

Dr. Martin Berzins, University of Utah

Developing Software for Multiscale Multi-Physics Modelling with Applications in Materials by Design.

Abstract: Improvements in parallel computer performance have made it possible to consider solving multi-scale multi-physics problems that were previously simply too large and complex. Examples being considered at the SCI Institute at the University of Utah include turbulent combustion problems with 10^{13} cells, large scale detonations and materials-by-design problems. At the same time, the architectural changes in proposed new machines that are being introduced, or are planned for the next decade, have created a degree of uncertainty for software that has not been present for the last decade or so. In this talk, we describe one approach based on dynamic task-graphs that is seen as a likely candidate for exascale computers. This approach is implemented in the Utah computational framework. While task-graphs provide many advantages, they are not in themselves sufficient to achieve performance on the largest systems today. A number of enhancements are required to deliver scalability on these machines. Scalability results from machines such as DOE's Titan and Mira will be shown. Extension of this approach to multiscale materials by design will be described, together with the challenges that it poses. The extension exascale-type architectures will be described as much as this is possible.

Bio: Martin Berzins is a multi-disciplinary Computational Science researcher whose research cuts across Applied Mathematics, Computer Science and Engineering and is focused on the development of partial differential equations software for solving challenging engineering problems from a variety of applications on extreme-scale computers.

He is a Professor of Computer Science in the School of Computing and in the Scientific Computing Imaging Institute at the University of Utah and a Visiting Professor at the University of Leeds. He graduated in Mathematics at the University of Leeds in 1978 and obtained a Ph.D. in Numerical Analysis there in 1982. From 1982 until 2002 he was a Lecturer, Senior Lecturer, Reader, Professor in Scientific Computing and finally the Research Dean for Engineering at the University of Leeds. He was also the co-founder of the Computational PDEs unit at Leeds. Dr. Berzins is a Fellow of the Institute for Mathematics and its Applications in the UK and a Chartered Mathematician.

In 2003 he moved to the University of Utah, where he was Associate Director (2003-2005) and then Director of the School of Computing (2005-2010). From 2005 until 2014 he was co-Editor in Chief of Applied Numerical Mathematics. In 2012 he became Recipient Program Manager of the US Army Research Laboratory Collaborative Research Alliance in MSME (Multiscale multi-disciplinary Modeling of Electronic Materials), that brings together nine universities in undertaking electronic materials by design. In 2013 he became the Computer Science lead in the DOE NNSA PSAAP2 Carbon Capture Multidisciplinary Simulation Center at the University of Utah.