Numerical Algorithms and Libraries for Exascale NAL-X

ISC20 Workshop Proposal

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1 Motivations

Due to hardware technology scaling with the ongoing manycore and accelerators revolution in heterogeneous chip design, the existing numerical algorithms and software model are breaking down. Indeed, there is currently a fundamental mismatch between the underlying hardware architecture with high thread concurrency and the software deployment of numerical libraries for scientific applications, which rely on the traditional bulk synchronous programming model. Ideally, numerical software in scientific computing should first squeeze single-node performance by efficiently running on manycore architectures with processor counts sharing a common memory in the hundreds. Programming and extracting performance from these advanced architecture chips may not be straightforward. Algorithmic solutions such as fine-grained computations, communication/synchronization-reducing, and mixed precision algorithms represent some of the most critical key ingredients to employ moving forward with extreme-scale computing.

This half-day workshop brings together experts who lead efforts in developing innovative numerical algorithms and scalable software libraries for high performance computing on today's architectures and the upcoming Exascale systems.

Below are the main themes of the workshop:

- High performance direct / iterative solvers
- Mixed precision algorithms exploiting low-precision hardware
- Synchronization-reducing and communication-avoiding algorithms

- Performance optimizations for accelerated / hybrid architectures
- Numerical libraries for large-scale scientific applications

2 List of Confirmed Speakers

All the following presenters have confirmed their attendance upon acceptance of the workshop at ISC20:

- Hartwig Anzt, KIT, Germany. Hartwig is Helmholtz-Young-Investigator Group leader at the Steinbuch Centre for Computing at the Karlsruhe Institute of Technology (KIT), working mainly on Fixed-point methods for numerics at Exascale (FiNE). Hartwig Anzt has a long track record of high-quality software development. He is author of the MAGMA-sparse open source software package and managing lead of the Ginkgo numerical linear algebra library. Hartwig Anzt is a co-PI of the PEEKS project and the xSDK project inside the software technology effort of the US Exascale Computing Project (ECP).
- Alfredo Buttari, CNRS, France. Alfredo is the Principal Investigator of the SOLHARIS project that aims at developing algorithms, programming models and scheduling methods that improve the scalability of sparse linear algebra solvers and, in general, of scientific computing libraries, on large scale parallel hand heterogeneous supercomputers.
- Laura Grigori, INRIA, France. Laura is a senior research scientist at INRIA in France, where she leads the Alpines group, a joint group between INRIA and the J.L. Lions Laboratory, Sorbonne University, in Paris. She leads several projects on preconditioning, communication avoiding algorithms and associated numerical libraries for large scale parallel/multicore machines.
- Daniel Grünewald, ITWM Fraunhofe, Germany. Daniel Grünewald leads efforts on GaspiLS, a scalable linear solver library for the Exascale age and it is industry proven in CFD and FEM simulations. The effort are part of European project INTERTWinE that addresses the problem of programming-model design and implementation for the Exascale.
- David Keyes directs the Extreme Computing Research Center at the King Abdullah University of Science and Technology (KAUST), where

he was the founding Dean of the Division of Mathematical and Computer Sciences and Engineering in 2009 and currently serves in the Office of the President as Senior Associate for strategic priorities and institutional partnerships. He works at the interface between parallel computing and partial differential equations and statistics, with a current focus on scalable algorithms exploiting data sparsity in the context of the HiCMA software library.

- Ulrike Meier Yang, LNL, USA. Ulrike leads the Mathematical Algorithms and Computing group in the Center for Applied Scientific Computing at LLNL. She leads the xSDK4ECP (Extreme-scale Scientific Software Development Kit for the ECP) project, which is part of the Software Technologies component of the ECP.

3 Vendor Panel

Following the presentations, the workshop will conclude with a moderated panel composed of experts from major industrial vendors in the context of hardware/software co-design: Sarah Knepper from Intel, Fabrice Dupros from ARM, and Harun Bayraktar from NVIDIA. We are still in the process of approaching Cray/HPE, Fujitsu, NEC and AMD.

The idea of the panel is to hear the vendor perspective on their own initiatives and efforts in facilitating hardware/software co-design, on the roadmaps of their numerical libraries, and on their plans for sustainable software ecosystems at the dawn of Exascale computing.

4 Workshop Agenda

We provide below the tentative agenda of the half-day workshop:

- 9:00-9:05 Welcome and introduction by the workshop chairs
- 9:05-9:30 Ulrike Meier Yang
- 9:30-9:55 Daniel Grünewald
- 9:55-10:20 Laura Grigori
- 10:20-10:40 Hartwig Anzt
- 10:40-11:00 Alfredo Buttari

- 11:00-11:30 Coffee Break
- 11:30-11.55 David Keyes
- 11:55-12.55 Vendor Panel
- 12:55-13:00 Concluding remarks

5 Targeted audience

- Researchers and engineers working on HPC applications and performance optimizations.
- Domain scientists and computer scientists interested in learning latest updates on major numerical libraries.
- Research software engineers and systems administrators with an interest to support their institutions' software infrastructure by installing and providing alternatives for scalable numerical libraries.

6 Estimated attendance

40-50

7 Expected outcome

- Develop a website to gather the workshop details and to publish all presentation slides.
- Enhance research collaborations between academic and industrial partners.
- Build a momentum to organize a regular ISC'xy workshop, form a steering committee, and eventually set up peer-reviewed paper proceedings for future NAL-X workshops.