

Dynamic Domain Decomposition for 3D PIC simulation with Adaptive Mesh Refinement

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With a rapid growth in the number of processors in the supercomputers of late, parallelizing the existing stand-alone codes and their optimization for massively parallel architecture are in imminent demand. Among many numerical methods that have been ported to such environments, Adaptive Mesh Refinement is one of the challenging examples for parallelization mainly because its inhomogeneous and variable grid distribution across multiple processors. As with the case with AMR, a traditional PIC method also suffers from the similar issue when simulating highly inhomogeneous plasmas on parallel computers. A conventional domain decomposition scheme which assigns an equal and stationary space to each processor, gives rise to an imbalance in the computational cost, resulting in a significant reduction in total parallel performance.

A suite of new simulation techniques in the present work are developed in aim to overcome this problem inherent to both AMR and PIC methods by dynamically decomposing a simulation space into subdomains, and to propose a scalable program design that can still be viable for the massive number of processors. This decomposition is carried out in such a way that the number of particle loops that each processor carries is equalized, based on the fact that this quantity is roughly proportional to the computational cost in AMR-PIC code. The second feature included in this parallelization task is the 3D decomposition based on the Z-ordering [1]. This algorithm has merits in that a 3D problem can be virtually reduced into a 1D problem, so that more isotropic 3D decomposition can be achieved than the conventional raster sequencing can. Another notable feature is the autonomic space managing system, in which each process determines its own domain without delegating a master process. This proposed paradigm is particularly necessitated for the high number of processors, where a single process can no longer orchestrate an entire simulation space.

Some initial results computed with these new key functions implemented to a 3D AMR-PIC code are shown, together with parallel benchmarks to demonstrate its scalability.

[1] Morton, G. M., "A computer Oriented Geodetic Data Base; and a New Technique in File Sequencing", Technical Report, Ottawa, Canada: IBM Ltd., 1966