

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

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EXECUTIVE SUMMARY:

FIGURE 1: A weak scaling study for (a) fast Fourier transforms, and (b) multigrid-based partial differential equation solvers. The relative efficiency for Coarray Fortran and MPI on Blue Waters are shown in red and blue, respectively. [1]

This project had two foci. First, we aimed to demonstrate that Coarray Fortran (CAF) offers petascale performance that is comparable to or better than the best that MPI-3 has to offer. Both CAF and MPI-3 have also been shown to outperform MPI-2 by a substantial margin. In doing and publishing this work we found efficient implementation strategies that work well for any one-sided messaging paradigm.

Second, we studied two-fluid turbulence in molecular clouds. The turbulent plasma that makes up a molecular cloud is predominantly made 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. This results in a modified turbulence. Such two-fluid turbulence has special signatures. We studied the special signatures and showed that it matches observed isophotologous lines from molecular clouds.

INTRODUCTION

We are at the threshold of a new data-rich and simulation-rich era in star-formation studies. The new generation of infrared instruments will give us a new vista into chemical processes involved in star formation. Observations show that star formation takes place in a partially ionized plasma. Furthermore, Balsara [1] showed that it is very important to represent the plasma as two fluids, one made of neutral molecules and the other made of ions that are threaded by a magnetic field. Previous studies were analytical or restricted to low resolution. This research used higher model resolution to study this phenomenon. Additionally, we have NSF funding to test different highly scalable paradigms for the formation of young stars (protostars) on extremely scalable platforms.

METHODS & RESULTS

Scalability Study

In 2013–2014 we generated a very extensive comparison of Cray’s Coarray Fortran (CAF) standard with MPI-3 for a range of partial differential equation applications. Both CAF and MPI-3 are novel programming paradigms and it would greatly help the community to have their capabilities documented and published. 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 carried out a weak scalability study and reported our results in Garain, Balsara, & Reid [2].

Fig. 1 shows the results of weak scaling on Blue Waters for fast Fourier transforms (FFT) and multigrid applications ranging from 8 to 65,536 cores. CAF and MPI-3 kept up with each other across the entire range of processors. We further found that both CAF and MPI-3 were more than twice as fast as MPI-2 when approaching large numbers of processors with one-sided communication. This showed the value of these

novel programming paradigms when computing at scale.

In Garain, Balsara & Reid [2] we documented best practices for using CAF and MPI-3 for the community. We also showed that CAF code is much easier to write and maintain, and the simpler syntax made the parallelism easier to understand. Educational lectures on CAF were developed as part of this work and are freely available from our website [3].

Two-Fluid Turbulence Simulations

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 [4,5] and have also contributed to the theses of graduate students Meyer and Burkhart. Both have successfully landed jobs based on their computational skills.

Recent observations of differences in the linewidths between neutral and ionized tracers have led to the suggestion that ambipolar diffusion affects the turbulence in M17 [6]. Fig. 2 from Li & Houde [6] shows observed velocity dispersions as a function of length for the HCN molecule (black) and the HCO⁺ ion (red). The dashed lines trace turbulent spectra. The velocity dispersion in the ions was lower than that in the neutrals on smaller scales, providing evidence for dissipation via ambipolar diffusion on small scales. The dissipation scales found by Li & Houde [6] were consistent with theoretical estimates of Alfvén wave dissipation by ion-neutral drag [2,7].

WHY BLUE WATERS

Our NSF-funded work required us to develop CAF-based adaptive mesh refinement (AMR) applications and demonstrate their scalable performance on high-end parallel supercomputers. We developed a CAF-based AMR magnetohydrodynamics application that worked extremely well with Cray’s CAF compiler as well as Intel’s CAF compiler. Our scientific goal was to do several two-fluid simulations of star formation, which take many more time steps (and therefore more compute time) than a single fluid simulation. Neither the scaling nor the two-fluid turbulence portions of this research would have been possible without the high-end computational resources that only Blue Waters

can provide, and both are eminently suited to Blue Waters. In particular the Blue Waters technology enables very efficient one-sided communication.

PUBLICATIONS

Garain, S., D. S. Balsara, and J. Reid, Comparing Coarray Fortran (CAF) with MPI for several structured mesh PDE applications. *J. Comput. Phys.*, 297 (2015), pp.237–253, doi:10.1016/j.jcp.2015.05.020.

Garain, S., D. S. Balsara, and J. Reid, Comparing Coarray Fortran (CAF) with MPI for several structured mesh PDE applications. *J. Comput. Phys.*, 297 (2015), pp.237–253, doi:10.1016/j.jcp.2015.05.020

Meyer, C., D. S. Balsara, B. Burkhart, and A. Lazarian, Observational Diagnostics for Two-Fluid Turbulence in Molecular Clouds As Suggested by Simulations. *Mon. Not. R. Astron. Soc.*, 439 (2014), 2197, doi:10.1093/mnras/stt1893.

Burkhart, B., A. Lazarian, C. Meyer, D. S. Balsara, and J. Cho, Alvenic Turbulence Beyond the Ambipolar Diffusion Scale. *Astrophys. J.*, 805:2 (2015), 118, doi:10.1088/0004-637X/805/2/118.

FIGURE 2: Observed velocity dispersions as a function of length for the HCN molecule (black) and the HCO⁺ ion (red). The velocity dispersion in the ions was lower than that in the neutral molecules. [5]

