characteristics during turn-on for studying novel effects based on wave function phase manipulation, and as an alternative research path to simulating dissipation and nonlocal scattering. Time-resolved quantum transport simulations are performed with the semi-empirical tight binding method. Initial work shows that this approach is valid up to about 1 mV/ps, corresponding to a few GHz in realistic transistors.

Self-assembled quantum dots are highly strained heterostructures with optoelectronic applications, such as infrared photodetectors, intermediate band solar cells, optical amplifiers, and quantum dot lasers. A universal behavior in terms of strain magnitude and profile is observed in atomistic strain simulations of dots with different shapes and materials. Atomistic strain simulations are more accurate but more expensive than analytic continuum solutions. Simulations on Blue Waters showed that both techniques indicate that the strain depends on the aspect ratio of the dot, and not on the individual dimensions. This has allowed for the formulation of a compact model of strain effects on self-assembled quantum dots.

Multi-quantum well LEDs have carrier flow through complex quantum states and the NEGF (non-equilibrium Greens function) approach has been used to model nitride-based diodes that provide blue mid-to-high power light. Strong electron-electron/phonon scattering thermalizes carrier distribution in the wells. A multiscale approach models the barriers in non-equilibrium with the wells in equilibrium. Simulations of 120 nm long devices show IV characteristics matching experimental results when accounting for temperature differences and external resistance. This research has revealed how p-side wells provide higher radiative recombination, supporting experimental evidence, due to more deeply filled electronic states, leading to a stronger overlap in the electron-hole densities.

WHY BLUE WATERS

In many cases the work could not be accomplished in a reasonable amount of time without Blue Waters, and for larger simulations the work could not be accomplished on other available systems. Blue Waters staff provide **exemplary** support and user outreach to guide system usage, help with issues as they arise, and assist with code performance and scaling. In particular, they have provided custom scripts and permissions to facilitate management of an allocation with a large research group.

NEXT GENERATION WORK

A next-generation Track-1 system will enable efficient reliability predictions of modern nanodevices—a crucial milestone in their design. Atomistic deviations due to statistical and fabrication fluctuations can have increasingly large effects on a device's operation as devices are scaled, and it is imperative to have a strong grasp on these phenomena in the coming years.

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COMPRESSIBLE LARGE EDDY SIMULATION OF A FILM-COOLED STAGE-ONE NOZZLE AT DIFFERENT FREESTREAM TURBULENCE LEVELS

Allocation: Innovation and Exploration/300 Knh
PI: Gregory M. Laskowski[1]
Co-PI: Gustavo Ledezma[2]
Collaborators: Qiqi Wang[3], ZJ Wang[4], James Kopriva[1], Rathakrishnan Bhaskaran[2], Lawrence Cheung[2], and Umesh Paliath[2]

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EXECUTIVE SUMMARY

Gas turbines are the backbone of aircraft propulsion. Therefore, technologies that improve the fuel efficiency of these turbines can have a significant impact on the U.S. economy and can substantially reduce polluting emissions. The quest for greater turbine efficiency has led to increased firing temperatures, subjecting turbine components to extremely high temperatures. One common technique for abating these temperatures is film cooling, which bleeds cool air from the compressor stage of the engine and discharges it through small holes in the turbine blade walls, providing an insulating layer of cool air. The focus of this project is to investigate the impact of freestream turbulence on film cooling, including mixing, turbulence decay, and boundary layer development.

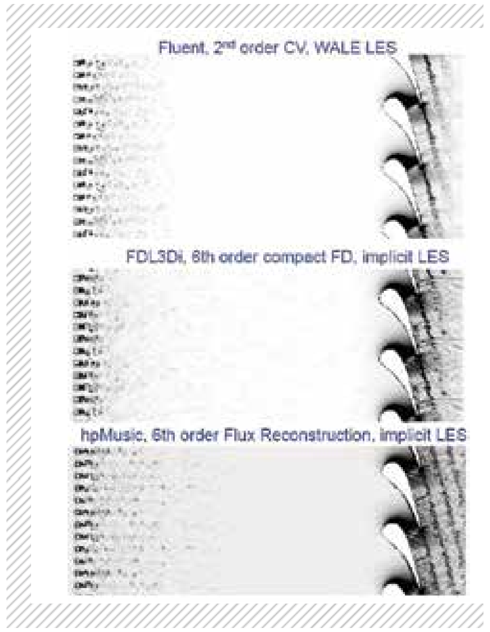

FIGURE 1: Numerical schlieren for an uncooled transonic vane and 6% turbulence intensity (a) unstructured 2nd order solver (b) structured 6th order solver (c) unstructured 6th order solver.

INTRODUCTION

Because of their power density and efficiency, gas turbines are, and will continue to be, the backbone of narrow- and wide-body aircraft propulsion. According to the Federal Aviation Administration, the United States alone consumed approximately 35.6 billion gallons of aviation fuel in 2012. Technologies that can further improve fuel efficiency can have a significant impact on the U.S. economy while reducing emissions.

The modern high-bypass turbofan engine is based on the Brayton cycle. Air is ingested in the engine and passes through the fan. A majority of the airflow bypasses the core of the engine to increase propulsive efficiency. The core flow is compressed, increasing total pressure (Pt) and total temperature (Tt). Fuel is added and burned in the combustor, increasing Tt and slightly reducing Pt, and the flow is expanded through the turbine, reducing Pt and Tt. Work extracted by the turbine drives the compressor. The turbine also drives a fan at the front of the engine in order to increase the mass flow through the engine, thus increasing the propulsive efficiency. In order to improve thermal efficiencies the turbine inlet temperature and compressor pressure ratio have historically increased with time.

The need for higher turbine efficiencies to reduce fuel consumption keeps pushing the firing temperature up. As a result, all components in the high-pressure turbine (HPT) are subject to extremely

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.

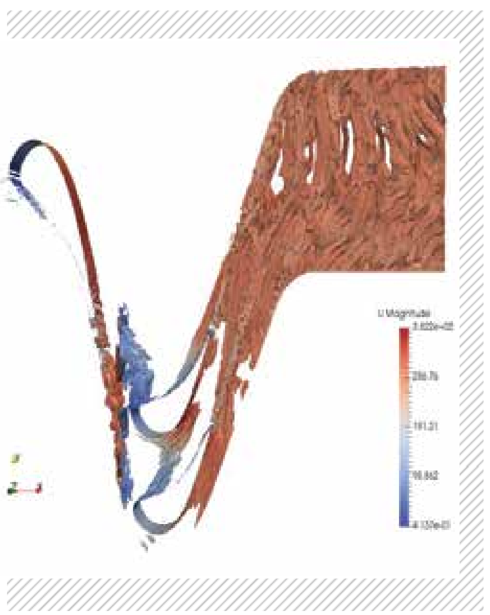

FIGURE 3: Setting the stage for a stage analysis with a high-pressure turbine stationary vane and moving blade.

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