What are the Opportunities and Challenges for a new Class of Exascale Applications?

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Abstract. The U.S. Department of Energy's (DOE) Exascale Computing Project (ECP) is a partnership between the DOE Office of Science and the National Nuclear Security Administration. Its mission is to transform today's high performance computing (HPC) ecosystem by executing a multi-faceted plan: developing mission critical applications of unprecedented complexity; supporting U.S. national security initiatives; partnering with the U.S. HPC industry to develop exascale computer architectures; collaborating with U.S. software vendors to develop a software stack that is both exascale-capable and usable on U.S. industrial and academic scale systems, and training the next-generation workforce of computer and computational scientists, engineers, mathematicians, and data scientists. The ECP aims to accelerate delivery of a capable exascale computing ecosystem that will enable breakthrough modeling and simulation (M&S) and data analytic computing (DAC) solutions to the most critical challenges in scientific research, energy assurance, economic competitiveness, and national security.

Applications ready and able to address challenge problems of U.S. interest are the driving force behind the ECP, hence the ECP is responsible for ensuring exascale application readiness and delivering scalable science and engineering performance. The vision of the ECP Application Development effort is to enhance the predictive capability of M&S and DAC applications of high priority to the DOE and other U.S. agencies through requirements-based development of physical models, numerical algorithms and methods, and exascale software. This includes integration of crosscutting co-designed software technologies, exascale system readiness and utilization, and demonstration of exascale challenge problem capabilities.

Given these challenges, tremendous opportunity nevertheless exists for science-based computational applications that can deliver, through effective exploitation of exascale HPC technology, breakthrough M&S and DAC solutions that yield high-confidence insights and answers to the nation's most critical problems. While reflecting on some of my own person R&D experiences, I will survey these application opportunities, with a particular focus on CFD applications, where I will also touch upon challenges, decadal challenge problems, and prospective outcomes and impact.