

REPORT

2019 Summer School and Workshop Parallel Computing in Molecular Sciences

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EXECUTIVE SUMMARY

A three and a half-day summer school was held with the primary goal of educating and training a new generation of graduate students and postdocs in molecular sciences with advanced high-performance parallel computing skills on the computing architectures of today and tomorrow. The summer school was held August 5-8, 2019 at Stony Brook University, Long Island, NY. 20 graduate students and postdocs participated. The workshop was supported by the Molecular Sciences Software Institute, the DOE ASCR ECP Project, IACS at Stony Brook and LBNL.

INTRODUCTION

The needs of molecular science place increased emphasis on achieving high performance on massively multicore heterogeneous computer architectures. A single desktop already consists of a dozen or more computer cores, while departmental compute clusters of tightly coupled 100s of compute nodes are also readily available. Emerging architectures on the horizon, with hundreds of non-uniform cores in a single “node” and hundreds of thousands of nodes connected in a non-uniform topology, will further widen the gap between the preparation of a typical junior scientist and the frontier of discovery in computation and data. We address these opportunities and challenges by bringing together the academic molecular science community and the Department of Energy (DOE) computing organizations and projects that have deep experience and skills at the forefront of HPC.

The goal of this summer school and workshop is to transfer and develop skills in parallel computing for molecular sciences, and to expose the next generation of science leaders to the state-of-the-art high-performance scientific computing on modern massively parallel architectures such as the exascale architectures coming online in the near future. These summer schools are essential for workforce development.

The primary organizers of the summer school and workshop are:

- **Bert de Jong** - Lawrence Berkeley National Laboratory
- **Robert Harrison** - Institute of Advanced Computational Science at Stony Brook University and Brookhaven National Laboratory, **MolSSI Board of Directors**
- **Ed Valeev** - Virginia Tech
- **Carlos Simmerling** - Laufer Center for Physical and Quantitative Biology at Stony Brook University

WEBSITE AND RECRUITMENT

The summer school and workshop details were announced on its website and the MolSSI website/email list:

<https://sites.google.com/lbl.gov/parcompmolsci/>

<https://molssi.org/2019/04/15/summer-school-and-workshop-2019-parallel-computing-in-molecular-sciences/>

Additional outreach was done at invited talks of the organizers. Applications were solicited of interested postdocs and graduate students. Out of the applications, 20 participants were selected. A list of the participants and affiliations can be found in Appendix A. Unfortunately, only 15% of the participants were women.

AGENDA, SPEAKERS AND TOPICS COVERED AT SUMMER SCHOOL

The list of speakers for the summer school are listed in Appendix B. A detailed agenda for the summer school can be found on the website below.

<https://sites.google.com/lbl.gov/parcompmolsci/home/schedule-and-people>

We would like to pursue a more diverse speaker pool for the next edition of this event.

PUBLICITY

The pictures below show the group and lecture session taken at the summer school.



OUTCOMES AND CONCLUSIONS

A clear conclusion drawn from the summer school and workshop is that there is a significant gap in training the next-generation of software developers in the field to fully exploit parallel computing in chemical sciences. Participants, many with no parallel computing training, or limited to basic programming classes, were highly engaged and enthusiastic about the summer school, and many see as an essential training that they were missing. It is essential to teach students parallel computing concepts early, allowing them to better reason about algorithms and coding strategies. The need for parallel computing training in chemical sciences was reinforced by the informal feedback we received directly from many of the participants.

FUNDING RESOURCE UTILIZATION

Funding resources consisted of a MolSSI/NSF grant of \$15,000 plus in-kind funding of workshop coordination resources, the DOE ASCR ECP commitment of \$15,000, a \$5,000 contribution from IACS at Stony Brook. A \$100 registration fee per student was used to ensure the students were serious in attending.

Nearly all of the funds were used to provide travel awards and housing for the graduate student and postdoc participants, and for breakfast, lunch and refreshments. Students were housed in Stony Brook dormitories, which led to a very cost-effective summer school. A rough (rounding) breakdown of the costs is below:

Food and lodging	\$4,685
Travel	\$5,355
Travel awards	\$3,500

MoISSI funds effectively covered the costs for all participants. IACS provided funds for the conference dinner and transportation.

SUMMARY AND FUTURE PLANS

A three and a half-day summer school was held with the primary goal of educating and training a new generation of graduate students and postdocs in molecular sciences with advanced high-performance parallel computing skills on the computing architectures of today and tomorrow. The summer school was held August 5-8, 2019 at Stony Brook University, Long Island, NY. 21 graduate students and postdocs participated. The workshop was supported by the Molecular Sciences Software Institute, the DOE ASCR ECP Project and IACS at Stony Brook. These summer schools are essential for workforce development.

Looking into the future, the organizing team would like to organize the summer school and workshop annually, alternating between the east coast and west coast. The first summer school was at Berkeley, CA, the second was at Stony Brook University. The team has already received a funding commitment from DOE ASCR ECP for 2020. A request for MoISSI will be made. Additional funding resources will be pursued (for example via commercial sponsorships) to allow a larger group of postdocs and graduate students to participate.

The team will also further increase the diversity, increased participation by students/postdocs from underrepresented groups, in the participant pool through targeted advertising and diversification of the speakers.

The training and exercise materials from this summer school will be converted into an online resource and potentially a new textbook that can be used in academia going forward.

ACKNOWLEDGMENTS

This research was supported by the Exascale Computing Project (ECP), Project Number: 17-SC-20-SC, a collaborative effort of two DOE organizations—the Office of Science and the National Nuclear Security Administration—responsible for the planning and preparation of a capable exascale ecosystem—including software, applications, hardware, advanced system engineering, and early testbed platforms—to support the nation's exascale computing imperative. Additional support was provided by the NSF funded Molecular Sciences Software Institute (MolSSI), AICS at Stony Brook and LBNL.

The team would like to acknowledge the hard work by Kortni Lindsey, Megan Gaskill and Jeanette Cooper at Virginia Tech to help in the organization of the event.

Appendix A: Complete list of participants

First name	Last name	Institution	First name
Malik	Abdul	Texas Tech University	Malik
Steven	Ayoub	California State University Northridge	Steven
Sathwik	Bharadwaj	Worcester Polytechnic Institute	Sathwik
Hyeji	Choi	Stony Brook University	Hyeji
Zach	Glick	Georgia Institute of Technology	Zach
Kent	Gorday	University of California Berkeley	Kent
Reza	Hemmati	Auburn University	Reza
Adrian	Hurtado	Stony Brook University	Adrian
Aaron	Mahler	Duke	Aaron
Sean	Mascarenhas	Stony Brook - IACS	Sean
Sehr	Naseem Khan	University of North Texas	Sehr
Rajat Kumar	Pal	CUNY	Rajat Kumar
Suehyun	Park	Georgia Tech	Suehyun
Lauren	Prentis	Stony Brook University	Lauren
Janos	Sarka	Texas Tech University	Janos
Natalia	Sizochenko	Dartmouth College	Natalia
John	Stoppelman	Georgia Institute of Technology	John
Chuan	Tian	Stony Brook University	Chuan
Zhe	Wang	Virginia Tech	Zhe
Robert	Wexler	Princeton University	Robert

APPENDIX B: SUMMER SCHOOL SPEAKERS

Summer school speakers:

- Ed Valeev – Virginia Tech
- Taylor Barnes – MoISSI/Virginia Tech
- Robert Harrison – Stony Brook (**MoISSI Board of Directors**)
- Lingda Li - Brookhaven National Laboratory
- David Cerutti – Rutgers University