Using Roadrunner to Model Shock Breakout in Supernovae and National Ignition Facility Experiments

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Thermal X-ray transport is an important physical component in phenomena, such as supernova explosions and inertial confinement fusion, where hot, radiating material is tightly and nonlinearly coupled to the radiation it emits. The time-implicit method for simulating thermal X-ray transport, Implicit Monte Carlo (IMC), approximates small-timescale absorption and reemission with a scattering process that is numerically stable but very computationally intensive [1].

The Jayenne IMC Project [2] was one of the early adapters for assessing the IBM Cell Broadband Engine (Cell BE) architecture for LANL's Roadrunner Project during the years 2005 to 2007. The Roadrunner supercomputer architecture increases a standard Opteron cluster's floating point throughput by an order of magnitude with Cell BE processors. The early Cell BE-enabled version of the Jayenne Project stand-alone code, Milagro, adapted a limited set of capabilities to test the feasibility of scientific simulations on the Cell BE architecture. The Jayenne Project codes are general-capability IMC codes with multiple data-decomposition parallel schemes; multiple geometries of R, RZ, XYZ; multiple frequency treatments, and a Random Walk method for speeding up the code in thick diffuse regimes, all of which can be run as the radiation-only stand-alone Milagro code or as the Wedgehog package for operator-split inclusion in a multiphysics application code. The first Milagro-Cell BE code was RZ-geometry, multigroup frequency treatment, replicated-geometry parallelism only, and absorption/reemission without physical scattering [3]. That first version showed speedups of up to eight on a radiation flow problem.

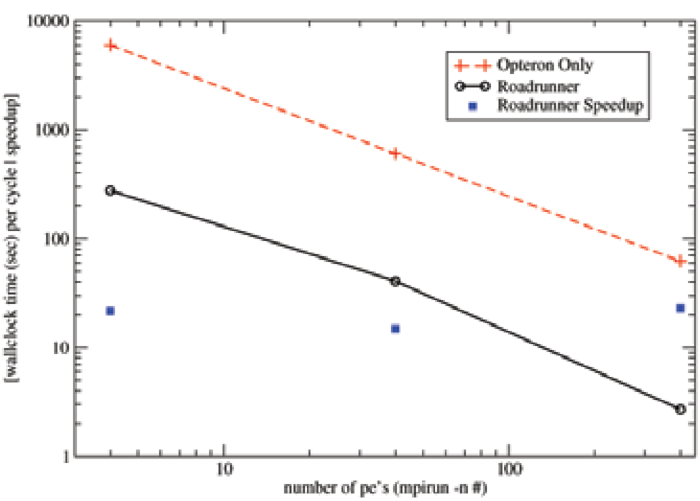

Fig. 1. Roadrunner and Opteron-only runtimes per cycle and Roadrunner speedups for a simple radiation-only problem.

Since then, several additional Jayenne Project capabilities have been adapted to the Cell BE architecture, including domain-decomposition parallelism, physical scattering, the Random Walk speedup technique, and extension to the Wedgehog interface for radiation-hydrodynamics simulations via LANL's Cassio code, which models radiation, electrons, and ions independently in a nonequilibrium fashion.

The first comparison of this new Roadrunner-ready code with the standard version was on a simple radiation-only, steady-state, infinite homogeneous problem that, over time, remains at its initial temperature. Given that only the IMC particle transport utilizes the Cell BE chips, and that this problem is almost 100% particle transport, this problem represents an upper limit of the speedups with this version of Cassio/Wedgehog. The runtimes per cycle and speedups are both shown in Fig. 1, with speedups in the range of 15-22.

Our Roadrunner Open Science run focused on using the Cassio code to model the shock breakout in a supernova explosion. The engine of a supernova explosion is buried deep within the exploding star. Initially, the photons in the star are trapped in the outward flowing explosion. But as this explosion shock hits the surface of the star, the photon mean free path increases dramatically, allowing the photons to lead the explosion. This shock "breakout" is the first burst of photon radiation seen in the explosion and has now been observed in a number of supernovae. Until now, all models of this shock breakout were either limited to 1D simulations using flux-limited diffusion or equilibrium calculations that assumed the matter and radiation spectra were described by a single temperature.

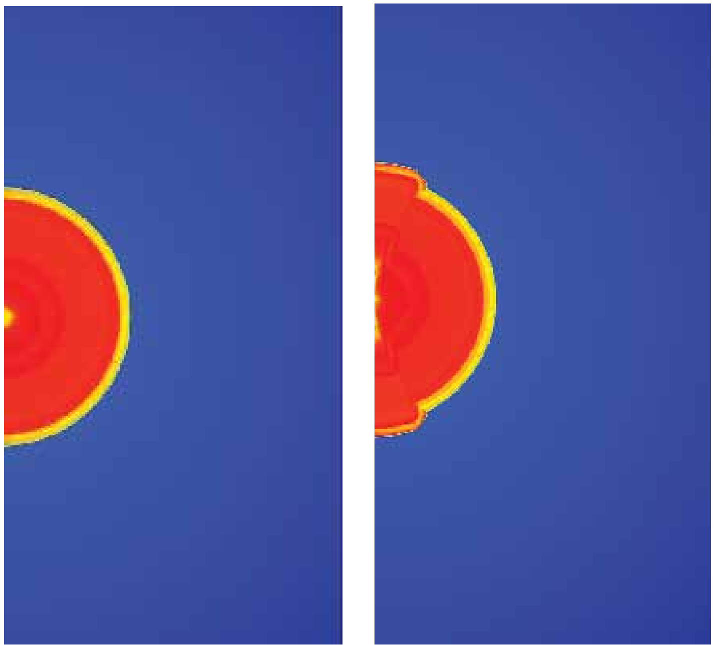

Fig. 2. Plot of the radial velocity structure (red denotes strong outward velocity, blue is zero velocity) of the shock breakout from two different supernova explosions: a symmetric explosion (left) and an asymmetric bipolar explosion based on the asymmetries studied in Hungerford et al. (2003).

Our calculations mark the first nonequilibrium radiation-hydrodynamics calculations of a supernova explosion in 2D, and the first-ever radiation hydrodynamics calculations of shock breakout with a higher-order transport scheme.

In Fig. 2, two of our calculations just after shock breakout show the velocity structure (colored by the magnitude of the radial velocity) for a symmetric and an asymmetric explosion using the bipolar explosion paradigm discussed in Hungerford et al. in an effort to match the asymmetries observed in supernova 1987A [4]. There is growing evidence that many core-collapse supernovae have such asymmetries. But without detailed spectral calculations, it will be difficult to determine the exact nature of the asymmetry. Our simulations mark the beginning of such precision comparisons of theory and observations. The NASA Swift satellite has begun an active observing program to observe shock breakout, and we are working closely with this team to couple theoretical models to the observations. This effort is a key aspect of the SciDAC (DOE's Scientific Discovery through Advanced Computing program) priorities identified in nuclear astrophysics and will be part of the upcoming SciDAC science competition.

This capability is also being used to simulate experiments on the National Ignition Facility (NIF). For this calculation on 32 processors, the standard version of the code took 37 hours to run. Running the same input deck on the Roadrunner version took about 5 hours, yielding an overall speedup of seven. Figure 3 shows the running wallclock time for each code version.

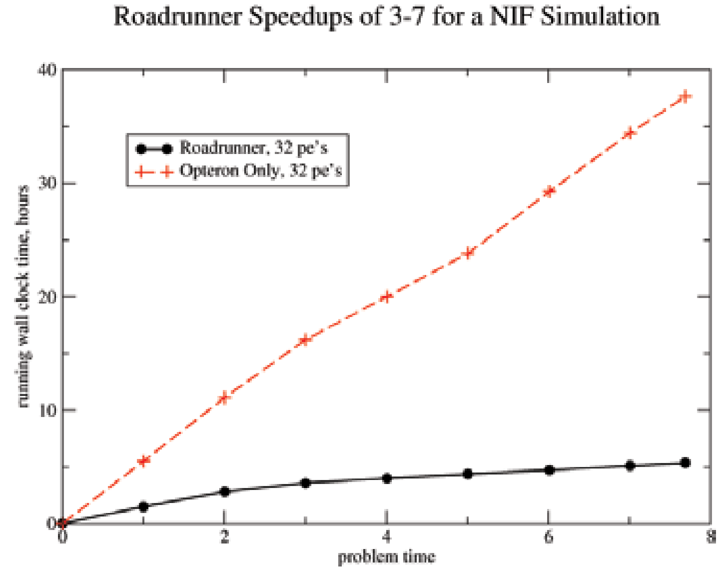

Figure 3. Cumulative wallclock times over the duration of a NIF experiment simulation for 32 processors on both Roadrunner and Opteron only. Cumulative Roadrunner speedups are about three early in the problem, and seven at the end of the problem.

As we look beyond Roadrunner to the next generation of heterogeneous architectures, we will look to speed up a greater fraction of the overall computation and develop new methods that were maybe too compute-intensive to consider before Roadrunner, but that now might make sense.

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[2] T.J. Urbatsch, T.M. Evans, "Milagro Version 2, An Implicit Monte Carlo Code for Thermal Radiative Transfer: Capabilities, Development, and Usage," Los Alamos National Laboratory report LA-14195-MS (Jan. 2005).
[3] T.M. Kelley and P.J. Henning, "Adaptation of Milagro Implicit Monte Carlo to the Roadrunner Hybrid Architecture," in *ADTSC Science Highlights* 2008, Los Alamos National Laboratory, LA-UR-08-1960.
[4] A.L. Hungerford, C.L. Fryer, M.S. Warren, *Ap. J.*, **594**, 390 (2003).

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