

Fourth ISC HPC Applications in Precision Medicine Workshop (HAPM20)

Co-located with ISC 2020

Workshop Motivation

High-performance computing has become central to the future success of precision medicine. Catalyzed by the dramatic increase in the volume of research and clinical data available through sequencing and advanced imaging techniques, clinical data available through medical records and mobile health devices, research data from automated platforms, combined with molecular simulations and the rapid adoption of deep learning approaches has created a convergence shaping the frontiers of computing and precision medicine. New approaches to drug discovery, data sharing, aggregation and safeguards, clinical deployment, and use of machine learning models in research and clinical contexts have identified new challenges and opportunities in these rapidly evolving frontiers. The growth of opportunities to incorporate HPC in precision medicine applications continues to accelerate, exemplified by a very successful EU funded CompBioMed Conference held in September 2019 and pervasive presence of HPC applications at the recent SC19 conference including the room-filling (capacity limited at 82) Fifth Computational Approaches for Cancer workshop, along panel discussions, Birds-of-a-feather meetings and the selection of the use of HPC to study RAS biology as the best paper at the conference.

Synergies between experiments and theory in precision medicine research are often complicated by the lacking availability of primary data. Given the growing use of predictive models in multiple forms, especially in the context of deep learning and AI, large volumes of reliable and well annotated information are needed to establish a ground truth for training, for evaluation and even for validation of models. During the workshop, connections will be made across the communities, discussing platforms and possible ongoing solutions to facilitate development, referencing and exchange of experimental data and computational results.

The most recent Third HPC Applications of Precision Medicine workshop held at ISC19 was a tremendous success, building on the growing participation and interest in the first two workshops. The participants resoundingly are in support of a fourth workshop. Further, as efforts have been underway to broaden the interest in HPC applications of precision medicine, ISC is well positioned to provide the ongoing hub for collaborative discussion, drawing from across Europe as well as North America and Asia. The HPC Applications in Precision Medicine workshop aims to bring together the international computational and life sciences communities to share experiences, examine current challenges, and explore future opportunities for applications of high-performance computing in precision medicine.

Impact on ISC Conference

The workshop favorably impacts the ISC conference by attracting a growing community of life science participants to the conference. Conversations with life science professionals confirms interest in learning more about and increasing use of high-performance computing and applications in their efforts. Continuing the workshop as part of the ISC conference provides an opportunity to attract both the new and established life science and HPC communities looking to better support applications in medicine. The participants truly are looking forward to continued workshops as well as broadening the participants as the critical mass of attendees grows.

The workshop is specifically aiming to increase commercial participation in the ISC conference, attracting pharmaceutical and health companies with an interest in expanding the use of HPC to

accelerate critical business research and development efforts. The strength of the interdisciplinary draw for the workshop is confirmed in the slate of presenters in the first three workshops, initially invited and now predominantly selected from submitted abstracts.

Workshop Organizing Committee for HAPM20

The workshop organizing committee is spearheading the identification of presenters from across Europe, US and Asia. The committee was strongly supported by colleagues in both identifying, recruiting and selecting the slate of presenters for past workshops and has support for the same in developing the program for the 2020 workshop.

Eric Stahlberg – Frederick National Laboratory for Cancer Research

Jan Nygard – Cancer Registry of Norway

Marco Berghoff – ETH Zurich

Thomas Steinke – Zuse Institute Berlin

The workshop organizing committee continues to establish a growing program committee to support the organizers in developing the 2020 workshop program, including review and selection of submitted papers.

Tentative Workshop Program Committee

Sunita Chandrasekaran - University of Delaware

Peter Coveney – University College London

Bertil Schmidt, University of Mainz, Germany

Erin Crowgey, Nemours Children Hospital

Paul Macklin, Indiana University, USA

Jonathan Ozik, Argonne National Lab

Kshitij Srivatsava, Oak Ridge National Lab

Dave Richards, Oak Ridge National Lab

Fernanda Foertter, Nvidia

Target Audience

The workshop is expected to attract those developers, researchers, academic investigators, and commercial interests with interests in discussing cutting-edge computational problems in precision medicine, issues and opportunities for providing access to data, opportunities for incorporation of new technologies and solutions, and those seeking to develop new collaborations. The workshop will also attract computational and data scientists, health professionals, industry and others with recognized need for HPC solutions in precision medicine applications spanning large data, secure data, simulation, machine learning across the life sciences and health industries.

Prior workshops in related areas continues to attract a cross-disciplinary target audience to the workshop with expertise spanning HPC, machine learning, bioinformatics, parallel programming, big data, computer systems architecture, FPGAs, physics, biomedicine, cancer, precision medicine, deep learning, pathology, virology, GPU computing, computational physics, multiscale modeling, pattern recognition, software development, aerospace/computational fluid dynamics, crystallography, mathematics, storage, computer science, structural biology, IT infrastructure, protein structure, visualization, and systems biology.

Workshop Program

The workshop program is expected to provide a balance between invited presenters, presenters for accepted papers and panel discussions. Invited presenters will be selected with notable expertise in HPC applications in precision medicine, machine learning, novel architectures and large data management.

Call for Papers - The call for papers will seek submissions including the use of HPC in precision medicine, technologies with potential to accelerate HPC applications in precision medicine, use of machine learning in precision medicine, frontiers of HPC applied to life sciences, as well as special topical emphasis on cross-organization data access and sharing, predictive model access and sharing, reproducibility requirements in medical applications, adoption of HPC applications in clinical workflows, composite model and ensemble approaches. Topics from prior year workshops including use of synthetic data, multiscale modeling of biology and disease, data access and ground truth validation will be incorporated in the call.

The format for the program is projected to be:

Morning session

- Keynote and invited talks
- Submitted paper presentations
- Interactive panel discussion on challenges and opportunities (coverage for contributions to whitepaper(s))

Afternoon session

- Morning session recap – useful for attendees unable to make morning session
- Invited talks
- Submitted papers
- Open discussion and working session on next steps (logistical next steps for subsequent meetings, workshops and details for whitepaper contributions)

Workshop Outcomes

The primary outcome for the fourth 2020 HPC Applications in Precision Medicine workshop builds on the community building accomplishments of the first three workshops. The fourth workshop will focus on building collaborations and working together to address critical data challenges and exploit opportunities for accelerating adoption of HPC in precision medicine applications. This will be accomplished through the following workshop outcomes:

- 1) Education and increase mutual awareness of HPC applications in precision medicine
- 2) Build collaborative connections among workshop attendees
- 3) Build the community with the collection of email addresses for future communications
- 4) Provide opportunity for updates to topical whitepapers related to opportunities for international collaborations addressing challenges and opportunities for HPC applications in precision medicine – these challenges and opportunities include cross-organization data access and sharing, predictive model access and sharing, reproducibility requirements in medical applications, adoption of HPC applications in clinical workflows, composite model and ensemble

approaches

4) Catalyze discussions on future workshops, forming the foundation for the future call for papers at the ISC20 workshop.

Note: Publication of slides used in presentations will be done to the extent possible and permitted by presenters. Slides from the Third workshop were posted at the ISC website.

Workshop Promotion

Promotion of the proposed workshop has already commenced, at the SC19 Computational Approaches for Cancer workshop and SC19 Impacting Cancer with HPC Birds of a Feather session, discussions were held with participants about the interest in continuing and expanding the workshop.

Emails gathered from prior workshops at the SC conference and past ISC workshops will be employed to directly target attendees with known interest.

Additionally, the workshop will be promoted through multiple digital means as well as word of mouth and personal contacts of workshop organizers and presenters. The workshop will be visibly promoted to the bioinformatics community, the precision medicine community, and the HPC community through various email distribution lists and through direct emails to prior participants. Specific avenues identified below:

- Bioinformatics and Computational Biology Communities – Posting at bioinformatics.org, distribution through ISCB (International Society for Computational Biology), and other bioinformatics conferences attended and community events.
 - Drug development conferences and communities
 - HPC, Computing and Data Science Community – Submit call for participation on HPCWire, IEEE and ACM websites. Mailing lists for SIAM and other societies will be employed.
- Information on the workshop will also be shared with industry representatives selected to present in the industry overview. Flyers and notices shared at conferences attended.

Workshop Abstract

High-performance computing has become central to the future success of precision medicine. Catalyzed by the dramatic increase in the volume of research and clinical data available through sequencing and advanced imaging techniques, clinical data available through medical records and mobile health devices, research data from automated platforms, combined with molecular and multi-scale simulations and the rapid adoption of deep learning approaches has created a convergence shaping the frontiers of computing and precision medicine. New approaches to drug discovery, data sharing, aggregation and safeguards, use of machine learning models in research and clinical contexts have identified new challenges and opportunities in these rapidly evolving frontiers. The Fourth HPC Applications in Precision Medicine workshop aims to bring together the computational and life sciences communities to share experiences, examine current challenges in access and availability of research and clinical data, sharing and integration of computational approaches, and discuss future opportunities for addressing these and other challenges, thus shaping the future for HPC applications in precision medicine.