Martinet (Visiting Researcher)
    - Runtime Environment
    - 2018.4.1-2019.3.31
  - Ksander Selim Ejjaaouani (Internship Student)
    - Programming Language Environment
    - 2018.1.22-2018.3.20

Human Resource and Training

- CEA-RIKEN HPC School
  - focuses on “advanced” topics
  - PhD students, young researchers
- 1st CEA-RIKEN HPC School @ MDLS, Saclay, France, Sept. 2017
  - Arm SVE, PiP, XcalableMP, MPC
- 2nd CEA-RIKEN HPC School @ R-CCS, Kobe, Japan, Jul. 2018
  - Boast, OpenMP SIMD, OpenMP Task

Summary …. not conclusion :-)

- In the middle of 5 years agreement (+ another 5 years?)
- A broad range of areas
  - Programming Language Environment
  - Runtime Environment
  - Energy-aware batch job scheduler
  - Large DFT calculations and QM/MM
  - Earthquake Related Issues of Nuclear Power Plant Facilities
  - Key Performance Indicators
  - Human Resource and Training
  - *Arm Performance Evaluation
  - *AI & Big Data
  - target: exa-scale/pre-exa-scale systems
    - Arm HPC
- Next HPC School will be hold in France
  - Jun. 2019
  - Arm HPC hackathon
  - We are looking forward to your participations