According to Caltech seismologist Jeroen Tromp, there are two challenges that petascale computation will enable researchers to address.

"The first will require harnessing the entire machine to do very high-resolution simulations" of seismic wave propagation across the entire globe, "a machine like that should get us into the 1 to 2 Hz range," which Tromp explains will provide unprecedented insight into the small-scale structure of our planet's interior.

For example, where the liquid outer core meets the solid lower mantle, "all kinds of things appear to be happening at that boundary," he says. The mantle appears to undergo a phase transition at this depth, changing its properties and behavior. "We would love to be able to really image that. "The fundamental question is: How does the planet work in terms of its physics and chemistry?"

The second grand challenge that petascale computing will enable researchers to address is "simulating phenomena down to a scale of 100 meters. By comparing these fine-grained simulations with current approximations, researchers will be able to determine whether those approximations are sufficient or, if they are not, how to improve the model to better capture what happens in the real world.

"We'll be able to get much closer to reality," Nolan says, which means understanding better where hurricanes will form and how their intensity can shift. "It simply comes down to better hurricane forecasting."

"Proteins are the miniature machines that do everything in the human body," says David Baker, a biochemist at the Howard Hughes Medical Institute at the University of Washington.

Understanding proteins—which ones perform which duties, how they operate, and what happens when they fail to function correctly—provides tremendous insights into the mechanics of life, the roots of disease, and how to better treat illness.

"The fundamental question is: How does the protein give it a unique function. Determining protein structures is lagging behind the generation of sequences. Baker arrives at protein structure predictions computationally, using his Rosetta code to look for the shape of lowest energy among the possible forms the protein can take. "The bigger the protein is—the more moving parts it has, essentially—the larger the number of possible states," he explains.

Baker likens the quest to searching for the lowest elevation on a plane's wing. "Many variables interact in these complex systems, and for other small-scale phenomena. Simulating phenomena down to a scale of 100 meters. By comparing these fine-grained simulations with current approximations, researchers will be able to determine whether those approximations are sufficient or, if they are not, how to improve the model to better capture what happens in the real world.

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"High-performance computing is central to Boeing's businesses. For example, the company uses tens of thousands of computational fluid dynamics (CFD) simulations to evaluate designs and systematically explore the possibilities of design improvements for its aircraft. "Computational excellence is an enabler to our ability to lead aerospace technology and product innovation to the marketplace," says Paul Fussell, senior manager of mathematical modeling for Boeing Engineering, Operations and Technology.

Using CFD to analyze the aerodynamics of the aircraft under certain conditions, like cruise or one-engine takeoff, is just the starting point. With petascale computing power, Boeing will be able to undertake much more complex simulations at much finer fidelity. Petascale simulations could include more extensive aerodynamics and would enable optimization considering several physics, rather than just one. For example, simulations could include wing structure as well as aerodynamics in order to better capture the complex interplay occurring as the plane's wing bends, influencing its aerodynamics, which affect the load and elastic response of the wing. With this computing capacity, Boeing could design better materials, consider structure and airframe, and study their response to dynamic loads.

"We always use all the computational capability on our machine to solve the most significant challenges we face. And the bar is always rising; we always imagine how we'll use the next increase in machine capability. We always know of more physics to consider or more design-spaces to explore," Fussell says.