DE LA RECHERCHE À L'INDUSTRIE

CEA and RIKEN HPC Collaboration

CEA と RIKEN HPC コラボレーション

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OUTLINE - 輪郭

- Motivations & objectives - 動機と目的
- Research topics - 研究テーマ
- Questions - 質問

動機と目的
Motivations & objectives

MOTIVATIONS & OBJECTIF -動機と目的

- HPC is a strategic asset for China, EU, Japan and USA.
  - Top500 is dominated by China and USA
  - Japan and France have a strong presence and impact in the HPC community
    - CEA and RIKEN public Research and Technological Organisations are major players
    - Working closely with HPC industrials - Fujitsu and ATOS

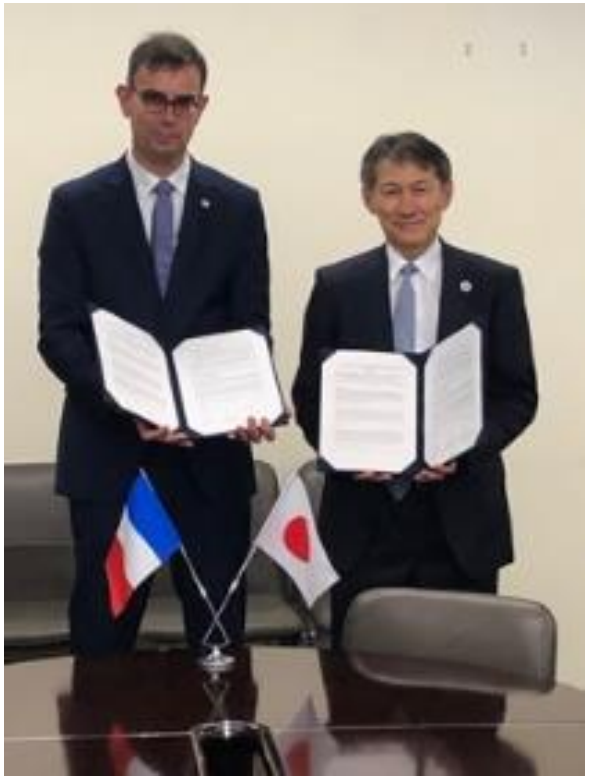
FUJITSU

Bull
atos technologies

MOTIVATIONS & OBJECTIF -動機と目的

- CEA and RIKEN HPC collaboration aims to promote and strengthen the HPC ecosystem
  - Middleware/Software Stack
  - HPC Applications
  - Common interest in HPC hardware and architecture - Strong focus on ARM architecture

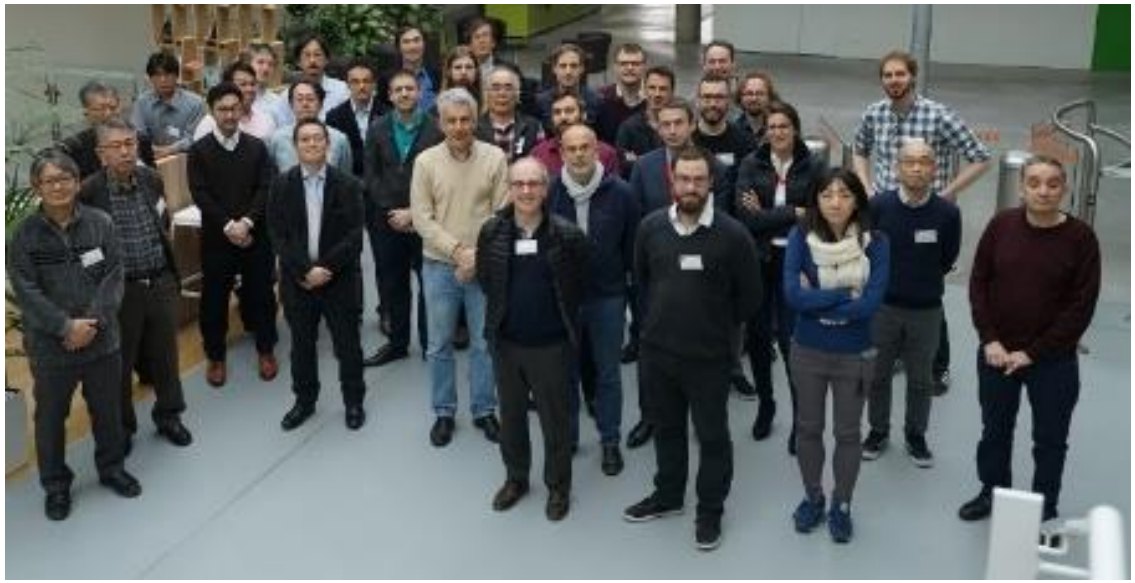
- Long term collaboration between CEA and RIKEN
  - CEA and RIKEN HPC Collaboration is part of an agreement between MESRI (Ministère de l'Enseignement Supérieur, de la Recherche et de l'Innovation) and MEXT(Ministry of Education, Culture, Sports, Science and Technology-Japan)
  - Initial Statement of Work was signed in January 2017 for 5 years
  - Current (amended) SoW signed in June 2019



MOTIVATIONS & OBJECTIF -動機と目的

- Programme management and life
  - Regular Face-to-Face and follow-up meetings
  - 2 plenary workshops per year
    - 1 in Japan, 1 in France
  - F2F meetings during SC and ISC conferences
  - Summer school every year
  - Master, PhD or post-docs students visits and exchanges

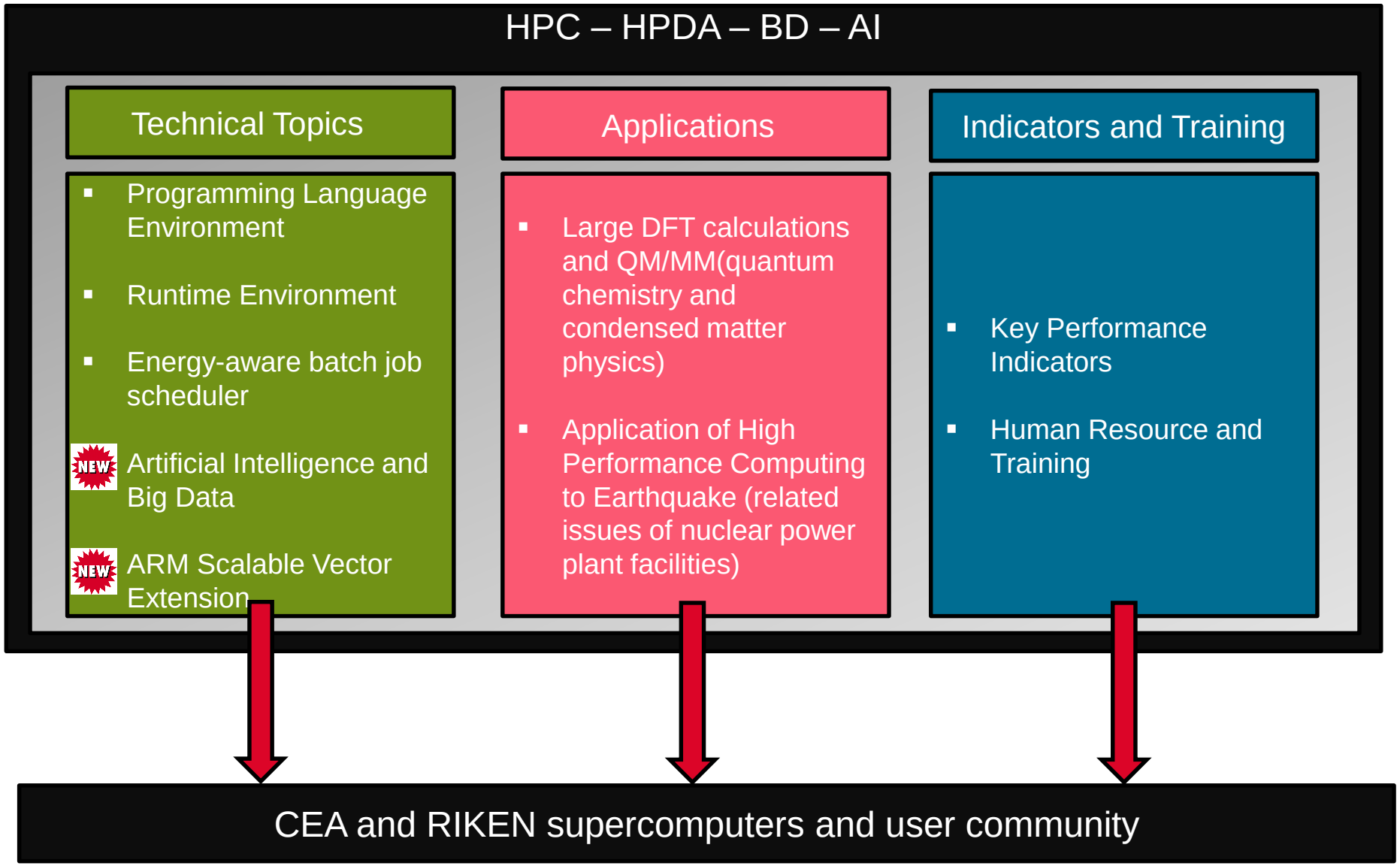
- About 40 researchers involved



研究テーマ
RESEARCH TOPICS

RESEARCH TOPICS - 研究テーマ

- 9 topics distributed under 3 pillars



RESEARCH TOPICS - 研究テーマ

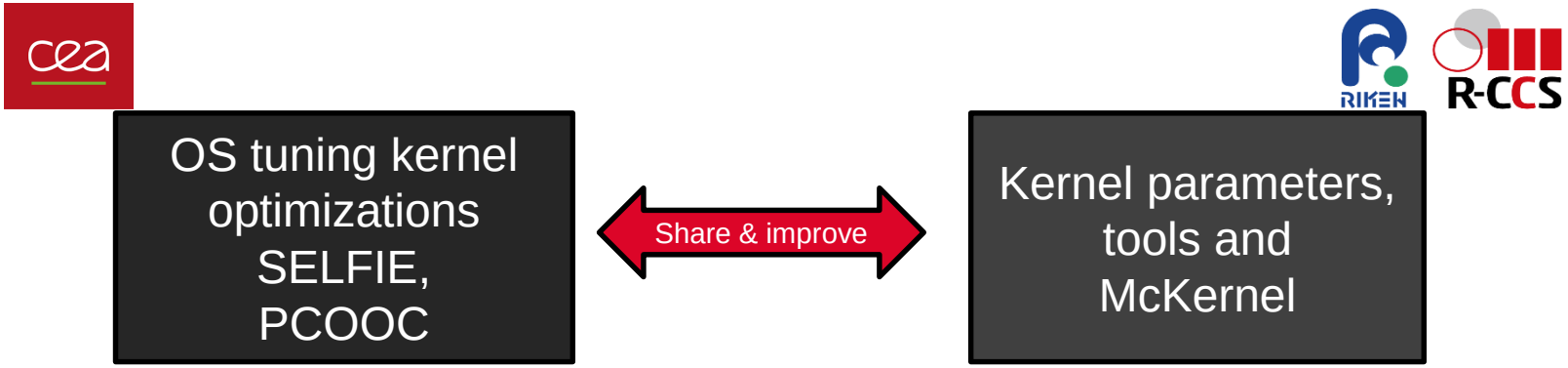
- Programming Language Environment
  - Focus on task-based parallel programming models and PGAS (Partitioned Global Address Space)
  - Address the next generation of manycore processor systems

  - Multi-Processor Computing (MPC)
    - Provide unified parallel runtime designed to improve the scalability and performances of applications running on clusters of (very) large multiprocessor/multicore NUMA nodes.
    - Provide implementations for the MPI, OpenMP and POSIX Threads standards

  - XcalableMP (XMP)
    - Directive-based language extension for scalable and performance-aware parallel Programming
    - Easy and fast development for parallel programs on distributed memory systems
    - Parallelization under "global-view model“
    - Co-array to use one-sided communication easily under "local-view model“
    - Combination of MPI and OpenMP

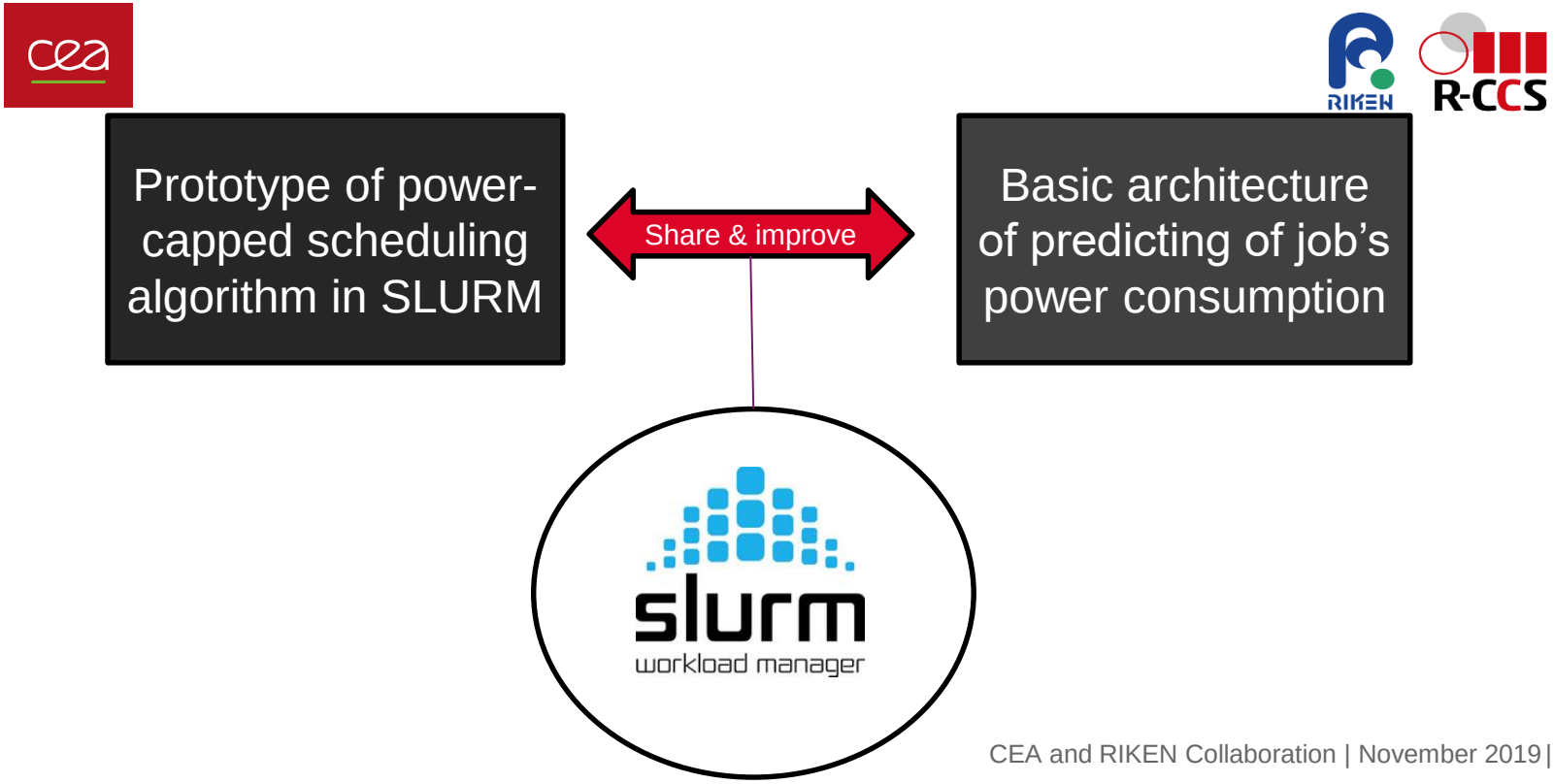
RESEARCH TOPICS - 研究テーマ

- Runtime Environment
  - Define a standard of the runtime environment settings (including libraries, kernel parameters and kernels) of supercomputers to improve portability of applications
  - Find optimal settings in terms of application performance
  - Working on several key technologies



RESEARCH TOPICS - 研究テーマ

- Energy-aware batch job scheduler
  - Develop framework of energy-aware job scheduling:
    - Prediction method of system power consumption and the energy-aware scheduling algorithm
    - Needs the prediction of each job's power consumption.



RESEARCH TOPICS - 研究テーマ

- Artificial Intelligence and Big Data
  - Strong focus on AI and Big Data in interaction with HPC for CEA and RIKEN
  - 3 main axis identified:

AI for predictive maintenance for HPC infrastructure operation	HPC for AI: how HPC technics and know-how could benefit to AI	AI for HPC: how AI could improve, accelerate classical HPC simulations or analysis
▪ Use of AI to optimize supercomputer exploitation ▪ Use AI simulations to automatically and quickly identify needs and upcoming events (e.g., failures etc.) related to the system	▪ Optimize AI applications and/or compute kernel on current and future architectures (namely x86, possibly ARM architecture and GPUs) ▪ Extension on Machine Learning (ML) and Deep Learning (DL) application portfolio ▪ HPC environment to welcome AI workloads: integration of AI software stack in current HPC software stack designs ▪ File system for HPC and Big Data	▪ Use of AI and/or High Performance Data Analytics (HPDA) for processing analysis (in-situ analysis) ▪ Use of ML or DL for meta-models and/or analytical in numerical simulation: Some HPC compute kernels on some applications might be replaced by ML or DL kernels to accelerate time to solution.

RESEARCH TOPICS - 研究テーマ

- ARM Scalable Vector Extension
  - Context of the European Processor Initiative (EPI) and RIKEN A64FX
  - Programming and tuning method to derive performance improvement by SIMD using Arm SVE;
  - Evaluating SW stack for porting and optimization in ARM environment
  - Study of ARM SW stack, provide feedback on porting applications on ARM and optimize critical runtime parts

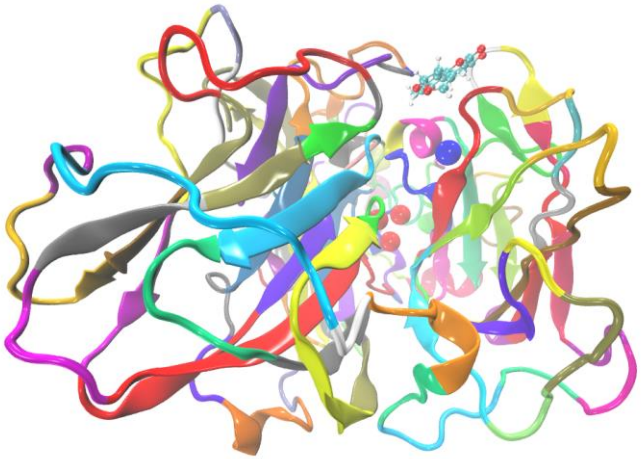
Set of applications, Human resources, Strong experience on ARM

Share & improve

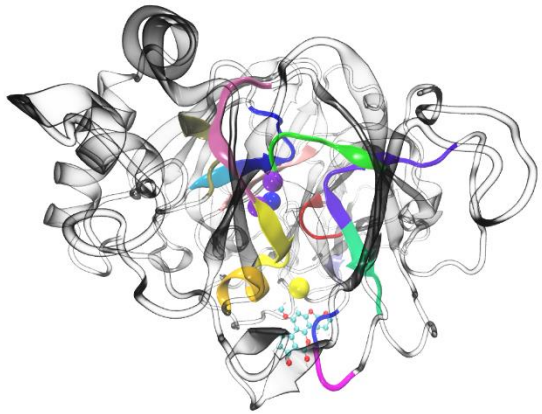
simulator to evaluate the processor A64FX performances and supercomputer access

RESEARCH TOPICS - 研究テーマ

- Large DFT calculations and QM/MM (quantum chemistry and condensed matter physics)
  - Develop new computational approaches based on a new massively parallel library to calculate the properties of large systems using linear scaling density functional theory (DFT) and QM/MM (Quantum Mechanics/Molecular Modeling)
  - Objective: automatic fragmentation of large molecules (proteins, toxins) to guide QM/MM calculations (split the system into a part near the active site described accurately i.e. QM) and a remaining part described coarsely (MM))



Autofragmentation of aflatoxin (toxin in nuts to destroy)



Fragmentation of aflatoxin near the reactive site

RESEARCH TOPICS - 研究テーマ

- Application of HPC to Earthquake
  - Related issues of nuclear power plant facilities
  - Active fault evaluation, seismic hazard assessment, soil-structure interaction (SSI), seismic structure response analyses, and probabilistic risk evaluation
  - Exchanging information in relation with the aforementioned topics and optimizing computing tools
    - Increase scalability and performance of the frameworks
    - Provide technical details about the programs and modules

Technical information on interface elements usable in FEM computing code to simulate foundation sliding and/or uplift (SSI), as well as on methodologies for probabilistic risk assessment

Techniques (e.g. fast solvers, etc.) well-fitted for nonlinear FEM HPC computations

RESEARCH TOPICS - 研究テーマ

- Key Performance Indicators
  - Defining proper methodology and metrics for KPIs (Key Performance Indicators) in the area of HPC systems.
  - What is a capable, useful and productive supercomputer?
  - What is a successful industrial supercomputer development?
  - Technical performance and efficiency (via proper benchmarking)
  - Programming productivity, ease of use, cost effectiveness of HPC systems
  - Impact of applications made possible in terms of scientific, industrial and societal outcomes
  - Simplified Sustained System Performance Metric (SSSP)
    - SSSP metric makes a performance projection of real applications based on a set of benchmarks
    - Extension of Sustained System Performance (SSP) metric developed at NCSA

RESEARCH TOPICS - 研究テーマ

- Human Resources and Training

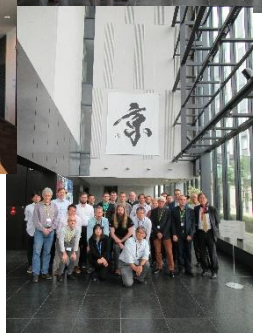
  - Develop the human resources to play an important role in HPC: Skill development

  - Organize seminars for the fundamental knowledge of HPC
    - France-Japan Summer/Winter schools with different focuses in HPC
    - Training workshops on advanced software developed in the RIKEN-CEA collaboration and on HPC tools (with hands-on XMP, MPC, ARM, and runtime, etc.)

  - Workshops on scientific topics of joint interest for CEA & RIKEN

  - Internship program for PhD students and masters students

  - Exchange and visits of young researchers and Post-doc



RESEARCH TOPICS - 研究テーマ

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ありがとうございました
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