FIGURE 2: Numerical schlieren for a cooled transonic vane at 6% and 20% turbulence intensity for unstructured second order solver.

high temperatures that, in many cases, exceed their melting point. One of the most common techniques to protect HPT components against the high thermal loads is film cooling, which bleeds airfoil cooling flow into the hot gas path so the coolant forms an insulating layer between the airfoil and the hot gases. The air used for film cooling is by-pass air from the late stages of the compressor. Therefore, there is a performance penalty due to the extraction of the cooling air that could instead have been used to extract work in the HPT.

The focus of this project is to investigate the impact of freestream turbulence on film cooling, including mixing, turbulence decay, and boundary layer development. In parallel, the investigation is evaluating the importance of higher order numerical schemes in capturing the turbulent mixing.

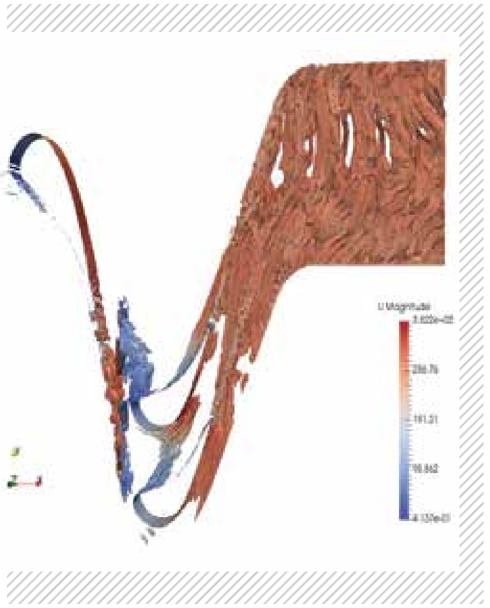

FIGURE 3: Setting the stage for a stage analysis with a high-pressure turbine stationary vane and moving blade.

METHODS & RESULTS

The availability of massively parallel computer environments has increased the popularity of scale-resolving computational fluid dynamics techniques such as direct numerical simulation (DNS), large eddy simulation (LES), and hybrid RANS-LES methods (HLES). Despite being computationally expensive, scale-resolved methods often bring significant improvements in accuracy over RANS (Reynolds-averaged Navier-Stokes) methods and provide an opportunity to understand the fundamental physics. LES resolves a significant part of the energy spectrum and models only the smaller, more dissipative subgrid scales present in the flow, resulting in accurate predictions of turbulent mixing.

For this study, we modified the uncooled turbine vane used by Arts and Rouvroit [1], adding a generic film-cooling hole shape based on Saumweber *et al.* [2] on the suction side of the vane. Figure 1 shows simulation results for uncooled geometry using second order unstructured Ansys Fluent v17, sixth order structured FDL3Di [3], and sixth order unstructured hpMusic [4]. Simulations for high and low levels of turbulence with the film cooling hole are ongoing (Figure 2).

WHY BLUE WATERS

Aero-thermal LES of turbomachinery problems at engine relevant Reynolds numbers is computationally intensive [5]. Physical testing has clearly shown that turbulence is an important contributor to turbulent mixing in aero-thermal applications of turbomachinery, but often testing is not capable of explaining the reason [1,2]. This is due, in part, to the range of length and time scales associated with turbulence and the challenges of measuring

single-point and multi-point correlations in high Reynolds number and high Mach number flows associated with rotating machinery. Simulations on Blue Waters are enabling us to replicate observations in physical testing while providing data that can provide insight into the mechanisms responsible for those observations.

NEXT GENERATION WORK

The current simulations are simplified to provide insight into the complex mixing of a single hole. In reality, the HPT airfoils are cooled by many holes. Furthermore, a high pressure turbine stage consists of a stationary airfoil (stator) and a rotating airfoil (rotor). The former turns the flow for the latter which extracts work to drive the compressor. Executing a cooled stage analysis would be the natural next step, followed by optimization of features. GE is collaborating with MIT to develop optimization capabilities in an LES framework [6], and preliminary simulations of a stator/rotor are ongoing (Figure 3).

PUBLICATIONS AND DATA SETS

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NUMERICAL STUDY OF THE MANY-BODY LOCALIZATION TRANSITION

Allocation: Illinois/50.0 Knh
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EXECUTIVE SUMMARY

We study the details of the many-body localization (MBL) transition and its adjacent phases in one-dimensional quantum spin systems through extensive numerical simulations using an exact diagonalization technique, which allows for the solution of the Schrödinger equation in finite spin chains. This transition is a formidable example of the breakdown of statistical mechanics in strongly interacting disordered systems, which do not thermalize.

Our main finding—using concepts from quantum information—is that in the vicinity of the critical point the system displays a mixture of localized and delocalized states, pointing to a highly nontrivial nature of the critical regime. We also find evidence in the probability distributions of matrix elements of local observables that in the regime of intermediate disorder, where the transport is subdiffusive, the generally assumed ansatz of the eigenstate thermalization hypothesis (ETH) in the scaling of the variance of these distributions as well as their shape has to be modified.

INTRODUCTION

While statistical mechanics usually assumes the presence of a heat bath, in the advent of cold atomic systems the study of completely isolated quantum systems has gained fundamental importance. In the absence of any coupling to the outside world, the dynamics of quantum systems are governed by the unitary time evolution described by the Schrödinger equation, and it is not clear how these systems would reach a thermal state. However, experiments of generic quantum systems point to a rapid thermalization. An important step towards an understanding of this phenomenon was the idea that quantum chaos leads to thermalization via the ETH [2,3,8]. While the ETH can explain thermalization in

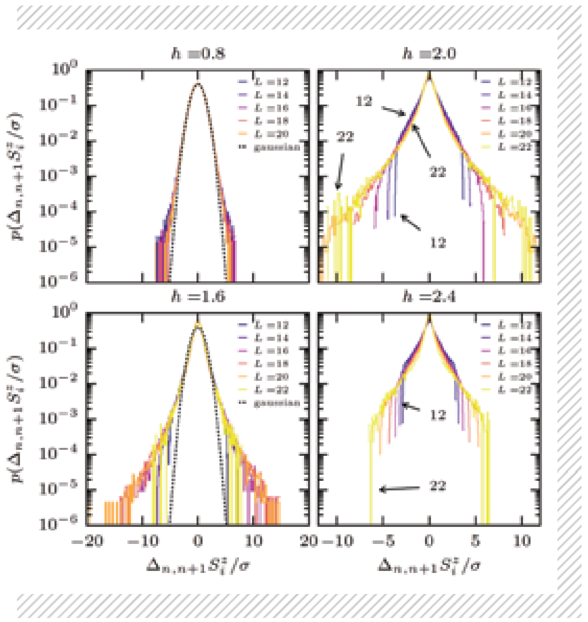

FIGURE 1: Probability distribution of the difference in local magnetization for states from the center of the spectrum of the random Heisenberg chain at disorder strength h. The distributions are normalized by their variance to compare their shapes for different chains of length L and their mean is zero. At weak disorder, the distributions are close to Gaussian and become increasingly non-Gaussian in the regime where transport is subdiffusive. The MBL critical point in this system is around $h_c \sim 3.7(1)$ [5].

many generic systems, noteworthy counterexamples have been discovered, one of which are many-body localized (MBL) systems [1], which violate ETH and do not thermalize.

MBL systems have been mostly explored in one dimension, due to the enormous computational complexity of the problem, caused by the exponential growth of the many-body Hilbert space, and the best-studied systems to date are interacting quantum spin chains with disorder (cf. e.g. [4,5]). In these, a transition between a thermal ETH phase and an MBL phase can be observed and the focus of our work lies in the transition and its vicinity to better understand how the thermalization mechanism breaks down at a critical strength of disorder. We use both concepts from ETH, mostly local operators like the local magnetization, and concepts from quantum information theory, like the entanglement entropy, to study the transition.

METHODS & RESULTS

We use state-of-the-art large-scale exact diagonalization techniques for the sparse Hamiltonian to obtain high energy eigenstates (cf. [5]), which are crucial for directly addressing the ETH. To leading order, local observables in the basis of eigenstates are required by the ETH to be diagonal matrices with Gaussian fluctuations around the mean (and around zero in the off-diagonal entries), whose variance vanishes exponentially with system size. We have studied the behavior of these matrix elements by a systematic study of the probability distributions of the local magnetization for various system sizes and strengths of disorder. This was achieved by calculating histograms of the matrix elements in the eigenbasis at zero energy transfer over a large number of eigenstates and realizations of disorder. Our main finding is that at weak disorder, the ETH ansatz is well-verified and the distributions are very close to a Gaussian distribution, whose variance scales with the exponential law in system size as predicted by ETH. However, at intermediate disorder, this is no longer true and the distributions become strongly non-Gaussian, while the variance of the distribution decreases slower than expected from ETH. In the MBL phase, ETH is violated and the variance of the (non-Gaussian) distributions does not decrease with system size, thus not leading to thermalization.

In ongoing work, we explore whether the deviation from the scaling of the variance from the ETH ansatz as well as the non-Gaussian distributions are linked to the subdiffusive transport, observed in the same parameter regime by previous studies [6, 7].

The MBL transition can also be addressed using concepts from quantum information theory, most prominently by the entanglement entropy (EE). The entanglement entropy can be viewed as the thermodynamic entropy of a subsystem if the rest of the system is considered to be the heat bath. This leads to the requirement from ETH, to the fact that thermodynamic entropies are extensive, and that if the system thermalizes, the EE has to scale by a volume law. Contrarily, in the MBL phase, this is explicitly broken and the EE displays an area law. We consider the transition between these two behaviors in our current work and develop a formalism based on general concepts (strong subadditivity of EE) that allows for a quantification of the EE scaling of single eigenstates in inhomogeneous systems. The erratic behavior of the EE as a function of subsystem size in disordered systems seems at first not to allow for such an analysis but we prove in [9] that in periodic chains, the EE is a concave function of subsystem size, if one averages over all cuts of the same length (cf. Fig. 2). By an extensive analysis of the probability distributions of the slope of this cut averaged EE as a function of subsystem size, we find that in the critical regime, a mixture of volume and area law states appears, which opens new questions about the nature of the MBL transition.

WHY BLUE WATERS

The numerical study of quantum many-body systems is an extremely hard problem that requires massive computational resources. Here, we consider disordered systems, which makes the problem harder by several orders of magnitude as one has to average over many configurations of disorder. The disorder corresponds basically to the effect of “dirt” on the system and is modeled by random potentials.

Solving the Schrödinger equation for one realization of such a dirty system already requires more than one node of Blue Waters for large systems and repeating this calculation for hundreds to thousands of configurations is only feasible on a massively parallel setup like Blue Waters.

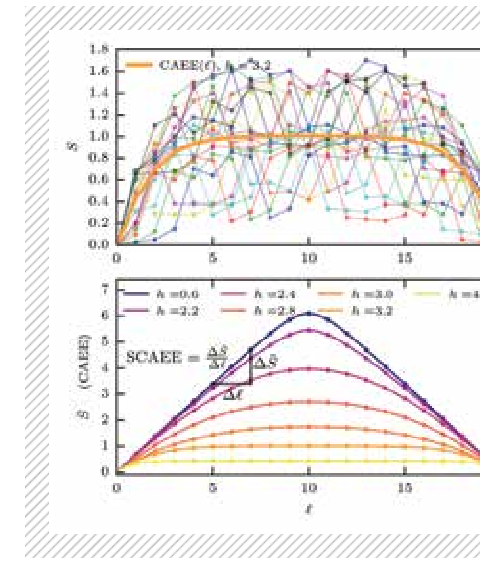

FIGURE 2: Top: Entanglement entropy as a function of subsystem size for one high-energy eigenstate of a random Heisenberg chain of length L=20 and at disorder strength h=3.2 for all possible left cut positions. The erratic behavior is completely removed by the average over all cut positions (CAEE). Bottom: Typical cut averaged EE curves for single eigenstates at various disorder strengths with well-defined slope (SCAEE).

PUBLICATIONS AND DATA SETS

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DNS AND STOCHASTIC STUDY OF THE RELATIVE MOTION OF HIGH INERTIA PARTICLES IN ISOTROPIC TURBULENCE

Allocation: NSF PRAC/1.77 mnh
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Collaborator: Rohit Dhariwal[1]

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EXECUTIVE SUMMARY

The objective of our research is to investigate the role of turbulence in driving the relative velocities and positions of inertial particles in isotropic turbulence. First, we studied the effects of turbulence on the relative motion of high-inertia particle pairs in isotropic turbulence. Accordingly, we performed direct numerical simulations (DNS), as well as Langevin simulations (LS) based on a probability density function (PDF) kinetic model for pair relative motion. Recently, we developed a stochastic theory that derives closures in the limit of high Stokes number for the diffusivity tensor in the PDF equation for particle pairs. The diffusivity contained the time integral of the Eulerian two-time correlation of fluid relative velocities seen by pairs that are nearly stationary. The two-time correlation was determined analytically using the