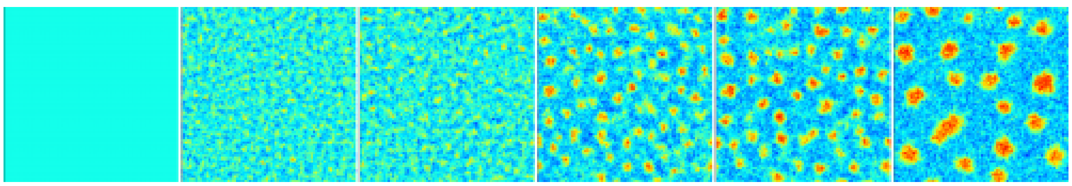
Mathematicians model fluids at the mesoscale

March 6 2015, by Julie Chao



These images show spinodal decomposition (liquid and vapor components separating out spontaneously) in a near-critical Argon system from a homogeneous initial condition into droplets suspended in a majority vapor phase.

When it comes to boiling water—or the phenomenon of applying heat to a liquid until it transitions to a gas—is there anything left for today's scientists to study? The surprising answer is, yes, quite a bit. How the bubbles form at a surface, how they rise up and join together, what are the surface properties, what happens if the temperature increases slowly versus quickly—while these components might be understood experimentally, the mathematical models for the process of boiling are incomplete.

The math whizzes at the Center for Computational Sciences and Engineering (CCSE) at Lawrence Berkeley National Laboratory (Berkeley Lab) are tackling this and many other similar problems head on. Along with Alejandro Garcia from San Jose State University and Aleksandar Donev from the Courant Institute, they are at the forefront of a neglected corner of the scientific world, building mathematical models for fluids at the mesoscale.

Here, mesoscale refers to the regime between the microscale, where physicists and chemists use molecular dynamics to characterize the motion of atoms and molecules, and the macroscale, where scientists and engineers apply continuum models to describe fluid flow that is observable with the naked eye.

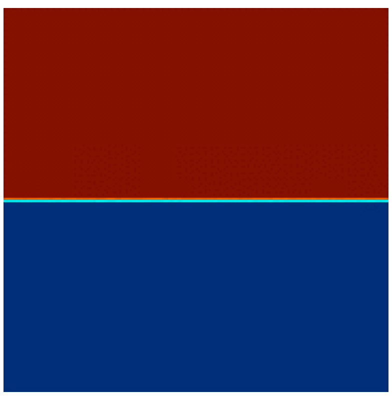
"Modeling fluids at the mesoscale is a relatively new area," said John Bell, principal investigator of the project looking at these phenomena. "The idea is to incorporate important physical effects at the microscale into continuum models. We're constructing equations that have the best of both worlds."

The potential applications are enormous. "A lot of interesting phenomena happen at these length scales, which range anywhere between nanometers and micrometers, and time scales, which range between nanoseconds and microseconds," said Anuj Chaudhri, a postdoctoral researcher in the group. "For example, phase separation, protein aggregation, entanglement in polymer dynamics, rheological response of complex fluids, self assembly, protein folding, and biofluid dynamics, just to name a few. A large part of how these fluids behave arises from their microstructure. It's important to understand their microstructure to be able to understand their macroscopic properties."

New models for new hydrodynamics

The field is called fluctuating hydrodynamics because it takes into account the movements, or fluctuations, of the atoms and molecules. "What is missing in the deterministic continuum models is the idea of fluctuations," Chaudhri said. "Looking at a glass of water, you don't see anything moving. But if you look under a microscope, at the microscale things are moving continuously. A lot of water's properties, such as its viscosity and thermal conductivity, are described by those individual motions which are only modeled as averaged properties in continuum equations."

Technically, molecular dynamics could be used to accurately model any fluid. However, no supercomputer would be able to run the models. "You can't model that many molecules," noted Bell. "You're limited to hundreds of millions of atoms at one time. But the number of atoms in a tiny speck of grain is 12 orders of magnitude larger. So you can barely do anything with it—we just don't have enough computational power."



This shows the development of a mixed-mode instability as a layer of salty water is placed on top of a horizontal layer of less-dense sweet water.

On the other hand, at such small scales the continuum models would give the wrong answers since the fluctuations are missing. So fluctuating hydrodynamics is needed to model fluid flow in these systems while still including the important physics.

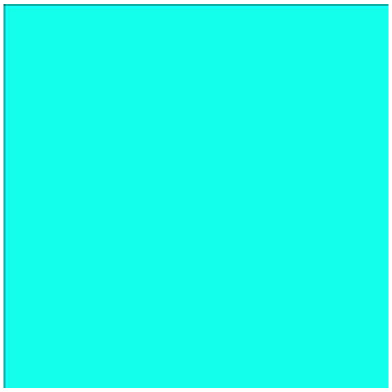
The model output can then be compared with actual experimental results. "That's how we are able to validate our models—they're able to predict phenomena you see in nature that you don't get with the standard continuum equations," Chaudhri said.

These Berkeley Lab mathematicians, including CCSE research scientist Andy Nonaka, are among a handful of people in the world working in this field. "This research is multidisciplinary and technically challenging, and requires expertise in fluid dynamics, statistical mechanics, mathematical modeling, and numerical approximation of stochastic systems," said Nonaka.

Low Mach number flows

CCSE is working on two thrusts, one for compressible fluids, including gases, and another for incompressible or so-called low-Mach number flows, which are flows where the effect of sound waves can be ignored because the flows are at much slower speeds than the speed of sound. "A low Mach number approach allows us to be a lot more computationally efficient and simulate low Mach number flows over much longer time periods using the same computational resources," Nonaka said.

Nonaka is co-author of a forthcoming paper titled, "Low Mach Number Fluctuating Hydrodynamics of Multispecies Liquid Mixtures," to be published in the journal *Physics of Fluids*, in which new numerical techniques were developed to create a sophisticated model for fluid mixtures.



This shows adiabatic expansion of super-critical Argon in a square cavity driven by boundary cooling. Modeling the formation of liquid and vapor phases and their interfaces is the first step in being able to model boiling water.

"We derived new equation sets to handle these low Mach number cases," he said. "We can now compute low Mach number flows where fluctuations have a significant impact on the physics much more efficiently. We can also model multicomponent fluids, where each fluid component has its own density and material properties."

Other applications include biological membranes and microfluidic devices. "Basically for any kind of device fabrication at the microscale, if there are fluids involved, you won't be able to model the physics of the fluids correctly without a method such as this," Nonaka said.

So why study boiling water?

So about that pot of boiling water – why is Chaudhri studying this? Multiphase fluids could play an important role in electronics. "One of the biggest areas right now is micro-nanoelectronics cooling," he said. "Think of your laptop—it can get very hot. How does one dissipate this heat? One idea is to use the process of phase change to ultimately carry the heat away. And the important physics to do this lies at the mesoscale."

Mathematically modeling the boiling of water is "a very, very complicated problem," he says. "So we're trying to build models to attack this problem fundamentally. We have gotten to the point where we have the necessary tools to tackle this effectively."

Multiphase problems also arise in metallurgy, as well as in making emulsions and suspensions; Chaudhri is now starting to look at electrolytes, which are chemicals that carry charge in a battery or fuel cell. "There are a lot of potential applications in industry," Chaudhri said. "We're building smarter and smarter models so we can tackle problems that can't otherwise be solved."

Provided by Lawrence Berkeley National Laboratory