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Interoperable Technologies for Advanced Petascale Simulations (ITAPS)

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1 Abstract

Our final report on the accomplishments of ITAPS at Stony Brook during period covered by the research award includes component service, interface service and applications. On the component service, we have designed and implemented a robust functionality for the Lagrangian tracking of dynamic interface. We have migrated the hyperbolic, parabolic and elliptic solver from stage-wise second order toward global second order schemes. We have implemented high order coupling between interface propagation and interior PDE solvers. On the interface service, we have constructed the *FronTier* application programer's interface (API) and its manual page using doxygen. We installed the *FronTier* functional interface to conform with the ITAPS specifications, especially the iMesh and iMeshP interfaces. On applications, we have implemented deposition and dissolution models with flow and implemented the two-reactant model for a more realistic precipitation at the pore level and its coupling with Darcy level model. We have continued our support to the study of fluid mixing problem for problems in inertial confinement fusion. We have continued our support to the MHD model and its application to plasma liner implosion in fusion confinement. We have simulated a step in the reprocessing and separation of spent fuels from nuclear power plant fuel rods. We have implemented the fluid-structure interaction for 3D windmill and parachute simulations. We have continued our collaboration with PNNL, BNL, LANL, ORNL, and other SciDAC institutions.

2 *FronTier* Component and Interface Services

2.1 *FronTier* Functions and Manual

A detailed manual for a user-friendly *FronTier* code [5] has been developed. This webpage contains synopsis of *FronTier* functions and sample driver codes which users can download and run for various benchmark testing problems. They can also be modified for simulations of different physical and scientific applications. The functions in the manual are divided into four levels: (a) beginner level for basic usage, (b) intermediate level for setting options of algorithms and data structures, (c) advanced level for setting more advanced options and for customizations, and (d) developer level for core programmers of the *FronTier* code. We also performed some bench mark study in comparison with other interface methods. Figure 1 and Figure 2 show the comparison with the level set method.

FronTier has adopted objective oriented programming method and many major functionalities have been modulized to allow users calling them with minimum knowledge of internal operation and coding. We have classified FronTier functions into the following categories:

(1). **Initialization**, including IO channels for computation and application parameters, such as dimension, domain, mesh, boundary and others; initialization of front interface; and initialization of front propagation and velocity related functions. We provided windows so that users can write their own functionalities to a specific application.

(2). **Query functions**, for users to obtain front interface entities including arrays of vertices, simplices, manifolds, and connectivity information.

(3). **Propagation Control functions**, including front advancement, redistribution and bifurcation as well as setting criteria for these operations.

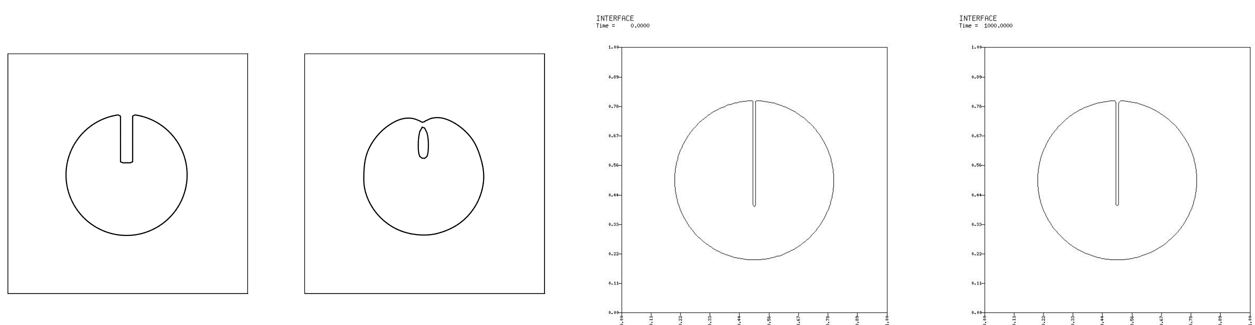
(4). **Front and subdomain interaction functions**. This set of functions allow users to couple the front propagation with PDE solvers through a set of conveniently designed window functions including locating neighboring points, setting up stencils and interpolating physical state variables. tem[(5).] **Output and data saving functions**. We provide a number of output functions for users to conveniently write to output files for post-processing. Our output formats include vtk files for VisIt and paraview, list file for geomview and output using HDF and GD packages.

We provide template codes with as few as 300 lines to demonstrate the application of *FronTier* with different initialization and velocity functions including examples to show different mesh operations: redistribution, merging and bifurcation. Figure 3 shows three examples of *FronTier* functionalities.

2.2 Higher Order Parabolic and Elliptic PDE Solvers

The incompressible Navier-Stokes solver has become one of the most important component of the *FronTier* service. Our study has been focused on the high order geometric algorithms and its coupling with the parabolic and elliptic PDE solvers.

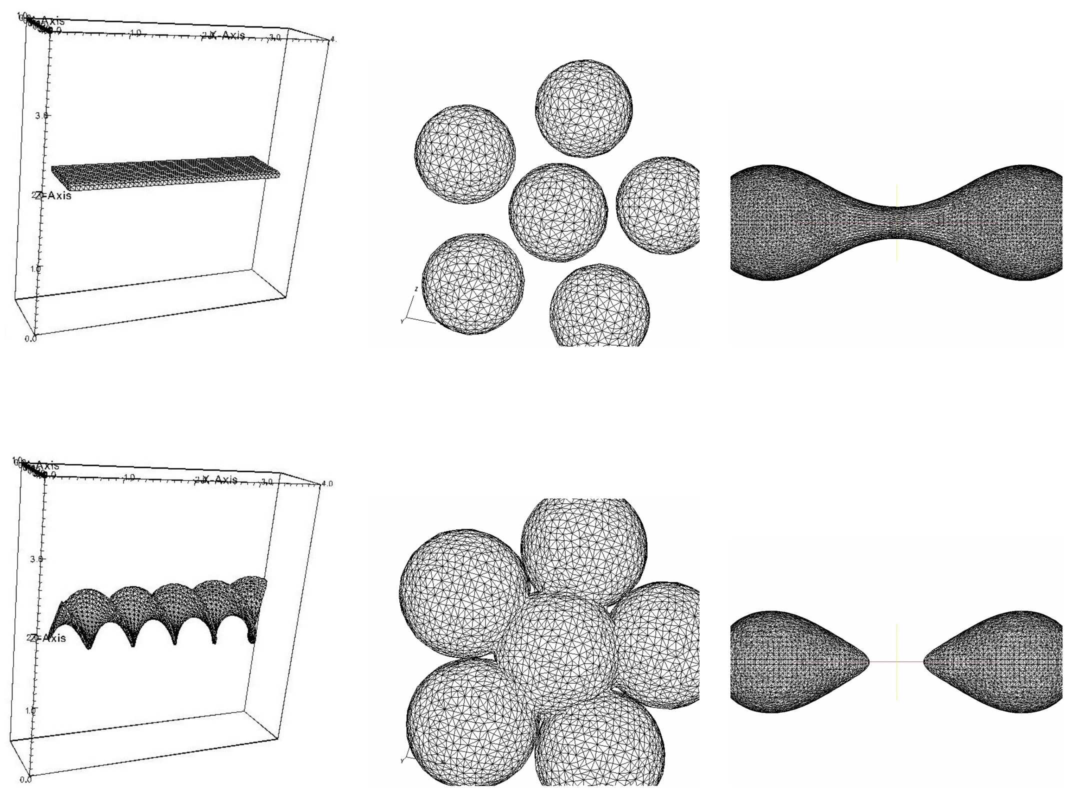
The high-order geometric algorithms are important in *FronTier* to allow the numerical errors in the interface computations no greater than those from the high-order incompressible fluids solvers. They are also important for better conservation in front tracking and mesh generation and improvement of complex and evolving geometries. Achieving high-order accuracy over discrete surface triangulations is a challenging task. We have previously developed accurate and robust algorithms for computing normals and curvatures based on weighted least squares approximations. We have integrated these high-order algorithms into *FronTier* and have undergone extensive testing. Recently, we further extended the method to perform high-order interpolaton and surface reconstruction, and integrated these new algorithms into *FronTier* to improve the accuracy of node redistribution. These new capabilities are currently being tested. We are also generalizing the framework to compute high-order surface integration, which is useful for computing conservative variables in front tracking.



$\theta = 0$ $\theta = 26\pi$ $\theta = 0$ $\theta = 2000\pi$

Figure 1: Benchmark test of Zalesak's slotted disk in rotational velocity field. Left two plots: level set method using the 5th order WENO solver, 13 revolutions. Right two plots: front tracking with 4th order Runge-Kutta ODE solver, 1000 revolutions. Both tests have an underlying rectangular grid of 128^2

Figure 2: Reversal test of a 3D interface in deformation velocity field. The three plots in the left are computed in the 64^3 mesh, and the three right plots are in the mesh of 128^3. For each set, from left to right are $t = 0,\ 1.5,\ 3$ respectively.



Mesh twisting | Mesh merging | Mesh bifurcation

Figure 3: Three examples of the 3D dynamic surface evolutions using the *FronTier* library. From left: mesh twisting, mesh merging and mesh bifurcation.

2.3 *FronTier* and AMR

We continued the development of AMR capability in the *FronTier* code. Our focus is on the three dimensional coupling and the design of a code interface with different AMR libraries including Overture and Samrai. The parallel re-partition and CPU control system will also be implemented to the *FronTier*

-AMR operation for load balancing.

Initial experimental work in *FronTier* and AMR was done with the Overture AMR package. Overture specific calls were placed throughout the code. For code maintenance and modularization reasons this model was reworked. *FronTier* 's AMR usage has been completely redesigned in oder to make calls to wrapper AMR code that can be filled with any block structured AMR package. Wrappers for the Overture package are completely functional and in use. Wrappers for the SAMRAI code are being written and tested.

The inclusion of SAMRAI in the *FronTier* library will introduce the AMR coupling code in a logical and staged set of patches. Each patch set will ensure all algorithmic functionalities in the non-AMR front tracking remain unchanged. Also physics examples have been written for the AMR coupled front tracking code and they are used for code verification and validation.

The 2D AMR code has stabilized. All AMR and front tracking coupling codes that involve front communication and surgery between patches are fully functional. This code is currently at a production level, for example, running in large mesh sizes for diesel jet simulations. The 2D AMR code is currently undergoing smaller changes and testing in initialization and boundary condition codes, in order to ensure proper functionality in all 2d problem types. 3D *FronTier* -AMR code has also been developed.

2.4 Advanced Multi-thread Parallelization

High performance computing is moving toward multi-core platforms. The multicore solution becomes more popular due to the fact that it is becoming harder to scale single-core processors while trying to maintain the heat and power envelope necessary to make systems practical. Multicore is no longer a scaling issue, but rather a requirement to meet growing performance requirements. Our objective is to adapt the *FronTier* to the new programming requirements using the OpenMP platform. The OpenMP portable and scalable framework supports multi-platform, shared-memory parallel programming. It targets SMP systems. It is a thread-oriented approach that maps well to existing hardware architectures. We add to *FronTier* some core elements include thread management, synchronization, and parallel control structures.

2.5 Other Progress in Component and Interface Services

The rich features and rapid development of *FronTier* made software engineering more and more important over time. During the past year, we have also enhanced the software engineering practices of *FronTier* development. In particular, we have set up a wiki page and bug tracking system for *FronTier* based on the Trac system developed by Edgewall software. In addition, we have set up an automatic code uilding and testing system, which compiles the *FronTier* on six different platforms and runs a number of benchmark problems every night. This system can detect compilation errors and changes in the solutions, and alert developers about potential bugs. These improved software engineering practices have helped to improve the productivity of our development team and the robustness of the *FronTier* library.

We have continued implementation, modification and testing of the ITAPS mesh interface. In particular, we have implemented most of the iMesh specifications and part of the iMeshP specifications. We have actively participated the iField design workshop and is in preparation for the new interface. In addition, we have designed the application programer's interface (API) for the *FronTier* library under its own name space.

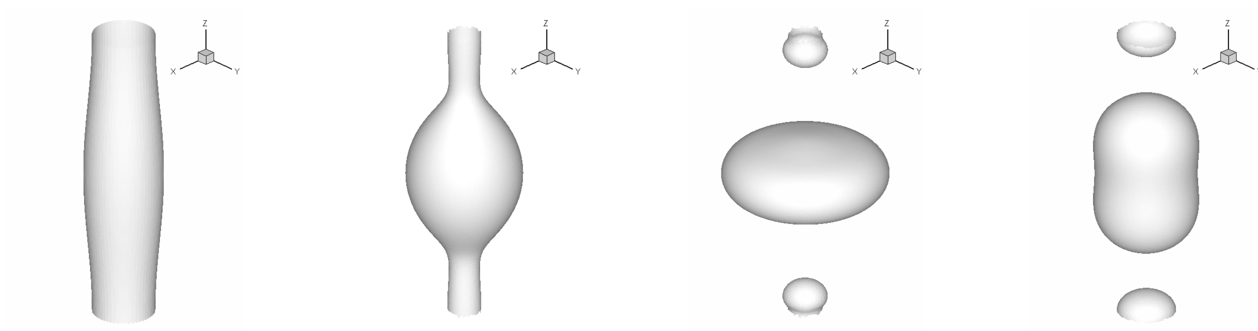


Figure 4: *FronTier* simulation of Rayleigh instability with newly upgraded point propagator and high order curvature algorithm.

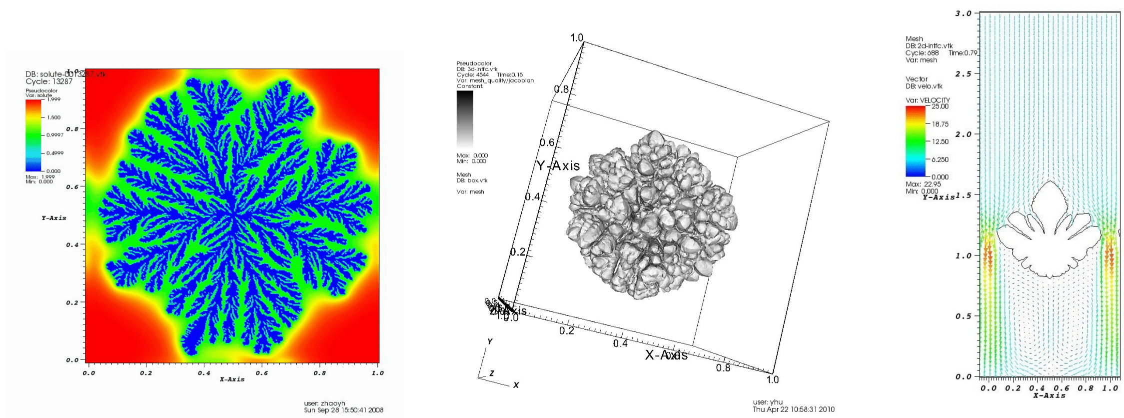


Figure 5: Front tracking on the simulation of solute precipitation. The left two plots are 2D and 3D crystal formation without fluid flow. The right is the coupled simulation of precipitation with subsurface flow.

3 Applications to Problems of DOE Interests

3.1 Application to SciDAC Subsurface Problem

We have established the computational platform for a precipitation and subsurface model. Figure 5 shows the simulation based on the *FronTier* subsurface code. The left two plots show the 2D and 3D cryatal formation and the right plot is a coupled simulation of precipitation with subsurface flow.

3.2 Two Reactants Precipitation in Pore Scale

We have also implemented a more realistic two reactant precipitation model and the coupling with the Darcy scale model. The objective of this work is to study the realistic reaction-diffusion equations in a porous medium in two different orders of scale, namely the Pore-Scale and the Darcy Scale. These

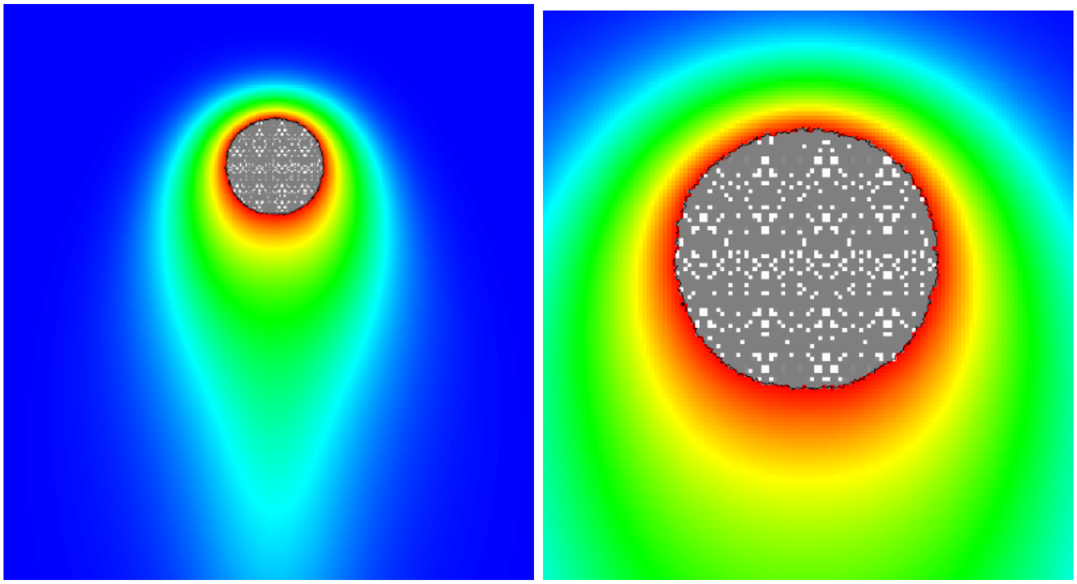


Figure 6: 2D dissolution with porous particle. It shows the dissolving interface, and the ratio of solute concentration and solubility of species A at time t=1.6.

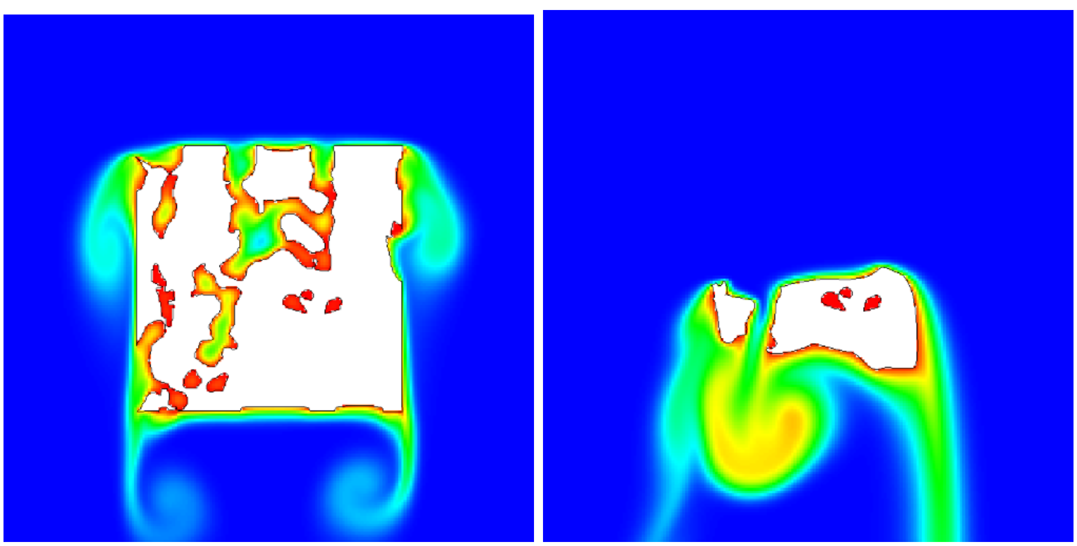


Figure 7: 2D dissolution with a multiphase material. It shows the dissolution interface, and the ratio of solute concentration and solubility of species A around the dissolving interface.

solutions are then coupled to the subsurface simulation.

Reaction-diffusion equations form an important class of semi-linear parabolic partial differential equations. These equations describe how the concentrations of the solutes change with respect to time and the spatial variables, under the influence of two processes, namely diffusion and chemical reaction.

The Reaction-Diffusion Equations can be represented in the general form as follows:

$$\frac{\partial \mathbf{q}}{\partial t} = \mathbf{D}\nabla^2 \mathbf{q} + \mathbf{R}(\mathbf{q}), \tag{1}$$

where $\mathbf{q}(\mathbf{x}, t)$ is a vector whose components are the concentrations of solutes under consideration, $\mathbf{D}$ is a diagonal matrix of diffusion coefficients and $\mathbf{R}(\mathbf{q})$ is a vector which accounts for the local chemical reaction.

In this work, we study the system at two different spatial scales, the Pore-Scale and the Darcy-Scale. The Pore-Scale model describes the diffusion and reaction processes on the microscopic level. It also describes the precipitation of the product of reaction once the local concentration reaches above a critical level, namely the equilibrium concentration. At this scale, the rate and the direction in which the crystal interface advances into the liquid is dependent on local pore geometry. The real dimensions associated with the Pore-Scale model depend on the particular system under consideration, and may be of the order of millimeters, centimeters or even meters depending on the realistic pore geometry. However, this does not pose any problems during the simulations as long as the ratio of dimensions in Pore and Darcy scale is maintained constant throughout.

The Darcy-Scale model considers the porous medium on macroscopic level and neglects the local effects of pore geometry. Typically, the system is viewed as a continuum, and the porosity ϕ is added to the mathematical model to account for the reduced permeability. Assuming that the ratio of Darcy-Scale to Pore-Scale is big enough and the precipitation rate is slow, the changes in porosity due to microscopic effects can be neglected. The functional relation between the porosity and the spatial variables, even under simplified scenarios, is still open to scientific investigation. The real dimensions at this scale are again dependent on the system under study, and may be of the order of meters or even kilometers if one is working on the field.

Alexandre M. Tartakovsky et al.[17, **?**] solve the system of equations with Smoothed Particle Hydrodynamics (SPH). Although SPH manages to avoid the difficulties usually encountered in front-tracking, studies (see [9, 7, 5]) have shown that front tracking gives more accurate results where there are sharp fronts to be tracked. This is the case with Pore-Scale model. Front tracking offers special advantages when the pore geometry is complex and when the front needs to be merged or bifurcated with considerable accuracy. Hence we propose to use front-tracking to study the system at Pore-Scale. Since there are no sharp fronts to deal with in Darcy-Scale, the accuracy of numerical solutions in this scale depends only on the consistency of the numerical scheme used. Our new code on two reactant diffusion model has been tested and ready for real time simulations.

3.3 Simulation of Dissolution

Dissolution is the opposite process of deposition. In the last two years, we have also extended our subsurface code to the application of dissolution of spent fuel in nuclear reactor. This work is in collaboration with Valmor F. de Almeida at Oak Ridge National Laboratory.

The dissolution of a solid particle is an industrially important application. It plays a crucial role in a variety of scientific, engineering, and industrial processes, such as porosity and permeability changes in hydrothermal system[?], suspension polymerization[?], melt extraction from Earth's upper mantle[?, ?, ?], geochemical self-organization[?], acid stimulation process[?], and environmental contaminant transport[?].

These applications usually involve multiple process like convection, diffusion, and reaction, which couple with chemistry , and heat and mass transfer. This work aims at a contribution to reliable numerical predictions of multi-phase processes. In this case, it is advantageous to be able to predict the detailed evolution of the initial shape of the solid particles to better estimate macroscopic parameters in coarser space-time scale models. In addition, improved understanding of the physical process in conjuction with experimental measurements are likely to be obtained from a modeling and simulation approach that captures the detailed evolution of the solid-liquid interface. Figure 6 and Figure 7 show two cases of the dissolution simulations using our *FronTier* phase transition module.

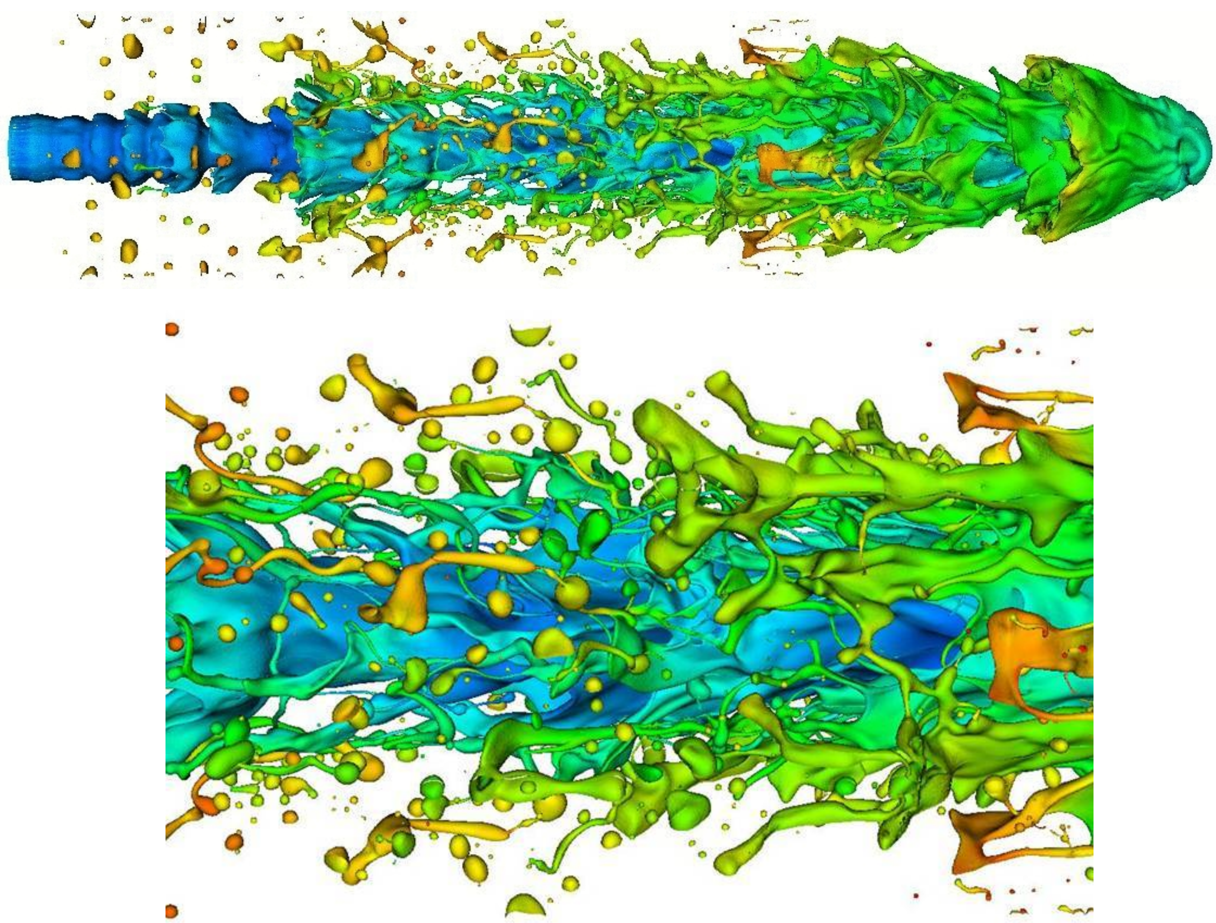


Figure 8: Liquid jet and the detail of the jet surface at the end of the simulation.

3.4 Simulation of Liquid Jet

We completed the simulation of 3D primary breakup on a fine grid using a Blue Gene/L computer with 4096 processors. The breakup of the liquid jet is predicted. The detailed structure in primary breakup such as droplets and ligaments are noticed in the results. Figure 7 is the simulation of Rayleigh

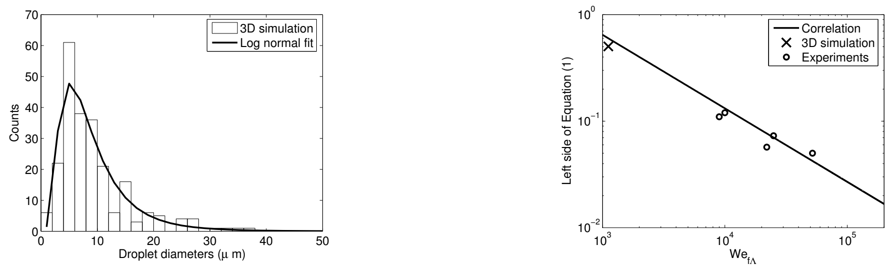
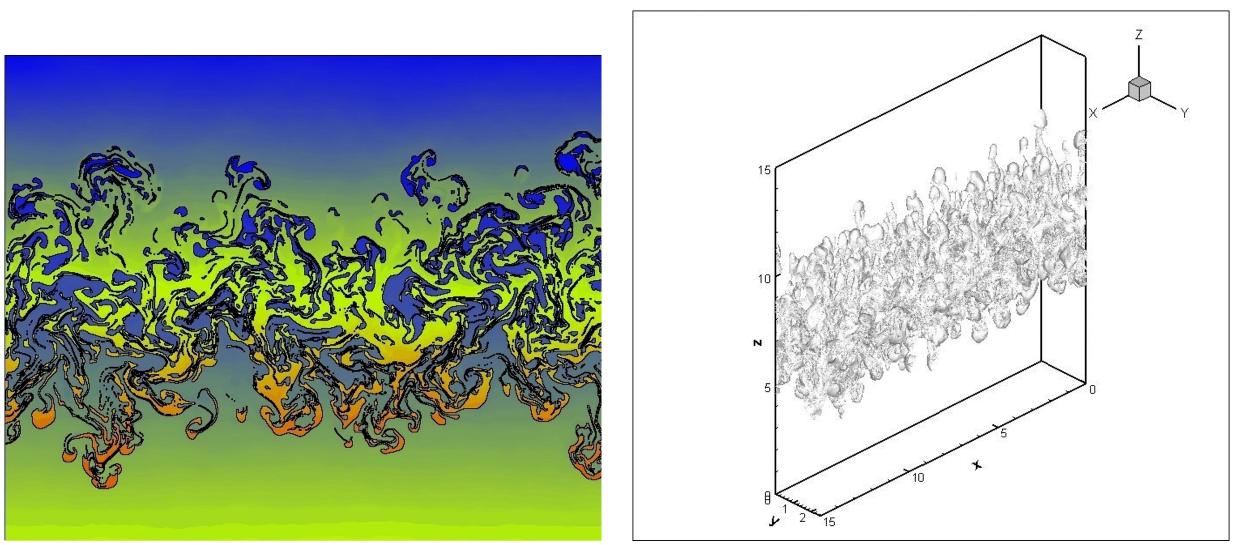


Figure 9: Left: Droplet diameter distribution from the 3d simulation. Right: The SMD from the simulation. We plot the correlation (left side of Equation (2)) vs. $We_{f\Lambda}$.



(a) (b)

Figure 10: Front tracking simulation of Rayleigh-Taylor Mixing. Left: a two dimensional evolution of fluid interface. Right: a case of three dimensional mixing fluid interface.

instability, which is one of the important mechanism in the jet break-up process. Figure 8 shows the jet fluid interface. Major features such as filaments and droplets are evident. The droplet size follows a log-normal distribution, which is consistent with experiments. We also find the agreement of the resulting SMD with Wu *et.al.*'s correlation [18], see Figure 9 for details.

$$SMD/\Lambda[1 + 0.04(\rho_g/\rho_f)(\bar{u}_0/\bar{v}_0')^2(\Lambda/SMD)^{2/3}]^{3/5} = 76(We_{f\Lambda})^{-0.69}, \quad (2)$$

Here Λ is the turbulence length scale, ρ_g and ρ_f are the gas and liquid densities, $\bar{u}_0$ and $\bar{v}_0'$ are the mean flow and radical turbulence velocity respectively. $We_{f\Lambda} = \rho_f \bar{u}_0^2 \Lambda/\sigma$ is the liquid Weber number based on the length scale Λ.

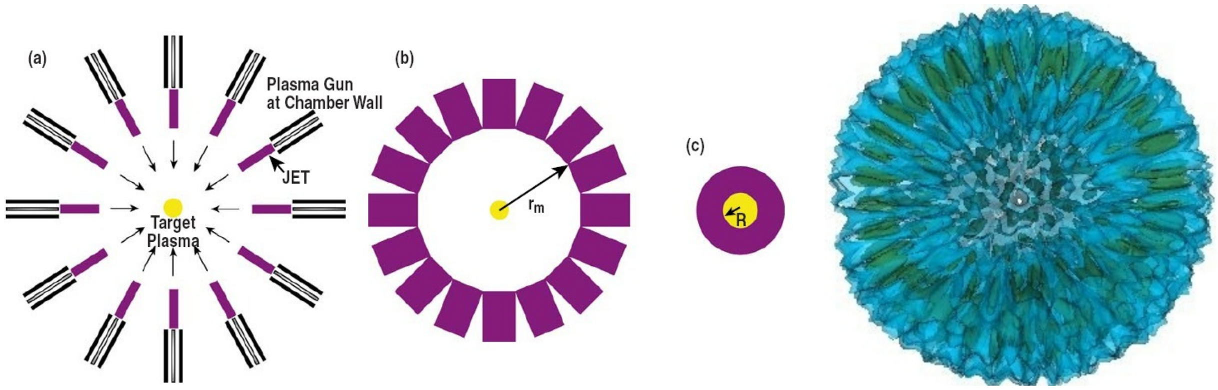


Figure 11: *FronTier* simulation of the implosion of plasma liner formed by the merger of 625 jets. Left three plots show the structure of the plasma liner, and the right shows the *FronTier* simulation results.

3.5 Formation and Implosion of Plasma Liners

ITAPS front tracking technologies have been used in computational studies of the plasma jet driven magneto-inertial fusion (PJMIF). In the PJMIF concept, a plasma liner, formed by merging of a large number of radial, highly supersonic plasma jets, implodes on the target in the form of two compact plasma toroids, and compresses it to conditions of the fusion ignition. By avoiding major difficulties associated with both the traditional laser driven inertial confinement fusion and solid liner driven MIF, the plasma liner driven magneto-inertial fusion potentially provides a low-cost and fast R&D path towards the demonstration of practical fusion energy. The goal of PJMIF simulations is to evaluate the method by estimating the fusion energy gain and to provide guidance for the plasma liner experiment being built at Los Alamos. In the first phase of research, we optimized the nuclear fusion gain in the liner . target parameter space via spherically symmetric simulations. Single and double-layer deuterium and xenon liners have been investigated as well as liners to be used in the PLX experiment. By varying target and liner parameters, the implosion process was optimized for maximum fusion energy gain and compared with theoretical predictions and scaling laws. In the most optimal setup, fusion ignition and energy gain of 10 was achieved with energy release of 10 GJ. Current work focuses on large scale 3D simulations of the propagation and merger of high Mach number plasma jets, the formation and implosion of liners, and compression of targets. The merger of 125, 144 and 625 jets have been simulated and the uniformity and Mach number reduction of the corresponding liners have been investigated. During late stages of the implosion, the Mach number of 3D liners was about half of that of spherically symmetric liners. The uniformity of the liner is critical for the reduction of Rayleigh-Taylor instabilities in the target while maintaining a high Mach number in the liner is necessary to achieve high target compression rates. Figure 11 shows the configuration for such simulation.

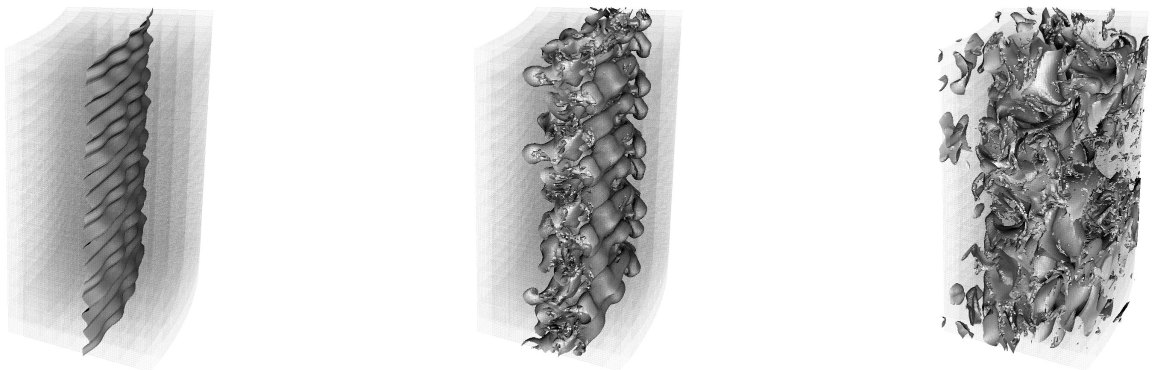


Figure 12: *FronTier* simulation on instability of turbulent Taylor-Couette Flow of two-fluid between Concentric Rotating Cylinders.

3.6 Reprocessing and Separation of Spent Nuclear Fuel

We simulate a step in the reprocessing and separation of spent fuels from nuclear power plant fuel rods. A contactor is a high speed rotating (Couette) two phase immiscible flow, whose goal is to produce a fine scale mixture of bubbles and droplets with a greatly extended surface area. The chemical reactions that drive the fuel separation occur on the interface between the two fluids, and the objective of this study is to simulate in sufficient detail to be able to estimate this surface area, and thus the fuel separation reaction rate. In Figure 12, we show a simulation (with modified physics, to render the problem more tractable) of a small segment of the contactor. Simulation courtesy of Hyunkyun Lim, based on the code front tracking *FronTier* .

4 Application to Non-SciDAC problems

4.1 Fluid-Structure interaction

On a broader impact of the SciDAC component development, we have also applied *FronTier* to scientific and engineering problems funded under other federal grants or proposed for other projects. One of these extensions is the fluid structure interaction and its application to airfoil and parachute dynamics [8, 10]. This project has been funded by the ARO. The fluid-structure interaction code has also been applied to the simulation of wind power generator.

Fluid structure interaction is a natural extension of the capabilities of *FronTier* . In the first year of the proposed work to ARO, we started the implementation of these extensions by including the interaction between fluid and rigid body and the interaction between fluid and deformable fabric surface. Our objective if to apply these extensions on two interesting and important applications to the ARO mission.

The study of parachutes involves the modeling and numerical implementation of unfolding cloth and its interaction with the surrounding fluid. The former is modeled by adding a new data structure and its associated functions to the *FronTier* library while the latter needs a high order incompressible fluid solver using the projection method. Figure 13 shows the simulation of a table cloth using the spring model on the *FronTier* platform.

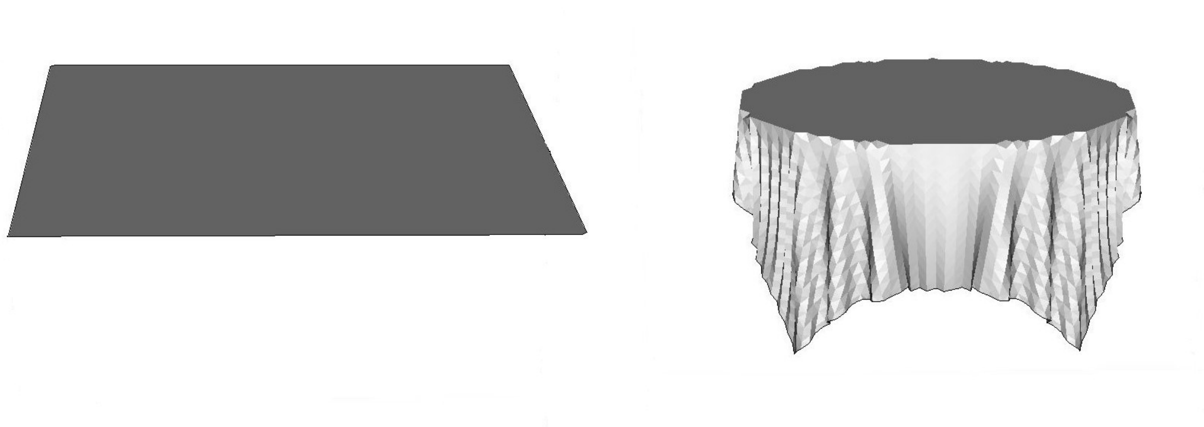


Figure 13: Simulation of a table cloth draping under the gravitational force. The fabric constraint automatically adjusts the parts of the cloth. The spring model of the fabric gives a realistic motion of the cloth. The characteristic eigen frequency for the fabric model in this simulation is $\sqrt{k/m} = 1000$ and the friction constant is $\kappa = 0.1$.

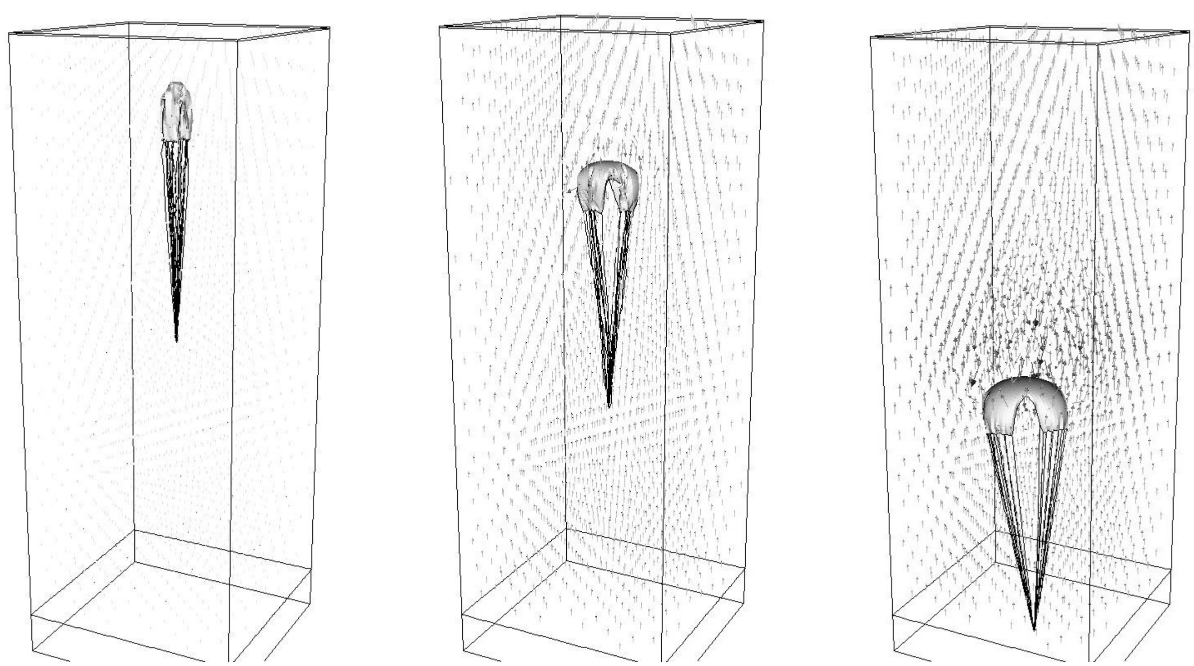
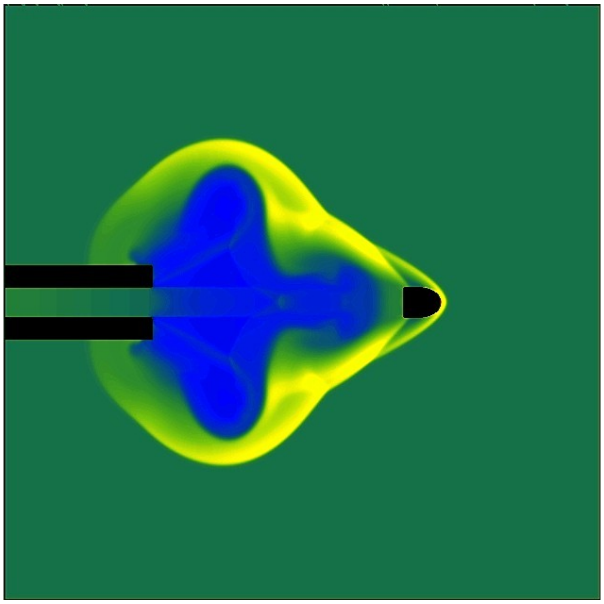
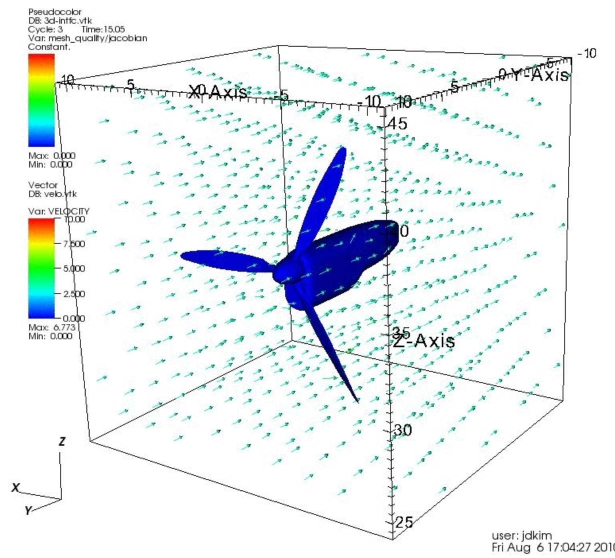


Figure 14: Cross parachute inflation for wind tunnel experiment. The initial shape is flat cross, the diameter is 1.27 m, the parachute has 20 suspension lines which are 1.27 m each. The simulation starts from a fully folded state and ended when the canopy is opened.

Although this seems to be a minor amendment to the data structure, it requires several major changes in handling the evolution of curves and surfaces. Many topological properties previously used for manifold interface can no longer be used for this new mesh type. We have modified some of the existing functions



Projectile



Windmill

Figure 15: Our compressible fluid solver uses the fifth order WENO scheme which can capture shock structure with high resolution. Our incompressible fluid solver is coupled with the CAD interface. The left plot is the simulation of a projectile fired from a cannon. The right plot shows the simulation of windmill power generator.

and created several new functions which use the geometrical properties alone to recognize and operate on the new entities of the interface. Another challenge to this new type of interface is to satisfy the constraint imposed to the mesh structure such as length (2D) or area (3D) conservation. Figure 14 shows the simulation of the cross parachute inflation using the coupled Navier-Stokes solver and the spring model code.

We have implemented data structure for and functionalities for mechanics of rigid body motion and added functionalities to import structure and parachute canopy from CAD data sets. This allows the front tracking to perform realistic simulation using the original design geometry for these studies. Figure 15 shows two fluid and rigid body interactions, the left is a projectile from a cannon and the right is a windmill.

4.2 Internet Sites

(1) Access to *FronTier* software for downloading:

http://sitsec.ams.sunysb.edu/trac/wiki/FronTier

(2) User manual:

http://www.ams.sunysb.edu/∼yli/front/html/modules.html

(3) *FronTier* examples:

http://www.ams.sunysb.edu/∼linli/FTruns/index.html

4.3 Networks and Collaborations Fostered

(1) Simulation of Diesel Spray: Valmor de Almeida (ORNL)

(2) MHD and Fusion: Roman Samulyak (BNL), Alice Ying (UCLA Fusion Center).

(3) Ground Water: Harold Trease, Timothy Scheibe and Alexandre Tartakovsky (PNNL)

(4) Fluid Mixing: David Sharp, Baolian Cheng, John Grove (LANL), H. C. Yee and B. Sjogree (LLNL)

(5) Nuclear Fuel Contactor Valmor de Almeida (ORNL)

4.4 Other

(a) **Software.**

The front tracking package *FronTier* is now available for distribution.

(b) **Educational Aids.**

This project has been incorporated with graduate education. The program has partially supported several graduate students, including two American students: Brian Fix, and Ryan Kaufman. These students have communicated with national labs using the knowledge and tools developed under this grant to assist research projects of DOE interests. Among these projects are shock and gravity driven instabilities (Los Alamos), combustion engine (Oak Ridge National Lab) and ground water precipitation (PNNL). One of our best former student (Wurigen Bo) has accepted an offer of post doctoral research fellow at Los Alamos National Lab.

We have organized a series of graduate student seminars introducing software development techniques, post-processing packages and skills for large scale parallel computation. These tutorials and workshops have been videotaped as an educational tools for new and incoming students.

We have encouraged graduate students to meet and interact with scientists at national labs through attending academic conferences and participating the ITAPS boot-camp for common geometry related user interface.

4.5 Personnel Support

Besides the one month summer support of the PI (Xiaolin Li), eight graduate students have been partially supported by the ITAPS grant. This includes Tulin Kaman on multi-thread testing, Yanhong Zhao and Sauranh Joglekar on subsurface probblem, Yijing Hu on iMesh testing and the subsurface code development, Yijie Zhou and Junya Kamiyasuhira on Navier-Stokes solver, Joungdong Kim on fluid-structure interaction, and Fan Zhang on general FronTier code development. There are matching supports for all the students through university TA lines and other grants including the one from the Army Research Office.

4.6 Publications

In References: [1, 4, 6, 11, 3, 13, 3, 12, 14, 16, 15, 13, 2, 9, 8, 10].

4.7 Conference Presentations

(1). *Front tracking on Fabric Modeling and Application to Parachute Dynamics*, Wuhan Institute of Physics, Chinese Academia Sinica, July 6, 2012.

(2). *Front Tracking and Application in Fluid Physics*, Departmental Colloquium, Beijing Normal University, July 4, 2012.

(3). *Front Tracking on Fabric Modeling and Application to Parachute Dynamics*, Departmental Colloquium, Shanghai Jiaotong University, July 3, 2012.

(4). *Lagrangian Front Tracking Method to Fluid Instability Problems*, Xiaolin Li, Department of Mathematics, National Taiwan University, Taipei, March 19, 2012.

(5). *A Spring Model and the ODE System for the Study of Fabric Surface and Its Application in Parachute Simulation*, Xiaolin Li, Joung-Dong Kim, and Yan Li, Department of Mathematics, National Sun Yat-sen University, Kaohsiung, Taiwan, March 21, 2012.

(6). *Front Tracking Method and Applications to Fabric Modeling and Parachute Simulation*, Xiaolin Li, Joung-Dong Kim, and Yan Li, Department of Mathematics, National Cheng Kung University, Tainan, Taiwan, March 22, 2012.

(7). *Front Tracking Method and Applications to Fabric Modeling and Parachute Simulation*, Xiaolin Li, Yan Li, I-Liang Chern, Joung-Dong Kim, East Asia SIAM Conference, Taipei, June 25, 2012.

(8). *Mathematics and Applications*, Sanya College, China, 4/18-4/22, 2011.

(9). *Front tracking and air foil simulation*, ICIAM, Vancouver, Canada, 7/21, 2011.

(10). *Front tracking and applications to physics and engineering problems*, Xiaolin Li, Departmental colloquium, Math Department, Wichita State University, April 2, 2009.

(11). *Front tracking on crystal formation and subsurface problem*, Xiaolin Li, IMACS World Congress, Athens, GA, August 4, 2009.

(12). *Front tracking on fluid structure interaction*, Xiaolin Li, AMS Sectional Meeting, New Jersey Institute of Technology, Newark, NJ, May 20, 2010

(13). *Application of front tracking, hyperbolic and beyond*, Xiaolin Li, HYP-10, Beijing, China, June 17, 2010.

(14). *Front tracking on convection dominated problems*, Xiaolin Li, SIAM Annual Meeting, Pittsburg, PA, June 15, 2010.

(15). *Physics of fluid interface instabilities and computation*, Xiaolin Li, TD Lee Lecture, Graduate School of Academia Sinica, Beijing, China, June 17, 2010.

(16). *Front tracking on Convection Dominated Problems*, Xiaolin Li, Peking University, Beijing, China, June 16, 2010.

(17). *Supercomputing and front tracking method*, Xiaolin Li, Wuhan University, Wuhan, China, June 21, 2010.

(18). *Partial differential equations and free boundary problems*, Xiaolin Li, Linyi Normal University, Linyi, China, June 28, 2010.

(19). *Front tracking and convection dominated problems*, Xiaolin Li, Zhejiang University, HangZhou, China, July 8, 2010.

(20). *FronTier and Applications Under ITAPS*, Xiaolin Li, Minisymposium, SIAM CSE, Miami, Florida, March 2-6, 2009.

(21). *A crashing tutorial of FronTier library*, Xiaolin Li, Minisymposium, SIAM CSE, Miami, Florida, March 2-6, 2009.

(22). *FronTier and Application to Stefan Problems, Precipitation, Phase Transition, and Pricing of American Options*, Xiaolin Li, Minisymposium, SIAM CSE, Miami, Florida, March 2-6, 2009.

(23). *On the Structure of Plasma Liners for Plasma Jet Induced Megnetoinertial Fusion*, Roman Samulyak, 52st Annual Meeting of the Division of Plasma Physics, November 8 - 12, 2010, Chicago, Il.

(24). *Simulation of Formation and Implosion of Plasma Liners for Magnetized Target Fusion*, Roman Samulyak, 51st Annual Meeting of the Division of Plasma Physics, November 2 - 6, 2009, Atlanta, Georgia.

(25). *Intrinsic rotation of pellet ablation clouds*, Roman Samulyak, 51st Annual Meeting of the Division of Plasma Physics, November 2-6, 2009, Atlanta, Georgia.

(26). *Simulations of Multiphase Flows in Nuclear Fusion Applications*, Roman Samulyak, Physics Department Colloquium, Stony Brook University, October 16, 2009, Stony Brook, NY.

(27). *Multi-Physics Simulations of the Failure of Fuel Rods During Accidents in Sodium-Cooled Fast Reactors*, Roman Samulyak, Workshop on Characterization of Advanced Materials Under Extreme Environments for the Next Generation Energy Systems, September 25-26, 2009, Brookhaven National Laboratory, Upton, NY.

(28). *Simulations of High-Intensity Pulsed Beam Targeting*, Roman Samulyak, Workshop on Applications of High Intensity Proton Accelerators, October 19-21, 2009, Fermi National Accelerator Laboratory, Batavia, IL.

(29). *Simulation of mercury targets for Neutrino Factory Muon Collider*, Roman Samulyak, MUTAC, April 68 2009, Fermi National Accelerator Laboratory, Batavia, IL.

(30). *ITAPS Based Software for Multiphase Flows in Nuclear Fusion Applications*, Roman Samulyak, SIAM Conference on Computational Science and Engineering, Roman Samulyak, March 2-6, 2009, Miami, Florida.

4.8 SciDAC Related Colloquia

(1). Updating meshes on deforming domains via the target-matrix paradigm, Patrick M. Knupp, Sandia National Laboratories, April 1, 2009.

(2). Shock Wave Propagation in Tissue and Bone, Randall J. LeVeque, April 22, 2009.

(3). Multi-scale simulations of multiphase flow and reactive transport in fractured and porous media, Alexandre Tartakovsky, acific Northwest National Laboratory, June 24, 2009.

(4). The Common Component Architecture for Scalable Scientific Software Engineering, Kostadin Damevski, Virginia State University, September 23, 2009.

(5). Petascale Adaptive Computational Fluid Dynamics, Min Zhou, Rensselaer Polytechnic Institute, Oct. 28, 2009.

(6). Sensitivity Analysis, Uncertainty Quantification and Multiscale Modeling of Complex Systems, Guang Lin, Pacific Northwest National Laboratory, September 8, 2010.

(7). Challenges for Modeling and Simulation of Solvent Extraction in Nuclear Fuel Reprocessing, Valmor de Almeida, Oak Ridge National Laboratory, December 2, 2009.

(8). Computational studies for spatial dynamics of cell signaling with localized scaffold, Jinjie Liu, Xinfeng Liu, March 12, 2010.

(9). The Overlapping Yee FDTD Method on Nonorthogonal Grids, Jinjie Liu, Delaware State University, March 17, 2010.

(10). Computational method for simulating two-phase gel dynamics, Jian Du, University of Utah, March 26, 2010.

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