Title: Computational Science at the Argonne Leadership Computing Facility

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Abstract: The goal of the Argonne Leadership Computing Facility (ALCF) is to extend the frontiers of science by solving problems that require innovative approaches and the largest-scale computing systems. ALCF’s most powerful computer -- Mira, an IBM Blue Gene/Q system -- has nearly one million cores. How does one program such systems? What software tools are available? Which scientific and engineering applications are able to utilize such levels of parallelism? This talk will address these questions and describe a sampling of projects that are using ALCF systems in their research, including ones in nanoscience, materials science, and chemistry. I will also present the allocation programs available to U.K. researchers and the international community. Lastly, I will present some information about the future ALCF systems, Theta and Aurora.