THE COMPLEXITIES OF HIGH REYNOLDS NUMBER TURBULENCE

PI: P.K Yeung[1]
Co-PIs: A. Majumdar[2], R.D. Moser[3], D. Pekurovsky[2], and J.J. Riley[4]
Collaborators: B.L. Sawford[5] and K.R. Sreenivasan[6]

[1]Georgia Institute of Technology
[2]San Diego Supercomputer Center
[3]University of Texas at Austin
[4]University of Washington
[5]Monash University
[6]New York University

EXECUTIVE SUMMARY

A half-trillion-grid points simulation of turbulence performed on Blue Waters has provided clear evidence of extreme events where local measures of the deformation and rotation of local fluid elements are much stronger than and have topological properties different from previous understanding. More recently, a substantial algorithmic change in the interpolation of fluid particle velocities on a distributed domain has allowed us to track the motion of some 300 million fluid particles at an affordable cost, both forward and backward in time. Small-scale intermittency is examined as a function of scale separation in space, and through statistics taken along the trajectories of a large collection of fluid particles, taken singly or in pairs. The effects of extreme events are of special interest. New progress is also made for the study of turbulent mixing of passive scalars of very low molecular diffusivity, using a dual-resolution algorithm based on a highly scalable compact finite-difference scheme for the scalar fields.

INTRODUCTION

Fluid motions in many fields of science and engineering are typically turbulent, with disorderly fluctuations over a range of scales. One of our fundamental objectives is to understand the nature of intense fluctuations, which are highly localized in time and space, and to use this understanding to address the effects of fine-scale intermittency [1] in applications. As reported in a recent publication, we have observed the robust existence of "extreme events" where dissipation rates and entropy fluctuations occur at magnitudes as large as $O(10^5)$ times the mean, are nearly coincident in space, and have topological features different from conventional thought. Since these extreme events are localized in space they are important in various flow phenomena dominated by the small-scale motions in turbulence.

Much of the reason for the importance of turbulence itself is enhanced mixing and dispersion of fluid elements with distinct properties or other entities such as heat, chemical species, or passive contaminants carried in the flow [2,3]. For example, examination of fluid particle trajectories going backward in time provides crucial information on how entities originally far apart in space are brought together, which is an important question when disease agents in the environment are involved. The effectiveness of mixing is dependent on a coupling between advective transport by the velocity field and molecular diffusion, which may be strong or weak depending on the nature of the diffusing substance or property. Current work with Blue Waters includes the analysis of recent data and conduct of new simulations, with the latter designed to address both dispersion and mixing in parameter regimes difficult to reach without resources of the magnitude provided on Blue Waters.

METHODS & RESULTS

The only technical approach capable of truly capturing extreme events localized in both time and space is direct numerical simulation, in which we solve exact equations for conservation of mass and momentum. Because of the focus on small scales, we consider isotropic turbulence on a 3D periodic domain. Although Fourier pseudo-spectral methods for this type of geometry are communication-intensive, remote memory addressing and topologically aware scheduling on Blue Waters have allowed us to perform a production $8{,}192^3$ simulation, which surpasses recent work in both the Reynolds number reached and small-scale resolution. The new simulation data have been analyzed from probabilistic, spatial and temporal viewpoints. Extreme events are seen to possess a spatial structure (Fig. 1) differing from conventional notions. Several numerical tests have confirmed these results are robust.

Given the instantaneous velocity field at a mixed set of grid points, the main task of tracking fluid particles is to calculate the particle velocity by interpolation from the velocity values defined at neighboring grid points. We use cubic splines interpolation which is fourth-order accurate and twice differentiable. For each particle, this scheme requires information at 64 grid points that, in general, will reside in different sub-domains and hence require communication. To reduce communication costs, we divide particles among message passing interface tasks dynamically, based on their instantaneous positions instead of the particle IDs. With this algorithm, we have tracked 300 million fluid particles and obtained values of all velocity gradients evaluated at the particle positions as well. Since the governing equations are not reversible in time, we study backward dispersion by post-processing of pairs and tetrads selected based on their final-time positions. Details of this backward-tracking procedure are given in Buaria, Sawford & Yeung (2015) and a Ph.D. thesis (D. Buaria, 2016). A long-standing challenge in the study of dispersion is the pursuit of so-called *Richardson scaling* which occurs at intermediate times long enough for the memory of initial conditions on pairwise separations to fade. This regime is difficult to reach and, especially for backward statistics, requires high Reynolds number—for which our $8{,}192^3$ simulation appears to be just sufficient for the classical scaling to materialize in a convincing manner.

For turbulent mixing, we are working with funding from the Blue Waters PAID subaward to simulate passive scalars at high Schmidt number (i.e. low diffusivity) which requires finer resolution than the velocity field. Previous works were usually limited in either the Schmidt number or the Reynolds number. However, our new collaborator T. Gotoh [4], has developed a new algorithm where the velocity field is computed on a coarser grid using pseudo-spectral methods, but the scalar field is computed on a finer grid using high-order compact finite difference methods. Compact finite difference methods have the advantage of inherently modest communication cost. Test runs to date performed with a new simulation code for this work are very encouraging in both scientific fidelity and performance.

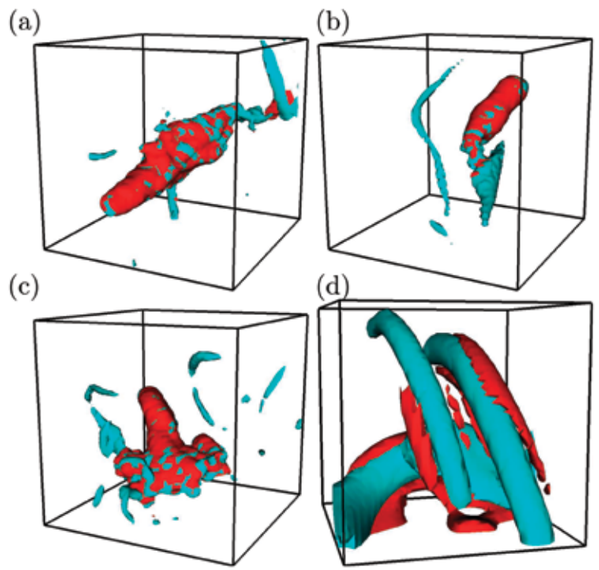

FIGURE 1: Perspective view of 3D color contour surfaces of intense dissipation (red) and entropy (cyan) from three $8{,}192^3$ snapshots (A,B,C), showing a structure distinct from sheets and tubes in image from $1{,}024^3$ at lower Reynolds number (lower right).

WHY BLUE WATERS

In general, an $8{,}192^3$ simulation is almost 16 times as expensive as one at $4{,}096^3$, but it is necessary (as verified by numerical tests) so that high-quality results can be obtained at sufficiently high Reynolds number. A large allocation of time on a multi-petaflops computer such as Blue Waters is thus vital. The outstanding level of support we received through the PRAC program has also been crucial. Generous provision of mass storage resources associated with Blue Waters has allowed us to build a petabyte-sized computational laboratory for answering long-standing questions in the study of turbulence.

NEXT GENERATION WORK

Possible future targets at similar or greater rigor include various turbulent flows subjected to other external influences such as buoyancy, solid-body rotation, or electromagnetic forces.

PUBLICATIONS AND DATA SETS

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LATTICE SCREENING AND OPTICAL PROPERTIES OF NOVEL PEROVSKITE PHOTOVOLTAIC MATERIALS

Allocation: Illinois/500 knh
PI: André Schleife[1]
Co-PI: Joshua A. Leveillee[1]

[1]University of Illinois at Urbana-Champaign

EXECUTIVE SUMMARY

Due to the extremely quick rise of their photoconversion efficiency, hybrid organo-metal-halide perovskites have recently garnered a large amount of attention as potential materials for efficient, cost-effective, and broadly applicable next-generation photovoltaics. However, the influence of excitonic effects on optical absorption and exciton binding energies in these materials is not well understood. In particular, lattice and free-carrier contributions to dielectric screening are currently under investigation. Spin-orbit interaction plays an important role in these materials as well. We use many-body perturbation theory to compute optical properties and an approximate approach to explore the influence of lattice screening. Our results show that when all these effects are taken into account, very good agreement with the experiment is obtained. This work constitutes the **first** step towards a full, first-principles treatment of these effects that will be broadly applicable for material design of novel photovoltaics.

INTRODUCTION

Hybrid organo-metal-halide perovskites of the form ABX_3 have recently garnered a large amount of attention [1]. In this formulation, A is an organic cation, B is a metal cation, and X is the halide anion. Elements such as B={Pb, Sn, Ge} and X={I, Br, Cl} have been investigated, and CH_3NH_3 is of large interest for A. As a result of their exceptional optical absorption, these materials were used as dye sensitizers. However, current interest is attributed to the quick rise of photo-conversion efficiencies to more than 20% within a few years. The high photo-conversion efficiency of prototypical $CH_3NH_3PbI_3$ needs to be understood to successfully design materials with better performance or improved stability.

For successful device engineering, detailed knowledge of the electronic structure and optical properties is needed. In particular, the influence of excitonic effects on optical absorption and exciton binding energies is not well understood. Exciton binding energies are important because

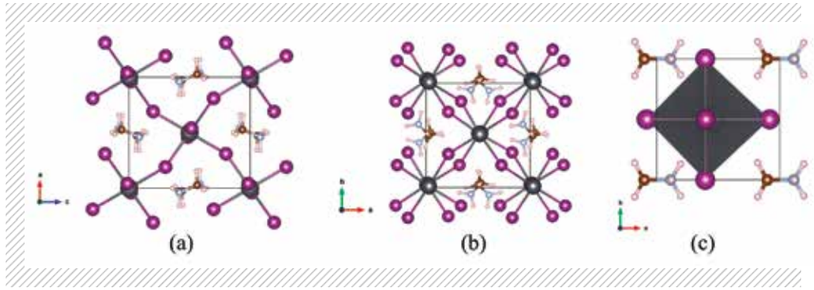

FIGURE 1: Unit cells of the low-temperature orthorhombic phase (a), the room-temperature tetragonal phase used in operational devices (b), and the high-temperature cubic phase (c).

they critically determine how efficiently electrons and holes can be separated in a photovoltaic device. Concurrently, a fundamental understanding is needed because excitonic effects and binding energies sensitively depend on the screening of the electron-hole interaction in the material. Better understanding will influence general first-principles models and could lead to an efficient, cost-effective, and broadly applicable set of materials for next-generation photovoltaics.

METHODS & RESULTS

We study optical properties using first-principles, theoretical spectroscopy based many-body perturbation theory [2]. We compute optical absorption spectra by solving a Bethe-Salpeter equation for the optical polarization function. Single-particle energies in the excitonic Hamiltonian are approximated using a generalized-gradient approximation for exchange and correlation. The spin-orbit interaction is approximately included for orbital energies of collinear spins, but not for wave functions used to compute Coulomb matrix elements. Using this approach on Blue Waters, we can accomplish the numerical challenge of converging the optical absorption spectra on Brillouin zone sampling.

The potentially large influence of lattice screening on the electron-hole interaction makes the description of these materials particularly challenging. We employ an approximate technique by Bechstedt et al. to incorporate the influence of lattice polarizability [3]. Experimental work has determined the static dielectric constant to be in the range of 30 to 32 [4], but even values as large as 1,000 were reported [5]. The approximation used here is merely the first step towards a **more sophisticated**, first-principles approach to clarify the influence of free-carrier and lattice screening.

We compute the optical-absorption spectra of three different polymorphs of $CH_3NH_3PbI_3$: the low-temperature orthorhombic phase, the room-temperature tetragonal phase used in operational devices, and the high-temperature cubic phase (Fig. 1). Our results for the cubic phase in figure 2 indicate a significant influence of the spin-orbit interaction due to heavy lead (Pb) atoms in the material. We also find a significant influence of the lattice screening on the optical-absorption spectra. If the lattice contribution is fully taken into account, excitonic effects are strongly reduced, and the spectrum approaches the density function theory result.

We find very good agreement with an experimental result [6], indicating that not only is lattice screening is important, but also that our approximate

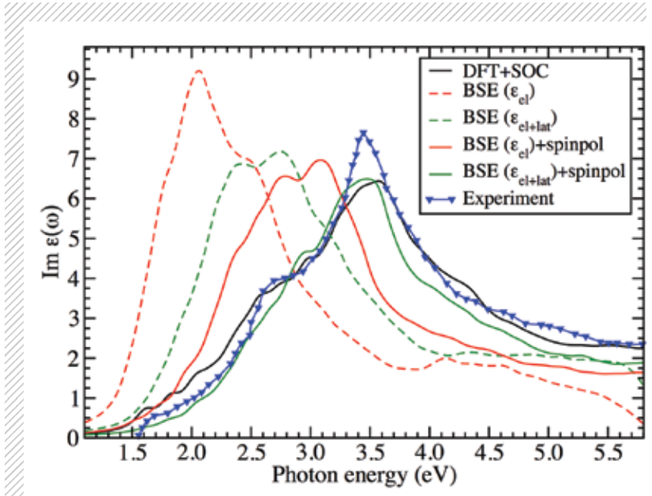

FIGURE 2: Imaginary part of the frequency-dependent complex dielectric function of $CH_3NH_3PbI_3$ computed using different levels of theory is compared to data from experiment.