Lattice QCD in HPC

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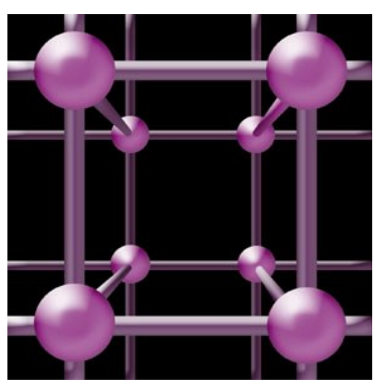
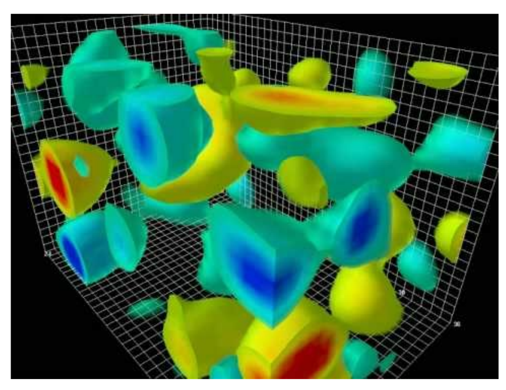
Introduction

Understanding the structure and interactions of subnuclear particles represents the main challenge for today's nuclear physics. These subnuclear particles are made of quarks and their behavior is described in principle by quantum chromodynamics (QCD) which cannot be solved analytically. Lattice QCD is a 4-D discretized version of QCD that can be solved numerically.





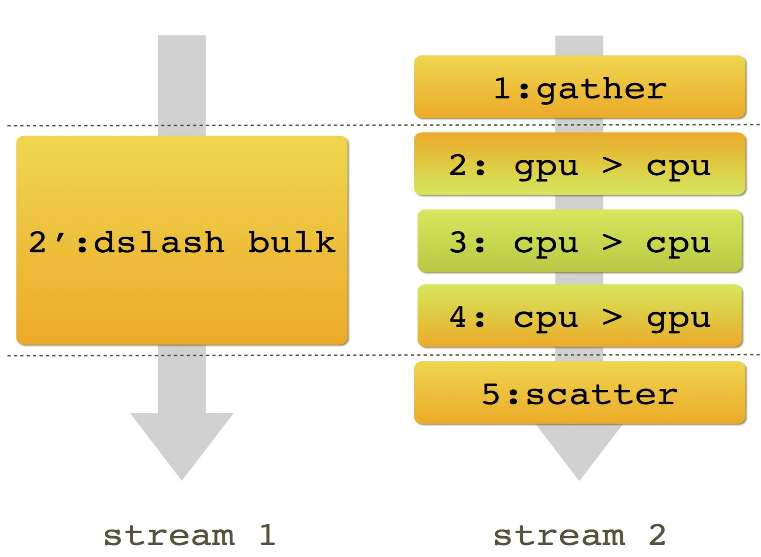
We study the structures of particles by placing them in an external electric field. In particular, we calculate their polarizabilities, which describe their rigidity in response to field. We also study particle interaction by computing the phase shift pattern which describe how those two particles interact with each other.

Computations

The core routines in our calculations are vector routines and the multiplication of a large sparse matrix called Dslash, **D.**

$$\mathbf{D}\,|\psi\rangle = |\varphi\rangle \qquad \alpha|\psi_1\rangle + \beta|\psi_2\rangle = |\varphi\rangle$$

- Routines are local i.e. communication only between neighbors
- Parallelization is natural
- Single-instruction, multiple-data (SIMD) paradigm



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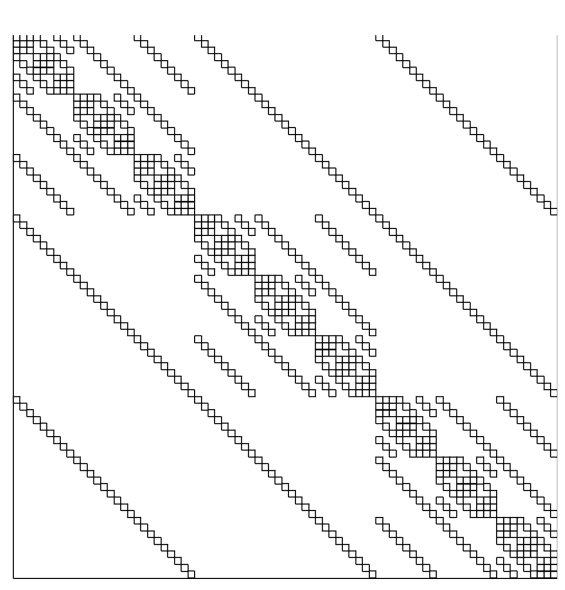
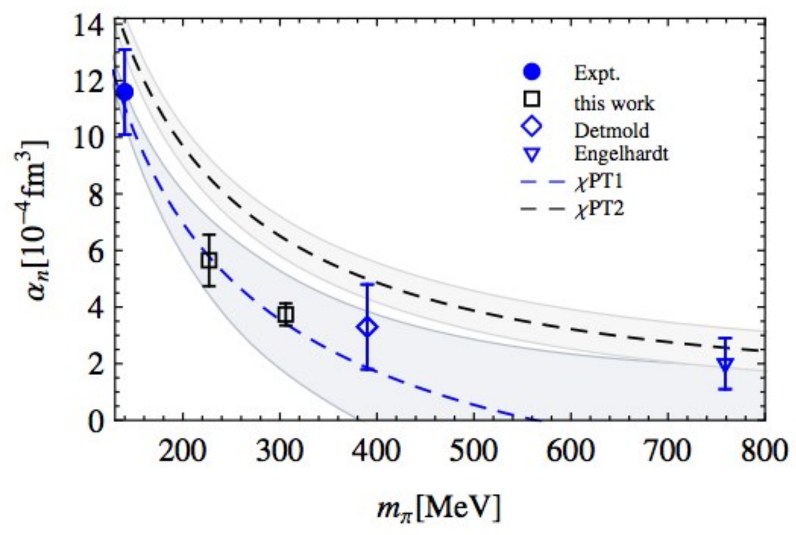
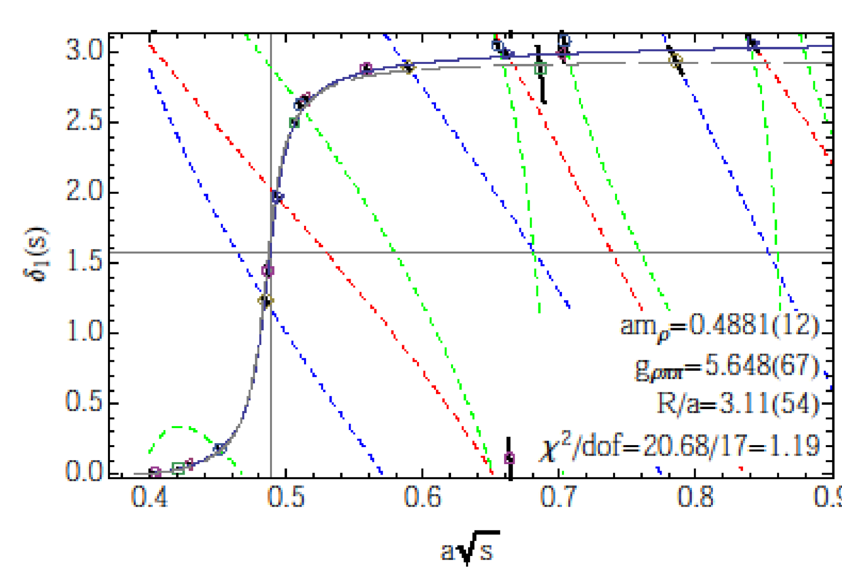


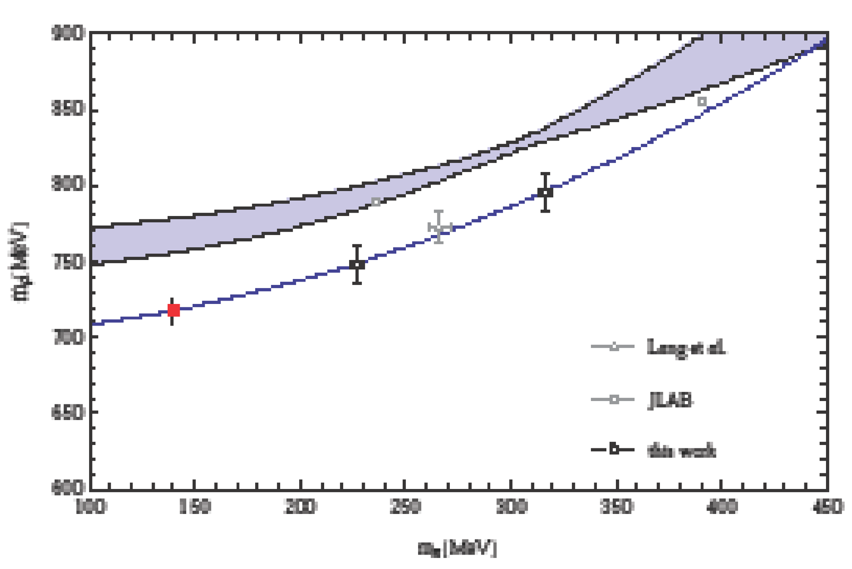
Neutron Polarizability



An electric field is used to probe the internal structure of particles. The reaction of particles to an external electric field gives us information about the underlying structure of the particles. Here we present a study of the neutron polarizability from Lattice QCD calculations and chiral perturbation theory. **Computational cost**: 4 million CPU-hours + 800,000 GPU-hours.

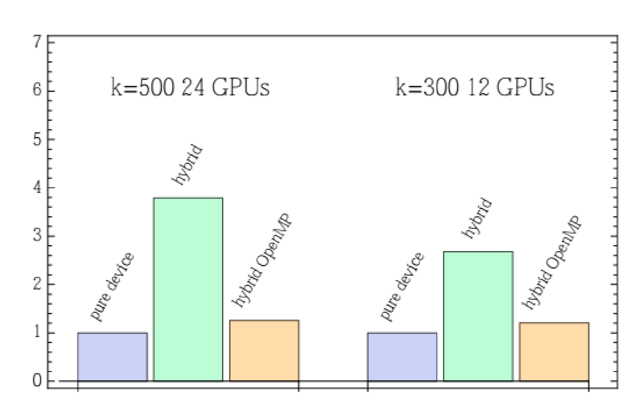
Two-pion Scattering

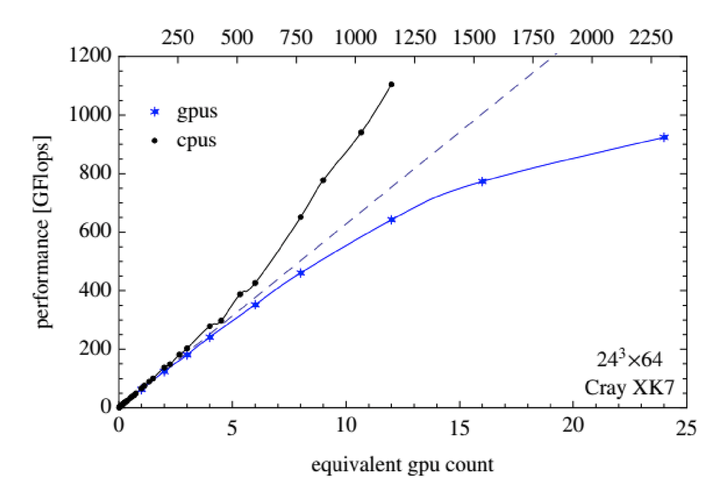




Two pions with back to back momentum collides with each other elastically. Their phase shift pattern captures the interaction properties between these two particles. The phase shift also indicates the existence of a resonance when it changes from 0 to 180 degree. We present a lattice QCD calculation for two pions scattering phase shift. It requires about 350,000 CPU-hours and 1.5 million GPU-hours.

Performance





The left panel shows the timings of eigensystem calculations for different operation modes: vectors residing in GPU memory, mixed CPU and GPU memory, and mixed CPU and GPU memory with OpenMP. The tests were run on a Cray XK7 machine. The right panel shows the Dslash calculation performance for CPU and GPU codes on the same machine. The x-axis indicates the number of GPUs (lower edge) and number of CPU cores (upper edge). The scales are normalized so that they match at

Conclusion and Outlook

Lattice calculations are pushing the forefront of today's supercomputers. Our research is using the latest of GPU technology. An efficient implementations of the Dslash operator allows us to scale to large numbers of GPUs. We've used over 2 million GPU-hours thus far in the calculations of hadron structures and their interactions. Our ongoing research are replacing more parallel sections of the CPU codes with GPU codes to obtain larger speedup. In particular our codes utilize both GPU and CPU memory in an efficient way to address the issue of memory constraints on GPUs.

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