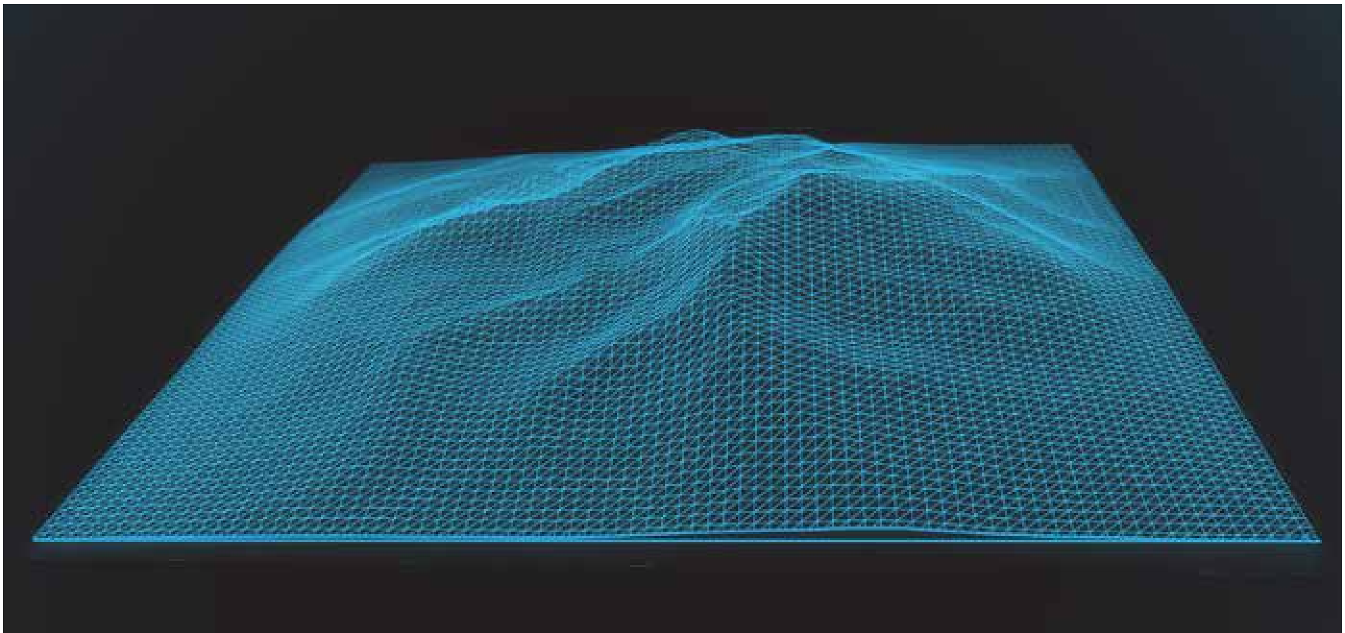

Advances in high accuracy, high performance scientific computing

There is a need for computational results with ever-increasing accuracy for the study of various geophysical, fluid dynamical, aeronautical, and astrophysical phenomena

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SCIENTIFIC computing is all-pervasive, with its applications ranging from weather prediction, geophysics, astrophysics, branches of engineering to genomics (as noted in the present-day context where the first task was to obtain the genome sequence for the viral pandemic). The relationship between computing and science is synergistic – with the former providing an orderly, formal framework which acts as an explanatory apparatus for the latter. While there is always an emphasis on creating Big Data for Analytics, there is an often overlooked aspect of extremely high accuracy scientific computing which is ready to solve many unsolved problems. One would like to emphasise that high accuracy scientific computing will play a similar role, as calculus did for growth of science in the 17th century. With the increasing availability of powerful computers the associated cost has diminished, making high quality/accuracy calculations possible in science and engineering.

Historically, high-precision scientific computing was conceived of as a mechanical calculator with gears, levers, and pulleys by Charles Babbage. While, this was ahead of its time in the concept, yet it led to high-precision manufacturing during the industrial revolution, making Britain a superpower. This serendipity of research, where the search for an accurate scientific calculator eventually led to high-precision manufacturing hub, highlights the need for investment in quality. In the context of scientific computing, the major ingredients needed for high-fidelity are the simultaneous achievement of sound mathematical formulation, very efficient computing hardware, and excellence in scientific software engineering.

The sound mathematical formulation is founded on the principles of mathematical physics, attributed to the calculus of Newton and Leibnitz, which has led to flourish in physical sciences from the 18th century onwards. Excellence in scientific computing started with pioneering works by Euler, Gauss, and Fourier, among many others. Coming together of sound conservation principles along with developments in numerical methodologies, enthused the pioneer in Richardson[1] who came out with the idea of successful weather forecasting, almost two decades before the first digital computer, ENIAC, made its appearance. Due to unavailability of methods for rigorous analysis, the method proposed by Richardson was not diagnosed to be unconditionally unstable. This attracted the attention of some of the finest minds of early 20th century, in anticipation of the arrival of computers. One of the groups led by von Neumann provided a theory of scientific computing in solving partial differential equations, in a classified Los Alamos Report[2] in 1947. The report was declassified much later in 1996, but the theory of von Neumann based on Fourier analysis has been the principle of computing for the next five decades.

The Fourier analysis primarily focused on preserving numerical stability, as noted in the report by the authors[2]: 'our concern here is with stability rather than with accuracy.' Unfortunately, this theory could not explain many phenomena, even for the simple model of one-dimensional wave propagation equation, for which an exact solution exists! The nature of this equation is an ideal tool to test the accuracy of any numerical method. Being a linear equation for the wave (signal), the von Neumann analysis assumed that the computed error follows the same dynamics! Recently this has been replaced by a consistent theory of scientific computing3 explained by using the same wave equation. The idea behind adopting this model equation has its roots in the theory of black swan, attributed to Scottish philosopher-educationist David Hume (see **Figure1**).

Figure1: The statue of Scottish philosopher David Hume, a leading thinker, philosopher and educationist of his time. It is ironic that in his own land, he is adorned with a traffic cone! Hume is credited with the theory of the black swan.

Simply stated, this theory critiques

the method of induction used in epistemology, which is based on a common European belief in the middle ages that all swans are white, as was the case in Europe. When settlers arrived in Australia and noted the presence of black swan, it prompted Hume to his famous theory that the existence of even a single black swan is sufficient to negate the hypothesis that all swans are white. In a similar fashion, the new theory of scientific computing3 does not assume the numerical error evolution for the model convection equation given by

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = 0 \qquad (1)$$

where c is the phase speed. Classical von Neumann analysis assumes the numerical error (e) to also follow Eq. (1). However, the proposed theory of scientific computing3 starting from the first principle considers the effects of spatial and temporal discretisations together, to arrive at an equation governing the error

$$\frac{\partial e}{\partial t} + c\frac{\partial e}{\partial x} = -c\left[1 - \frac{c_N}{c}\right]\frac{\partial u_N}{\partial x} - \int \frac{dc_N}{dk}\left[\int ik' A_0 [|G|]^{\frac{t}{\Delta t}} e^{ik'(x - c_N t)}\, dk'\right] dk - \int \frac{\ln|G|}{\Delta t} A_0 [|G|]^{\frac{t}{\Delta t}} e^{ik(x - c_N t)}\, dk \qquad (2)$$

where A0(k) is the initial amplitude given as a function of wavenumber (k). Based on the property of Eq. (1), this initial solution will propagate to the right at the speed c without any attenuation or dispersion. Thus, in this equation, G is the numerical amplification factor, which should have unit amplitude. The focus of von Neumann and Richtmeyer2 was to keep this always less than equal to unit value. Here, uN is the numerical solution obtained using the time step of Δt. While the details are available elsewhere,3 one can note the governing equation for error is driven by the terms on the right hand side, which are absent in von Neumann's theory. The moot point in scientific computing of Eq. (1) is that the constant phase speed (c) is no more a constant (cN = cN (k)) while one is computing it! This comes as a surprise to many computing professionals who may be in the field for decades.

Each of the terms on the right-hand side has distinct origin in Eq. (2). The first two terms on the right-hand side are sources of dispersion error. Despite its formidable appearance, this equation includes all error sources in computation. The spatio-temporal analysis of numerical methods can capture essential elements of error dynamics. The numerical methods which drastically reduce the sources of errors in Eq. (2) are called the dispersion relation preserving (DRP) methods, which are essential for all branches of physics and engineering dealing with signal propagation and wave phenomena.

Applications of dispersion relation preserving methods across multiple disciplines

There are instances across disciplines, where the physics is related to signal or wave propagation. In such cases, DRP methods are essential to retain high accuracy. This is equally important in direct numerical simulation (DNS) of fluid flow, which requires resolving all the present length scales. As an illustration, consider the generation of cyclonic disturbances in the Taylor-Green vortex problem. The flow with periodic boundary conditions admits an exact solution for the governing Navier-Stokes equation. However, small background disturbances (which could be inherent in computational framework) lead the exact solution to space-time dependent cyclonic structure, visualised in **Figure2**, obtained by solving the governing equation with DRP methods. The use of other methods leads to attenuation of disturbances without formation of the cyclonic structures, as visible on the top of Figure 2.

Figure2: Three-dimensional DNS of the Taylor-Green vortex with DRP methods, capturing coherent cyclonic structures

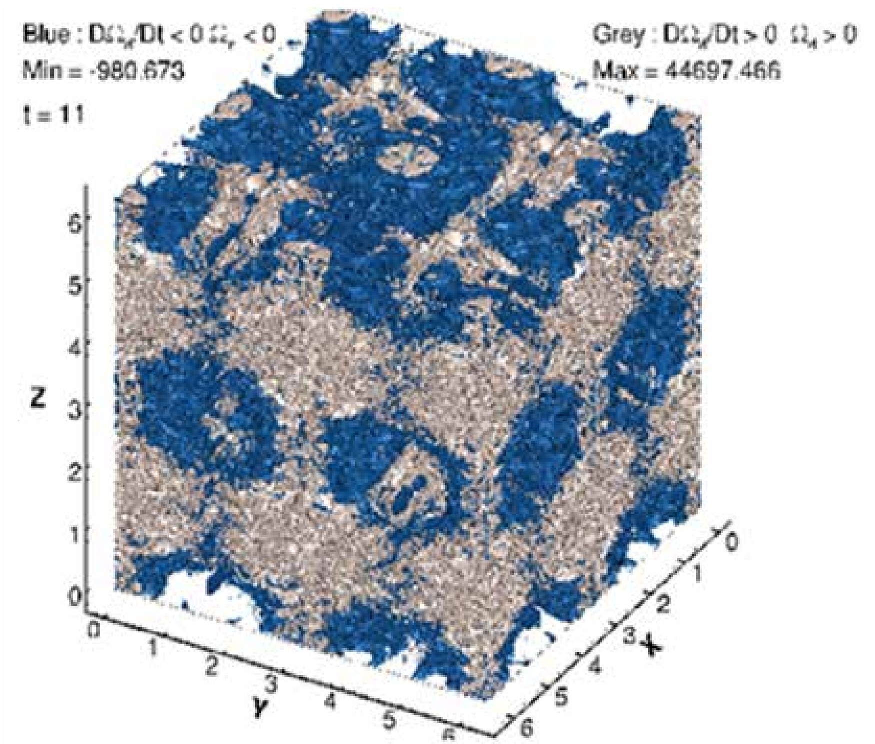
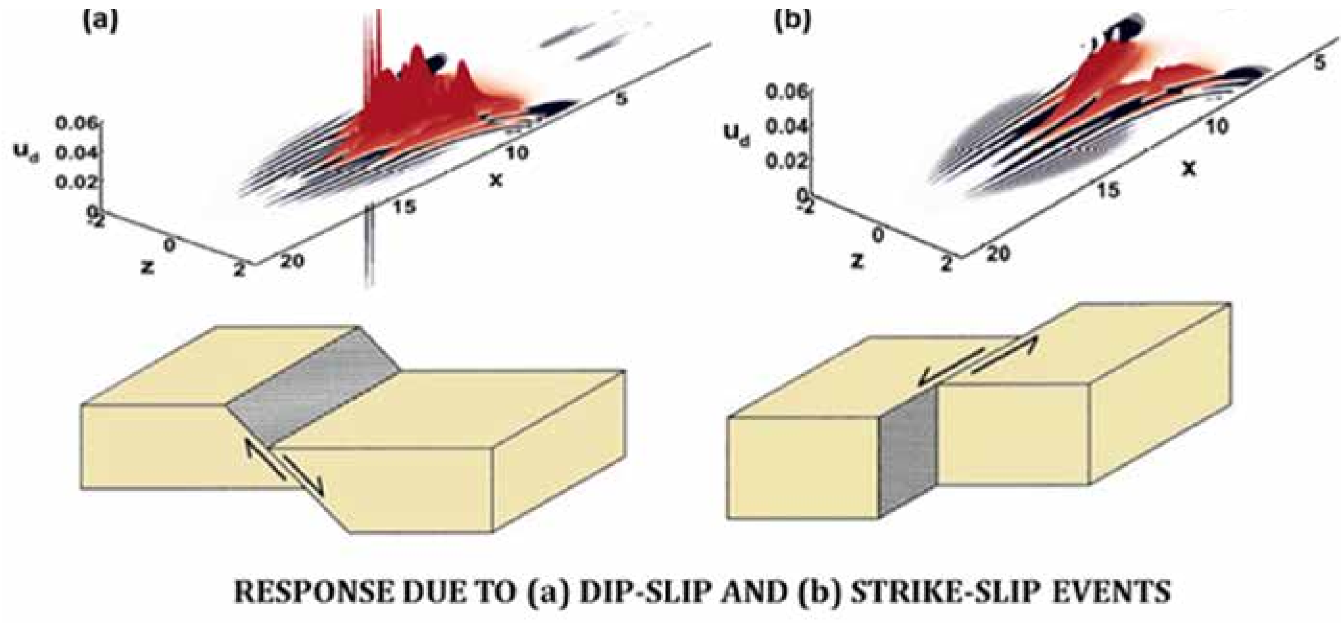


Figure3: Geophysical phenomena of tsunami explained by dip-slip and strike-slip events, by solving the Navier-Stokes equation using DRP methods



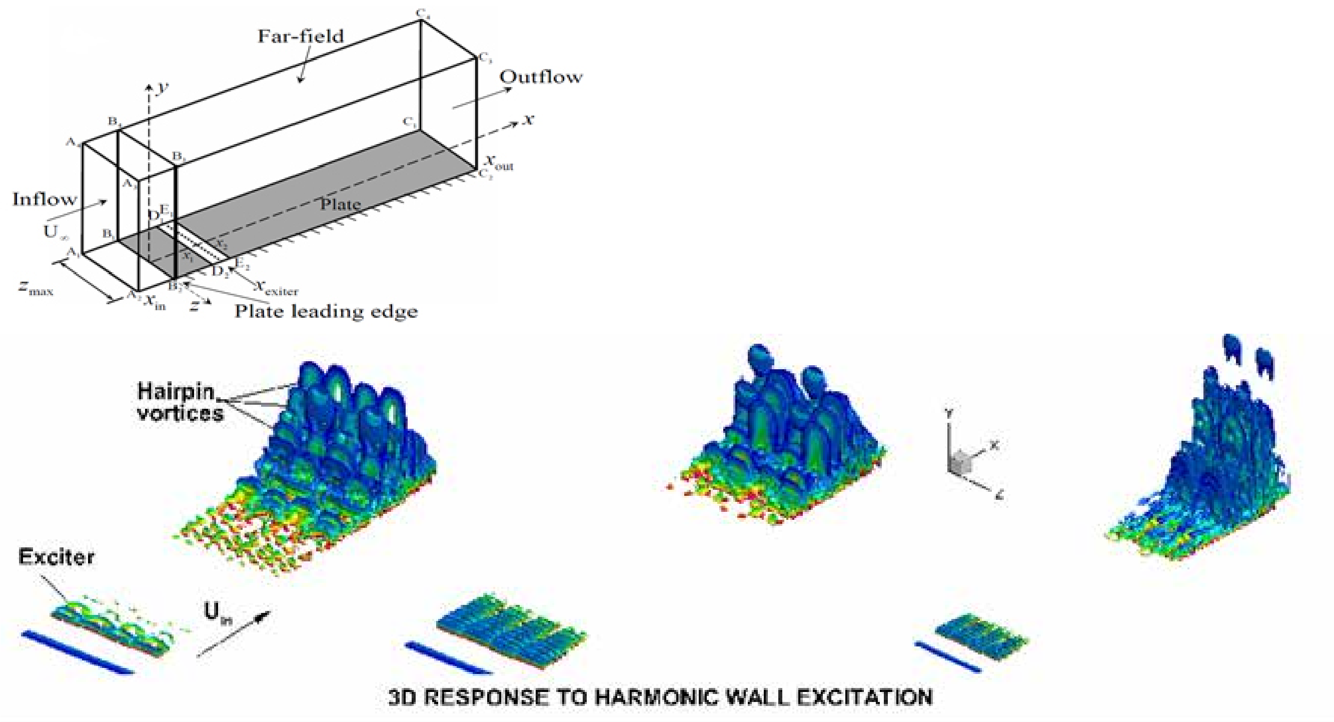
Physical mechanism behind formation of tsunami in geophysics

Devastations left in the wake of any tsunami makes one realise that the physical mechanism behind it is not completely understood by the scientific community even today. Although, earthquakes and continental tectonic plates relatively shifting are the triggers, it has left the lingering question: why don't all earthquakes cause tsunami even when the strength appears similar? To answer this, scientists at HPCL4 traced the events following earthquakes of two types: one caused by a vertical displacement, known as dip-slip event, and the other caused by a horizontal motion, called the strike-slip event (see **Figure3**). These events are shown in bottom of Figure3, and the nonlinear responses are shown on the top from DNS. It is clear that the effect of a dip-slip event is far more severe than its strike-slip counterpart. Tsunami waves are triggered by earthquakes following a dip-slip type of motion, even though the energy output of earthquake for these two events are same. Once again, the higher accuracy offered by the numerics show the occurrence of tsunami to be more likely with dip-slip events and not necessarily by strike-slip event.

Physical mechanism for transition to turbulence

Transition to turbulence is a classical problem of fluid dynamics, eluding many till date. It was the doctoral dissertation topic for Heisenberg and much later remained a topic of debate, till it has been solved in HPCL,5,6 showing that the unstable flows support a spatio-temporal wave front which causes turbulence in flows. As expected, this wave-packet requires a high accuracy DRP method to capture transition to turbulence. Some examples of the three-dimensional response to a system, excited at the wall, are shown in **Figures4** and **5**, with harmonic excitation and excitation due to Gaussian circular patch, respectively. The harmonic wall excitation leads to the formation of rows of hairpin vortices in Figure4. The Gaussian patch on the other hand, produces a wave-packet which eventually undergoes violent nonlinear breakdown. The differences in the disturbance evolution, even when both the flows are excited at the wall, highlight the sensitivity of the flow to the imposed excitation.6 Such sensitivity is captured by an accurate numerical method. The response to a vortex convecting outside the boundary layer is shown in **Figure6**, and is found to be much more susceptible to sudden and violent growth of the wave-packet like disturbance field, even when the initial disturbance is primarily two-dimensional. In this computation, the energy of the flow field migrates from large scale to smaller scales due to action of convection and diffusion. DRP methods capture the energy cascade by DNS. Commercial or open-source software are not capable of producing such detailed results. It is important to note that such DNS will be backbone of many future engineering solutions and will be used regularly.

Figure4: Three-dimensional response to a time-harmonic vortical excitation at the wall showing array of hairpin vortices forming the disturbance packet



Baroclinic instability by Rayleigh-Taylor mechanism

The Rayleigh-Taylor instability is an interfacial instability arising when fluids of different densities interact due to baroclinic vorticity generation, starting from the corners of the initial interface, as shown in Figure7. The setup is an isolated box containing air with different densities, initially separated by a non-conducting barrier. Rayleigh-Taylor instability is a complex instability and its examples include mushroom clouds formed in volcanic eruptions, nuclear explosions, and supernova explosions. Two structures which are commonly observed are the spikes (created by the denser fluid penetrating into the lighter one) and mushroom-shaped bubbles (created by lighter fluid penetrating into the heavier one), as indicated in **Figure7**. These structures are highly sensitive to the initial numerical

Figure5: Three-dimensional response to a Gaussian circular patch excitation at the wall showing disturbance propagation by a wave-packet like disturbance. Top frame shows the growing disturbance field, while the bottom frame depicts turbulent spots captured during nonlinear stages of transition to turbulence (flow is from right to left)

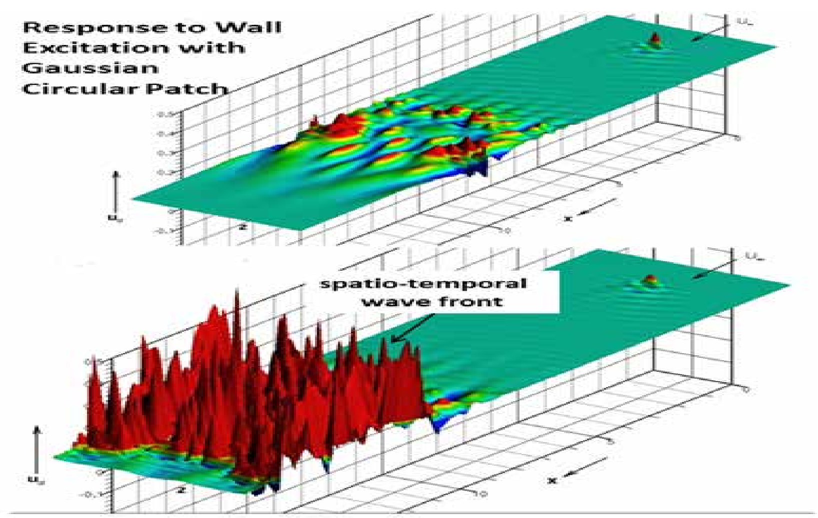
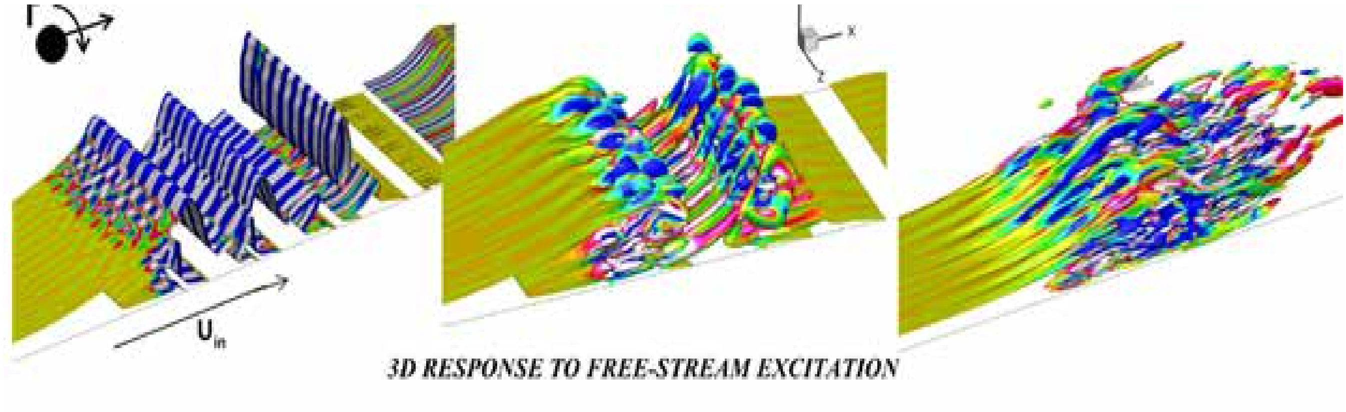


Figure6: Three-dimensional response to a vortex convecting outside the boundary layer showing wave-packet formation after initial two-dimensional response

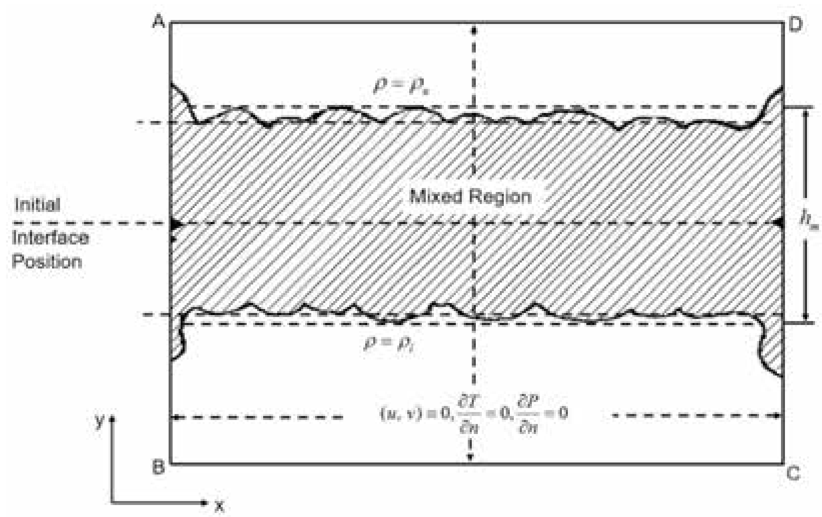


error triggering the instability[7] and often, computations of the Rayleigh Taylor instability miss their appearance by using a dissipative numerical method. The need for highly accurate, resolved simulations for capturing the instability events has been noted by Cabot and Cook[8] as, 'the availability of even more powerful computers has led to a somewhat ironic state of affairs, in that agreement between simulations and experiments is worse today than it was several decades ago.' The results in Figure7 have been obtained by using optimised DRP methods to solve the compressible Navier-Stokes equation, which retain high accuracy while providing superior performance.

Transonic flow and shock capturing

While performing computations of the transonic flow past an aircraft wing section, researchers face difficulties due to shocks in an unsteady flow. The use of highly accurate DRP methods is essential to draw comparisons with experiments.[9] The problem is with unsteady shock formation that interacts with the boundary layer. Most analyses involve time-averaging the flow to obtain the static shock instead, which is qualitatively different from the actual scenario of unsteady shock captured by accurately simulating the transonic flow field. A snapshot of such an unsteady flow is shown in **Figure8**, by solving the compressible Navier-Stokes equation with DRP methods for a high Reynolds number.

Figure7: Time-resolved three-dimensional simulations capturing essential events occurring during the Rayleigh-Taylor instability, using highly accurate numerical methods



The discussion so far would convince the reader that in studying various geophysical, fluid dynamical, aeronautical, and astrophysical phenomena, there is a need for computational results with ever-increasing accuracy. Any new insight can only be gleaned from carefully designed, accurate time-accurate simulations, backed up by rigorous analysis of numerical results. Advances in computing promise crossing over into exascale computing seamlessly. It is now all the more necessary that one does not compromise with accuracy while chasing performance. Creating big data followed by uncertainty quantification would not be the goal, instead one must usher a new revolution in creating the unrelenting battle using scientific computing for ad-

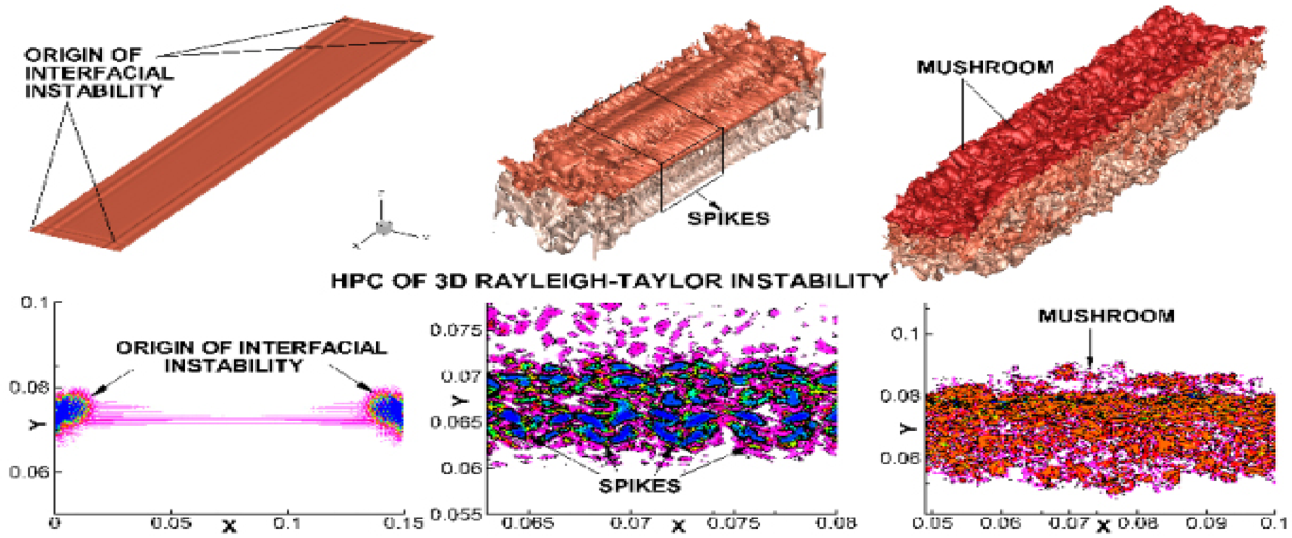
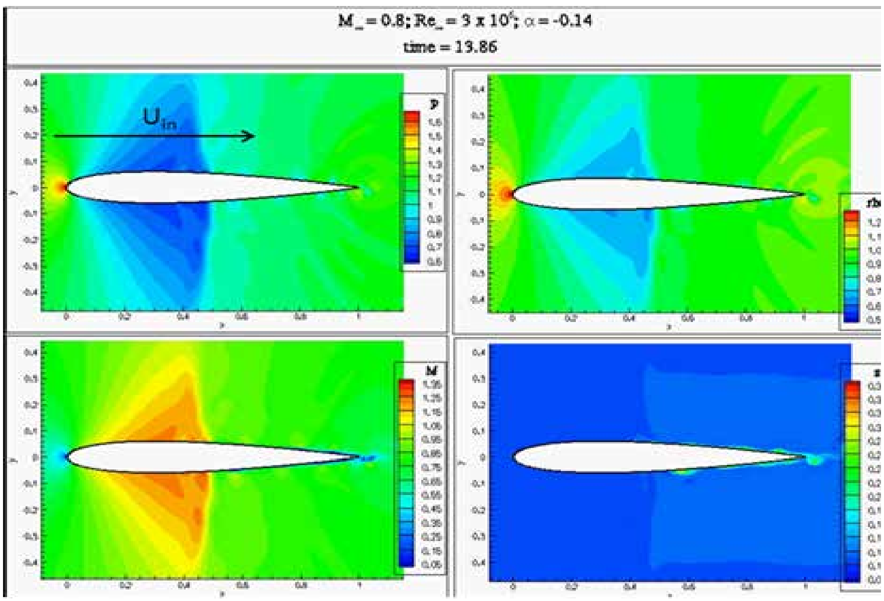


Figure8: Time-resolved DNS of the transonic flow past an airfoil capturing the unsteady shock interacting with the boundary layer, using DRP methods. Pressure, density, Mach number and entropy contours are plotted in these frames as a snapshot



vancement of science. In that respect, lots of progress has been made in this country.

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