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MAGNETOHYDRODYNAMIC SIMULATION: GALAXIES

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EXECUTIVE SUMMARY

Magnetized plasmas contribute to many phenomena in the universe, from stars and black hole jets to galaxy clusters. However, computational models of these plasmas require efficient use of vast computational resources. Implementing these models is further complicated by the growing number of architectures of upcoming machines. Most of these machines use different accelerators from different manufacturers, each with a different programming environment that normally requires a rewrite of the simulation code. In order to prepare for future supercomputers, the PI developed K-Athena, a conversion of the magnetohydrodynamics code Athena++ using Kokkos, a performance portability library, which allows one code base that runs efficiently on many computer architectures. In this work, the researcher used K-Athena on the GPUs on Blue Waters to study the transference between kinetic and magnetic energies in the magnetic turbulence by modeling the Taylor–Green vortex. The next step will be to develop physics-rich galaxy cluster simulations with magnetic fields, cosmic ray physics, and active galactic nuclei feedback.

RESEARCH CHALLENGE

Plasmas dominated by magnetic fields are ubiquitous in the universe. Scientists know from observations of synchrotron radiation that galaxy clusters, the largest gravitationally bound structures in the universe, host large-scale magnetic fields. Although the precise coupling of these fields and larger clusters is not yet understood, researchers know they influence cluster evolution. Magnetic fields generated within the active galactic nuclei (AGN), the supermassive black holes at the center of galaxy clusters, drive jets that carry energy out into the cluster, playing a key role in the quasistability of many clusters [1]. Cosmic rays, charged particles with relativistic velocities, stream along the magnetic fields and drive winds, carrying metals from stars and providing pressure support in the cluster [2]. Magnetic fields also couple to turbulence within the cluster gas through the small-scale dynamo effect, where small turbulent eddies wind up and grow magnetic fields, transporting small-scale kinetic energy into magnetic energy [3].

Although these effects have been observed, it is unclear how important they are in the evolution of galaxy clusters. Researchers can explore this, however, through simulation. Galaxy cluster simulations modeling the dark matter, gas dynamics, magnetic fields, and aforementioned effects would advance our understanding of galaxy clusters. However, such accurate models require the computational resources of next-generation supercomputers.

Most upcoming supercomputers, though, are moving to new hardware such as the GPUs on Blue Waters and other accelerators instead of the traditional CPUs. These accelerators use unique application programming interfaces (APIs), requiring codes to be rewritten for each API. To circumvent writing multiple codes, new tools such as RAJA, Kokkos, and additions to OpenMP allow for writing performance-portable code that executes efficiently across many hardware platforms. Taking advantage of these tools, the PI investigated creating a magnetohydrodynamics code that will be able to run on these upcoming accelerators. This led to the development of K-Athena, a conversion of the astrophysical magnetohydrodynamics code Athena++ [4] using Kokkos [5], a performance portability library, which attains high performance on CPUs and GPUs using thousands of nodes.

For this fellowship, the PI is using K-Athena on Blue Waters to study magnetic turbulence in the magnetized Taylor–Green vortex as the first application of K-Athena. The magnetized Taylor–Green vortex is a periodic initial field that decays into a turbulent flow. By modeling the vortex at high resolution, its energy spectrum can be measured to create simplified magnetic turbulence models. These models can be inserted into other simulations to account for turbulence below the simulation resolution. The next effort will be to add additional physics to K-Athena such as cosmic rays and AGN to do state-of-the-art galaxy cluster simulations on Blue Waters.

METHODS & CODES

Magnetized plasmas are expensive to evolve, requiring high resolution to accurately model many phenomena. Efficient usage of hardware is required to achieve these resolutions. To meet this challenge, the PI converted the existing Athena++ code using the Kokkos library [4] to enable high-performance runs on both CPUs and accelerators. Kokkos allows a single kernel to be compiled with OpenMP for CPUs, CUDA for NVIDIA GPUs, and other APIs for future machines.

The coding began using the plasma code Athena++ owing to its well-written structure and extremely efficient performance on CPUs [5]. The simple kernel design and robust data structures in Athena++ took minimal effort to incorporate Kokkos. The resulting K-Athena code runs near peak performance on state-of-the-art CPU and GPU machines using thousands of nodes.

RESULTS & IMPACT

This research using Blue Waters is just beginning. Results have already shown K-Athena performs on a variety of supercomputers, but simulating the Taylor-Green vortex on Blue Waters will be its first scientific application. By simulating magnetized turbulent flow with high resolution, this research will capture enough of the energy spectra to be able to extrapolate the effects of turbulent flows far below the simulated resolution in magnetized plasma simulations. Accounting for the turbulent cascade and small-scale dynamo effect will be crucial for modeling accurate galaxies and galaxy clusters with magnetic fields. These turbulence models will be used in next-generation astrophysical and cosmological simulations, consequently helping constrain the properties of dark matter and dark energy.

WHY BLUE WATERS

These magnetic turbulence simulations and idealized galaxy cluster simulations using the GPU-accelerated K-Athena code are well served by Blue Waters (BW). The resolution and scale of the simulations require large computational resources that are only available on a few supercomputers, including BW. The large number of GPU nodes on the BW system allows the simulations to use less energy and fewer resources. Additionally, the BW staff were very helpful in providing suggestions for compiling code to run at the best performance.

As a fourth-year Ph.D. student in astrophysics, Forest Glines works under the direction of Brian O'Shea at Michigan State University. He expects to receive his degree in April 2021.