Advancing the Materials Science of Concrete with Supercomputers

Adding to industry knowledge using complex and interactive simulations of rheology and hydration

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Simulations on supercomputers are used to enhance our understanding of complex systems such as global weather patterns, nuclear explosions, the birth of galaxies, molecular structure, and the rheology and hydration of concrete. These simulations are our current best representations based on fundamental physical, chemical, and mathematical principles.

Why does concrete need to be simulated on a supercomputer? Concrete is arguably, from a materials science point of view, the most complex material produced by humankind with distinct, important, and random structural features on length scales ranging from nanometers to hundreds of millimeters. It has many mineralogical phases; its behavior is time dependent; it's formed from natural materials whose properties are quite variable; and it's sensitive to its surrounding environment, which of course drastically varies around the world. For such a material, reliably and optimally manufacturing its constituents, mixing and placing the actual concrete, and then guaranteeing the appropriate finished properties are great challenges. Simulating this complex material is an even greater challenge.

Correctly modeling the rheology and hydration of concrete can help solve many problems that continue to bother the concrete industry. The National Institute of Standards and Technology (NIST) has made progress on these two problems by using massively parallel computers that drive advanced scientific models. This work has required sophisticated physical science to develop the models and sophisticated computer science and hardware to run the models effectively. Basic insights from these models will drive the development of more accurate and reliable standard measurement techniques.

This supercomputer-based research is closely coupled to NIST's Virtual Cement and Concrete Testing Laboratory (VCCTL) consortium, which was established in 2001 to bring concrete industry engineers and scientists together with NIST researchers to accelerate the development of a virtual testing software environment, mainly working at the micrometer-millimeter scale.[1] In its ninth year, the VCCTL project has recently been awarded the U.S. Department of Commerce Silver Medal "for creating the unprecedented capability to predict the performance of concrete—the key material used in the U.S. physical infrastructure." The consortium has also won two Department of Energy (DOE) Office of Advanced Scientific Computing Research (OASCR) awards for excellence in 3-D visualization of the cement and concrete models described herein.

RHEOLOGY AND HYDRATION MODELS

Modeling the rheology (flow) of concrete is very difficult because fresh concrete is composed of particles that range from less than 1 μm to 10 mm in size. Our multiscale models simulate flow at different length scales by adding particles to a representative matrix fluid that

models the particles' behavior. At the smallest scales of interest, water is the matrix fluid, and cement powder is added to the water to model a cement paste. The cement paste then becomes the next continuum matrix fluid, to which sand particles (and air voids) are added to model a mortar. The mortar's flow properties are input into a flow model of concrete, where fresh mortar is the matrix fluid and coarse aggregates are the inclusions.

Particle shape at all length scales must be considered when predicting flow properties. For example, riverbed aggregates are somewhat rounded but crushed aggregates can be angular with faceted sides; this shape difference affects the rheology. The same holds true at the cement particle scale. Our computational models are based on novel methods for modeling fluid flow.[2,3] We've developed models that simulate flow at the particle scale, taking into account variable particle shape and size, forces between particles in a dense suspension, and matrix fluids having complex flow properties.

The hydration of cement paste depends on the cement particle size distribution; cement mineralogy; the water-cement ratio; the presence of any chemical admixtures such as retarders, accelerators, or high-range water-reducing admixtures; and curing conditions such as temperature and relative humidity. A model of cement hydration must be able to predict the rate of hydration and the development of the binder structure as a function of all of these variables. The hydration process involves combining the diffusion of molecules in solution with 20 or more chemical reactions. Most of the reactions are not well understood, and there is some debate about their reaction mechanisms. In addition, hydration reactions occur at the nanometer scale but eventually give rise to micrometer-scale solid features in the microstructure that must also be accurately modeled so that setting time and mechanical and transport properties can be computed.

To address these challenges, we have developed a kinetic cellular automaton model that simulates the first few hours of cement hydration, when the chemical and microstructure changes are most pronounced. This model simulates the fully coupled diffusion and reaction phenomena, and we have used it to gain insight into reaction mechanisms and their influences on structure development in concrete binders at early ages. Other related models exist for simulating later-age structure and property development.

Fig. 1: Two highly parallel machines that have been used in the NIST simulation program: (a) Columbia, a cluster of 24 SGI Altix machines, each containing 512 processors, maintained by the National Aeronautics and Space Administration (NASA); and (b) Intrepid, an IBM Blue Gene/P with 163,840 processors, maintained by Argonne National Laboratory. Time on these machines was awarded to us by the NASA National Leadership Computing System initiative and by the DOE Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program, respectively. The machines are identified only to adequately describe the project—the identification is not an endorsement or recommendation by NIST, nor does it mean that the equipment is necessarily the best available for the purpose

MODELS AND COMPUTER SCIENCE

Both of the aforementioned models have been designed to run on large multiprocessor (also known as highly parallel) machines (Fig. 1). To use a "parallel" computer, a large computation must be split up into smaller parts with each part run by a separate processor. In principle, this can speed up the program by a factor equal to the number of processors used, although in practice there are always practical limitations. We could not run models that were large enough for concrete without the power of parallel algorithms and parallel computers.

For both models, we are simulating a physical system, contained in a 3-D volume; we are moving the simulation forward in time by small time steps. The algorithms use the local conditions (such as chemical concentrations and fluid velocities) surrounding any particular point in the model volume to predict the state of the system at that point for the next time step. This means that we can divide the simulation volume into subvolumes that are

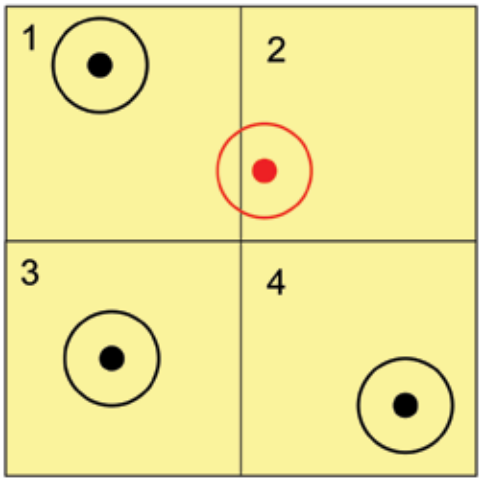

Fig. 2: A schematic picture of how a parallel computer with four processors treats the hydration or rheology models described in this article. The processors are numbered 1 to 4, and the squares are the regions they control. The points represent sample locations where data are updated as the simulation progresses. The circles represent the surrounding region from which information is drawn to update the data points in the models

each controlled independently by a single processor. So, for example, if we're running a simulation on 1000 processors, we can arrange these processors into a 10^3 size mesh, where each processor handles one subvolume, potentially speeding the computation by a factor of 1000.

Figure 2 shows a simple four-processor (potential speed-up of four times) setup in two dimensions. Each processor controls its own square area, and the points are some places where data is generated and updated at each time step. The circles around the points denote the local region that affects how the data at the point changes. The black points and their surrounding regions are totally within a processor's subvolume, so it has all the information it needs to predict its next time step. However, the red point has its data region crossing the boundary between processors, so Processors 1 and 2 will need to pass information back and forth to update the data at the red point, reducing the increase in speed to something less than a factor of 4. Because of this communications overhead, high-speed networks for information flow are a crucial part of supercomputing; and because communication rates are usually slower than computation rates, the real speed-up is typically less than the number of processors. In fact, as we use more processors to simulate a particular system, each processor's subvolume becomes smaller and at some point, adding more processors to a simulation will no longer improve the execution time because the overhead of interprocessor communication outweighs the benefit of having more processors to do the work.

In the flow model, both the fluid and the suspended inclusions (cement, sand, or gravel) are composed of smaller particles. As mixing forces are applied, the fluid particles and the inclusions begin to move within the volume. As these particles move within the simulation volume, they pass from one subvolume (or processor) to the next. The location and velocity of each particle are then updated based on the forces computed. The fluid stress on each inclusion and the total system stress are computed to give global rheological variables that can be compared to experiments.

When simulating cement hydration and setting, a cement paste system (cement particles and water) is represented by a 3-D voxel (volumetric picture element) digital image grid, and chemical components such as the various minerals, water, and dissolved species in solution are modeled as small cells of concentration at points of the grid. On each simulation time step, both diffusion of mobile species and chemical reactions can occur at each voxel.

The diffusion of mobile species is accomplished by random movements of those components between neighboring grid points, and chemical reactions are considered at each voxel. Chemical and structural changes in the system are tracked by updating the number of cells of each type at the end of every time step.

In addition, the model keeps track of the net heat released by the reactions; the solution composition, including pH; and the setting time. Updating diffusion and reactions at a grid point requires only localized information about the system around that point. Neighboring processors therefore require only as much communication with each other as necessary to exchange information about neighboring points at their subvolume boundaries.

MODELS AND VISUALIZATION

A *lot* of data comes out of these 3-D, multiprocessor simulations. Fully understanding the output of a supercomputer-based concrete flow or cement hydration simulation is a difficult problem that requires high-performance visualization and analysis. In the field, trying to look through fresh concrete is not easy, and with only simple-minded visualization of model outputs, researchers will end up fruitlessly "sticking their head into a bucket of concrete." Our team meets this challenge using a state-of-the-art immersive visualization environment (IVE). To understand immersion, consider the following analogy: looking at 3-D data on an ordinary computer screen is like looking at goldfish in a bowl; using an immersive system is like swimming with the goldfish at the scale of the goldfish.

The NIST IVE consists of hardware and software implemented to create a virtual laboratory. In this laboratory, the researcher is immersed into a qualitative and quantitative environment with tools for visualization, analysis, and measurement (Fig. 3). The system consists of three projectors (two rear projection, one top down)

arranged behind three 3.05 x 3.05 m (10 x 10 ft) square left, right, and floor screens arranged in a corner of a cube. Active stereo glasses produce 3-D images. A third, and very important, hardware component is location tracking. This subsystem tracks the direction and orientation in which a single user is looking. This information is used to update the 3-D images being generated in real time.

From the three screens, this user perceives a fused visual experience of being surrounded by the data. Within the physical constraints of the screen surfaces, the user can walk around and through the data representation. Using this environment allows the researcher to interact virtually with the system under study in ways that are physically impossible.

The creation of an immersive application requires collaboration between the physical scientist with knowledge of the application and the computer scientist with knowledge of the visualization techniques. The challenge is to find a graphical representation that "speaks" to the research scientist and facilitates new understanding through interactive navigation, analysis, and measurement in the virtual environment. A successful application will either confirm or contradict the scientist's preconceived notions. Both outcomes have benefits and point the way to future progress.

CONCRETE FLOW RESULTS

Figure 4 shows a snapshot of a visual simulation of aggregate flow inside (transparent) cement paste. Navigation in the immersive environment provides insight into the behavior of the flow. The system allows the researcher to "swim around" inside the concrete flow.

A technique recently implemented on the NIST system allows the researcher to focus on an area of interest while still providing visual context. In Fig. 5, the aggregates carrying low stress are shown as outline shapes while the aggregates carrying most of the stress are solid. This technique allows the researchers to focus on interesting high-stress areas while providing an overall view of the visual context, which is crucial for understanding. Isolated images without a visual context are not very instructive and can even be misleading.

Using this kind of visualization and further analysis of the supercomputer data, the concrete flow model has provided insight on how particle shape and size distributions can strongly influence rheological properties like yield stress (which inversely correlates to slump) and viscosity at cement paste, mortar, and concrete length scales. For example, in the case of a cement paste, it has been noted in the field that replacing a fraction of the cement with ultrafine fly ash can reduce yield stress. From large-scale simulations, it became clear that the reduction of yield stress was due to changes in how stress is transmitted throughout the suspension. When

Fig. 3: A user in the NIST IVE interacting with a 3-D simulation *(photo courtesy of Denease Anderson, NIST)*

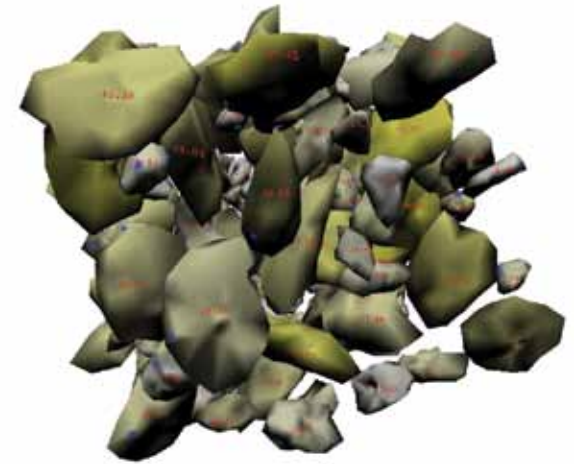

Fig. 4: Simulation of coarse aggregate flowing inside a fresh mortar. The numbers on the aggregates indicate shear stress levels exerted via the fluid and the other aggregates

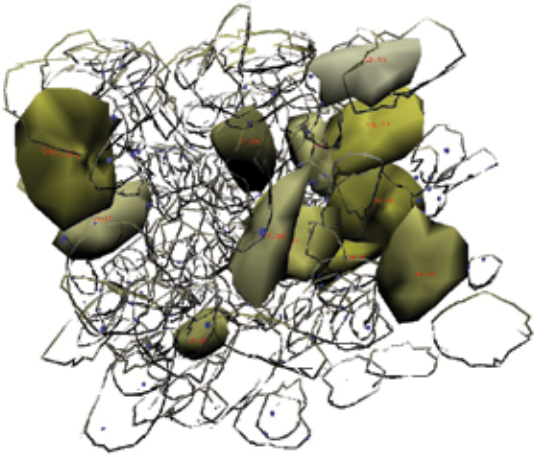

Fig. 5: This is the same simulation of coarse aggregate flowing inside a fresh mortar as in Fig. 4, with only the most highly stressed coarse aggregates shown. The rest are represented by only a wire frame to give context

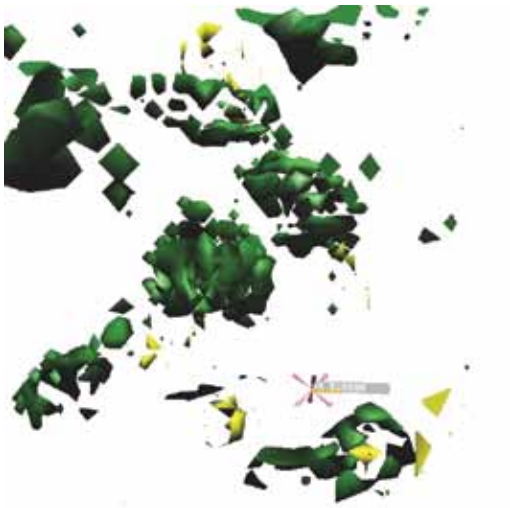

Fig. 6: Calcium sulfate and calcium aluminate phases during initial cement hydration at a very early age, when chemical admixtures added to change setting behavior can often be effective

shearing during mixing, pumping, and flowing, stress can be transmitted via compressive and extensional forces; and the transmission of stress in compression can make a significant contribution to the apparent yield stress.

The ultrafine fly ash is smaller than the cement particles and also round in shape. The model, with its detailed particle-level data and visualization, has shown that the inclusion of such particles makes it more difficult to establish "stiff" networks or chains of particles that can lead to jamming, making it harder to transmit stress in compression (that is, you can push a rod but not a rope). As a result, cement particles move about each other more easily, resulting in lower yield stress and viscosity. A similar result was found for higher-scale models of concrete where the matrix fluid is now a mortar and the solid inclusions are the coarse aggregates.

Our current simulations are investigating the effectiveness of different size gradations (aggregates at the concrete scale and cement particles at the paste scale) on viscosity and yield stress, which will lead to technical data that can be used to optimize these gradations for concrete flow. Because the models can handle any kind of external geometry, we also plan to simulate flow in common concrete rheometers using reference materials to obtain fundamental rheological parameters using standard measurements that can be used to optimize and control concrete placement.

CEMENT HYDRATION RESULTS

Microstructures generated by our 3-D cement hydration model can be interactively visualized and analyzed at any time in the simulation. Figure 6 is a snapshot from an interactive visualization of a hydration run at a very early stage of the hydration process. Only the important calcium sulfate and calcium aluminate phases are shown.[4] Using a virtual interactive tool, the sulfate ion concentration in solution can be measured at any spot in the pore space. For this example, the probe returns a value of 0.01039 mol/L at the point sampled. The availability of a concentration probe makes it possible to visualize concentration gradients and to determine, for example, whether calcium sulfate carriers are spatially distributed well enough in the cement to prevent undesirably rapid aluminate reactions. As the researcher probes the data, the numerical values are continuously displayed. Depending on the application requirements, the values can be saved for later use or dynamically fed to a separate process for real-time analysis.

The hydration model has been used to gain insights into the mechanisms that control the induction period of cement hydration, which is the time crucial to the placement and finishing of fresh concrete. The setting time of concrete is determined primarily by the length of the induction period, which can be controlled by the addition of chemical admixtures. Systematic design of admixture molecules will be made possible through a better understanding of the chemical processes that control the length of the induction period. The hydration model has been used to confirm that the induction period is controlled by the rate of growth of calcium-silicate-hydrate[5] and has also shown that the nucleation of calcium hydroxide plays an important role in determining the rate of that growth and the end of the induction period.[6]

Work is now beginning on simulating the mechanism by which calcium sulfate controls the aluminate reactions in portland cement and prevents flash setting. Proper sulfate balance is crucial to control setting, especially when mineral admixtures are present. With these insights, we will be able to predict the optimum sulfate level in cement and determine the answers to questions such as why does undersulfation strongly retard hydration?

PROSPECTUS

At sub-μm length scales, scientists have recently made strides in unraveling the structure and properties of C-S-H gel, the glue that holds concrete binder together at the nanometer and molecular scale via molecular modeling.[7] A framework is currently being built for connecting all these realistic models at different length scales and linking them to the macroscopic scale where engineering properties of concrete such as fresh concrete rheology, setting, mechanical properties, and transport properties can be computed as a function of time. We are already thinking of modeling degradation processes in concrete—this next step is not too far off. This approach of combining physical science and computer science—powered by supercomputers, interpreted by sophisticated visualization, and applied at many length scales—requires intense

and sustained effort, producing important results at present and leading to great promise for the future—especially as supercomputers keep on growing in size, speed, and availability.

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Selected for reader interest by the editors.

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