Recipient:
Dr. Fredrick Johnson
SC-21.1/Germantown Building
U. S. Department of Energy
1000 Independence Avenue
Washington, DC 20585

DOE ID: #DEFC0201ER25461

FINAL REPORT

Terascale Simulation Tools and Technologies

Principal Investigators:
Xiaolin Li
University at Stony Brook

Reporting Period:
August 15, 2001 – August 14, 2006

Recipient:
Research Foundation
University at Stony Brook
Stony Brook, NY 11794-3366

Unexpended Funds: \$656

1 Findings and Significance

We report the development of front tracking method as a simulation tool and technology for the computation on several important SciDAC and SciDAC associated applications. The progress includes the extraction of an independent software library from the front tracking code, conservative front tracking, applications of front tracking to the simulation of fusion pellet injection in a magnetically confined plasma, the study of a fuel injection jet, and the study of fluid chaotic mixing, among other problems.

The objective of the TSTT center is to facilitate the use of advanced mesh tools for increasingly complex and realistic simulations of PDE-based applications. Numerous software tools are available to help manage the complexity of these simulations, including computer-aided design systems used to represent the geometry of the computational domain, mesh generation tools to discretize those domains, solution adaptive methods (AMR) to improve the accuracy and efficiency of simulation techniques. Here we emphasize numerical and software tools for tracking a dynamically moving front.

Numerical simulations can be performed more efficiently using the latest technologies. The TSTT Center has developed interoperable and interchangeable mesh, geometry, and field manipulation tools that are of direct use to the DOE SciDAC applications. The premise of our technology development is that advanced mesh, geometry and field services can be provided as libraries that can be used with minimal intrusion into application codes. During SciDAC-1, the TSTT team developed and deployed a number of advanced technologies — including the *Frontier-Lite* front tracking library [11], the *Mesquite* mesh quality improvement toolkit [4], and unstructured mesh refinement [38] and mesh swapping tools — that provide ample

evidence of the viability of this approach. Moreover, we combined these *component services* in an interoperable manner to provide new *integrated services* such as AMR-front tracking, parallel adaptive loop libraries, and combined geometry-mesh modification tools for use in shape optimization applications.

Critical to the TSTT interoperability goal is the development of common interfaces that provide data-structure-neutral access to mesh, geometry, and field information. These interfaces provide access to all TSTT services in a uniform way and are fundamental to creating interoperability for the integrated services. Moreover, a uniform interface allows easier experimentation with different, but functionally similar, technologies to determine which is best suited for a given application. The development of such interfaces requires creating a consensus among a large group of mesh, geometry, and field experts. This is a difficult technical and sociological challenge that would have been impossible without the collaborative environment fostered by the SciDAC program. It is this integration of a wide range of DOE and university mesh-related technologies under a common interface that distinguishes TSTT as a center.

2 FronTier-Lite, An Software Library for Interface Tracking

A general purpose software package for the geometry and dynamics of an interface has been extracted from the FronTier code developed by the principal investigator and colleagues. The code is downloadable from the web, and is accompanied by a web based testing and evaluation site as well as a web based documentation. When coupled with graphics packages such as HDF, Geoimview, or Paraview, the evolution of the moving front can be

easily converted into movies. We have made significant improvements to the robustness of the Front Tracking package, especially in the 3D handling of topological bifurcations.

A major new algorithm called Locally Grid Based tracking (LGB), which combines the best features of two previous 3D tracking algorithms is introduced in this software package. It combines the robustness of grid based tracking with the accuracy of grid free tracking, and thus it is a significant improvement to both of these algorithms.

We have assessed the performance of the package, in comparison with publicly distributed interface codes (the level set method), with published performance results (volume of fluid (VOF) and other methods) and with previous versions of front tracking. In comparison with the level set method, we used the fifth order WENO scheme for the convection of the level set function, while for the front tracking code, we used the fourth order Runge-Kutta method for the point propagation. Benchmark cases include the rotation of a slotted disk and an ellipse moving in a swirling velocity field. In both of these tests, the front tracking showed enduring correctness of the front topology and resolution while the level set broke down at an early time. Figure 1 shows a comparison test for a rotating slotted disk.

In comparison with the VOF method, we have applied the deformation velocity field acting on a sphere. The front tracking code gives a solution superior both qualitatively and quantitatively (Figure 2) to that of the VOF method, especially when the interface is stretched to become narrow and thin, [6].

Figure 1: Comparison of slotted disk simulation using high order methods. The upper sequence shows the result of the level set method using the fifth order WENO scheme and the lower sequence shows the result of front tracking using the fourth order Runge-Kutta method.

Figure 2: Reversal test of 3D interface in double vortex velocity field. The reference rectangular mesh is 64^3 .

3 Conservative Front Tracking

Conservative front tracking 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 implemented a fully conservative front tracking algorithm for an N -dimensional system of nonlinear conservation laws.

The new algorithm is based on the divergence form of the conservation law in a space-time domain. Consider a system of conservation laws in N spatial dimension in differential form

$$\frac{\partial U}{\partial t} + \nabla \cdot F(U) = 0, \quad F = (f_1, f_2, \dots, f_N) \quad , \quad (1)$$

where $U \in R^p$ and $f_j(U) = (f_{1j}(U), \dots, f_{pj}(U))^T \in R^p$ are defined in a spatial domain $\Omega \subset R^N$.

Integrating (1) in a time-space domain $\mathcal{V} \subset R^{N+1}$, we obtain the integral form of (1),

$$\int_{\mathcal{V}} \left(\frac{\partial U}{\partial t} + \nabla \cdot F(U) \right) d\mathcal{V} = 0 \quad . \quad (2)$$

By the divergence theorem, we have

$$\int_{\partial \mathcal{V}} (U, F(U)) \cdot n dS = 0 \quad . \quad (3)$$

The finite difference method presented here is an explicit finite volume integration scheme based on the integral form (3).

Assume a space-time discretization $\{\mathcal{V}_i\}$ which conforms to the space-time interface (see Figure 3) as U evolves in one time step from t_n to t_{n+1} . We solve (3) explicitly in this region. We define each $\mathcal{V}_i$ as a space-time control volume, and $\partial \mathcal{V}_i = D_i^n \cup D_i^{n+1} \cup \hat{S}_i$ with D_i^n , D_i^{n+1} , and $\hat{S}_i$ meeting at most at their boundaries. Here D_i^n and D_i^{n+1} are the boundary surfaces of $\mathcal{V}_i$

Figure 3: An example of 3D space-time interfaces joining two sequential time steps.

at time level n and $n+1$ respectively, and $\hat{S}_i$ is the complementary boundary surface of $\mathcal{V}_i$. Dividing the calculation of the integral (3) into three parts over D_i^n , D_i^{n+1} and $\hat{S}_i$ respectively, we have

$$|D_i^{n+1}|\overline{U}|_{t_{n+1}} = |D_i^n|\overline{U}|_{t_n} - \int_{\hat{S}_i} (U, F(U)) \cdot n dS, \quad (4)$$

where

$$\overline{U}|_{t_n} = \frac{1}{|D_i^n|} \int_{|D_i^n|} U(x_1, \dots, x_N, t_n) dx_1 \dots dx_N$$

and

$$\overline{U}|_{t_{n+1}} = \frac{1}{|D_i^{n+1}|} \int_{|D_i^{n+1}|} U(x_1, \dots, x_N, t_{n+1}) dx_1 \dots dx_N$$

are cell averages, $|D_i^n|$ is the face area of D_i^n , $|D_i^{n+1}|$ is the face area of D_i^{n+1} , and n is the outward normal of $\hat{S}_i$. Therefore, $\overline{U}|_{t_{n+1}}$, is the solution to (4) at time t_{n+1} .

To calculate $\overline{U}|_{t_{n+1}}$, we first need to determine the space-time control volume $\{\mathcal{V}_i\}$. Then we calculate the fluxes defined on the surfaces of $\mathcal{V}_i$, so

that we can apply (4). Works on this important improvement of the front tracking method have been published in [25, 32, 33].

4 Fuel Injection for the ITER

The injection of frozen pellets of deuterium and tritium is considered the major mechanism for refueling of the Tokamak nuclear fusion reactors. This problem is significantly important for the International Toroidal Experimental Reactor (ITER). However, challenging problems remain to be solved before achieving accurate numerical simulations of pellet ablation. The required level of detail in modeling is not available in standard MHD codes for fusion plasmas. Qualitatively new simulations are also required to estimate the efficiency of the recently proposed methods of laser ablation (rocket) and gyrotron driven pellet acceleration. If successful, these methods will achieve pellet velocities of the order of kilometers per second, and deposit the pellet material deeply into the plasma in ITER. The goal of our work is to develop mathematical models and numerical algorithms, and perform numerical simulations of processes associated with the injection of frozen deuterium-tritium fuel pellets in the tokamak. TSTT Front Tracking technology is a critical part of our computational model for tokamak fueling.

We have developed a 2D axisymmetric model for pellet ablation in the tokamak based on the front tracking MHD code for low magnetic Reynolds number free surface flows [37]. The system of MHD equations in the low magnetic Reynolds number approximation is a coupled hyperbolic-elliptic system in geometrically complex moving domain:

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{v}), \quad (5)$$

$$\rho \left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) \mathbf{v} = -\nabla P + \mathbf{J} \times \mathbf{B}, \quad (6)$$

$$\rho \left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) e = -P \nabla \cdot \mathbf{v} + \frac{1}{\sigma} \mathbf{J}^2 - \nabla \cdot \mathbf{q}, \quad (7)$$

$$\nabla \cdot \sigma \nabla \phi = \nabla \cdot \sigma (\mathbf{v} \times \mathbf{B}), \quad \left. \frac{\partial \phi}{\partial \mathbf{n}} \right|_{\Gamma} = (\mathbf{v} \times \mathbf{B}) \cdot \mathbf{n}, \quad (8)$$

$$P = P(\rho, e), \quad \mathbf{J} = \sigma (-\nabla \phi + \mathbf{v} \times \mathbf{B}). \quad (9)$$

Here $\mathbf{v}$, ρ and e are the velocity, density and the specific internal energy of the fluid, respectively, P is the pressure, $\mathbf{B}$ is the magnetic field induction, $\mathbf{J}$ is the current density distribution, σ is the fluid conductivity, and ϕ is the electric field potential, satisfying the Poisson equation with Neumann boundary condition (8). An external heat source $-\nabla \cdot \mathbf{q}$ represents the electron heat flux in the pellet ablation problem.

We have developed a numerical method for solving such a system and corresponding parallel software. In an operator splitting approach, we solve the hyperbolic subsystem (5) - (7) using the hydrodynamic package of the FronTier code. The elliptic problem (8) is solved using either a mixed finite element discretization on a triangular (tetrahedral) mesh dynamically conforming to the moving interface, or the embedded boundary discretization [30] on the rectangular mesh. The embedded boundary method is based on the finite volume discretization in rectangular grid cells, and irregular cells adjacent to the interface. The irregular domain is embedded in the rectangular Cartesian grid, and the solution is treated as a cell-centered quantity, even when these centers are outside of the domain. This ensures that the conditioning of fluxes is relatively unaffected by small cell volumes. The conservative second order accurate fluxes are calculated on every irregular cell boundary. The method fits very naturally to the internal structure of the FronTier code since one of its major interface propagation algorithms, the

grid based tracking [6], explicitly constructs irregular cells adjacent to the interface. The implementation of elliptic solvers in the FronTier code can be beneficial not only to MHD. It can also enable the explicit treatment of viscosity for highly viscous fluids (when the explicit inclusion of the parabolic viscous terms limits the time step due to the Courant-Friedrichs-Lewy (CFL) stability condition), and the incompressible formulation of the fluid dynamics equations within Chorin’s projection method, both for multifluid problems with discontinuity interfaces. The linear systems resulting from the embedded boundary discretization are solved using parallel iterative solvers, including algebraic multigrid (AMG), and preconditioners implemented in PETSC [2] and Hypre packages.

Since the method of front tracking allows the study of multiphysics phenomena in multiphase systems characterized by strong discontinuities in physical properties of the system components, it is ideally suitable to the pellet ablation problem. In our computational model, explicit interfaces separate the solid pellet from the ablated gas, and the cold, dense, and weakly ionized ablation cloud from the highly conducting fusion plasma. Realistic equations of state are employed in different geometrical regions corresponding to different states of matter. The code is capable of simulating the transition of deuterium in the pellet from a solid to a liquid state under high ablation pressures. A surface ablation model is used on the pellet surface. An electronic heat flux model for the calculation of the thermal energy deposition in the ablation cloud and on the pellet surface uses analytical approximations to the solution of the kinetic equation [29]. Atomic physics processes in the ablation cloud such as dissociation, recombination, and ionization are taken into account by the EOS model for weakly ionized plasmas. Using this model, we have performed studies of the pellet ablation physics, pellet ablation rate

and the lifetime in the magnetic field, and compared with analytical predictions and previous numerical simulations. The 1D version of the model is in excellent agreement with the scaling laws and ablation rate predicted by the NGS model [36]. The 2D axisymmetric simulations agree with results of MacAulay [35], and Ishizaki et al. [29]. Our work goes beyond these studies and calculates properties of the ablation channel in magnetic fields. Shapes of the ablation cloud at early time in magnetic fields ranging from 0 to 5 Tesla are depicted in Figure 4. For the first time, we have performed simulations leading to the calculation of ablation rates in magnetic fields [1]. In the future, we will use a 3D model of the pellet ablation for the study of striation instabilities. These instabilities are presently not well understood.

Figure 4: FronTier simulation of the formation of pellet ablation channels in magnetic fields ranging from 0 (left) to 5 Tesla (right). Temperature distributions are shown.

5 Turbulent Mixing

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 cured the first problem [15, 15, 14, 8], excess numerical mass diffusion, and by enhancements to this software, we also address the second problem, insufficient physics models for physical mass diffusion and/or physical surface tension, see [34]. The result is complete agreement or nearly so in the match of simulation to experiment for Rayleigh-Taylor mixing.

6 Diesel Fuel Injection and Jet Atomization

We have studied the cavitation and atomization of high speed liquid jets in combustion applications. In the design of a fuel injector, the characteristics of the spray are crucial variables to improve the engine performance and reduce the pollution. Despite substantial theoretical and experimental efforts, many of the atomization mechanisms remain untested and the mechanisms of atomization 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 the spray formation. The phase transition is governed by the compressible Euler equations with heat diffusion. The phase boundary in one dimension is modeled as a tracked interface

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} = 0, \quad (10)$$

where $U = [\rho, \rho u, \rho E]^\tau$, $F(U) = [\rho u, \rho u^2 + P, \rho u E + uP - \kappa \frac{\partial T}{\partial x}]^\tau$, ρ denotes

density, u velocity, P pressure, $E = u^2/2 + \epsilon$ is the specific total energy, ϵ is the specific internal energy, κ is a coefficient of thermal diffusion, and T is temperature. Integrating the conservation equations (10) across the interface, we obtain the balance equations for the mass, momentum, and total energy, respectively:

$$[\rho u] = s[\rho] \quad , \quad (11)$$

$$[\rho u^2 + P] = s[\rho u] \quad , \quad (12)$$

$$[\rho u E + u P - \kappa \nabla T] = s[\rho E] \quad . \quad (13)$$

We also postulate that the temperature is continuous across the phase boundary. Therefore, the interfacial temperatures of the vapor and liquid are equal

$$T_l = T_v = T_s \quad , \quad (14)$$

where T_s is the interface temperature. To complete the formulation we need to provide an equation for either the interface temperature T_s or the mass flux M . Denoting the equilibrium pressure at temperature T by $p_{\text{sat}}(T)$, the net mass flux of evaporation is found from the kinetic theory

$$M = \alpha \frac{p_{\text{sat}}(T) - p_v}{\sqrt{2\pi RT}} \quad . \quad (15)$$

We have developed an iterative phase boundary propagation algorithm. It generalizes the numerical methods for finding the contact discontinuity of a Riemann problem, and introduces a subgrid model for finding the interface temperature. In the phase boundary problem, velocities and pressures are discontinuous across the phase boundary, and satisfy the above interface conditions.

These numerical models have been used to simulate cavitation, jet breakup, and spray formation. The disturbance of the cavitation bubbles produced

upstream significantly impact the downstream jet breakup. These vapor bubbles grow and break the jet surface, forming spray and droplets. For the details of the simulation and algorithms, see [40] and Fig. 5.

Figure 5: FronTier simulation of the liquid jet atomization. Left: mixed phase flow in nozzle. Right: atomization and spray.

Figure 6: FronTier simulation on crystal growth of solute on solid surface.

7 Other Applications

We introduce briefly some other applications, led by or with important contributions from other institutions, under the TSTT Center:

- **AMR Front Tracking.** In SciDAC-1, TSTT researchers merged the front tracking code *FronTierLite* with the AMR code Overture to create a combined, AMR-front tracking capability needed by fusion, groundwater, combustion, and astrophysics applications. This code was created in 2D, although both components function in 2D and 3D.
- **Virtual Microbial Cell Simulator (VMCS).** TSTT mesh generation and discretization technologies were used in simulations that provided new scientific insight into the flocculation behavior of *Shewanella* in oxygen rich environments by confirming that there is an oxygen gradient from the edges of the floc into the center. This collaboration with PNNL computational biologists has resulted in the development of the VMCS which is targeting DOE bioremediation problems in heavy metal waste.
- **Subsurface Problem.** SBU has started collaboration with T. Scheibe and Harold Trease at PNL in the application of the front tracking code to the simulations of reactive transport and precipitation problem. A simulation platform has been built for comparison with the results obtained by Tartakovsky et al [39] on crystal-like growth of solute on solid surface. Figure 6 shows a simplified front tracking test on such problem. More accurate simulations on both 2D and 3D are underway.

7.1 Publications Resulting from DOE Support

The publications (listed in the references section), supported from the completed grant were:

- 2001: [5, 18, 19];
- 2002: [15, 17, 23, 22, 21];
- 2003: [8, 13, 24, 26, 31];
- 2004: [9, 10, 27];
- 2005: [12, 16, 28, 3, 7, 11];
- 2006: [32, 33, 40, 6, 14, 20]

8 References

- [1] R. Samulyak and T. Lu and P. Parks. A hydromagnetic simulation of pellet ablation in electrostatic approximation. *Nuclear Fusion*, 47:103–118, 2007.
- [2] S. Balay, W. Gropp, L. McInnes, and B. Smith. PETSc users manual. Technical Report ANL-95/11 - Revision 2.1.1.
- [3] W. Bo, B. Cheng, J. Du, B. Fix, E. George, J. Glimm, J. Grove, X. Jia, H. Jin, H. Lee, Y. Li, X. Li, X. Liu, D. H. Sharp, L. Wu, and Yan Yu. Recent progress in the stochastic analysis of turbulent mixing. *Contemporary Mathematics*, 2005. In Press. Stony Brook University Preprint Number SUNYSB-AMS-05-18, Los Alamos National Laboratory LAUR Number LAUR-05-7102.
- [4] M. Brewer, L. Diachin, P. Knupp, T. Leurent, and D. Melander. The Mesquite mesh quality improvement toolkit. In *Proceedings of the 12th International Meshing Roundtable*, pages 239–250, 2003.
- [5] B. Cheng, J. Glimm, X. L. Li, and D. H. Sharp. Subgrid models and DNS studies of fluid mixing. In E. Meshkov, Y. Yanilkin, and V. Zhmailo, editors, *Proceedings of the 7th International Conference on the Physics of Compressible Turbulent Mixing, (1999)*, pages 385–390, Sarov, Nizhny Novgorod region, Russia, 2001. RFNC-VNIIEF.
- [6] Jian Du, Brian Fix, James Glimm, Xicheng Jia, Xiaolin Li, Yunhua Li, and Lingling Wu. A simple package for front tracking. *J. Comp. Phys.*,

213:613–628, 2006. Stony Brook University preprint SUNYSB-AMS-05-02.

- [7] S. Dutta, E. George, J. Glimm, J. Grove, H. Jin, T. Lee, X. Li, D. H. Sharp, K. Ye, Y. Yu, Y. Zhang, and M. Zhao. Shock wave interactions in spherical and perturbed spherical geometries. *Nonlinear Analysis*, 63:644–652, 2005. University at Stony Brook preprint number SB-AMS-04-09 and LANL report No. LA-UR-04-2989.
- [8] S. Dutta, E. George, J. Glimm, X. L. Li, A. Marchese, Z. L. Xu, Y. M. Zhang, J. W. Grove, and D. H. Sharp. Numerical methods for the determination of mixing. *Laser and Particle Beams*, 21:437–442, 2003. LANL report No. LA-UR-02-1996.
- [9] S. Dutta, J. Glimm, J. W. Grove, D. H. Sharp, and Y. Zhang. Error comparison in tracked and untracked spherical simulations. *Computers and Mathematics with Applications*, 48:1733–1747, 2004. University at Stony Brook preprint number AMS-03-10 and LANL report No. LA-UR-03-2920.
- [10] S. Dutta, J. Glimm, J. W. Grove, D. H. Sharp, and Y. Zhang. Spherical Richtmyer-Meshkov instability for axisymmetric flow. *Mathematics and Computers in Simulations*, 65:417–430, 2004. University at Stony Brook preprint number AMS-03-13.
- [11] B. Fix, J. Glimm, X. Li, Y. Li, X. Liu, R. Samulyak, and Z. Xu. A TSTT integrated FronTier code and its applications in computational fluid physics. *Journal of Physics: Conf. Series*, 16:471–475, 2005.

- [12] E. George and J. Glimm. Self similarity of Rayleigh-Taylor mixing rates. *Phys. Fluids*, 17:054101–1–054101–13, 2005. Stony Brook University Preprint number SUNYSB-AMS-04-05.
- [13] E. George, J. Glimm, J. W. Grove, X. L. Li, Y. J. Liu, Z. L. Xu, and N. Zhao. Simplification, conservation and adaptivity in the front tracking method. In T. Hou and E. Tadmor, editors, *Hyperbolic Problems: Theory, Numerics, Applications*, pages 175–184. Springer Verlag, Berlin and New York, 2003.
- [14] E. George, J. Glimm, X. L. Li, Y. H. Li, and X. F. Liu. The influence of scale-breaking phenomena on turbulent mixing rates. *Phys. Rev. E*, 73:016304–1–016304–5, 2006.
- [15] E. George, J. Glimm, X. L. Li, A. Marchese, and Z. L. Xu. A comparison of experimental, theoretical, and numerical simulation Rayleigh-Taylor mixing rates. *Proc. National Academy of Sci.*, 99:2587–2592, 2002.
- [16] J. Glimm, J. W. Grove, Y. Kang, T. Lee, X. Li, D. H. Sharp, Y. Yu, K. Ye, and M. Zhao. Errors in numerical solutions of spherically symmetric shock physics problems. *Contemporary Mathematics*, 371:163–179, 2005. University at Stony Brook Preprint Number SB-AMS-04-03, Los Alamos National Laboratory number LA-UR-04-0713.
- [17] J. Glimm, J. W. Grove, X. L. Li, Yingjie Liu, and Zhiliang Xu. Unstructured grids in 3D and 4D for time-dependent interface in front tracking with improved accuracy. In B. K. Soni et al., editor, *Proc. 8th Int. Conf. Num. Grid Generation in Comp. Field Simulations*, pages 179–188. 2002. LANL report No. LA-UR-02-0893.

- [18] J. Glimm, J. W. Grove, X. L. Li, W. Oh, and D. H. Sharp. A critical analysis of Rayleigh-Taylor growth rates. *J. Comp. Phys.*, 169:652–677, 2001.
- [19] J. Glimm, H. Kirk, X. L. Li, J. Pinezich, R. Samulyak, and N. Simos. Simulation of 3D fluid jets with application to the muon collider target design. In *Advances in Fluid Mechanics III*, volume 26, pages 191–200. WIT Press, Southampton, Boston, 2000.
- [20] J. Glimm and X. L. Li. Recent progress in turbulent mixing. In M. Legrand and M. Vandenboomgarde, editors, *Proceedings of the 10th International Workshop on the Physics of Compressible Turbulent Mixing, 17-21 July, Paris France*, 2006. Stony Brook University Preprint SUNYSB-AMS-06-13, In Press.
- [21] J. Glimm, X.-L. Li, and A.-D. Lin. Nonuniform approach to terminal velocity for single mode Rayleigh-Taylor instability. *ACTA MATHEMATICAE APPLICATAE SINICA*, 18:1–8, 2002.
- [22] J. Glimm, X.-L. Li, and Y.-J. Liu. Conservative front tracking in higher space dimensions. *Transactions of Nanjing University of Aeronautics and Astronautics*, 18, Suppl.:1–15, 2001. Proceedings of International Workshop on Computational Methods for Continuum Physics and Their Applications (IWCCPA), Nanjing, China.
- [23] J. Glimm, X.-L. Li, and Y.-J. Liu. Conservative front tracking in one space dimension. *Contemporary Mathematics*, 295:253–264, 2002. Proceedings of the Joint Summer Research Conference on Fluid Flow and Transport in Porous Media: Mathematical and Numerical Treatment. Report SUNYSB-AMS-01-16.

- [24] J. Glimm, X.-L. Li, Y.-J. Liu, Z. L. Xu, and N. Zhao. Conservative front tracking with improved accuracy. *SIAM J. Numerical Analysis*, 41:1926–1947, 2003.
- [25] J. Glimm, X.-L. Li, Y.-J. Liu, and N. Zhao. Conservative front tracking and level set algorithms. *Proc. National Academy of Sci.*, 98:14198–14201, 2001.
- [26] J. Glimm, X. L. Li, W. Oh, A. Marchese, M.-N. Kim, R. Samulyak, and C. Tzanos. Jet breakup and spray formation in a diesel engine. In *Proceedings of the Second MIT Conference on Computational Fluid and Solid Mechanics*. Cambridge, MA, 2003. SUNY Stony Brook preprint No. susb-ams-02-20.
- [27] J. Glimm, X.-L. Li, and Z.-L. Xu. Front tracking algorithm using adaptively refined meshes. In *Proceedings of the 2003 Chicago Workshop on adaptive Mesh Refinement Methods*. 2004. the Lecture Notes in Computational Science and Engineering, ISSN: 1439-7358.
- [28] James Glimm, M.-N. Kim, X.-L. Li, R. Samulyak, and Z.-L. Xu. Jet simulation in a diesel engine. In *Computational Fluid and Solid Mechanics 2005*. Elsevier Science, 2005.
- [29] R. Ishizaki and et al. Two-dimensional simulation of pellet ablation with atomic processes. *Phys. Plasmas*, 11:4064–4080, 2004.
- [30] H. Johansen and P. Colella. A cartesian grid embedded boundary method for poisson’s equation on irregular domains. *J. Comput Phys*, 147:60–85, 1998.

- [31] L. Li, J. Glimm, and X.-L. Li. All isomorphic distinct cases for multi-component interfaces in a block. *J. Comp. Appl. Mathematics*, 152:263–276, 2003.
- [32] J.-J. Liu, J. Glimm, and X.-L. Li. A conservative front tracking method. In F. Asakura, H. Aiso, S. Kawashima, Matsumura A, S. Nishibata, and K. Nishihara, editors, *Hyperbolic Problems: Theory, Numerics, and Applications*, pages 57–62. Yokohama Publishers, Osaka, Japan, 2006.
- [33] Jinjie Liu, Hyun-Kyun Lim, James Glimm, and Xiaolin Li. *J. of Sci. Comp.*, 2006. In Press. Stony Brook University preprint number SUNYSB-AMS-06-04.
- [34] X. F. Liu, E. George, W. Bo, and J. Glimm. Turbulent mixing with physical mass diffusion. *Phys. Rev. E*, 73:056301–1–056301–8, 2006.
- [35] A. K. MacAulay. Geometrical, kinetic and atomic physics effects in a two dimensional time dependent simulation of ablating fuel pellets. *Nuclear Fusion*, 34:43–62, 1994.
- [36] P. Parks and R. J. Turnbull. Effect of transonic flow in ablation cloud on lifetime of a solid hydrogen pellet in a plasma. *Phys. Fluids*, 21:1735–1741, 1978.
- [37] R. Samulyak and Y. Prykarpatsky. Richtmyer-meshkov instability in liquid metal flows: influence of cavitation and magnetic fields. *Mathematics and Computers in Simulations*, 65:431–446, 2004.
- [38] M. S. Shephard, J. E. Flaherty, K. E. Jansen, X. Li, X.-J. Luo, N. Chevaugneon, J.-F. Remacle, M. W. Beall, and R. M. OBara. Adap

- tive mesh generation for curved domains. *J. for Applied Numerical Mathematics*, 53(2-3):251–271, 2005.
- [39] A. Tartakovsky, P. Meakin, T. Scheibe, and R. West. Simulation of reactive transport and precipitation with smoothed particle hydrodynamics. *J. Comp. Phys.*, 21, 2006.
- [40] Z. L. Xu, M. Kim, W. Oh, J. Glimm, R. Samulyak, X. L. Li, and C. Tzanos. Discrete bubble modeling of unsteady cavitating flow. *International Journal for Multiscale Computational Engineering*, 2006. Accepted. SB Preprint Number: SUNYSB-AMS-05-08.