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FronTier and Applications under TSTT

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Summary

We report several important developments of the front tracking method and its use in science and engineering applications under the TSTT project. Recent progress includes the development of a stand-alone front tracking software library, conservative front tracking algorithms, applications of front tracking to the simulation of fusion pellet injection in a magnetically confined plasma, along with studies of a fuel injection jet and fluid chaotic mixing, among other problems.

Front tracking is a Langrangian method for propagating a moving manifold through the use of marker particles which represent the interface. It is distinguished from the classical marker particle method in that the particles are located only on the interface, rather than in a volume region near the interface and by the connection of the particles to each other to form a triangulated mesh (3D) or piecewise linear segments (2D) of the interface. It is thus significantly faster than other particle methods since fewer particles are used per cell.

A new software library for tracking the geometry and dynamics of a moving front has been extracted from the previously developed FronTier code. This code is more modular than its predecessor and easily inserted into application codes. In addition, it contains a major new algorithm, Locally Grid Based tracking, which combines the robustness of grid-based tracking with the accuracy of grid-free tracking, and is thus a significant improvement to both of these algorithms. The package also includes other methods such as the level set method to allow for easy comparison among techniques. This freely available library is accompanied by web-based testing, documentation and evaluation.

Another recent development includes conservative front tracking. This method increases the order of convergence for the truncation error at a discontinuity and therefore converges faster than ordinary tracking or than untracked algorithms to the physical solution. We have formulated a fully conservative front tracking algorithm for an N-dimensional system of nonlinear conservation laws and implemented it in 1D, 2D and 3D. The new algorithm is based on the divergence form of the conservation law in space-time cells.

We have applied the enhanced front tracking code to study a number of applications and we highlight two here.

Cavitation and atomization of high speed liquid jets in combustion applications: In

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the design of a fuel injector, the spray characteristics are crucial in improving engine performance and reducing pollution. Despite substantial theoretical and experimental efforts, many of the atomization mechanisms remain untested and are still a research issue. Thus, direct numerical simulations are critical for improving spray predictions, understanding atomization mechanisms and providing input to spray combustion models for predictive modeling of diesel engine combustion. We have studied the influence of cavitation on spray formation, in which phase transition is governed by the compressible Euler equations with heat diffusion. In a recent collaboration with Valmor de Almeida (ORNL), the FronTier simulation of droplet spray is combined with the KIVA code at Los Alamos to study of diesel engine efficiency.

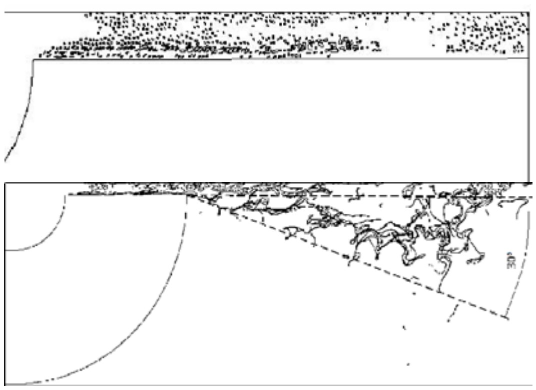

Figure 1. Simulation of the diesel injection jet using the front tracking code. Above; vapor bubbles of fuel in the nozzle. Below: formation of the fuel spray.

Turbulent mixing of acceleration driven fluids causes potential degradation of the performance of an ICF capsule. Acceleration by a steady driving force, known as the Rayleigh-Taylor mixing problem, is a specific and prototypical special case. Until recently, most simulation codes disagreed with experimental measurements for even the most basic diagnostic, the overall mixing rate, by a factor of two. Several explanations have been offered for this fact, the one we favor being that the simulations are hampered by excess numerical mass diffusion and insufficient physics models. Using TSTT developed front tracking software, we addressed this problem by implementing the models of realistic physical mass diffusion and physical surface tension. The result is complete agreement or nearly so in the match of simulation to experiment for Rayleigh-Taylor mixing.

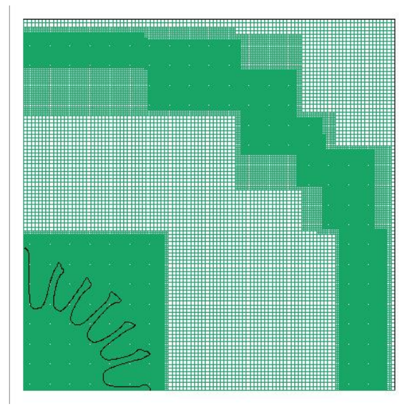

Figure 2. A combined operation of AMR by Overture and tracking by FronTier in the simulation of supernova circular Richtmyer-Meshkov instability.

Development of interoperability between FronTier and other software codes in DOE laboratories is also an important task in our agenda. We have merged the front tracking code with the LLNL AMR code of Overture to create a combined, two and three-dimensional AMR-front tracking capability needed by fusion, groundwater, combustion, and astrophysics applications.

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