Scaling a high energy laser physics application (VBL) using MPI and the RAJA portability layer

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ABSTRACT

LLNL is a world leader in designing and maintaining high energy lasers, built upon decades of leadership in the modeling of high energy laser systems. Here we present initial results for a parallel mini-app based on the National Ignition Facility's (NIF) Virtual Beamline (VBL)[1,2] code, a single-node laser physics modeling engine. Recent advances in ultra-intense short-pulse laser systems are driving us to develop massively parallel laser physics capabilities similar to the laser physics code Miró[3] (an MPI-only implementation) to support the multi-order increase in time/space resolution needed for these types of broadband, chirped-pulse amplification lasers. Here we present a demonstration of our new scalable simulation code architecture using MPI and the RAJA Portability Layer[4]. This hybrid parallelization approach promises to bridge the gap in resolution allowing us to deliver future simulations with the requisite physics fidelity at an unprecedented scale.

1. INTRODUCTION

Modeling laser systems to predict energetics, wavefront, near- and far-field beam profiles, and damage risk is essential to designing, operating, maintaining and improving complex laser systems. At LLNL, the focus has been on the design and operation of the National Ignition Facility (NIF) which is a 192 beam, 1.8 MJ laser system, the most energetic and largest laser facility on earth. To meet the modeling needs of new laser designs like the Advanced Radiographic Capability (ARC)[5] and High-Repetition-Rate Advanced Petawatt Laser System (HAPLS)[6] the mission of the current physics modeling code, the Virtual Beamline (VBL), has been expanded to include new capabilities such as modeling of chirped or broadband beams, depolarization effects, diffraction gratings, interactions with under-dense plasmas and thermal effects in the frequency converters.

The current VBL code has been written as a single node application. The parallelism enabled by shared memory application level threads in modeling the beam's interaction with optical components has been sufficient for the spatio-temporal memory footprint of typical NIF class laser simulations. The code supports split-step propagation using a discrete Fast Fourier Transform (FFT) algorithm, models complex coupled nonlinear material effects. The physics models for common optical components include many time and/or space independent calculations yielding rich parallelization opportunities. The drive for advanced physics capabilities will require significant increases in the spatial and temporal resolution – pushing past the limits of single node shared memory computing.

2. Approach

We wrote a 'mini-app' version of the single node VBL code to prototype the parallelization scheme and validate the physics results. The mini-app reads in a realistic source term for the laser beam with amplitude and phase, propagates the beam through vacuum, nonlinear materials, and through an amplifier which simulates gain amplification using the standard Frantz and Nodvik scheme.[7] The 'mini-app' utilizes the HDF5 library[8] to read and write the contents of the electric-field to disk for visualization, validation, and analysis. A key part of the 'mini-app' approach has been to validate the physics results in a controlled fashion to ensure reproducibility and agreement with the current single node implementation. In addition to distributing the representation of the electric field and parallelizing the calculations on the field, we took advantage of performing loop fusions and altered the programming paradigm to trade CPU cycles for less memory accesses.

We designed into the 'mini-app' the ability to compare parallel decompositions using MPI along any spatial and/or time axis. This is critical for prototyping new physics algorithms which may have differing resolution constraints in time than space. We present here only our initial scaling results splitting the MPI tasks along the y-dimension which is how the single node VBL implementation schedules its application level threads.

After validating the physics simulation computations against the baseline application, we converted our 'mini-app' from an MPI-only application to a hybrid application using the RAJA portability framework which provides a common interface to heterogeneous compute resources. With a minimal code footprint, we are able to use RAJA to express traversals over the spatio-temporal grid. In the poster we will show example loop transformations and report results of running MPI only, using RAJA with MPI and threads, and using RAJA with MPI, threads and GPUs.

3. Evaluation and Analysis

Our initial results are shown in Figures 1, 2 and 3. In Figure 1, we show that the mini-app is able to take advantage of parallel computing to solve a laser physics problem at a high enough resolution to resolve the interference pattern caused by 150 micron phase aberrations. Figure 2 shows our MPI strong and weak scaling results. While there is still more performance tuning to be done, these results represent a dramatic improvement to our existing capabilities.

Figure 3 shows how the mini-app is able to take advantage of multiple types of node-level parallelism through OpenMP or CUDA.RAJA allows us to write one code that supports both OpenMP and CUDA and choose between them by how we select the policy. We investigated hand-coded routines for a transpose and gather operation because their performance was lower than expected and were able to get significantly better performance. We are working with the RAJA development to determine how these improvements can be expressed using RAJA.

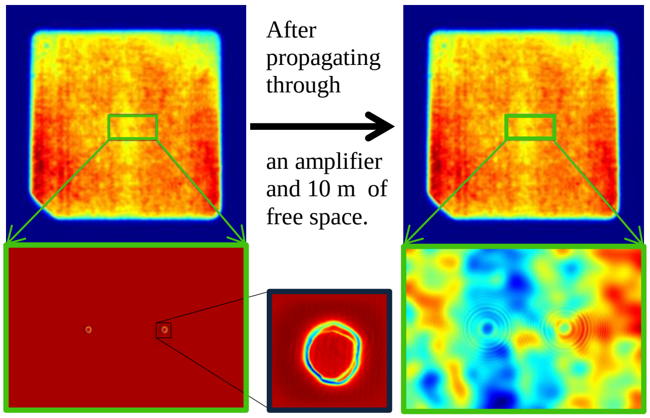
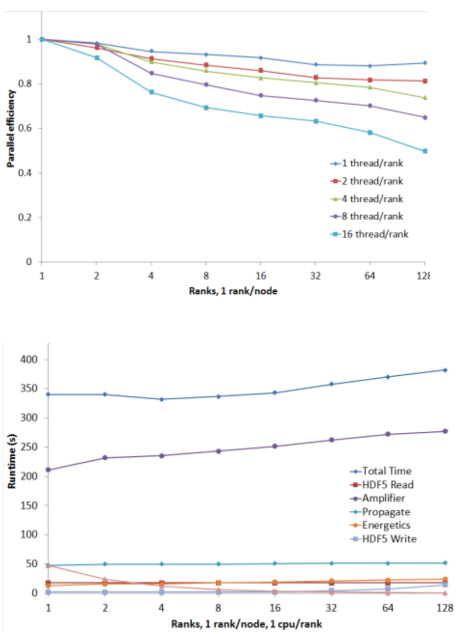
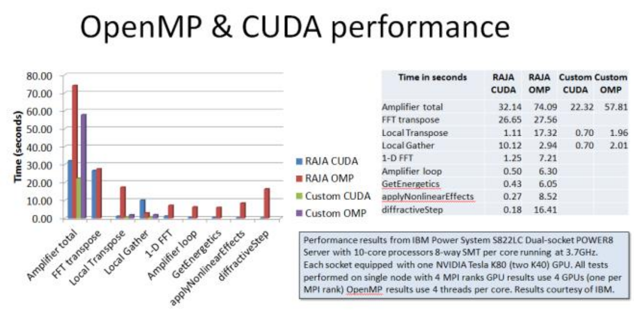


Figure 1*: VBL mini-app simulating a single time slice $2^{16}x2^{16}$ spatial beam profile of a 1.8 MJ NIF shot after applying two characteristic optics defects (lower left, center) and propagating through an amplifier and 10 meters of free space, producing diffraction waves in the fluence (right).*



Increasing ranks or thread/rank gives speedup in all cases. With one thread (MPI only), PE is at or above 90%. Speedup from 1 rank, 1 thread to 128 ranks, 16 threads is over 200x. Split-step amplifier (FFT) is limiting factor in scaling. HDF output starts to become a problem with increasing ranks. Amplifier setup speedup is due to fixed size of amplifier with increasing ranks.

Figure 2: VBL mini-app performance results on Livermore Computing's Syrah machine.



Time in seconds	RAJA CUDA	RAJA OMP	Custom CUDA	Custom OMP
Amplifier total	32.14	74.09	22.32	57.81
FFT transpose	26.65	27.56		
Local Transpose	1.11	17.32	0.70	1.96
Local Gather	10.12	2.94	0.70	2.01
1-D FFT	1.25	7.21		
Amplifier loop	0.50	6.30		
GetEnergetics	0.43	6.05		
applyNonlinearEffects	0.27	8.52		
diffractiveStep	0.18	16.41		

Figure 3: Compares RAJA OpenMP, RAJA CUDA results and in some cases hand-coded versions.

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