The Dust Between Us and the Big Bang
Frontera Startup Request

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We are requesting 4477 SUs on Frontera in order to do a performance study in advance of our upcoming *Pathways* request.

The simulations that will be in the full proposal are part of an effort to observe gravitational waves from the Big Bang. Gravitational waves generated at the beginning of the Universe leave an imprint in the polarization of the cosmic microwave background (CMB). The CMB is the oldest light observable in the Universe, and gives us a snapshot of its very early stages. Observing the polarization of the CMB will give us a measurement of gravitational waves that were produced at the formation of the Universe. Unfortunately, the dusty plasma in our own Milky Way also produces polarized light that is brighter than the primordial signal. Our simulations will study the polarization properties of the light from the plasma in Milky Way type galaxies. Understanding this polarization is essential for its removal from future measurements of the CMB.

For the full proposal, we will perform two studies. One will target small scale structures using simulations of driven magnetized turbulence. The other will target large scale features and variation by simulating isolated galaxies. Our scaling study will reflect these two use cases.

The code we will use is Enzo (Bryan et al. 2014; Collins et al. 2010), an open source code that has been used for a number of astrophysics applications (Abel et al. 2002; Correa Magnus et al. 2023). Enzo is an adaptive mesh refinement (AMR) code that dynamically adds resolution elements as the system requires it. We will use the constrained transport (CT) module (Collins et al. 2010) that conserves the divergence of the field to machine precision. It uses FFT-based gravity for the root grid and multigrid relaxation for gravity on fine grids. The base MHD solver is a higher order Godunov method.

There are three major numerical systems that need to be profiled: the hydro solver, the gravity solver, and the AMR machinery. The hydro solver alone is entirely local, and has been demonstrated to scale quite well. The gravity solver uses an additional FFT to solve the gravity which will have its own scaling properties. Finally the AMR machinery that communicates the solution between coarse and fine patches scales less well than the other two. We will thus perform three suites of weak scaling with the three dominant packages. The MHD suite will use only the MHD solver; the Gravity suite will use MHD and gravity; and finally the AMR suite will incorporate AMR as well as MHD and gravity. In practice the AMR grid layout is chaotic. For simplicity and reproducibility we will use three levels, with the two refined regions covering half the box length (1/8 of the total volume), keeping the same number of zones per level. None of the main numerical packages have costs that depend on the state of the gas, so we will use uniform density and temperature for all simulations.

The cost of the scaling study, SU, is found as

$$SU = t_{\rm wall} N_N \tag{1}$$

$$t_{\rm wall} = \frac{N_Z N_U}{\zeta} \frac{1}{N_C}, \tag{2}$$

where ζ is the performance of the code in zone-updates/core-second, N_Z is the number of zones, N_U is the number of updates, N_C is the number of cores, and N_N is the number of nodes. The performance, ζ, is in principle independent of the size of the problem, and only depends on the numerical package used. This is unknown on Frontera, and its measurement is in fact the purpose of the scaling study. To estimate the cost of the scaling study, will use the values obtained from previous scaling studies on *Stampede 2*, which will be somewhat lower than Frontera but will give the right ballpark.

We will use 56 cores per node and fixed work of 64^3 root grid zones per core. The number of root grid zones will be 256^3, 512^3, 1024^3 and 2048^3. Since 56 is not a power of 2, this leaves one node underutilized for each run, which will not impact our results much. We will take 100 root grid time steps for each of our simulations. For the AMR suite, each subgrid takes on average two steps per parent. Since all three levels have the same number of zones, this

Table 1: The request broken down by physics suite (first colums). N_Z is the number of root-grid zones. The number of cores per node will be 56, and 64^3 zones per grid will be used. ζ is the performance of the code in zone-updates per core-seconde, here estimated on *Stampede 2*. $N_U = 100$ is the number of root grid updates.

suite	N_Z	Nodes	ζ	SU
MHD	256^3	2	1.0×10^5	0.15
MHD	512^3	10	1.0×10^5	0.73
MHD	1024^3	74	1.0×10^5	5.39
MHD	1536^3	247	1.0×10^5	17.99
MHD	2048^3	586	1.0×10^5	42.67
Gravity	256^3	2	1.3×10^4	1.10
Gravity	512^3	10	1.3×10^4	5.52
Gravity	1024^3	74	1.3×10^4	40.82
Gravity	1536^3	247	1.3×10^4	136.26
Gravity	2048^3	586	1.3×10^4	323.27
AMR	256^3	2	1.2×10^4	8.50
AMR	512^3	10	1.2×10^4	42.48
AMR	1024^3	74	1.2×10^4	314.33
AMR	1536^3	247	1.2×10^4	1049.18
AMR	2048^3	586	1.2×10^4	2489.15
			Total SU	4477.53

is equivalent to 700 steps of one level. This number of time steps was chosen to account for the inevitable repetition of the suite as we optimize our build for Frontera.

Table 1 shows a breakdown of the cost of the scaling study, and includes the value of ζ used for each suite. The first column shows the package; the MHD solver, MHD with Gravity, and AMR with MHD and Gravity. The second column shows the number of zones per run, the third column shows the number of nodes to be used, the fourth column shows the anticipated performance, ζ, and the final column shows the total cost.

References

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