New mathematics accurately captures liquids and surfaces moving in synergy

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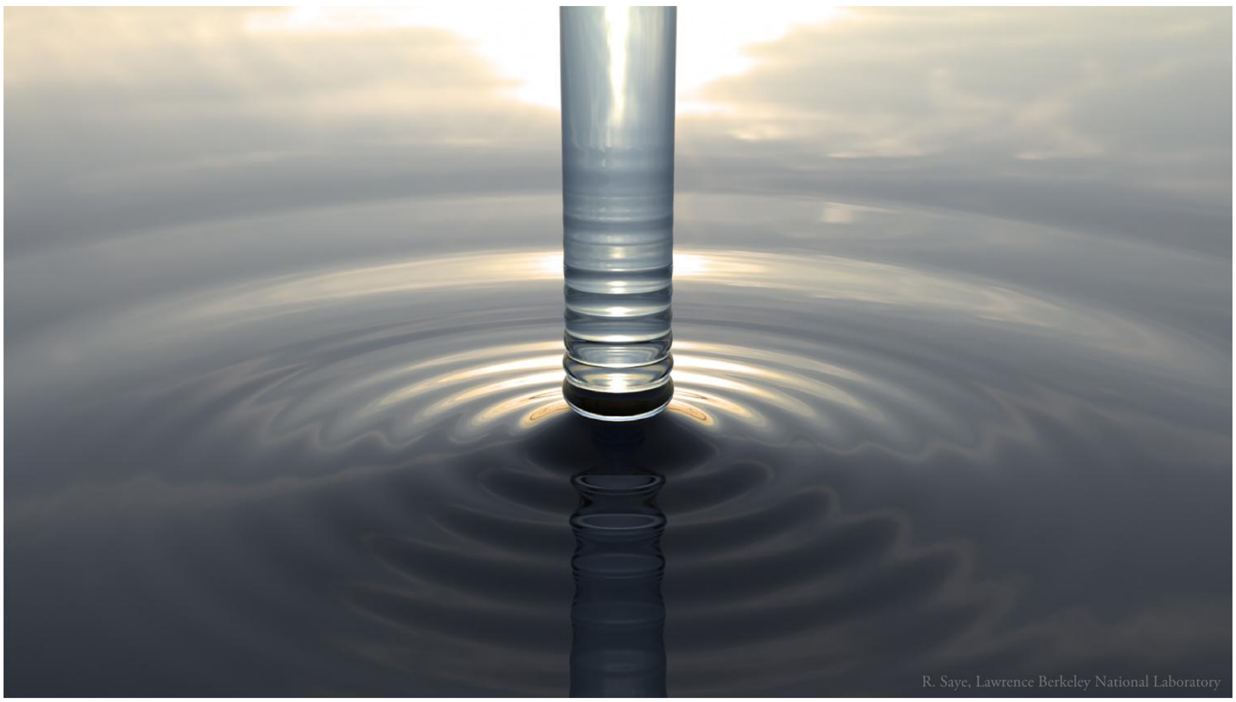

Algorithms developed by researchers facilitate the accurate computational modeling of intricate fluid-interface phenomena, such as ripples in a liquid jet impinging on a reservoir of water (shown in this illustration). Credit: R.I. Saye, Lawrence Berkeley National Laboratory

Gas bubbles in a glass of champagne, thin films rupturing into tiny liquid droplets, blood flowing through a pumping heart and crashing ocean waves—although seemingly unrelated, these phenomena have something in common: they can all be mathematically modeled as interface dynamics coupled to the Navier-Stokes equations, a set of equations that predict how fluids flow.

Today, these equations are used everywhere from special effects in movies to industrial research and the frontiers of engineering. However, many computational methods for solving these complex equations cannot accurately resolve the often-intricate fluid dynamics taking place next to moving boundaries and surfaces, or how these tiny structures influence the motion of the surfaces and the surrounding environment.

This is where a new mathematical framework developed by Robert Saye, Lawrence Berkeley National Laboratory's (Berkeley Lab's) 2014 Luis Alvarez Fellow in Computing Sciences, comes in. By reformulating the incompressible Navier-Stokes equations to make them more amenable to numerical computation, the new algorithms are able to capture the small-scale features near evolving interfaces with unprecedented detail, as well as the impact that these tiny structures have on dynamics far away from the interface. A paper describing his work was published in the June 10, 2016 issue of *Science Advances*.

"These algorithms can accurately resolve the intricate structures near the surfaces attached to the fluid motion. As a result, you can learn all sorts of interesting things about how the motion of the interface affects the global dynamics, which ultimately allows you to design better materials or optimize geometry for better efficiency," says Saye, who is also a member of the Mathematics Group at Berkeley Lab.

"For example, in a glass of champagne, the motion of the little gas bubbles depends crucially on boundary layers surrounding the bubbles. These boundary layers need to be accurately resolved, otherwise you won't see the slight zig-zag pattern that real bubbles take as they float to the top of the glass," he adds. "This particular phenomena is important in bubble aeration, a process used widely in industry to oxygenate liquids and transport materials in liquid chambers."

High-Order vs. Low-Order

By solving the Navier-Stokes equations, researchers can gain insights into how fast a fluid is moving in its environment, how much pressure it is under and what forces it exerts on its surroundings, among other things. The results can also shed light on how all of these characteristics influence each other.

But solving these complex equations can be computationally challenging. Thus, over the years, researchers have devised a wide range of methods to simplify the equations as well as their numerical solution. One such widely used simplification is to model liquids, and in some cases gases as well, as incompressible.

According to Saye, most existing methods for solving incompressible fluid flow problems coupled to moving boundaries and surfaces are "low-order" methods. Conversely, the interfacial gauge methods that Saye developed are "high-order" methods.

"High-order methods are in some sense more accurate. One interpretation is that, for fixed computing resources, a high-order method results in more digits of accuracy compared to a low-order method. On the other hand, it is often the case that you only need a handful of digits of accuracy in your simulation. In this case, a high-order method requires less computing power, sometimes significantly less," Saye explains.

In addition, low-order methods for fluid interface dynamics tend to introduce "numerical boundary layers" into the calculated results. These lead to imperfections, a bit like film grain or noise in a photograph. It means you cannot closely examine and precisely analyze the fluid dynamics right next to the interface.

"What happens at the interface, such as the film of a soap bubble or the surface of a propeller, affects the large-scale dynamical structures in the surrounding environment," says Saye. "Low-order methods work well when everything is smooth, but you need a high-order method when you have intricate dynamics, when things are moving very fast, or if there are small-scaled features in the interface."

With cheaper computational models and increased resolution capabilities, researchers can study more complex phenomena, like how to optimize the shape of a propeller blade, the formation and destruction of foams, the resolution in modeling the boundary layers in blood flow in pumping hearts and the ejection of ink droplets in consumer inkjet printers.

Because his primary interest was to achieve a high level of resolution, it never really occurred to Saye to take a low-order method and improve on it. "I wanted to make these numerical algorithms significantly more accurate" he says. "When I thought about it that way, I realized that I needed a whole new technique to solve the equations."

His solution was to apply gauge methods to solve the incompressible Navier-Stokes equations. "Gauge methods are about the freedom one has in choosing variables in the equations," says Saye. "So I essentially used these ideas to rewrite the Navier-Stokes equations in a way that is more amenable to developing very accurate simulation algorithms."

He adds that gauge methods are in some ways a generalization of "projection methods"—well known and widely successful methods in the field of computational fluid dynamics, pioneered by Berkeley Lab Mathematician Alexandre Chorin in the 1960s.

"I am very fortunate to have been supported by Berkeley Lab's Luis Alvarez Postdoctoral Fellowship," Saye adds. "It has been instrumental in allowing me the flexibility to dedicate myself to my own research endeavors."

More information: Interfacial gauge methods for incompressible fluid dynamics, *Science Advances*, advances.sciencemag.org/content/2/6/e1501869

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