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Multiscale/Multiphysics Modeling of Concrete Structures

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Concrete structure modeling is not easy. Cement concrete has a complex microstructure, which is still not completely elucidated. A lot of study has been carried out in cement concrete materials and structures modeling. The microstructure of concrete contains random features over a wide range of length scales, from nanometers to millimeters, with each length scale presenting a random composite. In its engineering uses, concrete is considered as a uniform material at the length scale of meters. Concrete research topics include complex failure processes, such as, atomic scale cementitious hydration, micro-pore structure formation and moisture transport in microstructure, calcium ion transport and leaching, chloride ion transport and corrosion, durability prediction of damaged structural concrete and service life of structural concrete. These phenomena are scaled in a bottom-up manner from atomic to continuum scale.

Concrete behaviors, unfortunately, are hard to be addressed from continuum scale calculations. They include the influence of atomic scale debonding, micro scale buried interfaces, small size internal material defects and interactions that may control the macro scale structures. In order to achieve this, atomic scale models are employed to quantify relevant nano-mechanical, chemical and physical quantities. Researchers in nano-mechanics field have achieved exciting results both from characterizations and simulations. The advanced characterization technologies employed includes X-ray CT technology, scanning electron microscope, transmission electron microscope, and X-ray diffraction. Promising results have been made in modeling and simulation field, too. They use molecular simulation to model the real atomic structure of C-S-H and predict materials properties, e.g. elastic constants and strength.

However, molecular simulation is constrained by time and length scale limits. Even with the support of the most updated supercomputer, the molecular simulation size is still hard to represent a 1 millimeter sample. In addition, the representative volume element size in continuum method often ranges from centimeter to meter. There is a gap between molecular simulation and real structural scale. Basically, macroscopic characters of concrete structures rely on micro-pore structures and chemo-physical states that influence performance durability. In turn, chemo-physical states of substances in nano or micro pores are greatly associated with structural mechanics with damages induced by loads and weather actions. Material properties follow from their atomic and microscopic structures and exhibit different properties at different scales. For example, the range of the microstructure of concrete, from nanometers (C-S-H) to micrometers (cement paste) to millimeters (mortar and concrete) to meters (real structure) covers nine orders of magnitude in size. The multiphysics effects of various materials include cement hydration, moisture equilibrium, constitutive law of hardened cement paste, and chloride equilibrium, etc. In order to simultaneously solve this multiscale/multiphysics problem, each event needs to be sequentially processed. To fully model every effect, over 50 nonlinear governing equations need to be solved.

Thus, to fully represent cement concrete behaviors a single scale modeling method is hard to address the cross-scale complex behavior from material scale to structural scale. To look at a problem simultaneously from several different scales and levels of detail is a more mature way of doing modeling. In this regard, two sub-fields of structural mechanics and material science have been investigated to combine micro and macro features together. In this method, features are investigated from a sequential manner, named hierarchical approach. Results from micro scale are transmitted to a higher scale, and then perform single scale calculations to gain macro scale results. Current studies include carrying out bottom-up atomic and micro texture predictive simulations. Computational algorithms are integrated to approaches from statistical mechanics and chemistry to provide quantitative predictions of structural properties of cementitious materials across different time- and length-scales. We have recognized that the link between materials and structures (from atomic to continuum) is critical to come up with accurate models of the behavior of concrete structures.

The sequential approach, however, only represents the cross-scale interaction in a discrete bottom-up way, and there is no top-down effect can be integrated in data transition. Moreover, the computational efficiency is limited by the discontinuous data passing between scales. In comparison to hierarchical approach, the concurrent approach offers a fundamental change in the way we handle modeling. It connects physical, chemical, and mechanical features from atomic to continuum scales in a homogeneous way. It provides a powerful tool to connect structural applications to basic material science and comes up with a cross-scale view to modeling, by focusing on the different levels of physical laws and the relations between them. Consequently, the interaction of the constituents is accounted for by transition from the nano, micro, macro scale and vice versa.

For mustscale modeling on crack growth problem, the concurrent multiscale approach will need to set two different suitable scaling models. Specifically, the region near the crack tip, where classical elasticity theory is insufficient for characterizing nonlinear physical behaviors. We may introduce the molecular model such as embedded atomic model to address the crack tip dislocation and debonding process. In the far field, where the continuum model is sufficient for modeling, we may employ the conventional finite element model to address the stress-strain field. The interface region between molecular model and finite element model should be treated by advanced crossing scale technology. Note that the interface region is named a bridging scale domain which is set to transmit force and energy.

For multiscale modeling on C-S-H atomic structure for understanding their nanostructure-property correlations, we may introduce the two scales models: molecular dynamics model and coarse-grained model. For lattice interaction, the binding site can be treated by molecular dynamics model, whereas a coarse-grained

model is used to describe the C-S-H structure except the binding site. The interface region between lattice model and coarse-grained model, where transmits force and energy, needs to be handled by advanced crossing scale technology.

From the discussion presented in this editorial, concrete structures can be modeled at various degrees of complexity and at different scales. Multiscale modeling provides a framework, based on fundamental principles, for constructing computational models of such phenomena, by examining the connection between cement concrete models from different scales. Therefore, to model and predict behaviors of cement concrete structures, this editorial proposes an interesting research topic of concurrent multiscale paradigm to model the cross-scale behaviors of stone-based materials and connect it to the structural scale properties in a concurrent manner.