COMPARING CAF AND MPI-3 AND SIMULATING MOLECULAR CLOUD TURBULENCE WITH TWO-FLUID MHD

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EXECUTIVE SUMMARY

This project has three foci. First, we plan to demonstrate that Coarray Fortran standard offers petascale performance that is comparable to or better than the MPI-3 standard has to offer. Both CAF and MPI-3 have also been shown to outperform the MPI-2 standard by a substantial margin. In doing this work, we also found efficient implementation strategies that work well for any one-sided messaging paradigm. Second, we wish to study two-fluid turbulence in molecular clouds. The turbulent plasma that makes up a molecular cloud is predominantly made up of neutral molecules that are threaded by ions that gyrate around a strong magnetic field. The ions and neutral fluids are coupled, but not perfectly, which results in a modified turbulence. We have also extended our two-fluid studies to relativistic two-fluid plasmas that are made of electron-positron fluids.

INTRODUCTION

Observations show that star formation takes place in a partially ionized plasma. Furthermore, Balsara [1] showed that it is critical to represent the plasma as two fluids, one made up of neutrals and the other made up of ions that are threaded by a magnetic field. Previous studies were analytical or restricted to low resolution. Thanks to the availability of Blue Waters, we have been able to carry out large-scale studies of two-fluid turbulence computationally. These have been documented in two recent papers [2,3] and have also contributed to the graduate theses of both Chad Meyer and Blakesley Burkhart, both of which are currently employed based on their computational skills.

METHODS & RESULTS

The first task that we undertook in the 2014-2015 timeframe was to generate a very extensive comparison of Cray's CAF standard with MPI-3 for a range of partial differential equation (PDE) applications. Both CAF and MPI-3 are novel programming paradigms, and it would greatly help the community if their capabilities were documented and published. We are also required to carry out this task as part of our NSF funding (NSF-ACI-1307369; NSF-DMS-1361197). Both CAF and MPI-3 provide for one-sided, non-blocking messaging, which should make them especially well-adapted to exploit Cray's SHMEM library middleware. We have carried out such a weak scalability study and report our results in Garain, Balsara & Reid [4].

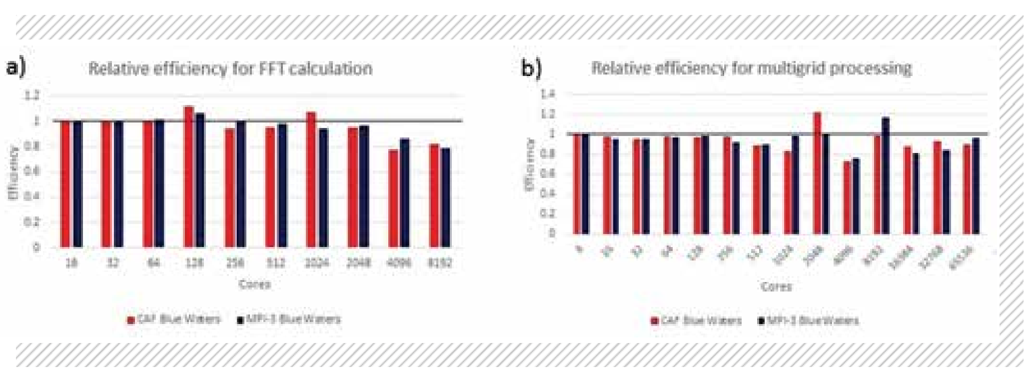

FIGURE 1A, B: From Garain, Balsara & Reid (2015), show a weak scaling study for FFT and Multigrid-based PDE solvers respectively. The relative efficiency for CAF and MPI on Blue Waters is shown in red and blue colors respectively.

WHY BLUE WATERS

Fig. 1 shows the results of weak scaling on Blue Waters for Fast Fourier Transform (FFT) and multigrid applications ranging from 8 to 65,536 cores. Blue Waters is the only available machine on which we can demonstrate this level of extremely scalable performance. We observe that CAF and MPI-3 can keep pace with each other across the entire range of processors. We further find that both CAF and MPI-3 are more than twice as fast as MPI-2 when one approaches large numbers of processors. This observation shows the immense value of these novel programming paradigms when computing at scale. Furthermore, this study would not have been possible without Blue Waters. In Garain, Balsara & Reid [4] we also document best practices for using CAF and MPI-3 for the community. We also show that CAF code is much easier to write and maintain, and the simpler syntax makes the parallelism easier to understand. Educational lectures on CAF were also developed as part of this work and are freely available from our website (http://www.nd.edu/~dbalsara/Numerical-PDE-Course).

NEXT GENERATION WORK

Electron-positron plasmas are very common in strongly relativistic environments, like the atmospheres of pulsars or black hole accretion disks. Thus developing a highly parallel capability to simulate such plasmas is crucial, and was achieved in the work of Balsara, Amano, Garain and Kim [5]. It is thought that the gamma-ray flares from the Crab pulsar are due to rapid magnetic reconnection events. Fig. 2 shows the results of such a simulation from Blue Waters. These are early results stemming from a very productive new direction.

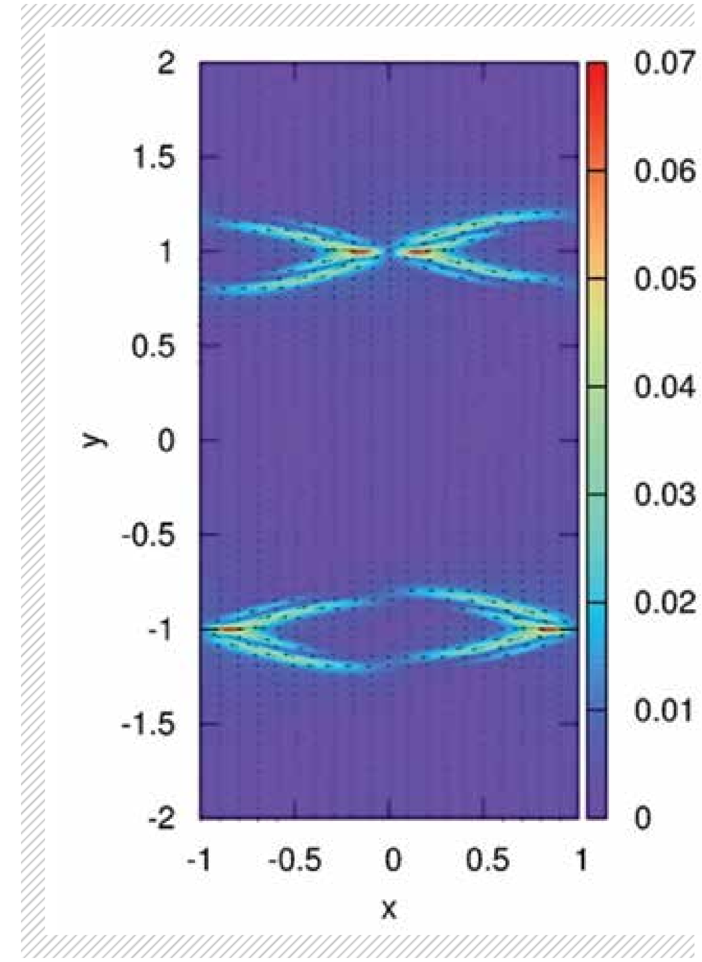

FIGURE 2: Showing the velocity field for reconnection in an electron-positron plasma from Balsara et al. (2016).