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David Daniel, Patricia Fasel, and George Zagaris  
Large-volume sky surveys have accessed the Universe’s vast temporal and spatial expanse via a remarkable set of measurements. Interpretation of these cosmological observations requires large-scale numerical simulation and modeling. Addressing analysis workflow complexity is as important as running the underlying extreme-scale simulations. Here, the authors discuss how the Hardware/Hybrid Accelerated Cosmology Code framework addresses these challenges.

24 Experiences from Leadership Computing in Simulations of Turbulent Fluid Flows  
Myoungkyu Lee, Rhys Ulerich, Nicholas Malaya, and Robert D. Moser  
PoongBack is a turbulence simulation code that helps create realistic simulations of turbulent flows. PoongBack includes a new parallel 3D FFT kernel and shows excellent scalability up to 786,432 cores. Using Mira at the Argonne Leadership Computing Facility, PoongBack achieved direct numerical simulation at $Re = 5,200$, and generated approximately 140 Tbytes of data.

32 Real-Time Stochastic Optimization of Complex Energy Systems on High-Performance Computers  
Cosmin G. Petra, Olaf Schenk, and Mihai Anitescu  
A scalable approach computes in operationally-compatible time the energy dispatch under uncertainty for electrical power grid systems of realistic size and with thousands of scenarios.

44 Scientific Discovery in Fusion Plasma Turbulence Simulations at Extreme Scale  
William Tang, Bei Wang, and Stephane Ethier  
Extreme-scale plasma turbulence studies offer new insights on confinement scaling in magnetic fusion systems by using powerful, world-class supercomputers to run simulations with unprecedented resolution and temporal duration. The studies also shed light on how the turbulent transport of heat and particles in the plasma and the associated confinement scale from present-generation devices to much larger ITER-size plasmas.

54 Quantum Dynamics Simulation of Electrons in Materials on High-Performance Computers  
André Schleife, Erik W. Draeger, Victor M. Anisimov, Alfredo A. Correa, and Yosuke Kanai  
An implementation of Ehrenfest non-adiabatic electron-ion dynamics demonstrates high scalability on two different leadership-class computing architectures. The implementation accurately calculates electronic stopping power, which characterizes the rate of energy transfer from a high-energy particle to electrons in materials. It has the potential to yield other scientific insights using quantum dynamics simulations at the electronic structure level.

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Driven by community needs, the Extreme Science and Engineering Discovery Environment (XSEDE) project substantially enhances the productivity of a growing community of scientists. XSEDE’s integrated, comprehensive suite of advanced digital services federates with other high-end facilities and with campus-based resources, serving as the foundation for a national e-science infrastructure ecosystem.

For more information on these and other computing topics, please visit the IEEE Computer Society Digital Library at www.computer.org/csdl.
Formal Verification of a Gravity-Induced Loss-of-Consciousness Monitoring System for Aircraft
Seonmo Kim, Wonhong Nam, Hyunyoung Kil, and Myunghwan Park

Gravity-induced loss of consciousness (GLOC) due to blood draining away from the brain is one of the main reasons for many high-gravity maneuvering aircraft accidents, with many pilots losing their lives. This article presents a case study to verify a GLOC monitoring system by using a model-checking technique.

Large-Scale Parallel Simulations of 3D Cell Colony Dynamics
Maciej Cytowski and Zuzanna Szymarska

Biological processes are complex and involve many unknown relationships and mechanisms at different scales. Achieving a simulation scale that corresponds, for instance, to clinically detectable tumor sizes is still a huge challenge. A novel, high-performance computational approach enables simulations of 3D cell colony dynamics at a previously unavailable tissue scale.

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