Performance and Scaling for Athena

Since ATHENA uses an unsplit, explicit update, parallelization with MPI using domain decomposition is straightforward and efficient. ATHENA has been carefully benchmarked on a variety of large-scale computing systems, including a Cray XT-3 at Sandia National Lab (RED STORM), a Cray XT-5 at NICS (KRAKEN), a Sun Magnum at TACC (RANGER), and two Dell Clusters at TACC: STAMPEDE and STAMPEDE 2. In all cases, it has shown nearly perfect scaling out to large numbers of cores, for standard 3D MHD test problems (e.g., propagation of magneto-sonic waves in three dimensions).

Here, we perform scaling tests for the numerical setup specific to the problem we propose to solve, MHD turbulence calculated in the shearing box approximation, with non-ideal MHD terms that result from low-ionization (see main document). Our setup includes specialized shearing-periodic boundary conditions along one dimension to account for Keplerian shear external to the domain, an orbital advection algorithm to solve the MHD equations separately from the Keplerian shear, a mass-conservation algorithm that invokes a global exchange of information between all processors, and a super-time-stepping approach to minimize the impact of some of the non-ideal terms on reducing the time step. We have run this particular configuration on both the Skylake (SKX) nodes and the Knights Landing (KNL) nodes on STAMPEDE 2 as we now describe.

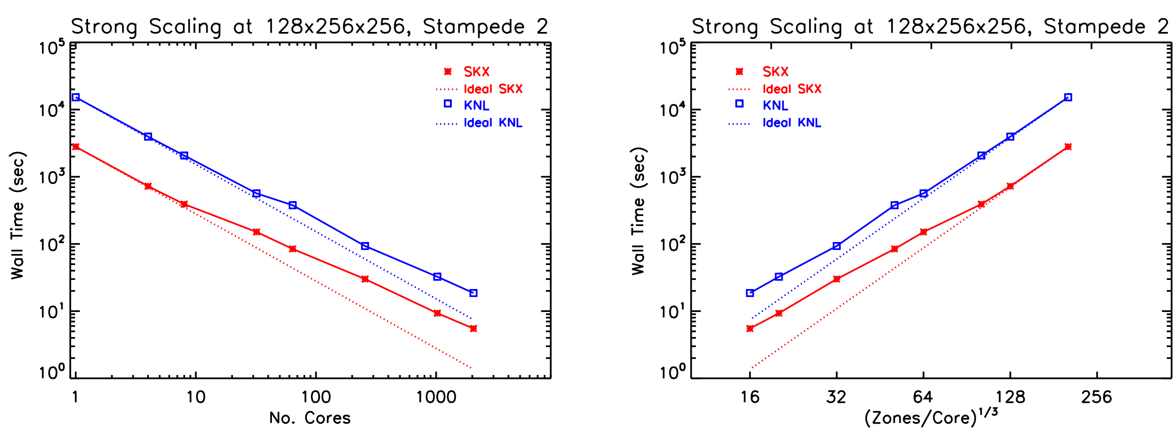

Fig. 1.— Strong scaling of ATHENA on STAMPEDE 2 for the MHD shearing box problem run at a resolution of $128 \times 256 \times 256$ zones. The left plot shows the wall time versus the number of cores, whereas the right plot shows the same data, but plotted as wall time versus zones per core. The strong scaling is close to ideal (dotted line) for all domain decompositions, departing from ideal around 32 cores for both the KNL and SKX nodes. The performance of ATHENA is better on SKX than KNL by a factor of 3–4 for ≥ 32 cores.

The strong scaling for this problem with $128 \times 256 \times 256$ total zones is shown in Fig. 1. In setting the number of cores per node, we chose the maximum available number of cores per node for all but one node (in the case that the total number processors is not evenly divisible by this maximum core number).[1] ATHENA exhibits scaling close to ideal (dotted line) for this particular setup on both SKX and KNL nodes. The code begins to depart from ideal scaling around 32 cores on both the KNL and SKX nodes. The SKX nodes are a factor of 3–4 faster than the KNL nodes for ≥ 32 cores.

As outlined in the main document, our simulations will be carried out at a higher resolution than presented in Fig. 1. However, this resolution ($256 \times 512 \times 512$) is too large for the KNL nodes; we encountered memory errors when attempting to run this resolution on these nodes. The SKX nodes, on the other hand, have more memory than the KNL nodes and can handle this resolution. The strong scaling of this same setup for the higher resolution is shown in Fig. 2.

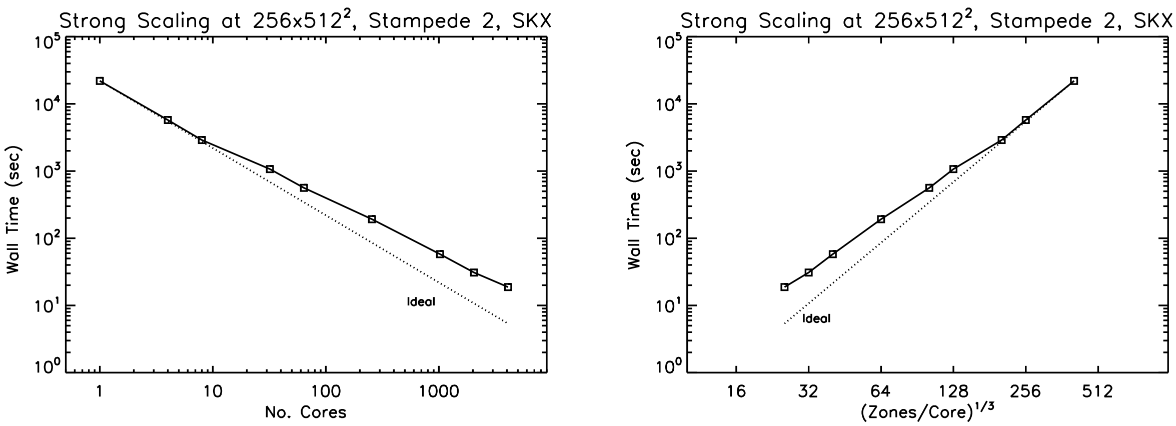

Fig. 2.— Strong scaling of Athena on Stampede 2 SKX nodes for the MHD shearing box problem run at a resolution of $256 \times 512 \times 512$ zones. The left plot shows the wall time versus the number of cores, whereas the right plot shows the same data, but plotted as wall time versus zones per core. The strong scaling is close to ideal (dotted line) for all domain decompositions, departing from ideal around 32 cores.

From this strong scaling, we take a nominal value of 16×32^2 zones per core (i.e., the point with the minimum wall time). While the strong scaling has departed from ideal scaling at this value, this is the number of zones per core in our proposed simulations, which has been chosen to increase the throughput of our runs on Stampede 2 at the expense of a slight efficiency hit. The weak scaling is shown out to 4,096 cores on SKX nodes in Fig. 3. For reference, we also include this data in the Table. Athena maintains scaling above 85% out to 4,096 cores; this excellent scaling makes Athena an ideal tool with which to carry out the high resolution simulations proposed here. Given this excellent scaling, in addition to the faster performance of Athena on SKX nodes and the higher memory of these nodes, we propose to carry out all of our simulations on the SKX nodes.

[1] We found a slight improvement in performance when choosing a constant number of cores per node. However, if we choose a constant number of cores per node (e.g., 32 cores per node on the SKX nodes) this will ultimately require more nodes to be used in our production runs (e.g., 128 SKX nodes in the case of 32 cores per node, as opposed to 86 SKX nodes when maximizing the number of cores per node). Thus, to reduce the number of SUs requested, we choose to use the maximum number of cores per node, as described here.

Table: Weak Scaling Data for MHD Shearing Box Simulations on the SKX Nodes

No. Cores	No. Nodes	Total Zone-Cycles / Second	Zone-Cycles / CPU-Second	Efficiency (Relative to 64 Cores on 2 Nodes)
64	2	6.74×10^6	1.05×10^5	1.0
256	6	2.47×10^7	0.97×10^5	0.92
512	11	5.01×10^7	0.98×10^5	0.93
1,024	22	9.78×10^7	0.95×10^5	0.91
2,048	43	1.89×10^8	0.92×10^5	0.88
4,096	86	3.67×10^8	0.90×10^5	0.85

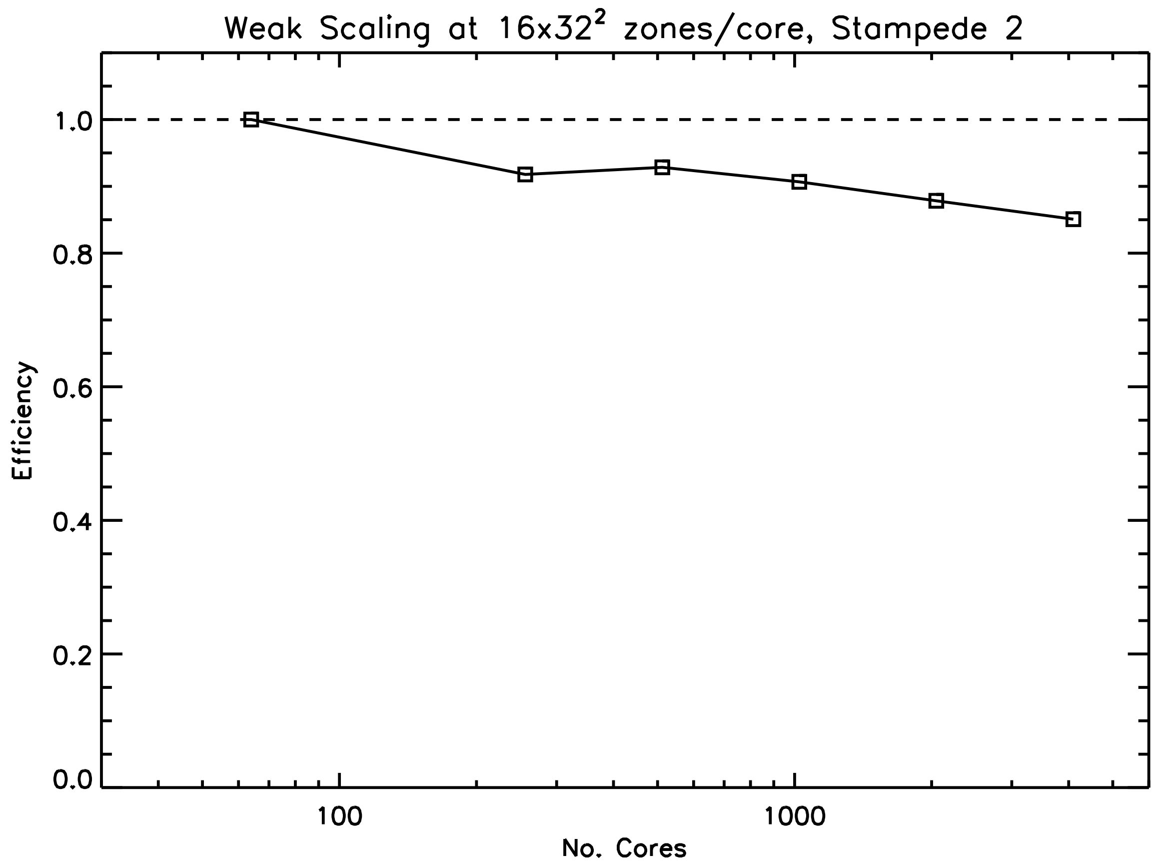

Fig. 3.— Weak scaling of Athena on Stampede 2 SKX nodes for the MHD shearing box problem at the fiducial 16×32^2 zones per core. The efficiency is measured relative to 64 cores (2 nodes) to remove the unavoidable performance hit associated with the introduction of internode communication at > 1 node. The scaling is very good, remaining better than 85% out to 4,096 cores.