

# High Performance Computing and High-Level Programming Concepts for Hyperbolic PDE Codes

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## Abstract

We propose to host a workshop at KAUST focused on hyperbolic PDE solvers. The workshop will aim at combining modern solution techniques for hyperbolic problems with high performance computing tools to enable efficient computation and visualization, including massive distributed-memory parallelism and many-core acceleration, while enabling advanced algorithmic technologies like adaptive mesh refinement and implicit solution techniques, using the Python scripting language. Workshop sessions will primarily be devoted to producing useful software by extending, adapting, and developing numerical algorithms, as well as assisting application scientists in applying the software to problems of interest. The proposed workshop is unusual in that it is focused primarily on working sessions (rather than lectures only) and in the combination of different but complementary disciplines that will be brought together.

## Introduction

A wide range of physical phenomena involve wave propagation and are modeled with hyperbolic PDEs. These models must be solved by computational methods, and their solution is often very expensive due to the presence of multiple scales in space and time, the appearance of shock singularities, or the need to resolve very fine wave or material structures. Such models are used to solve problems in seismic waves, magnetohydrodynamics, oceanography, porous media flow, atmospheric flow, and numerous other fields essential to KAUST's research agenda.

The development of numerical software is increasingly important in scientific research and is essential in utilizing KAUST's resources and establishing KAUST as a world leader in computational science. Recently, a team of scientists centered at KAUST (in collaboration with others in Europe and North and South America) has developed a new massively parallel solver for general hyperbolic PDEs (PyClaw) that leverages a range of existing software and libraries. The software is unique in both design and capability. The development of the parallel code was the Master's thesis work of Amal Alghamdi, a female KAUST student from Jeddah.

Alghamdi's initial development work catalyzed a KAUST-hosted five-day workshop in March 2011. That "[HPC]<sup>3</sup> Workshop" was focused on further development of the parallel wave solver. The workshop was unusual in format: the first two days were devoted to introductory lectures and tutorials, but during the remainder of the workshop participants worked in small teams on focused scientific software projects. Unlike many scientific activities, which require long lead times and iteration of ideas, software development is well suited to being done in "sprints" at workshops of this kind.

The workshop was highly successful by various measures. Besides generating new sustained collaborations (an indirect benefit of any successful scientific meeting), the 'working' part of the workshop directly generated several substantive advances, including a GPU-enabled wave propagation solver, a parallel, very-high-order WENO wave propagation solver, and initial development of a domain-specific language for hyperbolic PDE solvers. Each of these advances has led to a publication already submitted or in preparation. Furthermore, the workshop attracted significant attention from

the applied mathematics community and was recently the focus of a feature story in *SIAM News*, the periodical of the world's leading applied math professional society.

The purpose of the present proposal is to host another [HPC]<sup>3</sup> workshop at KAUST. The format and scope will be similar to those of the highly successful first workshop. Our hope is that with the support of KAUST Global Collaborative Research, we will be able to broaden and extend the impact of this workshop on a regional and international level.

## Goals and Objectives

The principal objectives of this workshop are:

1. Bring together experts in the areas of the workshop themes: hyperbolic PDE solvers, wave propagation applications, scientific software development, high performance computing, visualization, and Python programming, in order to share knowledge and generate new collaborations.
2. Develop new features and functionality in the PyClaw software framework
3. Apply the algorithms in PyClaw to solve problems of interest to KAUST researchers, particularly in seismic exploration and flooding

The goals of this workshop are tightly focused, allowing a substantial portion of the workshop to be devoted to letting the participants work in teams on development of specific applications of the PyClaw software that are relevant to them, as well as core functionality important for extending PyClaw to these domains. This “vertical integration” approach allows us to bring software developers, mathematicians and computational scientists, industrial partners, and application scientists all to the same table. The PyClaw project promises to open new horizons in the dissemination of tools and techniques to the computational science community.

The workshop is designed to leverage several of KAUST's unique strengths. Researchers from GCR partners are included in the organizers, speakers, and participants. Talents of KAUST's computational faculty will be focused through the collaborative lens provided by GCR to bear on scientific and industrial applications of strategic interest to the University, including seismic wave modeling and flooding, both of which are the subject of major new AEA collaborative projects (in partnership with UT and Stanford, respectively). The workshop themes of visualization and high performance computing will leverage KAUST's unique resources, in close coordination with members of the supercomputing and visualization core labs, who will participate in the workshop.

## Agenda

The workshop will take place February 4-8. Similar to last year, the first two days will be largely devoted to lectures and tutorials while the final three days will be devoted to project development work in small teams. Each morning will include a keynote lecture by an internationally renowned expert on a topic of interest to a wide audience of KAUST researchers.

Since it is not useful to prepare all details of the agenda until attendees are confirmed, please refer to last year's agenda for an idea of what will be done: <https://sites.google.com/site/hpc3atkaust/program>.

## Invited Speakers

The invited speakers include leading researchers in numerical methods for hyperbolic PDEs, visualization, high performance computing, and scientific software development, as well as KAUST researchers whose research targets wave propagation problems. The speakers are diverse in terms of training, location, and career type, which will be beneficial in terms of bringing together new ideas and generating interdisciplinary collaborations that wouldn't happen outside of an event like this.

- David Keyes KAUST, MCSE

- Hans Petter Langtangen *SIMULA/Univ. of Oslo*
- Marsha Berger *Courant Institute - New York University*
- Tobias Weinzierl *TUM*
- Aslan Kasimov *KAUST, MCSE*
- Tariq Alkhalifa *KAUST, PSE*
- Dave George *US Geological Survey*
- Jeff Stuart *UC Davis*
- Carsten Burstedde *University of Bonn*
- Hank Childs *Lawrence Berkeley National Lab*
- Sorin Mitran *UNC - Chapel Hill*
- Andreas Kloeckner *Courant Institute - New York University*
- Jed Brown *Argonne National Lab*

## Participants

Additional workshop participants will include researchers from KAUST and around the world in areas related to the workshop, as well as a number of KAUST students. We aim for a total of about 40 participants (10 international speakers, 10 other international invitees, and 20 KAUST participants) who will be involved in the workshop full-time throughout the week. In addition, the lectures will be open and it is expected that they will attract large audiences (the keynote talks were attended by about 50-70 last year).

## Technical Organizing Committee

The technical organizing committee members are:

- David I. Ketcheson, *KAUST MCSE Division* (Committee chair)
- Aron Ahmadi, *KAUST Supercomputing Lab*
- Randall J. LeVeque, *Univ. of Washington*
- Kyle T. Mandli, *Univ. of Texas Austin*

## Plan for evaluating and disseminating results

The [HPC]<sup>3</sup> workshop we held last year at KAUST attracted an unusual amount of attention for an event of its size – it was featured in two news articles with a worldwide audience and has already led to some submitted scholarly works. Furthermore, the principal outcome of the workshop was scientific software that is open source and freely distributed, with the number of users increasing significantly following the workshop. A workshop of this kind can have a powerful direct impact on a much broader audience than just the attendees, since the software developed at the workshop is a tool for researchers around the world. Evaluation of the meeting was performed by soliciting feedback from the participants, which was overwhelmingly positive but also included some useful criticisms that have been incorporated into plans for the sequel.

Results of the [HPC]<sup>3</sup> 2012 workshop will be disseminated in a similar way, probably including publication of scholarly works and articles in professional periodicals or websites and, most importantly, continued distribution of powerful open source software for solving hyperbolic PDEs. Effectiveness of the workshop will be evaluated by distributing an evaluation form to participants on the final day of the workshop.