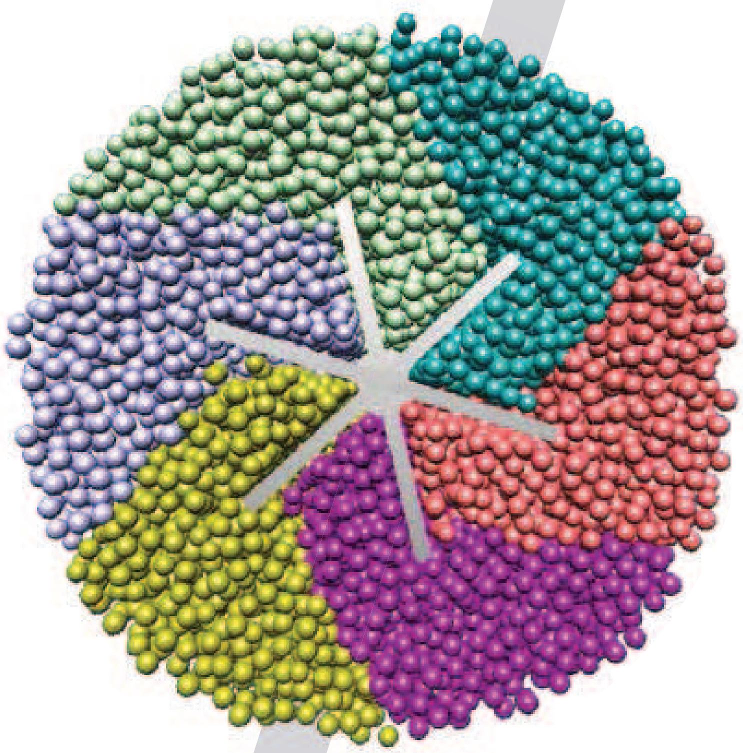
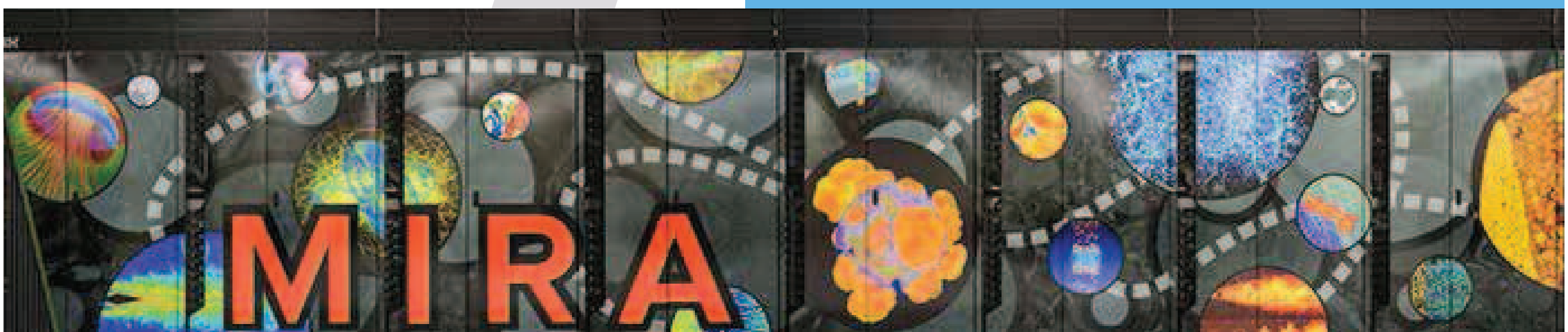
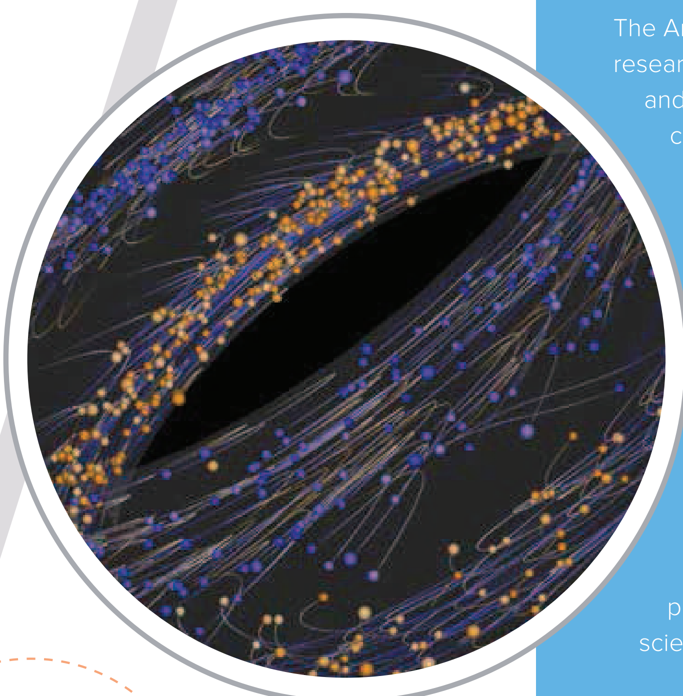
ARGONNE **LEADERSHIP COMPUTING** FACILITY

2013 SCIENCE HIGHLIGHTS



Argonne NATIONAL LABORATORY





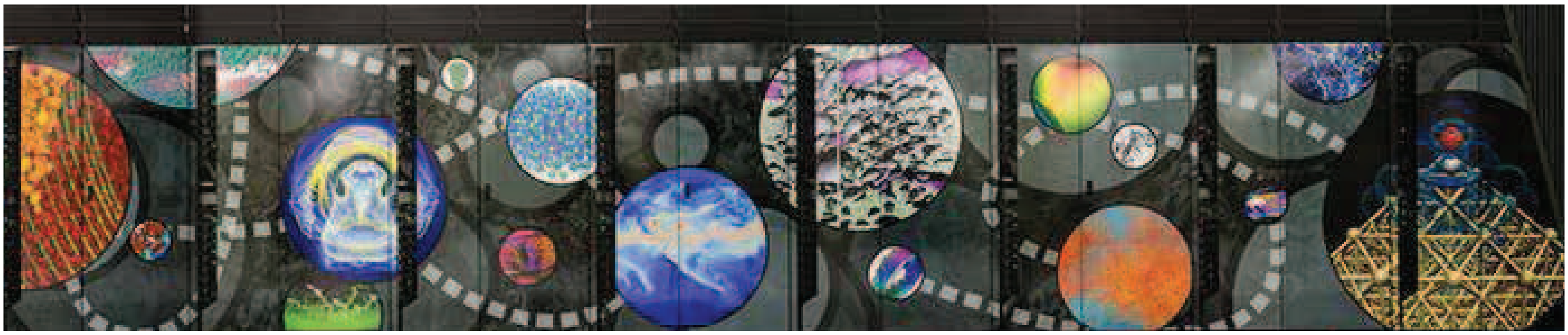
ABOUT **ALCF**

The Argonne Leadership Computing Facility provides researchers from national laboratories, academia, and industry with access to high-performance computing capabilities to enable breakthrough science and engineering. Supported by the U.S. Department of Energy Office of Science, the ALCF is one of two leadership computing facilities in the nation dedicated to open science.

MISSION

The ALCF's mission is to accelerate major scientific discoveries and engineering breakthroughs by designing and providing world-leading computing facilities in partnership with the computational science community.

{MIRA} AN ENGINE FOR DISCOVERY



The advent of petascale supercomputers allows researchers to conduct calculations and simulations on unprecedented scales, and the ALCF houses one of the fastest in the world. An IBM Blue Gene/Q supercomputer, Mira went into production on April 9, 2013. Its architecture is the result of a co-design collaboration between Argonne National Laboratory, Lawrence Livermore National Laboratory, and IBM Research.

Capable of carrying out 10 quadrillion calculations per second, Mira's enormous computational power can be attributed to a symbiotic architecture that combines novel designs for fine- and coarse-grain parallelism with corresponding network and I/O capabilities that redefine standards in supercomputer processing and networking.

With the ability to employ 10 times as much RAM and 20 times as much peak speed in floating-point calculations, Mira has far exceeded the capabilities of its immediate predecessor Intrepid, an IBM Blue Gene/P.

An escalation in Mira's node-level parallelism increases the number of tasks a node can perform. Each compute node has 16 processing cores supported by simultaneous multi-threading (SMT), which allows a core to run four simultaneous threads of execution—all adding up to 64 simultaneous tasks per node. This is further enhanced by quad processing extensions (QPX), which allow for single instruction multiple data (SIMD) operation on each thread. With this, Mira can execute eight floating-point operations with a single instruction.

This type of high-level computing would not be achievable without an equally highly structured communications network, such as Blue Gene/Q's 5D torus interconnect. Designed to provide greater bandwidth and lower latency relative to a 3D torus, more information can be relayed simultaneously and faster.

Buttressing the main architecture are custom features that help the user access and modify data more efficiently.

- The L1 cache prefetcher greatly reduces the time spent waiting for memory access and allows applications to run better by predicting and delivering data that the user needs before it is actually requested.
- Atomic operations ensure that data is read and written correctly when accessed by multiple threads simultaneously. These are implemented in the L2 cache rather than at the processor core, which dramatically reduces their cost.
- Transactional memory manages the concurrent use of multiple threads, protecting against conflicting operations in the atomic region and correcting for it. It is the first such hardware in a commercial supercomputer.

The Blue Gene/Q system demonstrates the major benefits that can be gained from innovative architectural features that are developed with a deep understanding of scientific computing requirements. Such an approach is already leading researchers down the path toward exascale computing. Making it possible to perform computations 100 times faster than today's most powerful computers, these machines will truly prove themselves engines of discovery.

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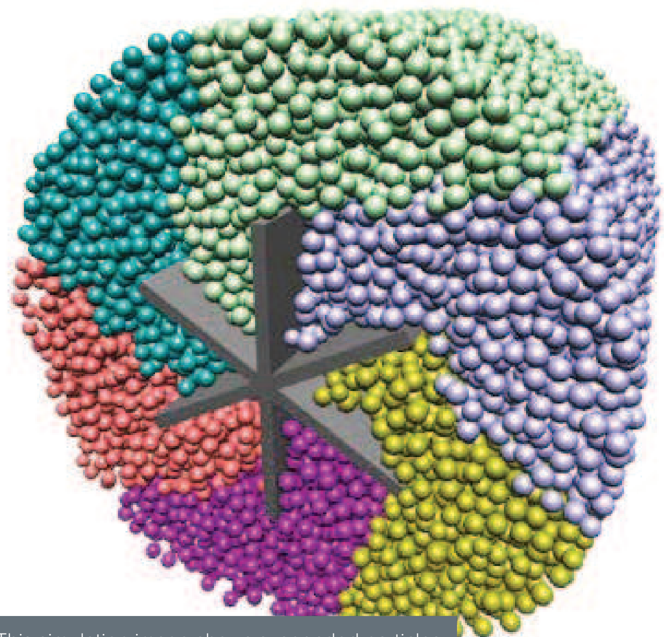
High-Fidelity Simulation of Complex Suspension Flow for Practical Rheometry

Highly versatile and stone-like in strength, concrete is the most widely used fabricated building material, representing a multibillion dollar industry. Researchers from the National Institute of Standards and Technology (NIST) are using ALCF supercomputers to conduct large-scale simulations to advance the materials and measurement science of concrete.

Given the critical importance of concrete to our nation's infrastructure, there is broad interest in making it a more sustainable material by improving its strength and durability, reducing the amount of greenhouse gas created during its production, and by finding new ways to recycle it. Architects also continue to push for enhanced workability that will allow concrete to flow more easily into increasingly intricate forms. These and other improvements require that scientists first find a way to accurately and reliably measure the viscosity of concrete.

Due to the complex nature of concrete, which is a dense suspension comprised of water, cement, and an aggregate, such sand or gravel, it is a challenge to accurately measure its rheological properties. Led by researchers from NIST, this project aims to advance the measurement science of concrete and to gain a fundamental understanding of how it flows. By simulating the flow of concrete in virtual rheometers, researchers are addressing the problem of relating measured quantities (e.g., torque and angular velocity measurements) to fundamental rheological properties (e.g., viscosity versus strain rate).

Researchers are combining data from these large-scale simulations with theoretical work and physical experiments to create Standard Reference Materials (SRMs) for concrete to allow for more accurate viscosity measurements. SRMs are certified and issued by NIST for use in quality control, regulatory compliance, product development, and scientific research for a wide variety of materials, including steel, rubber, and plastics. The NIST research team is currently running simulations that will feed into the development of SRMs to calibrate rheometers for mortar (cement and sand) and concrete (mortar and gravel). The mortar SRM is expected to be available soon.



This simulation image shows suspended particles in a rheometer for NIST's proposed mortar SRM. The spheres, which are color coded by their starting location in the rheometer, are suspended in a cement paste with properties derived from NIST's cement paste SRM.

Image Credit
Nicos Martys and Steven G. Satterfield, National Institute of Standards and Technology

IMPACT » **The development of Standard Reference Materials (SRMs) will enable accurate predictions of the flow of concrete, which is essential to exploring the use of new, more environmentally friendly ingredients for concrete mixtures. Additionally, the SRMs will help to improve the workability of concrete by creating standardized measurements that will allow builders to request a specific concrete formulation with reliable, repeatable results.**