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Guest Editorial

Special Section on Exascale Computing for Fluids Engineering Applications

The exascale computing project[1] of the department of energy initiated in 2016 and ending in December 2023 aimed at developing applications and a supporting software ecosystem able to run on the department of energy exascale (10^{18} calculations per second) supercomputers: Frontier (Oak Ridge Leadership Computing Facility) and Aurora (Argonne Leadership Computing Facility) for the Office of Science and El Capitan (Livermore National Laboratory) for the National Nuclear Security Administration. These exascale supercomputers are based on hybrid – also called heterogeneous – computer architectures that use graphics processing units as accelerators to the central processing units at scales greater than or equal to 10,000 nodes. Frontier and El Capitan use advanced micro devices (AMD) technologies, and Aurora uses Intel technologies. Frontier is currently the fastest supercomputer in the world with 1.6 exaflops (top500.org).

The impact of exascale computing on fluids engineering applications is capacity and accuracy. Exascale computing for computational fluid dynamics (CFD) allows unprecedented resolution (that is finer mesh resolution) in complex geometries with higher order spatial and temporal discretization methods. For turbulent flow, it means direct numerical simulation can now achieve larger Reynolds number. It also enables CFD to be used in multiphysics simulations including, among others, reactive flow with chemistry, materials deformation, fluid–structure interactions with energy transfer, and radiation transport, thus, increasing overall accuracy and prediction of engineering systems for energy and national security applications. It also means that one can perform more simulations to generate large training datasets for Artificial Intelligence and Machine Learning algorithms to better represent underlying physics, to develop surrogate models that bridge scales, and to ultimately accelerate and increase accuracy of fluids engineering simulations.

In this special section, five research projects funded through exascale computing project with applications relevant to fluids engineering are highlighted ranging from incompressible flow to compressible flow and single to multiphase flows in simple to complex geometries:

- Energy Exascale CFD Simulations with the Spectral Element Method
- Exascale CFD in Heterogeneous Systems
- PeleMP: The Multiphysics Solver for the Combustion Pele Adaptive Mesh Refinement Code Suite
- Toward polydisperse flows with MFIX-Exa
- Performance Portable Graphics Processing Unit Acceleration of a High-Order Finite Element Multiphysics Application

In these articles, the authors described what computer science and software technologies they had to adopt and how they had to adapt them to prepare their CFD and multiphysics applications codes to run on exascale architecture and achieve performance that will enable fluids engineering breakthroughs in future computational science campaigns.

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