

HPC User Forum Update

Interviews with HPC Community Leaders: Irene Qualters, Los Alamos National Laboratory

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IN THIS UPDATE

After the global pandemic forced Hyperion Research to cancel the its 2020 HPC User Forums, we decided to reach out to the HPC community in another way – by publishing a series of interviews with select HPC thought leaders. Our hope is that these leaders' perspectives on HPC's past, present and future will be interesting and beneficial to others. To conduct the interviews, Hyperion Research engaged insideHPC Media. We welcome comments and questions addressed to Steve Conway, sconway@hyperionres.com or Earl Joseph, ejoseph@hyperionres.com.

This interview is with Irene Qualters, who serves as the Associate Laboratory Director for Simulation and Computation at Los Alamos National Laboratory. She previously served as a Senior Science Advisor in the Computing and Information Science and Engineering (CISE) Directorate of the National Science Foundation (NSF), where she contributed to strategic leadership in new directions for the CISE Directorate and played a leadership role in interagency, industry, and academic engagements to advance computing. Qualters also served on the Science and Technology Committee of the LLNS/LANS Board of Governors. Prior to her NSF career, Qualters had a distinguished 30-year career in industry, with a number of executive leadership positions in research and development in the technology sector. During her 20 years at Cray Research, she was a pioneer in the development of high performance parallel processing technologies to accelerate scientific discovery. Subsequently as Vice President, she led Information Systems for Merck Research Labs, focusing on international cyberinfrastructure to advance all phases of pharmaceutical R&D. She has a M.S. in Computer Science from the University of Detroit and a B.S. from Duquesne University.

The HPC User Forum was established in 1999 to promote the health of the global HPC industry and address issues of common concern to users. More than 75 HPC User Forum meetings have been held in the Americas, Europe and the Asia-Pacific region since the organization's founding in 2000.

IRENE QUALTERS INTERVIEWED BY DOUG BLACK, insideHPC

Black: Hi, I'm Doug Black, editor-in-chief of insideHPC, and as part of our Hyperion Research series of interviews today we are talking with Irene Qualters. She is Associate Laboratory Director for Simulation and Computation at Los Alamos National Laboratory. Irene, thanks so much for joining us today.

Qualters: Thanks, Doug. It's a pleasure to be here.

Black: I understand you run a rather sizeable organization within Los Alamos. If you could, tell us about some of the project work that your group is doing and some of its more exciting potential implications.

Qualters: I've been involved in HPC for a long time and I've watched its evolution in a variety of scientific disciplines. One of the things that is particularly interesting and challenging for me is that Los Alamos represents a very broad scientific and HPC-relevant scope. This includes research that is entirely open. We've been quite active within my group, within collaborating groups across the laboratory, with academic scientists worldwide, and with other laboratories in pursuing, for example, research associated with Covid. That covers areas such as the genetic structure of the virus, how it infects and how contagious it is, as well as vaccine development. And that's just one area. We also have groups that are working with global climate simulation; our area of expertise is particularly associated with sea ice and ocean modelling. As we enter a no-analog area in terms of where we as planet have been before, the implications, not just on the geophysical phenomena, but on the societies, on their security as changes happen with sea level, with the biological makeup of the oceans - all of these are areas that we are interested in and involved in with others.

We also have a very significant mission, which has to do with ensuring the safety and efficacy of the U.S. nuclear stockpile. There, too, the challenges for the future are taking us into a no-analog space where materials under pressure and over time have to be understood, and we need to be able to do prediction. In many cases we do not have the experimental data to support the theory and the computational models that we're using. So, it matches well with my background and my personal interests.

Black: As I understand it, throughout your career you've really worked at the convergence of advanced computing and scientific discovery. In that context, share with us your thoughts about where HPC is headed. Are there trends that have you particularly excited? Are there areas of concern?

Qualters: As we look at the evolution of AI, both bringing in what is being learned from the outside and bringing in our own bent on AI, such as physics-informed AI and trustworthy AI, I think there's enormous opportunity. There are challenges I see, but I see a bright future. I don't know exactly what form it will take but I'm not worried about it from the bigger picture perspective. I'm confident that as long as we stay with one foot in what our communities need from us, as well as one foot in how technologies are evolving, I think things will go very well for us in the future.

Black: Tell us your thoughts on the biggest changes HPC has helped bring about in your various fields of research.

Qualters: I think the advance of modelling and simulation has been phenomenal and I think that we should lay claim to that. That's really important and I don't see that going away. I see that the needs

will continue to advance, particularly, as I said, as we go into areas where instruments may not be capable of giving us insight into atomic-level phenomena in the physical sciences, for example.

Black: We also hear about bringing AI into simulation. That sounds tremendously powerful. Tell us a little about how you got involved with HPC in the first place.

Qualters: I was really fortunate to leave graduate school at a time when supercomputing was really quite nascent. I joined a very young startup company called Cray Research at a time when it had fewer than 100 employees, and I was probably among the youngest. To be able to join a group that has very senior, very experienced people that have broad and deep knowledge - that's really a career-forming change, because one can see how mathematics influences physics influences computing. That was really my start. It gave me both the confidence and experience to be able to engage others in other disciplines and to be excited and stimulated and confident about doing that.

Black: How did your career evolve from there so that you got to Los Alamos?

Qualters: There were two major steps in between. One was at Merck Research Labs, and it was an interesting time because molecular dynamics was really evolving and maturing as well, frankly, as some of the early stages of AI. We were looking for signal detection in clinical trial data. That was really also a shaping event. I did a brief stint in a startup company that ended up being acquired by NVIDIA. Finally, I spent over nine years at the National Science Foundation, again, reinforcing that cross-disciplinary collaboration and engaging with others to really look at challenges that are at the horizon level and making sure that the role of computing continued to advance in a way that could affect all of those disciplines. That was a good fit for Los Alamos, given the breadth of research in their history with codesign and how theory, simulation, and experiment all interact with one another. It really is a good match and I'm excited about the challenges that we're engaged in and how we're going about it, the scientific integrity used to go about pursuing that knowledge.

Black: Great stuff. Thanks so much for joining us today. It was a pleasure speaking with you.

Qualters: Thanks, Doug.

About Hyperion Research, LLC

Hyperion Research provides data-driven research, analysis and recommendations for technologies, applications, and markets in high performance computing and emerging technology areas to help organizations worldwide make effective decisions and seize growth opportunities. Research includes market sizing and forecasting, share tracking, segmentation, technology and related trend analysis, and both user & vendor analysis for multi-user technical server technology used for HPC and HPDA (high performance data analysis). We provide thought leadership and practical guidance for users, vendors and other members of the HPC community by focusing on key market and technology trends across government, industry, commerce, and academia.

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