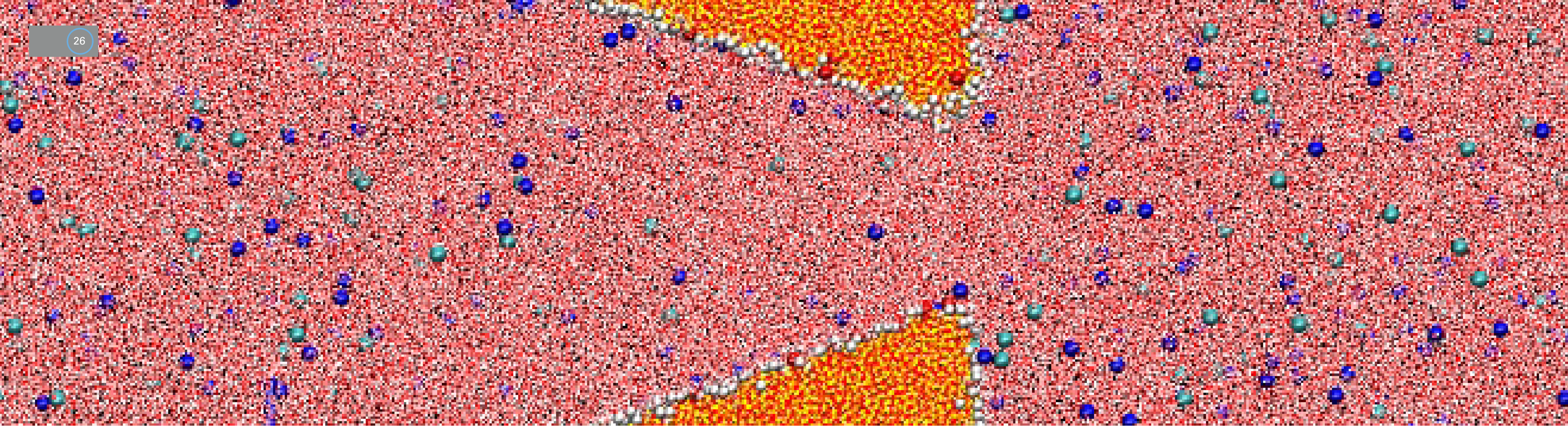

Fully atomistic simulations of electroosmotic flow in a "nano-nozzle" device.

ELECTRICAL DOUBLE LAYERS

Singer performs simulations of electroosmotic flow

Many biological molecules and common surfaces carry an electrical charge. For example, DNA has a strong negative charge, and so does an amorphous form of silicon dioxide known as silica, the material most people recognize as "glass." A charged molecule or surface, along with the electrically compensating layer of ions in the adjacent solution, is known as the electrical double layer (EDL).

"Interest in the EDL has never waned for roughly a century, and today that interest is especially intense because of the importance of EDL dynamics in nanoscale devices, especially for biomedical applications," said Sherwin Singer, Ph.D., professor of chemistry at The Ohio State University.

In these devices, electric fields are used to manipulate biological fluids in tiny channels. A voltage applied parallel to the surface forces the ions to move with the field. This, in turn, causes electroosmotic flow (EOF), fluid flow induced by the moving ions. EOF can be harnessed to control the transport biological fluids in micro- and nano-scale lab-on-a-chip devices. The goal is rapid, point-of-care screening of patients for biomarkers identifying heart disease or cancer.

Singer's group uses the computational resources at the Ohio Supercomputer Center to perform detailed atomistic studies in complex device configurations that have not been explored to this point.

"Departure from the slit pore leads to a complex interplay between non-uniform charge density and pressure gradients," Singer explained. For example, the Singer group has been able to perform fully atomistic simulations of EOF in a "nano-nozzle" device.

The work also has bearing on fundamental scientific issues. Before such atomistically detailed work was possible, scientists who study substances that are microscopically dispersed evenly throughout another substance, or colloids, could rely only on "effective" continuum models. These continuum models have to be invoked with contradictory assumptions to explain different experiments.

For example, to account for electroosmotic fluid flow, continuum theories give sensible predictions only if water adjacent to the surface is assumed to be immobile. At the same time, the ion current would disagree with experiment, unless ions in that same layer flowed virtually unimpeded. Realistic, atomistic modeling of that surface layer at OSC reveals that water and ions are mobile right up to the surface and explains why different and contradictory "effective" models were needed to fit the data.

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