Simulation of Turbulent, Compressible, Astrophysical Flows at the Petascale

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Over the last year, my research team has been restructuring our PPM codes for simulating turbulent, compressible, astrophysical flows so that we can take advantage of the emerging petascale computing platforms. The principal challenge has been to exploit ever larger numbers of processors without scaling the size of the computational grid beyond several billion cells. This has involved a restructuring of the computation and the fundamental data upon which it operates. Our codes now involve updating of subdomains of the grid by teams of 8 to 64 CPU cores, with the kernel computation for a single CPU core implemented as the complete update for a single 1-D pass of the algorithm for a tiny grid chunk of just 4^3 or 6^3 cells (depending upon the particular algorithm). Despite the small size of such a grid chunk, the computation is the most efficient we have so far achieved, and the necessary data context in the cache memory is less than 100 KB. These computations do not require more than 32-bit accuracy, and hence they can be implemented for the new generation of multicore processors with specialized “media extensions” that provide full vector speeds (20% of peak for CPU cores capable of multiply-adds and 50% of peak for other CPUs) for loops with as few as 16 iterations. Parallel implementations of these new PPM codes can exploit the new, very fine granularity of the gas dynamics computations to scale to systems with up to a million processor cores.

Present applications of these computing technologies involve studies of the helium shell flash in giant stars near the ends of their lives. These shell flashes lead up to the ultimate explosion of the outer convective envelopes of these stars to form planetary nebulae. To simulate the helium shell flash, multiple gas constituents need to be carefully tracked and their turbulent entrainment into the convection zone and subsequent burning and energy release simulated. Even petascale computers are not powerful enough to simulate these processes in all their complexity and detail over the year-long duration of a shell flash event. To make such simulations practical, processes such as the turbulent gas entrainment and mixing, that occur on small length and time scales need to be described by models rather than computed directly. Our team is using the Cray XT3 to perform detailed simulations of these small-scale phenomena on very fine computational grids of billions of cells. These large simulations are then used to test and validate modeling ideas. Using this approach, we have recently developed a new subgrid-scale model of compressible turbulence (see Woodward et al. 2006, at www.lcse.umn.edu/SciDAC2006). Present efforts are aimed at extending this model to describe entrainment and mixing of fresh hydrogen fuel into the helium shell convection zone of a giant star. Petascale computing platforms will enable “validation quality” simulations of such phenomena to be carried out in under an hour of machine time and simulations of the larger helium shell flash event, using models of these phenomena, to be performed in just days of computer time.