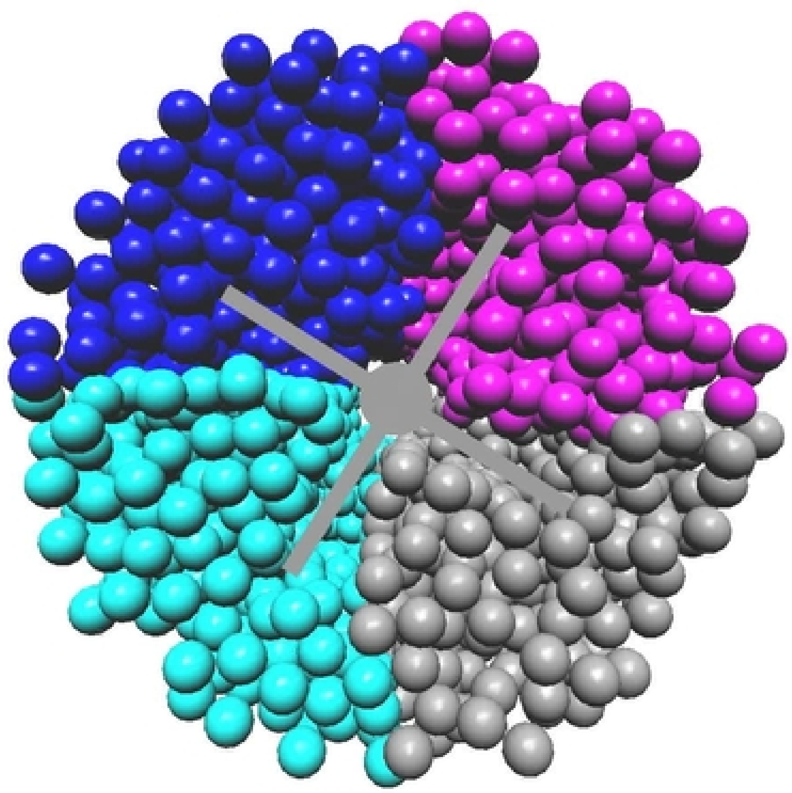
Supercomputer simulations yield method for predicting behavior of new concrete formulas

January 22 2015, by Chad Boutin



Just because concrete is the most widely used building material in human history doesn't mean it can't be improved. A recent study conducted by researchers from the National Institute of Standards and Technology (NIST), the University of Strasbourg and Sika Corporation using Department of Energy (DOE) Office of Science supercomputers has led to a new way to predict concrete's flow properties from simple measurements.

Concrete begins as a thick pasty fluid containing innumerable particles in suspension that can, ideally, flow into a space of nearly any shape, where it hardens into a durable, rock-like state. Its initial flexibility combined with its eventual strength has made it the material of choice for building everything from the ancient Roman Colosseum to the foundations of countless modern bridges and skyscrapers.

But concrete is not without its problems. For example, when concrete is pumped, it can jam in pipes, leading to time and cost overruns during construction. The particles can settle out, leading to structural problems after the concrete hardens. And a significant amount of energy is needed to create the cement that reacts with water to produce hardened concrete. This critical binding agent is manufactured at high temperatures in a kiln, a process that generates a great deal of carbon dioxide, a greenhouse gas. According to the World Business Council for Sustainable Development, worldwide cement manufacture is estimated to account for at least 5 percent of humanity's carbon dioxide emissions.

The industry can develop less energy-intensive concrete mixtures by replacing some of the cement with alternative materials like fly ash. However, these alternatives can require expensive chemical additives, and they also can have a range of effects on concrete flow. Ideally, the industry would like to tailor the use of these chemical additives, thus helping to assure the greatest use of alternative materials.

"We'd like to be able to design concrete that performs better on the job and doesn't demand so much energy to manufacture," says NIST computer scientist William George. "But what should we make it from? And what can we replace cement with? The answers will affect its properties. So we realized we needed to learn more about how suspensions work."

While it's a simple goal to describe, accomplishing it demanded some complex math and physics, and at the same time, an enormous amount of computer power to study how all the particles and fluid react as they are mixed. The NIST team was granted an INCITE Award that provided more than 110 million core hours at the Argonne Leadership Computing Facility. The ALCF supercomputers allowed them to simulate how a suspension would change if one or more parameters varied—the number of suspended particles, for example, or their size.

Suspensions have a remarkable property: Plotting two parameters—viscosity vs. shear rate (the latter refers to how neighboring layers of the fluid change velocity as it flows through a pipe)—always generates the same shaped curve as plotting them for the suspending fluid alone without added particles. This is true no matter what fluid is used. The curve just sits on a different location on the X-Y axis, as though someone had pushed it upwards or off to the side without otherwise altering its shape.

What the team unexpectedly found was the amount that the curves had to be shifted could be predicted based on the microscopic shear rates that existed between neighboring particles. Experiments at the University of Strasbourg confirmed the simulated results, which allowed the team to come up with a general theory of suspensions' properties.

"So now if you have a suspension that is made with a fluid that behaves a bit differently, you can still predict what its properties will be," George says. "You just have to measure the properties of the fluid that the particles are placed in, and you predict how the fresh concrete will behave."

The results should help accelerate the design of a new generation of high-performance and eco-friendly cement-based materials by reducing time and costs associated with R&D, George adds.

NIST is also using this new knowledge to create Standard Reference Materials for industrial researchers to calibrate concrete rheometers—instruments used to measure the flow of complex fluids—for material development. Ultimately, this could help expand the use of alternative materials. While it is not yet known whether these alternatives will fit the bill, the team's research could eventually help industry researchers zero in on the best new recipes.

More information: M. Liard, N.S. Martys, W.L. George, D. Lootens and P. Hebraud. "Scaling laws for the flow of generalized Newtonian suspensions." *Journal of Rheology*, 58, 1993 (Nov/Dec 2014 issue), DOI: 10.1122/1.4896896

Sika Corporation: usa.sika.com/

Provided by National Institute of Standards and Technology

Citation: Supercomputer simulations yield method for predicting behavior of new concrete formulas (2015, January 22) retrieved 25 April 2024 from https://phys.org/news/2015-01-supercomputer-simulations-yield-method-behavior.html