Getting down to basics - new technology will make it possible

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The goal is to produce large-scale, first-principle simulations of ion hydration and phosphoryl transfer signaling reactions--two fundamental processes that occur, respectively, in the environment and in the human body, but are little understood.
The processes themselves are not similar, however, and normally they would not be discussed in the same conference let alone the same presentation, yet they do share one thing in common: scale.

"This is as big as it gets in modeling," says John Weare, with 500-plus atoms to be scrutinized in any one simulation. By contrast, projects undertaken a few years ago may have modeled 20 or 30 atoms in a simulation.

Advancements in computational capabilities have made such monumental tasks possible. The central idea, Weare continues, is that "real life is large" and these multiscale projects illustrate "what we can do now that we couldn't do before."

In addition to simulating complex behaviors with "many many particles," Weare's team devotes about 40 percent of its efforts to developing algorithms and code to be implemented on a new generation of high-performance machines and architecture that is still on the horizon.

"There's a new wind blowing in science," Weare reports. "New equipment means new solutions are possible--we can get computers to solve really hard chemical problems, and that's changed how we

approach theory. It's a different paradigm."

Source: Pacific Northwest National Laboratory