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DEVELOPING SCIENTIFIC RESEARCH CODES FOR EFFECTIVE UTILIZATION OF LEADING HPC PLATFORMS

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ABSTRACT

Decades of advancements in mathematical models, numerical algorithms and computing capabilities have brought many complex non-linear problems that occur in science and engineering closer to understanding through simulations. The increased resolution and modeling fidelity comes with an increase in the complexity of developing and managing advanced simulation software. The model of a few researchers working in isolation with their own tools, though still used extensively in many academic communities, is not well suited to address present day challenges in developing scalable computing codes for High Performance Computing (HPC) platforms. A solution to the effective utilization of HPC resources could be the development of sophisticated, scalable, and robust *community codes* that are designed to cover the needs of a broader community of researchers, where various groups contribute to enhance the range of applicability. Today there are some successful cases where the integration of science and code teams lead to a collection of publicly released software (i.e. FLASH[1], NAMD[2], SAMRAI[3], etc.). Other communities have made less progress. The CFD community, for example, is hampered by the limited availability of scalable computational codes. This limits the use of HPC resources by the community.

The development of a well-managed reliable code is an important requirement for cost efficient utilization of HPC resources by a wider user base. This may include not only the simulation software but also the support software, such as data analysis, performance management, etc. The degree of sophistication and complexity of codes running on high-end HPC platforms necessitates attention to software engineering practices, such as version control, coding standards, unit tests and verification processes, documentation, etc. To address these challenges a cultural shift is probably necessary for scientists to realize the advantages of code reusability, verification and maintainability when an integrated computing approach is used.

The proposed mini-symposium will focus on how to address these challenges. We will invite keynotes and presentations from developers and users of *codes* that have transformed the simulation and modeling capabilities in their respective research communities. It will provide

a forum for sharing hard-won knowledge about what is successful, and what is not successful. Furthermore, bringing together practitioners from many relevant research fields will provide attendees with a unique opportunity for exploring and initiating interdisciplinary collaborations towards leveraging other efforts in their own research.

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