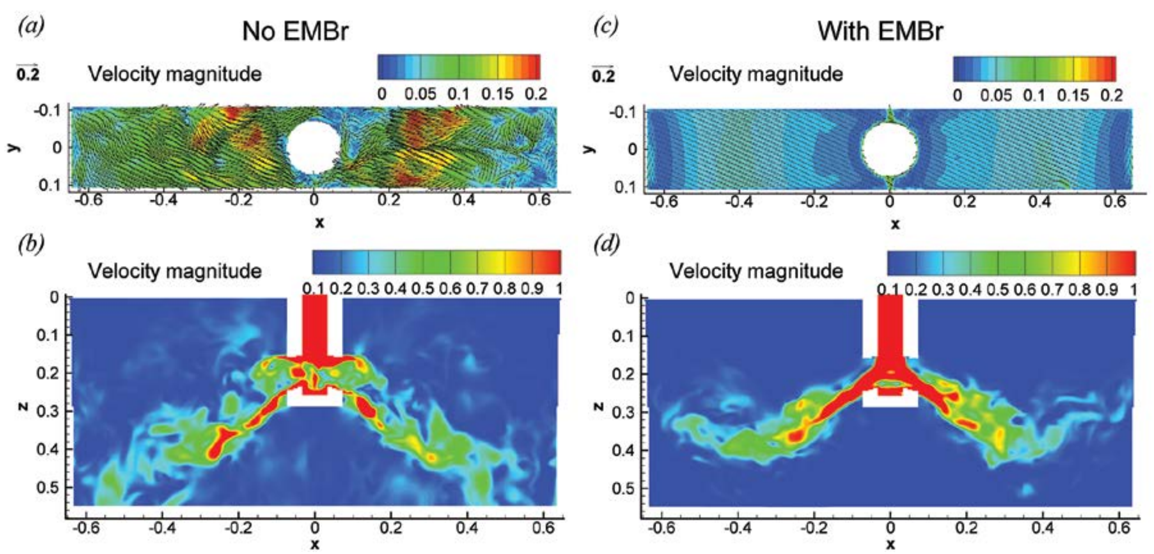

FIGURE 4: Predicted velocity in a horizontal plane near the top surface (top) and in the middle vertical plane of the caster mold (bottom) for cases without (left) and with (right) an external magnetic field.

of the caster (casting speed 1.5 m/min). Applying an EMBr field greatly lowered the velocity near the top surface, which can lead to problems of meniscus freezing in which the steel around the three-phase perimeter solidifies into detrimental hook structures that capture inclusions and bubbles. Figs. 4b and 4d show velocity in side views. Applying EMBr deflected the jets upward, but the flow in the top region was reduced by the dampening effect of the field. The steel plant that was experiencing this problem improved quality by lowering the field strength towards the top of the mold and increasing the casting speed.

WHY BLUE WATERS?

The in-house multi-GPU code CUFLOW was developed and tested on Blue Waters XK nodes and good speed-up was obtained. Less than two days were required for a 30 s LES simulation of flow in a caster domain with 14.1 million cells (based on a 100-time-step test run with an average time step size Δt=0.0005 s). Preliminary results showed that ANSYS-FLUENT also scales well on Blue Waters for this problem. To resolve turbulent flow in the real caster, complete with thousands of bubbles, is only feasible with petascale computing such as Blue Waters.

As another part of this project, transient thermal-stress models of the solidifying dendritic microstructure will be applied to investigate strain concentration and the formation of longitudinal cracks in order to understand how to avoid cracks.

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LATTICE QCD ON BLUE WATERS

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EXECUTIVE SUMMARY:

Project goals include developing highly optimized code for the study of quantum chromodynamics (QCD) to carry out calculations that will have a major impact on high-energy and nuclear physics. We have optimized and used Chroma for the simulation of Clover quarks and MILC for the simulation of HISQ quarks. Our long-term objectives with HISQ quarks are to generate gauge configurations with physical-mass up, down, strange, and charm quarks, to use these configurations to calculate fundamental parameters of the standard model of high-energy physics, and to make precise tests of the standard model. The objective of our Clover fermion program is the determination of the excited mass spectrum of strongly interacting particles (hadrons) within QCD.

INTRODUCTION

The standard model of high-energy physics encompasses our current knowledge of the fundamental interactions of subatomic physics. It has successfully explained a wealth of data from accelerator and cosmic ray experiments over the past 40 years. However, it has been difficult to extract many of the most interesting predictions of quantum chromodynamics (QCD), those that depend on the strong coupling regime of the theory. The only way, from first principles and with controlled errors, is through large-scale numerical simulations. These simulations are needed to obtain a quantitative understanding of the physical phenomena controlled by the strong interactions, determine a number of the fundamental parameters of the standard model, and make precise tests of the standard model. Despite the successes of the standard model, high-energy and nuclear physicists believe that a more general theory will be required to understand physics at the shortest distances. Thus, QCD simulations play an important role in efforts to obtain a deeper understanding of the fundamental laws of physics.

METHODS & RESULTS

Our objective is to perform calculations of QCD, the theory of the strong interactions of subatomic physics, to the precision needed to support large experimental programs in high-energy and nuclear physics. We are using two formulations of lattice quarks. The highly improved staggered quarks (HISQ) formulation is being used to calculate fundamental parameters of the standard model, our current set of theories of subatomic physics, and to make precise tests of the standard model. In particular, the HISQ formulation is being used to calculate the masses of quarks, which are the fundamental building blocks of strongly interacting matter, and to determine elements of the Cabibbo–Kobayashi–Maskawa (CKM) matrix, which are the weak interaction transition couplings between quarks. The CKM matrix elements and the quark masses are fundamental parameters of the standard model and therefore of great interest. Furthermore, a major line of research within high-energy physics has been to determine the same CKM matrix element through different processes to look for inconsistencies that would signal a breakdown in the standard model. Until now, uncertainties in the lattice calculations have limited the precision of these tests. We aim to match the precision of our calculations to that of experiments.

Our first objective with the Clover formulation of lattice quarks is to perform a calculation of the mass spectrum of strongly interacting particles (hadrons). The determination of the excited-state spectrum of hadrons within QCD is a major objective for experiments and is a focus of the $310 million upgrade of Jefferson Laboratory. In particular, the GlueX experiment at Jefferson Laboratory will search for “exotic” mesons. These particles are a signature for new states of matter, specifically the presence of gluonic

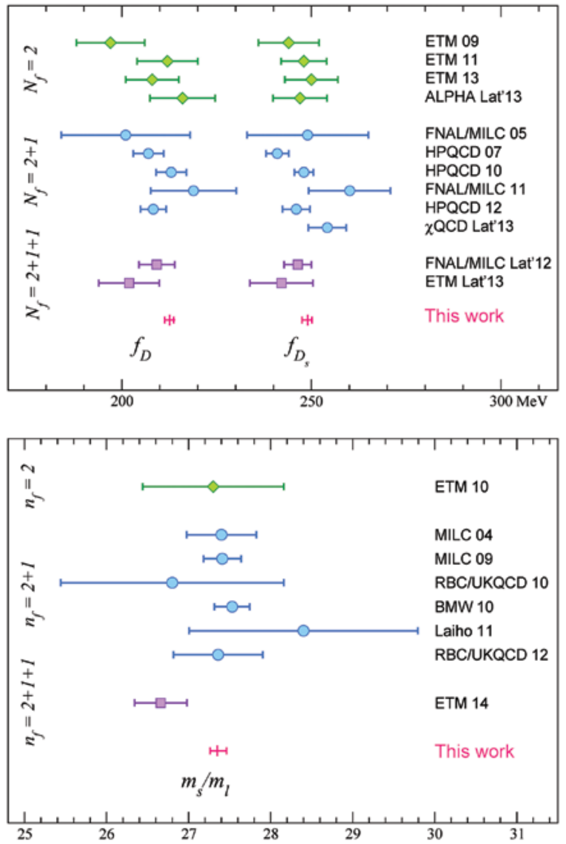


FIGURE 1: Comparison of our latest results for the leptonic decay constants f_D and f_{D_s} (top panel) and for the quark mass ratio m_s/m_l (bottom panel) with earlier lattice calculations. Results are grouped by the number of flavors of sea quarks from top to bottom: n_f=2 (green diamonds), n_f = 2+1 (blue circles), and n_f=2+1+1 (purple squares). Within each grouping, the results are in chronological order. Our new results are denoted by magenta pluses and labeled "This work".

degrees of freedom, predicted by QCD but thus far not clearly observed. The spectroscopy effort is intended to determine whether the equations of QCD do, in fact, realize the existence of such exotic states of matter. Because these predictions will be made before the experiments are performed, these calculations will provide crucial information about the decay signatures of such exotic states that will inform and guide the experimental searches.

Lattice QCD calculations have two steps. First, one generates and saves gauge configurations, which are representative samples of the QCD ground state. Then the gauge configurations are used to measure a wide range of physical quantities. Generating gauge configurations is the rate-limiting step and requires the most capable supercomputers available. The most computationally expensive component of the second step, the measurement routines, is to calculate the Green's functions for the propagation of quarks in the gauge configurations. For the light quarks, this calculation also requires highly capable computers.

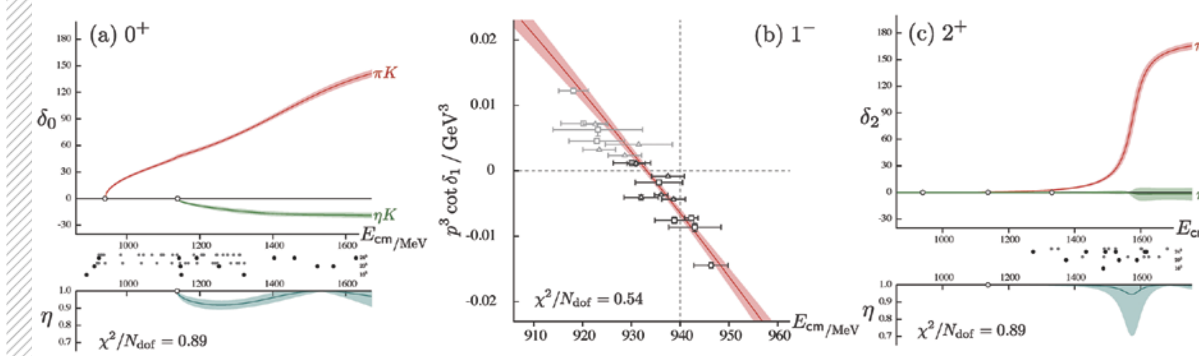
We have made major progress in our efforts to generate gauge configurations and quark propagators using Blue Waters, including the most challenging ensembles undertaken to date. The new HISQ configurations have been used to make the most precise determination to date of the decay properties of a number of mesons containing strange and charm quarks [1–6], which in turn have led to the evaluation of several CKM matrix elements that are important for tests of the standard model, and produced the most precise ratios among the up, down, strange, and charm quark masses [3]. The HISQ configurations have also been used in the study of gradient flow and scale setting [7,8]. Important advances have been made in the development of code for the generation of gauge configurations and quark propagators with the Clover formulation of lattice quarks [9].

WHY BLUE WATERS

Lattice QCD calculations have made major progress in the last few years with a limited number of calculations reaching precision of a fraction of a percent and techniques in place to determine many more quantities to this level of accuracy. Such precision is needed to test the standard model and for a detailed understanding of physical phenomena controlled by the strong interactions.

The advent of petascale computers, like Blue Waters, is playing a critical role in these advances. High-precision QCD calculations are enormous undertakings that require computers of the highest capability and capacity.

QCD is formulated in the 4D space–time continuum, which is translated to a 4D lattice, or grid, for computational purposes. One must perform calculations for smaller and smaller



lattice spacings across a fixed 4D space and extrapolate to the continuum (zero lattice spacing). Until recently, it has been too expensive to use the physical masses of the two lightest quarks (up and down), a known source of error. The computational cost grows roughly as the fifth power of the inverse of lattice spacing and also rises as the masses of the quarks decrease. Blue Waters enables us, for the first time, to carry out calculations with small lattice spacings and the masses of up and down quarks at their physical values. This has led to calculations of unprecedented precision.

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FIGURE 2: Results from [10] showing the scattering amplitudes of K-π and K-η mesons in isospin=1/2. The energy dependence of these scattering amplitudes is used to determine the resonance content of the spectrum. The left, middle, and right panels show the scattering amplitude of K-π (red), K-η (green), and K-π → K-η (lower panels) in l=0, 1, 2 waves, respectively. The points in between the panels are the energies determined from three different lattice sizes, and the curves are the parameterization of the scattering amplitudes with a resonance in J^P = 0^+ and 2^+, and a bound-state in J^P = 1^-.