



Nanoparticle haloing

In 2001, University of Illinois researchers, led by Jennifer Lewis, discovered a fundamentally new approach for tailoring the stability of colloidal suspensions, complex fluids used in numerous applications ranging from advanced materials to drug delivery. The researchers dubbed this technique nanoparticle haloing, a self-organizing process that imparts stability to naturally attractive colloidal microspheres, decorating their superficial areas with highly charged nanoparticles.

Erik Lijten, an assistant professor in the Department of Material Science and Engineering at the University of Illinois, was familiar with the work of Lewis and her colleagues and thought he could simulate it. This proved a daunting challenge because many complex fluids contain particles of widely different

sizes that also move at vastly different time scales. A simulation that faithfully captures both the motions of the faster small particles and the slower large particles would be extremely slow and impractical.

Lijten and graduate student Jiwen Liu developed a new simulation algorithm to crack this problem. Their algorithm generates a random pivot point, picks a particle for a point reflection, and pivots it 180 degrees to a new position. Any nearby particles, either within the field of influence of the pivoted particle's old or new position, are candidates for joining the cluster. These particles similarly pivot and contain their own field of influence.

In an effort to find a stable fluid phase, the team created a simulation box, which

contained 1-micron microspheres in a fluid. These spheres, left alone, clustered together in the fluid. The team then added smaller particles to the mix. As more small particles were added, the large particles no longer clustered, and a stable fluid phase occurred, as shown here. But, at some point, if even more small particles were added, the large particles clustered again.

Lijten has been running his simulations on Mercury, NCSA's TeraGrid cluster. NCSA's Performance Engineering and Computational Methods group is currently helping him optimize the code.

This piece, by NCSA's Herb Morgan, originally appeared in a longer form in data link, a newsletter for NCSA users.