



CSCS

Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre



東京工業大学

Tokyo Institute of Technology



ETH zürich



DAC Applications Working Group Update

Mark Straatsma (ORNL), Rio Yokota (Tokyo Tech), Tim Robinson (CSCS)

DAC Meeting, Lugano, Switzerland

June 2016



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Recap of actions from January 2016

General action items

Common portal to exchange documents between ADAC institutions

Github mechanism for code/libraries (Straatsma)

Establish ADAC project for access to compute resources

Presentations on github (Straatsma)

Monthly working group video conference calls (Straatsma, Robinson, Yokota)

- TiTech 22:00, ORNL 8:00, CSCS 14:00

near algebra libraries

Dmitry Liakh (ORNL): ExaTensor Library for Electronic Structure Applications

Thomas Schulthess (CSCS): Eigensolvers – distributed, accelerated LAPACK/SCALAPACK

Immediate

- Identify opportunities for codes in addition to current CAAR (Dirac, LS-Dalton, NWChem)
- Release ExaTensor intra-node component with documentation (Liakh)
- Identify users for ExaTensor at CSCS (Robinson), TiTech (Endo)
- Engage NTChem development team (Maruyama)
- Performance testing on Piz Daint (Liakh)

Near-term goals

- Discussion about the exposure of architectural details to the DSL users
- Start a discussion with LA library developers (Schulthess: Jack Dongarra)
- Engage the exascale computing project (Wells: Doug Kothe)

Classical force fields for biophysics applications

Arnold Tharrington (ORNL): Multi-Summation Method for Biophysics Applications

Rio Yokota (TiTech): Fast Multipole Methods for Biophysics Applications

Near-term goals

- Create common framework for general non-bonded force generation
- Engage with developers of main codes NAMD, GROMACS, AMBER, (Robinson) LAMMPS (Tharrington) (Schulthess to contact Klaus Schulten and Eric Lindahl)
- Organize workshop to define common API (Action: Robinson/Straatsma/Yokota)
- Define API for hierarchical methods

Longer term (1 year) goals

- Create a DSL based on the agreed upon API that implements:
 - PME (Robinson)
 - MSM (Tharrington)
 - FMM (Yokota)

Partnerships

- KAUST (Yokota: David Keyes)

Stencil libraries based applications

Takashi Shimokawabe(TiTech): Libraries for CFD Applications

Lucas Benedicic(CSCS): Gridtools and Python bindings

Naoya Maruyama(TiTech): Stencils and tree-based parallelism

Near-term goals

- Identify use cases, brief Jim Hack, Mark Taylor (Norman)
- Engage Aoki (Yokota)
- Distributed memory (Benedicic)

Data analytics libraries

Toshio Endo(TiTech): HHRT runtime for GPUs

Yutaka Akiyama(TiTech): Sequence matching libraries

Near-term goals

- Run GHOSTX-GPU and other use cases ORNL POC (Straatsma: Rangan Sukumar), CSCS POC (Robinson: Marcel Schoengens)
- Characterize HHRT performance on Titan (Wells, Endo, Tharrington)
- Model HHRT NVLINK performance (Endo)
- Explore hardware for data analytics frameworks (Straatsma: Arjun Shankar)

Longer term (1 year)

- General purpose framework



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update June 2016

Outstanding proposal CSCS: PRACE

The mission of PRACE is to enable high impact scientific discovery and engineering research and development across all disciplines to enhance European competitiveness for the benefit of society

PRACE 5IP WP7 proposal: *Applications Enabling and Support: Provision of Numerical Libraries for Heterogeneous/Hybrid Architectures*

Focus: **productisation and adoption of low-level numerical libraries targeting heterogeneous/hybrid architectures**

- (i) **Linear algebra libraries for distributed hybrid architectures.** Systematically extend Matrix Algebra on GPU and Multicore Architectures (MAGMA) library to distributed architectures. Adoption in community codes in materials science and electronic structure by providing access via a standard interface, hiding underlying implementation
- (ii) **Non-bonded interactions (Coulomb and Lennard-Jones potentials) in classical MD.** Develop a common API and tool for non-bonded interactions that can be plugged into widely-used community codes such as NAMD, GROMACS. Similar to comparable tools in linear algebra - implement different algorithms in the backend, e.g. PME, FMM.
- Further domains (e.g. climate, CFD) may be considered according to available effort and relevance to core approach

ca. 60 PMs if funded

Activities at ORNL

CAAR project for application DIRAC focuses on tensor algebra library for Summit

Portability project OLCF/ALCF/NERSC with MD as one application

- Hiring postdoctoral associate

ECP Co-Design Center Project plan with focus on Domain Specific Libraries for

- Tensor Algebra (ExaTensor)
- Integral Evaluation (ExaInt)
- Classical atomic forces and energy evaluation (ExaCafe)

Library update – Tokyo Tech/RIKEN/CSCS

Update since the January meeting

- Several video conferences between the CSCS GridTools team and RIKEN
 - CSCS: Thomas Schultess, Lucas Benedicic, Will Sawyer, Mauro Bianco, Paolo Crosetto, and Carlos Osuna
 - RIKEN: Hisashi Yashiro, Mohamed Wahib, and Naoya Maruyama
- Mutual interest between CSCS and RIKEN was identified
 - RIKEN's interest: Extending NICAM with high-level domain-specific tools for next-generation machines
 - CSCS's interest: Extending GridTools for icosahedral global climate models
- Three representative compute kernels in NICAM have been extracted and ported to C++ for evaluating GridTools

Plan after this meeting

- Implementing and evaluating the representative kernels with GridTools
- Face-to-face meeting on Wednesday at CSCS for more detailed planning
- 2-week stay at CSCS after this ADAC meeting by Mohamed Wahib (RIKEN) to get started with hands-on experiences

this morning's agenda

08:40. Update from Working Group leads

09:00. How to Think Exascale: Modernizing the LAPACK and Scalapack Libraries, Azzam Haidar (University of Tennessee)

09:30. The Development of the Electronic Structure Code LSDalton and its Library Requirements, Thomas Kjaergaard (Aarhus University)

10:00. Non Orthogonal Configuration Interaction on the Next Generation of Supercomputers, Remco Havenith (University of Groningen)

10:30. Break

10:50. Beyond ppOpen-HPC: Applications and Algorithms in the Post-K/Post-Moore Era, Kengo Nakajima (University of Tokyo, via Skype)

11:20. Past Algorithms and Future Libraries for Efficient Nonbonded Particle Simulations, Erik Lindahl (Stockholm University and KTH, via Skype)

11:50. Towards Large-Scale Quantum Chemistry with Second-Generation Density Matrix Renormalization Group (DMRG), Stefan Knecht (ETH-Zurich)

12:20. Working group lunch and break outs

