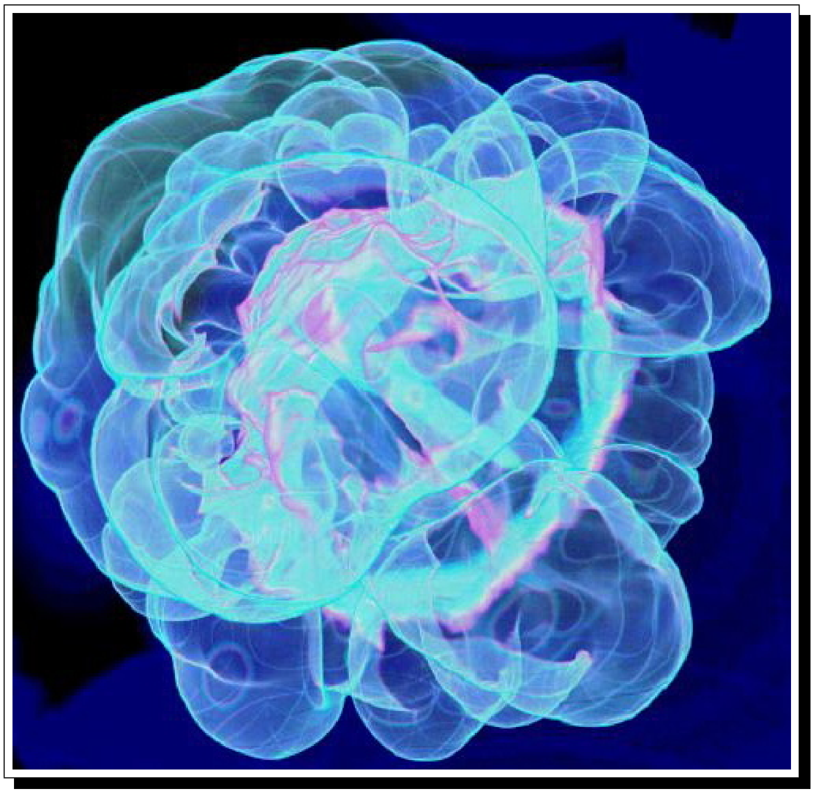
ASCI/ALLIANCES CENTER FOR ASTROPHYSICAL THERMONUCLEAR FLASHES
at
THE UNIVERSITY OF CHICAGO

YEAR 6 ACTIVITIES REPORT



October 2003

Abstract

We summarize the Year 6 activities at the University of Chicago Center for Astrophysical Thermonuclear Flashes. A detailed strategic plan for the next two years was developed and adopted early in the year.

Major milestones achieved by the code group include: (1) release of FLASH 2.3; (2) specification of FLASH 3.0, a significantly more powerful code that will enable developers in the community to contribute modules to FLASH with relative ease; (3) optimized an adaptive mesh multi-grid solver; (4) migrated physics modules to a second (new) branch of FLASH, so that they can be used with the implicit hydro solver; and (5) provided crucial support for the large-scale simulations carried out by the astrophysics group.

Major milestones achieved by the computational physics and validation group include: (1) implementation, testing, and application of the flame-capturing model required for the Type Ia supernova studies; (2) advances in validation work done together with experimentalists at Los Alamos National Laboratory, including a full-scale three-dimensional numerical model of the experiment; (3) implementation of the Hall MHD module in two and three dimensions, including a multi-grid solver for the Helmholtz equation; (4) implementation of the relativistic MHD solver; and (5) organization of an international meeting, "AMR2003: Chicago Workshop on Adaptive Mesh Refinement Methods." Progress was also made in developing the implicit hydrodynamic solver.

Major milestones achieved by the astrophysics group include: (1) completion of large scale 2-d and 3-d simulations of wind-wave mixing, and the extraction from these of the information required to construct a set of physically self-consistent sub-grid models for application to global one-dimensional nova models; and (2) completion of large-scale 3-d simulations of the deflagration-phase of Type Ia supernovae involving a Chandrasekhar-mass white dwarf. Progress was also made in studying the physics of X-ray bursts and in understanding flame physics.

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Contents

1 Introduction

The goal of the Flash center is to solve the long-standing problem of thermonuclear flashes on the surfaces of compact stars, such as neutron stars (X-ray bursts) and white dwarfs (novae), and in the interior of white dwarfs (Type Ia supernovae). The Center's scientific goal is realized through construction of a multi-dimensional, multi-physics, simulation code (the FLASH Code), which is able to carry out numerical simulations of the various aspects of the "Flash Problem."

The activities of the Flash Center involve scientists primarily located at the University of Chicago and Argonne National Laboratory, but also involve a number of collaborators at other universities and at the DOE DP laboratories. The Center if composed of five groups: Code, Computational Physics, Astrophysics, Computer Science, and Basic Physics.

In Year 6, we developed and adopted a detailed strategic plan for the next two years. We also released FLASH 2.3 and specified FLASH 3.0, a significantly more powerful code that will enable developers in the community to contribute modules to FLASH with relative ease. Scientifically, we provided a solution to the important problem of compositional mixing in novae, and made a scientific breakthrough in carrying out the first-ever simulations of off-center ignition in an entire white dwarf star. These achievements were made possible by crucial support from the Code group (e.g., in implementing a multipole gravity solver, parallel NetCDF, and in porting the FLASH Code to QSC) and from the Computational Physic group (e.g., in creating stable initial white dwarf models and in developing and implementing a flame capturing module).

2 Code

Participants: A. Dubey, W. Freis, B. Gallagher, K. Riley, D. Sheeler, A. Siegel (Group Leader)

2.1 Mission and goals

The Code Group is made up of software engineers with backgrounds in physics, applied math, and computer science. The role of the Code Group is to support the research of the Astrophysics Group by overseeing the maintenance, development, and design of the Center's flagship software—FLASH2. FLASH2 is an ambitious and far-reaching project, and each of these roles necessarily involves considerable direct input from both Astrophysics and Computational Physicists. Members from all groups contribute the future direction of the FLASH code in an open committee process, but it is the responsibility of the Code Group to harness these inputs and provide a tangible solution and project implementation plan. Members of all groups also help with debugging and support, but the code group attempts to minimize this burden by overseeing and organizing the process.

2.2 FLASHTEST

A major activity of the Code Group is to continue to develop and utilize the Center's sophisticated home-grown testing framework – FLASHTEST. FLASHTEST is the backbone of the group development process, automatically running over fifty tests several times a week on 10 different platforms. It is a highly extensible framework which allows developers to easily add new tests when new functionality is added to FLASH.

Our use of FLASHTEST has evolved of the past year to further diminish the burden on people outside of the Code Group. A Code Group member is assigned the responsibility of checking FLASHTEST results at the beginning of each day. If errors occur, this person must first try to solve the problem themselves. If that fails, the problems are discussed privately among the Code Group members. Finally, if it cannot be resolved, it is brought to the attention to the other Groups for assistance, with some guidance as to what/where the problem might reside.

The FLASHTEST software has also evolved considerably over the last year, with many tests added for new solvers, grid management, and performance. Also, the tests have been re-characterized as "essential" and "non-essential", helping us more easily manage failures. An email notification process is also in place, where those possibly responsible for a failure are automatically notified by email.

There are many other small feature enhancements. To gain a sense of these and to see how FLASHTEST works in general, our results are made public on the Flash web site: http://flash.uchicago.edu/˜tester/tests/

2.3 FLASH feature tracker

A major responsibility of the Code Group is to organize of and prioritize the huge number of pending tasks that are typical of any software project. These come from both in-house users as well as our growing external user community.

To manage all of this, the code Group has developed a FLASH-specific Feature Tracker built off of open-source software. Over the past year our understanding of how to use the tool has grown considerably. Users have become accustomed to logging there problem directly into our database, and a member of the Code Group has been assigned the responsibility of re-prioritizing and reporting on pending issues.

2.4 Repository management

Perhaps the most difficult high-level challenge for the Code Group is organizing the group development process. Having repository management (CVS) is not enough. With 10-20 developers working simultaneously at very different levels, a meeting schedule and communication hierarchies must be established to ensure a proper flow of development. The Code Group has spent a considerable amount of defining and refining this process.

Part of this includes a versioning system whereby external users can quickly benefit from bug fixes and additions to the code. Previously, FLASH was organized around point releases and occasional patches. Katherine Riley has developed a system where weekly builds can be automatically generated from CVS and posted on the website between point releases. This should significantly enhance the experience of our external users.

2.5 Other new work

In addition to overseeing the software process as described above, the Code Group has completed several significant longer-term projects described below. Over the past year we released FLASH version 2.4. A "what's new" list for the latest version can be found on our public online documentation http://flash.uchicago.edu. A number of these issues are described in detail below.

2.5.1 Optimized multigrid solver

Dan Sheeler has spent a considerable portion of his time rewriting and optimizing major portions of our native AMR multigrid solver. Implicit solvers typically perform and scale poorly on adaptive meshes, specifically because of load imbalances and the high cost of guardcell fills compared to a static mesh. Our goal was to 1) evaluate performance by establishing quantitative metrics ("slow compared to what") and 2) improving this performance when/where necessary.

Ultimately, Dan was able to improve our multigrid performance by a factor or 2–3, getting us to the regime where the self-gravity/hydro balance is close to 1-1 for many of our integrated simulations. His results will be presented in poster form at our upcoming site visit.

2.5.2 Parallel NetCDF I/O module

Consistent with Flash's philosophy of modular interchangeable parts, a second high-performance I/O module was added to the code. FLASH was previously based entirely on HDF5, but we considered it important to give our users alternatives—on some platforms another strategy might be more efficient, robust, etc.; they might be accustomed to a different I/O format.

Argonne had undertaken a project to create a parallel version of the popular NetCDFlibrary, and FLASH was one of its first trial applications. Brad Gallagher defined and implemented the NetCDFbindings for the FLASH I/O module. Additionally, he has written versions of FLASH post-processing tools (VIZ, etc.) to operate on the NetCDFoutput format.

FLASH has been fully tested with the new I/O format and it has reached production level on both the IBM SP2 machines (Frost, Blue Pacific, Blue Horizon) and the new Compaq Alphaserver Cluster (ASCI Q). Performance improvements are significant in some cases. These will be presented as both a poster at the upcoming site visit and written up for a future conference proceedings.

2.5.3 Runtime Visualization

FLASH has always included two separate runtime visualization models 1) a development version based on parallel vtk and 2) a production version based on a small, portable graphics library called GD.

The former is fully parallel and provides support for full 3d rendering. However, it is very difficult to use in an uncontrolled environment, and even harder to distribute in a portable production form. Its development is currently targeted for use with any in-house resources. The second version is currently limited to 2d (slices), and we have had to develop the parallel support ourselves, but it is easy to port and builds seamlessly with FLASH on all of our supported platforms.

As anticipated, in the past year with our huge volume of data being produced remotely the need for runtime visualization has come even more to the forefront of the Center. Alvaro Caceres (now very part-time in Code Group) has worked with Astrophysics and Computational Physics groups to continue to refine and extend our GD-based runtime visualization to fit the specific needs of our simulations. Additionally, he is completing a Python/Swig-based steering tool tailored specifically for FLASH that will make it easier for our users to monitor runs and access the images produced by the runtime visualization.

2.5.4 Scalability studies

As we increase the scale of our Astrophysics simulations an issue of growing concern for the code group is the scalability of our algorithms from hundreds to thousands and tens of thousands of processors. Furthermore, with the next generation of ASCI supercomputers designed in the 100K processor regime, an eye toward scalable algorithms is becoming critical.

To study FLASH scaling we have undertaken several projects. Anshu Dubey and Katherine Riley have done comprehensive tests on the largest machines (in terms of number of processors) that we can currently access. This includes Red, QSC, Seaborg, and MCR. Her experiments encompass both explicit and implicit numerics. Overall the results are very encouraging but they also point to some areas of potential concern. Details of her work will be presented as a poster at upcoming the site review.

Taking this a step further we have begun to develop a FLASH performance modeling tool that aims to model the performance behavior of FLASH on arbitrary architectures. The tool was originally conceived and developed by Jonathan Dursi. Katherine Riley is currently adapting and extending the tool to address issues of scalability, in particular on huge machines such as BG/L. Preliminary results will be used in to present the case for FLASH as a flagship BG/L testing application at the upcoming BG/L workshop in Reno.

2.5.5 Block redistribution algorithm

One of the principle potential bottlenecks to extreme scalability of FLASH is the AMR block redistribution algorithm—that is, the actual global algorithm that moves the blocks to new processors once a Morton curve is defined. This code is tricky to scale and can be written a number of ways, depending on tradeoffs such as memory vs. speed, clarity, testability, etc. To enable FLASH to run optimally on as wide a range of platforms as possible, a “smart” redistribution algorithm has been developed that makes such tradeoff decisions based on user hints and available machine resources. If memory is available, efficiency is increased dramatically; if it is not, the algorithm is still robust and functional. The code can dynamically choose which mode to run in within a given simulation.

It is our hope that this and other similar new algorithms will facilitate the transition to megaprocessor machines such as BG/L.

2.5.6 New generic solvers

The code group is responsible for programming or interfacing generic-type solvers to FLASH. Dan Sheeler has succeeded in improving our integration with the HYPRE linear and non-linear systems library from Livermore. Currently, HYPRE works well with FLASH on uniform meshes. Adding support for adaptivity is an ongoing project. Our hope is that CCA's development of an AMR multigrid component (under the direction of Phil Collela) will greatly simplify this integration, and provide a nice test-case for the use of high-performance components in scientific software.

Additionally, Dan Sheeler and Katherine Riley have worked to integrate IBEAM's PARAMESH-native linear-system-solve into the current version of FLASH. This is intended to be used for problems with radiation.

Anshu Dubey built the portable parallel fft library PFFT into FLASH and tested it to the point where it is ready for production. This could prove to be a very efficient tool for doing Poisson solves on uniform meshes.

Katherine Riley finished a beta version of her native optimized FLASH multigrid solver on a uniform mesh. It should be ready for production in the next several months.

Finally, Anshu Dubey implemented 2-d spherical multipole solver. It works as a submodule of multipole solver, with an algorithm that is different from the main module.

2.5.7 Implementation of portable logfile

During our efforts to collect reliable performance information, the Code Group became aware of the past year of the extreme inefficiency in our methods of sharing/reusing scaling information. FLASH provides a formatted performance summary for each run, but extracting this information and displaying, comparing, and sharing it is a manual process. This led us to consider developing a portable, parsable file format together with tools that can be used to, for example, manipulate, display, and compare them. The idea is that each FLASH run should produce a self-describing XML-type document from which all of the relevant performance information can be extracted. A difficult question that arises is: what is the minimum amount of information required to do this reliably? Wolfgang Freis has worked hard on developing such a self-describing format and implementing it within FLASH. His tool is currently in beta testing.

2.5.8 PARAMESH3

The newest version of our meshing package, PARAMESH3, contains dramatic improvements from the previous version, both in term of performance, features, and software engineering. Since FLASH is based on a home-cooked version of PARAMESH2 with many changes and FLASH-specific improvements, incorporating those changes and updating our version of PARAMESH was a considerable task. Katherine Riley (with help from PARAMESH developer Kevin Olson) worked hard to build the new version into FLASH. One of its major advantages is the ability to run in non-permanent guardcell mode, giving a big savings in memory footprint. These changes have just been completed and they are currently in beta testing.

In the future, we have committed ourselves to working in closer concert with the PARAMESH developers to avoid such a bifurcation in the future. To this end, several FLASH members were granted CVS access to the PARAMESH repository. We consider this a major step forward.

2.5.9 Unit tests

A major focus of FLASH software engineering over the next year will be the decreased emphasis on integrated testing in favor of unit testing (each module self-testing independently of every other module). Since there are module dependencies and code generation in FLASH, this requires some code refactoring. As a test-case, this was done for our equation-of-state module. Our PPM module has been completely rewritten by Bruce Fryxell and a unit test is being designed for it as well. Finally, Katherine Riley added a unit test to verify certain aspects of our AMR grid. All unit tests are currently being integrated into our FLASHTEST software.

2.5.10 FLASH benchmarks

As of last year, FLASH has not published any application benchmarks. Probably the biggest reason is that it is so difficult to define a benchmark that could provide any useful information—details of algorithms differ so much that it is very easy to draw misleading conclusions when making comparisons.

With the help of the other groups in the Center, led by Dan Sheeler the Code Group has put considerable emphasis on defining a reasonable set of tests and making a public platform-specific accounting of their performance. We expect a preliminary version of this page to be online by the time of the site visit.

2.6 Status of FLASH3

In addition to testing, support, maintenance, debugging, and significant short-term development, as described above, a principle responsibility of the Code Group is to lead the effort in defining the next generation of FLASH, which we refer to as FLASH3. Our general vision of FLASH3 is of a dramatically improved software architecture that will much more easily permit a special class of programmers (application developers) to understand and extend FLASH with minimal knowledge of the software internals. Together with this effort comes a FLASH Developers Guide as an extension to our current User's Guide. Also, FLASH3 must provide many of the tools and features that our in-house users have come to need for extremely high-performance simulations.

Our initial efforts resulted in a general list of improvements that define FLASH3 at the highest level. These were all agreed upon by a majority of those interested in voting. Specifically, we came up with the following ten compulsory items.

Required

- PARAMESH3.0 with full non-permanent guardcell support (Riley)
  -nearing completion
- complete unit testing framework for all modules (Siegel)
  -partially implemented – outstanding design issues
- increased componentization using variable set mappers (Weirs, Siegel)
  -partially implemented – outstanding design issues
- decouple driver/time-stepping strategy (Weirs, Siegel)
  -significant progress
- completely redesigned database API (Dubey)
  -design, but no implementation
- portable interactive 3d remote visualization package (Papka, Gallagher)
  -To be based on Argonne FLASHVIZ tool
- built-in memory diagnostics (Riley)
  -design, but little implementation
- support for XML-based standardized performance summary (Freis)
  -first attempt in beta testing
- independent distribution FLASH framework (Siegel)
  -design, but no implementation
- FLASH Developers Guide (Sheeler)
  -very little concrete progress

Still exploring

- 3d support for remote visualization
- FLASH code steering

While the compulsory list may not seem obviously ambitious on the surface, there is in fact a tremendous amount of very challenging work hidden in each item. Carrying out this work in simultaneously with our regular responsibilities, and in an environment with increasingly needed support for large production, is a principle challenge of the Center in the coming year.

Because of the exploratory nature of many of these changes and the implementation complexities that will necessarily accompany them, we developed a committee format to vote on API's, implementation, and code management strategy (in the face of such sweeping changes). Different group members (within any group) can take the lead and propose an API and optionally a partial implementation plan for one of the target items. These are read and discussed at the FLASH3 meetings, and we continue to iterate on design issues until we can reach some consensus. This is a difficult process as user needs often conflict with each other and with certain ideals and models of software engineering.

The result of this process is a set of guidelines and an implementation plan for FLASH3. This document should be available online at the time of the site visit.

2.7 New ports

FLASH has been successfully ported to the new Compaq Alphaserver Cluster (ASCI Q), the new Argonne Xeon-Myrinet Linux Cluster (Jazz), the LLNL Xeon-Quadrics Linux Cluster (MCR), and a smaller Cray SV1.

3 Computational Physics and Validation

Participants: V. Dwarkadas, T. Linde, T. Plewa (Group Leader), N. Vladimirova, G. Weirs.

3.1 Mission and goals

The Computational Physics and Validation group is responsible for selection, implementation, validation and verification of large computational modules for the FLASH code. Deployment of such new physics modules is required for advancing major astrophysics projects of the Flash Center. The group is also directly and indirectly involved in computer science aspects of the code by providing user expertise and data for the visualization, using experimental code modules developed by other groups, and extending code usage to new platforms to identify possible problems and assess usefulness of such platforms for production. To achieve these goals, the group members are closely interacting with astrophysicists, applied mathematicians, and computer scientists, and are directly involved in numerical simulations involving theoretical models as well as the experimental data.

3.2 Flame capturing method

Type Ia supernovae are believed to be explosive events associated with violent deaths of massive carbon-oxygen white dwarf members of close binary stellar systems [8]. The commonly accepted view is that the explosion is caused by a thermonuclear burning which begins subsonically in the region located close to the stellar center. The initial conditions near the ignition point are not well know. It is also possible that at some stage, the explosion transits from subsonic deflagration to a supersonic detonation.

Despite our limited knowledge, observational evidence strongly favors models which begin as deflagrations, subsonically moving burning fronts. Early numerical studies showed, however, that deflagrations moving with laminar flame speeds are too slow to power thermonuclear explosion and produce ejecta composition incompatible with observations. The extended, and now commonly accepted model, is based on realization that a flame front occupying a surface of the rising hot bubble of nuclear ashes will quickly become Rayleigh-Taylor unstable, get wrinkled, increase its surface and consequently rate of energy generation and "effective" speed. Such a turbulent flame model was first considered by Khokhlov [13]. Since thickness of the deflagration front is 6–8 orders of magnitude smaller than the star (thickness of the flame front is about 1–100 cm while the radius of a Chandrasekhar mass white dwarf is $\approx 2 \times 10^8$ cm), it is impossible to resolve the flame in direct numerical simulation and it is necessary to develop a suitable subgrid model.

To enable modeling white dwarf deflagrations with FLASH, Vladimirova, with contributions by Weirs, Plewa, and Robinson, developed a flame capturing (thick flame) model following prescription given by Khokhlov. Khokhlov's scheme was demonstrated to successfully account for several observed characteristics of Type Ia supernovae and its relative simplicity (when compared to level set or volume of fluid methods) makes it a primary choice for implementation. The numerical model includes a compressible flow scheme coupled with a advection-reaction-diffusion solver which describes spatial and temporal evolution if the subsonic flame front. Vladimirova's work provided initial analysis of the flame model, constructed an initial prototype, implemented and tested a complete set of modules into FLASH. Extensive testing included simplified KPP reaction rate [17] and original step-like formula of Khokhlov, tests with constant and variable flame speeds, laminar and turbulent prescriptions for evolution of the flame speed, and extensions to cylindrical and spherical geometry. One of the first applications of the model was study of initial stages of the Landau-Darrieus instability [18; 3; 23]. Figure 1 shows cusp formation in case of moderate ($\delta\rho/\rho = 2$) density jump.

Proposed future developments in the direction of flame modeling will include improvements and extensions to the existing thick flame model. More specifically, current implementation does not support variable composition of the unburned material and our studies are limited to a class of chemically homogeneous stellar models. Moreover, we are not accounting for subtle effects of nuclear statistical equilibrium which affects overall energetics of the explosion and is required to obtained a detailed chemical composition profiles of the ejected material.

Since we anticipate that the Astrophysics group will soon be obtaining realistic Type Ia SN explosion models, the next step will be to compare these models with observations. Dwarkadas and Plewa launched an initiative aimed at bringing capability of modeling of Type Ia SNe light curves top the Flash Center. Here the typical approach is to compute theoretical supernova light curves and their colors using ejecta structure obtained from the explosion model. This is usually done only during early expansion phases (the first few weeks) when the synthetic light curves and colors can be directly compared to the observations.

The accurate computation of the light curves involves multi-dimensional radiation transport and non-LTE conditions. We are not aware of existence of a complete production-quality three-dimensional supernova light curve code. We contacted several researchers in this field including Philip Pinto (U. Arizona) and Peter Lundqvist (Stockholm University). The most promising effort appears to be work of Peter Höflich (U. Texas) with whom we established a close collaboration. The first step in this collaboration is setting up a viable interface between the output from the FLASH Type Ia models and the input to Höflich's radiative transfer code. More progress in this direction is planned in 2004.

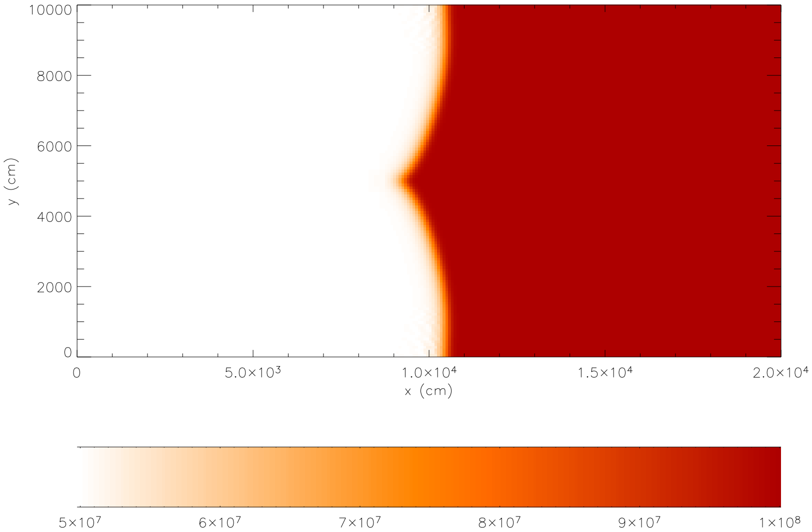

Figure 1: Cusp formation in the Landau-Darrieus problem. Density flowfield is shown at $t = 9 \times 10^{-3}$ s for initial density $\rho_{\mathrm{U}} = 5 \times 10^{7}\,\mathrm{g\,cm^{-3}}$; the density contrast is $\delta\rho/\rho = 2$.

3.3 Magnetohydrodynamic methods

The FLASH MHD module has been upgraded by Linde to include resistive, viscous, and heat conduction processes. All of these features became available in FLASH 2.3 released in June 2003. The viscoresistive part of FLASH has already been exercised by external users resulting in scientific publications [5]. Linde together with L. Malyshkin have started using these latest additions to study the two-dimensional magnetic reconnection problem proposed by S. Wainstein & Z. Mikic. Figure 2 shows the flux function at the height of the reconnection process while Figure 3 depicts corresponding current distribution.

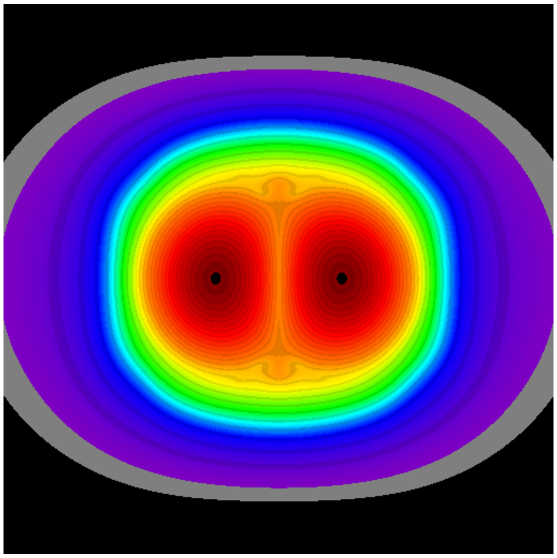

Figure 2: The flux function at the height of the reconnection process for the rosette initial field configuration.

The first version of fully relativistic MHD module has been implemented in FLASH. Although the module is missing full characteristic decomposition of the Jacobian, it successfully passed a series of tests on problems proposed by Balsara and Komissarov. Linde also incorporated a 2D Hall MHD module in FLASH. This development required construction of the Helmholtz solver for which the multigrid part of the code was used. Extensions to three dimensions are possible but will require development of an implicit solver. Linde and C. Zanni wrote a version of the MHD module for cylindrical geometry. The module was tested and the results for the jet acceleration will be presented in October 2003.

Progress was noted in research towards a consistent theory of Burgers turbulence in one dimension [2]. This work is being extended into compressible regime with perpendicular magnetic field. The ultimate goal of this project is to develop theory of compressible MHD turbulence in interstellar clouds. There are also concrete plans to begin a MHD validation study of the PPPL's magnetic reconnection experiment (MRX)

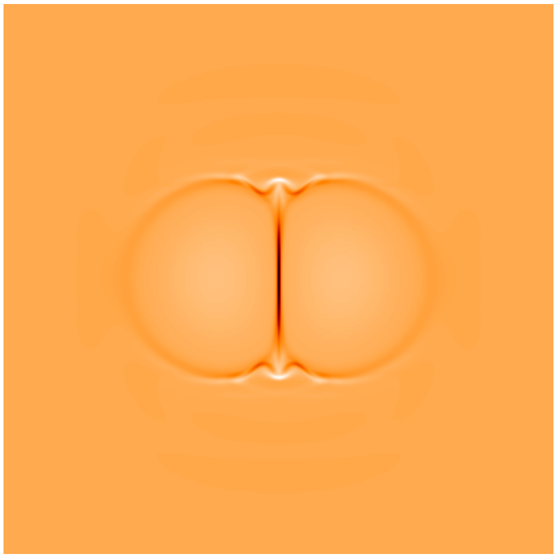

Figure 3: Current distribution at the height of the reconnection process in for the rosette initial field configuration.

and liquid metal wave experiments within the NSF Frontier Center.

3.4 Implicit methods for compressible hydrodynamics

The Barely Implicit Correction (BIC) method was chosen after determining the needs of the Astrophysics group and searching the literature for possibilities. BIC has the following properties, which make it a good choice for FLASH: only mild restrictions on the equation of state; no restrictions on the density distribution (such as incompressibility or hydrostatic background); only a scalar elliptic equation must be solved, as opposed to an elliptic system. The third feature is significant as we are still developing the capability to solve elliptic equations in FLASH. Finally, the authors claimed BIC would work with "any explicit base scheme," though they used Flux Corrected Transport (FCT) exclusively.

A prototype version of BIC was coded in one dimension, and eventually, it was found that only the FCT algorithm worked as a base scheme. Other explicit methods were unstable because they solve the mass, momentum, and energy conservation equations as a system, while FCT treats each independently; this allows FCT to advance the mass conservation equation at a time step independent of the sound speed. For ideal gases, the prototype code demonstrates that the stable time step for BIC is indeed independent of the sound speed, and BIC becomes more efficient than FCT for maximum Mach numbers below 0.2. At this point FCT and BIC have been implemented in FLASH. FCT has completed preliminary testing, and BIC is being debugged and tested; preliminary results are expected around mid-fall 2003.

3.5 Validation studies

In their validation efforts Dwarkadas, Plewa, and Weirs focused on collaboration with experimental hydrodynamics group led by Chris Tomkins and Robert Benjamin at Los Alamos National Laboratory. Several numerical models describing hydrodynamical evolution of the so-called single and double cylinder experiment were calculated in two dimensions allowing to quantify importance of only roughly known experimental parameters. These studies indicate that even though numerical models are capable of capturing overall morphology of the system, including velocity evolution, in cases of some experimental configurations single diagnostics used so far may not be sufficient for making meaningful comparisons. To facilitate such comparisons, extended three-fluid numerical models will be constructed. The group also obtained the first three-dimensional model of the whole experiment which indicates possible existence of three-dimensional effects (Widnall-like vortex instability). In what follows we present more detailed description of the experimental setups and numerical results.

The Los Alamos experiments involve planar collision of horizontally propagating planar Ma=1.2 shockwave with one or two cylinders of sulfur hexafluoride (SF_6) vertically flowing into a shock tube. Due to difference in densities between the shocked air and column material, the shock impact vorticity to be deposited along the surface of the gas cylinder. Once the shock has crossed the cylinder, the cylinder develops vortex rolls. Comparison between overall morphology and velocity distributions observed in experiment and in the numerical model provide measure of the code's accuracy.

The initial conditions for our numerical simulations are provided in the form of a TIFF image. The image is converted into the FLASH-readable format and carefully interpolated onto the initial computational grid. The maximum concentration of the SF_6 gas is not exactly known and is treated as an input parameter. The only other free parameter in our current models is numerical resolution controlled by changing the number of grid refinement levels (see below).

We have carried out a large number of two-dimensional two-fluid FLASH simulations to model the interaction between the shock and cylinder. During our early studies, we have found that use of a contact discontinuity steepener, an optional part of the PPM hydro solver, is responsible for creation of additional flows structures. No special treatment of contact discontinuities was used in the following studies.

Due to relatively small size of the gas cylinder, the shock-cylinder interaction problem is well suited for the adaptive mesh refinement code. To allow the AMR algorithm to track only essential flow structures, we have modified the grid refinement criteria by adding refinement based on the abundance of SF_6. Our simulations capture the details of the interaction and the formation and evolution of the vortex rolls in reasonable detail, but tend to give rise to more small-scale structure than is seen in the experimental results. As expected, the amount of structure increases with increasing levels of refinement indicating possible need for inclusion of viscous effects. Finally, to assess possible influence of nonuniform discretization on the flow we also ran a model in which we uniformly refined a rectangular region centered on the SF_6 column. This approach prevents creation of small-scale grid-induced numerical perturbations which results in spurious flow structures.

We have also obtained two medium resolution three-dimensional models of the shock-cylinder interaction. Primary target architecture for these simulations was the QSC OCF system at LANL. Modeling in three dimensions posed new problems since experimental diagnostics is essentially two-dimensional. For this reason we have created approximate initial conditions by assuming that the SF_6 gas will diffuse horizontally as it flows down from the tank through the shock tube. Thus the cross-section of the cylinder will increase along its length while the maximum concentration of SF_6 will decrease. Using an adaptive grid, we have been able to obtain equivalent resolutions up to $1024^2 \times 5120$.

The results of simulations of the single cylinder experiment were used by Michael Papka and Randy Hudson (both ANL) in their work on the visualization software FLASHVIZ. FLASHVIZ will serve as a portable parallel visualization platform for the FLASH code with volume rendering capability. An example of FLASHVIZ visualization is presented in Figure 4. The second set of LANL experiments involves two SF_6 cylinders. In this case there is one additional parameter, the distance separating the two cylinders, S_D, where S is the spacing between cylinders and D is their diameter. Original experiments have been carried out with 6 different values of this distance. For our study we selected only three cases: S_D=1.2, 1.5, and 2.0. The experimental data appears to contain a considerable background component, the amount of which is not exactly known and estimated to be around 5–10%. We calculated several models with different amount of background being subtracted (the procedure involves simple removal of constant amount of SF_6 from the image), and found that background has relatively small impact on the solution.

Previous analysis done at LANL indicated that in case of double cylinder experiment two regimes are present: one when the two cylinders are far apart and develop individual vortex rolls, and another when the two cylinders are so close that they behave as a single cylinder. Transition between the two regimes seems to occur around $S_D = 1.5$. In this case each cylinder is forming two individual vortices, but only one of these is well developed. When the distance between the cylinder is decreased to $S_D = 1.4$, a change by a mere 10%, the behavior clearly approaches that of a single cylinder. The FLASH solutions display qualitatively similar behavior.

For the case $S_D = 2.0$, we find that the cylinders undergo an additional global rotation about their centers, in agreement with the experiment. However, the rate of rotation seems to be different than observed in experiment. There are some early indications that the rate of this additional rotation depends on the maximum concentration of SF_6—one of the free parameters in our models.

Initial conditions for the experiments are taken with two different techniques, one using scattering from the water-glycol tracer, and another using Rayleigh scattering from the SF_6 gas itself. However, it is known that diffusion affects SF_6 to much higher degree than it does affect the water/glycol tracer. This directly influences our initial conditions through the experimental diagnostics. To correct for this effect, we started constructing three-fluid hydrodynamical models. The ability to model diffusion effects with FLASH will also allow us to put better constraints on the maximum concentration of SF_6. Also, a substantial progress was made in calculating temporal evolution of the column diffusion (work by Todd Dupont). This model will not only provide an insight into horizontal distribution of SF_6, but will also provide more realistic conditions for the next generation of three-dimensional models.

Figure 4: The flowfield density illustrates the vortex structure induced in a column of sulfur hexafluoride 825 μs after the passage of a Mach 1.2 shockwave. The shock induces vortical motions because of the misalignment between pressure and density gradients characteristic of the shockwave and the column material. Small-scale irregularities also develop because of fluid dynamic instabilities. The data is from a three-dimensional numerical simulation that was carried out using the FLASH code running on the ASCI Q machine. The initial conditions match experiments carried out at Los Alamos National Laboratory. FLASH is a parallel adaptive-mesh-refinement numerical hydrodynamics code developed at the ASCI Alliances Center for Thermonuclear Flashes at the University of Chicago. Visualization was produced using software developed in collaboration with Argonne National Laboratory.

Many of the simulations results obtained for a single- and double-cylinder experiment can be seen at the following URL,
http://flash.uchicago.edu/˜vikram/validation/index.html

Validation studies were recently extended (Weirs, Plewa) to include laser experiments conducted by Harry Robey, Bruce Remington, and their collaborators at the Lawrence Livermore National Laboratory. From three laser experiments, a two-mode Rayleigh-Taylor instability problem was selected for initial study. Preliminary study of initial conditions and computational requirements was conducted and numerical simulations of this problem will be undertaken later this year.

3.6 Other contributions

Greg Weirs, with partial contributions from other group members, spent considerable time on planning and developing changes to the FLASH software hierarchy, with the goal of making FLASH more flexible and more modular. There are two areas which have received the most attention. The first area is the transition to the "new branch," in which the high-level "driver" modules and compute-intensive "physics" modules are more clearly separated in terms of responsibilities and functionality. The main accomplishment was moving a version of the PPM module to the new branch; we view the PPM module as the most difficult to move. In the original branch, the PPM module handled many of the tasks now attributed to the driver modules, and extracting the proper functionality was nontrivial. The second area is the development of "mappers," which provide a formal mechanism for implementing transformations from one set of variables to another. The group members have played a leading role in defining what mappers should do and how they should be used. Weirs and Vladimirova also worked on implementing functioning prototype versions in FLASH.

The validation study represented the first example of use of the new code branch. Porting our single- and double-cylinder problem setups to the new branch required only minimal effort and proved the design successful. The group also promoted alternative to HDF5 I/O packages including NetCDF. This approach makes the code less dependent on and vulnerable to potential problems within HDF5 packages and inclusion of the NetCDFpackage offers generally faster parallel I/O option for the FLASH code. The Code group and the Computer Science group continue working on adding support for NetCDFacross FLASH visualization tools.

3.7 ASCI lab and other interactions

During 2003 the Computational Physics and Validation group was actively interacting with several group of researchers, including:

1. A. Bhattacharjee (plasma physics; UNH)
2. A. Burkert (star formation; MPIA, Heidelberg, Germany)
3. P. Colella (partial differential equations; LBNL)
4. R. Fitzpatrick (plasma physics; UT Austin)

5. S. Gopal (numerical hydrodynamics; Naval Research Laboratory)
6. J. Greenough (numerical hydrodynamics; LLNL)
7. P. Höflich (supernovae; UT Austin)
8. H. Ji (experimental plasma physics; PPPL)
9. A. Khokhlov (combustion; Naval Research Laboratory)
10. K. Kifonidis (supernovae; MPA Garching, Germany)
11. E. Oran (combustion; Naval Research Laboratory)
12. B. Remington (laser-driven hydrodynamics experiments; LLNL)
13. W. Rider (numerical hydrodynamics; LANL)
14. H. Robey (laser-driven experimental hydrodynamics; LLNL)
15. M. Różyczka (accretion disks; Copernicus Center, Warsaw, Poland)
16. C. Tomkins (experimental hydrodynamics; LANL)

A number of interactions also took place during meetings and conferences, some of them during the AMR2003 workshop organized at the Center, and included John Bell (LBNL), Attilio Ferrari (U. Torino, Italy), Rob Falgout (LLNL), Galen Giesler (LANL), Wolfgang Hillebrandt (MPA Garching, Germany), David Keyes (Columbia), Mark Marr-Lyon (LANL), Ewald Müller (MPA Garching, Germany, James Quirk (LANL), Brian Van Straalen (LBNL), Robert Weaver (LANL).

3.8 New arrivals

Beginning October 1, 2003, the group will be joined by Hua Pan, Institute of High-Performance Computing Center, Singapore. Dr. Pan will contribute his experience in solving weakly compressible problems and overset grid technology. He is expected to work closely with researchers at the Lawrence Berkeley National Laboratory towards adding low-Mach number flow modeling to the FLASH code.

4 Astrophysics

Participants: A. Alexakis[1], N. Boittin[2], E. Brown, A. Calder, J. Dursi[1], B. Fryxell, A. Heger, D. Lamb, B. Messer, A. Mignone[1], J. Morgan[1], F. Peng[1], K. Robinson, F. Timmes, R. Rosner, J. Truran (Group Leader), M. Zingale, J. Zuhone[1]

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[1] Graduate student

[2] Undergraduate student

4.1 Mission and goals

The astrophysics group has the responsibility to carry out the large-scale astrophysics simulations which are the heart of the Flash Center and to carry out the analysis and interpretation of the computational results in light of astrophysical observations.

4.2 Overview of astrophysics activities

The sixth year of astrophysics research has witnessed significant progress on several fronts. Development of the various physics modules required for the FLASH code has continued, as the thermonuclear reaction networks, stellar equations of state, and thermal transport coefficient modules (documented in the papers by Timmes [26], Timmes & Arnett [28], Timmes & Swesty [30], and Timmes [27]) have been complemented by modules for self-gravity and implicit diffusion that have been thoroughly tested and benchmarked. The Poisson solvers added to the FLASH code have been tested using the Jeans instability problem (for periodic boundaries) and the spherical collapse problem (for isolated boundaries), and are currently being utilized for our calculations of the deflagration of a Chandrasekhar mass white dwarf.

Flash Center astrophysical research is concerned with three explosive events arising from the accretion of matter onto the surfaces of compact stars in close binary systems. Nova explosions involve hydrogen thermonuclear runaways on the surfaces of white dwarfs. Type Ia supernovae involve the incineration of Chandrasekhar mass, carbon/oxygen white dwarfs. Type I X-ray bursts involve hydrogen/helium thermonuclear runaways on the surfaces of neutron stars.

The focus of Flash astrophysics activities over the past year has been on novae and Type Ia supernovae. The prime objective of the Center has been to carry out large scale, integrated, multi-physics simulations of these events. This work will be reviewed extensively in the following discussions. Analytic and numerical studies of X-ray bursts are also continuing, but large scale, integrated, multi-physics simulations of these events have not been a priority.

4.3 Studies of nova outbursts

Classical novae are a manifestation of thermonuclear runaways in accreted hydrogen/helium shells on the surfaces of white dwarfs in close binary systems (see, e.g., the review by Gehrz et al. [7]). Compelling observational data indicate that the material ejected by some classical novae can be significantly enriched in C, N,O, and Ne, by $\gtrsim 30\%$ by mass [21]. It was recognized early that such levels of envelope enrichment could best be explained by dredge-up of some of the underlying white dwarf matter, prior to the final stages of the thermonuclear runaway. The question of how this enrichment is realized has, however, challenged theory now for several decades (see, e.g., the review by Livio & Truran [20]), and constitutes a major roadblock to our understanding of the nova phenomenon. One of the more promising of the proposed mechanisms involves shear mixing [16].

Flash researchers have completed a systematic investigation of one promising mechanism for shear-induced mixing and envelope enrichment in nova white dwarf environments: a resonant interaction between large-scale shear flows in the accreted envelope and interfacial gravity waves [24]. The greater compositional buoyancy in the C/O white dwarf means that the interface sustains gravity waves. Miles [22] showed that in the presence of a shear flow (i.e., a "wind"), gravity waves with a group velocity matching a velocity in the shear flow are resonantly amplified. These waves eventually form a cusp and break. When the waves break, they inject, analogously to ocean waves, a spray of C/O into the H/He atmosphere. The source of the shear could arise from a number of mechanisms, including convection and the accretion process itself. We have explored the effects of such mixing with two dimensional models, in an attempt to demonstrate how the mixed mass depends upon the velocity of the flow, whatever its origin. From a suite of 2-d simulations, we have obtained a measure of the rate of mixing and the maximum mixed mass as a function of the wind velocity. Representative three dimensional simulations further reveal the characteristics of this mixing process. In the context of one dimensional models of nova outbursts, we then explored two scenarios for the mixing process and their implications for realistic models of nova explosions.

4.3.1 Breaking gravity waves: 2-dimensional studies

To calculate the amount of mass mixed by wave breaking as a function of time, we performed a suite of numerical simulations of wind-driven gravity waves in two dimensions. The initial configuration consisted of two stably stratified layers of fluids in hydrostatic equilibrium in a uniform gravitational field g. The upper fluid is composed of H/He at a density ρ_1; the lower fluid is composed of C/O at a density ρ_2. We impose a wind in the upper fluid given by

$$U(z) = U_{\max}(1 - e^{-z/\delta}), \tag{1}$$

where z is the vertical direction and $z = 0$ corresponds to the location of the initially horizontal interface; $U_{\max}$ is the asymptotic maximum velocity at $z \gg \delta$, and δ is the length scale of the shear boundary layer. This choice of wind profile was motivated by studies of the wind-wave resonant instability in oceanography [22].

Alexakis, Young, & Rosner [1] performed a linear stability analysis of the wave amplification for the novae problem. Here we apply those results to the conditions at the base of the white dwarf envelope. With the FLASH code, we were of course able to examine the full non-linear evolution of breaking waves. The equation of state is a gamma-law with index $\gamma = 5/3$, as appropriate for a degenerate, non-relativistic gas. We use periodic boundary conditions along the sides of the box, and hydrostatic boundaries at the top and bottom [32]. The wind profile is specified as an initial condition and in particular is not forced. For this study, we set the Mach number $\mathsf{Ma} = U_{\max}/c_{\mathrm{s}} = 0.5$, where c_{s} is the adiabatic sound speed. We considered four values of δ/H: 0.005, 0.01, 0.02, and 0.05, where $H = \gamma^{-1}c_{\mathrm{s}}^2/g$ is the pressure scale height. This choice varies the reciprocal Froude number $\delta g/U_{\max}^2$, which measures the available kinetic energy for mixing. The simulations were performed on a uniform mesh of resolution 1024×1024.

From the linear theory, the unstable modes have wave numbers $k \gtrsim g/U_{\max}^2$. Figure 5 shows fully developed waves breaking, generation of the "spray", and mixing of

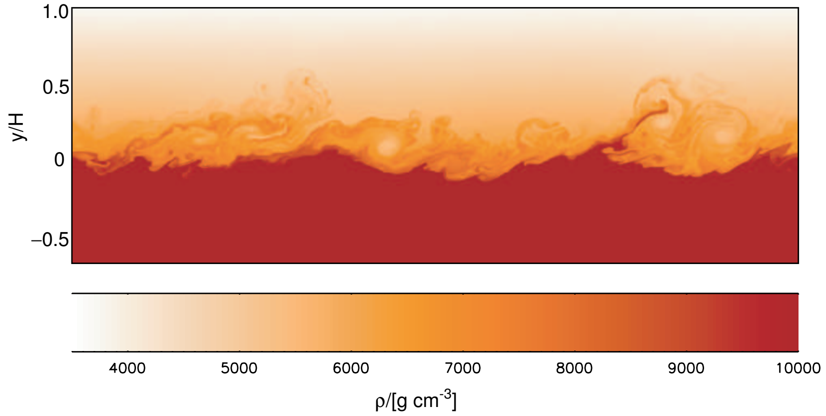


Figure 5: Breaking C/O waves, as determined by a two dimensional simulation. Gravity points toward the bottom of the figure, with the vertical distance y in units of the pressure scale height, as evaluated just above the interface. The color scale indicates the mass density in units of $\mathrm{g\,cm^{-3}}$.

the white dwarf substrate up into the atmosphere. The dominant wavelength that appears here is larger than the value that Kelvin-Helmholtz theory predicts but in agreement with Miles [22]. Mixing is not effected by overturning of the wave but rather by the wind breaking off the tip of the wave. Figure 6 shows the resulting mixed layer at a later time; the black lines, from bottom to top, are contours of the carbon mass fraction at 0.5, 0.2, and 0.02, respectively. The contour at 0.5 corresponds to the carbon mass fraction of the underlying white dwarf, while the smaller contour values indicate how far outward into the accreted material the white dwarf substrate is mixed. The contour at 0.2 shows the formation of a region that contains most of the initial enrichment.

Figure 7 shows the surface mass density of carbon-oxygen in the mixed layer averaged over the horizontal direction. The "mixed" layer is defined here as the layer in which the carbon mass fraction is between 0.49 and 0.01. The C/O is mixed rapidly until it saturates; further mixing occurs on diffusive timescales. Our two-dimensional simulations show, for the range of parameters examined, that the total mass of white dwarf material that becomes mixed is independent of the length scale δ. The rate of mixing, i.e. the initial slopes of the curves in Figure 7, does however show some dependence on δ. Using dimensional analysis and the numerical results, we find that for a fixed density ratio $\rho_1/\rho_2 = 0.6$ the total mass per unit area, $dM_{\rm CO}/dS$ mixed into the H/He saturates at

$$\frac{dM_{\rm CO}}{dS} = \alpha_2 \frac{U_{\rm max}^2}{g} \rho_{\rm WD}, \tag{2}$$

where α is a non-dimensional constant that we determine from our simulations to be $\simeq 0.06$. The timescale to reach saturation is far shorter than the timescale of either the accretion phase ($> 10^4$ yr) or the pre-peak convective phase (~ 100 yr) of a typical

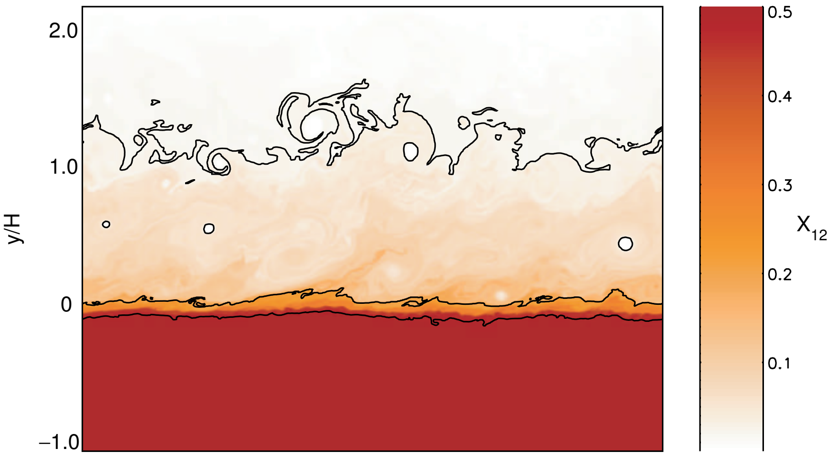


Figure 6: Mass fraction of ^{12}C for $\delta/H = 0.04$ after $t = 3500\delta/U$. The vertical dimension is scaled to the pressure scale height H, as evaluated just above the interface. The contours for ^{12}C mass fractions of, from the top, 0.02, 0.20, and 0.49 are shown. The color scale indicates the ^{12}C mass fraction.

classical nova.

4.3.2 Three dimensional simulations

To test the two dimensional assumption and verify the behaviors we have obtained in three dimensions, we performed three-dimensional simulations on a $(256)^3$ effective grid. The phase space explored in our 2-d and 3-d simulations is identified in Figure 8. Due to the numerical cost of three-dimensional simulations, only three runs were made. The first run (Case A) was chosen so that the evolution of a single mode was studied in a box the size of one wavelength. This run showed the three dimensional structure that appears as the wave becomes nonlinear. In particular the wave remained two dimensional at initial times but as the wave began to overturn three dimensional structures became present, especially at the cusp of the wave and at the "spray" distribution. The surface corresponding to a carbon mass fraction 0.125 enrichment of the envelope is shown in Figure 9.

For the other two cases, a larger box was chosen and a multi mode perturbation was imposed. The first of the two (Case B) was for a strong wind and the second one (Case B) for a weaker wind. Each box was chosen to be large enough so that the amount of mass mixed per unit area is not effected by it. The first run of stronger wind gave similar results to that of the equivalent 2-D case. Although, the structure of the mixed layer in the 3D case was different than the 2-D case, the total amount of mass that was mixed was very close.

The final run with the weaker wind did not yield significant mixing, and no cusp

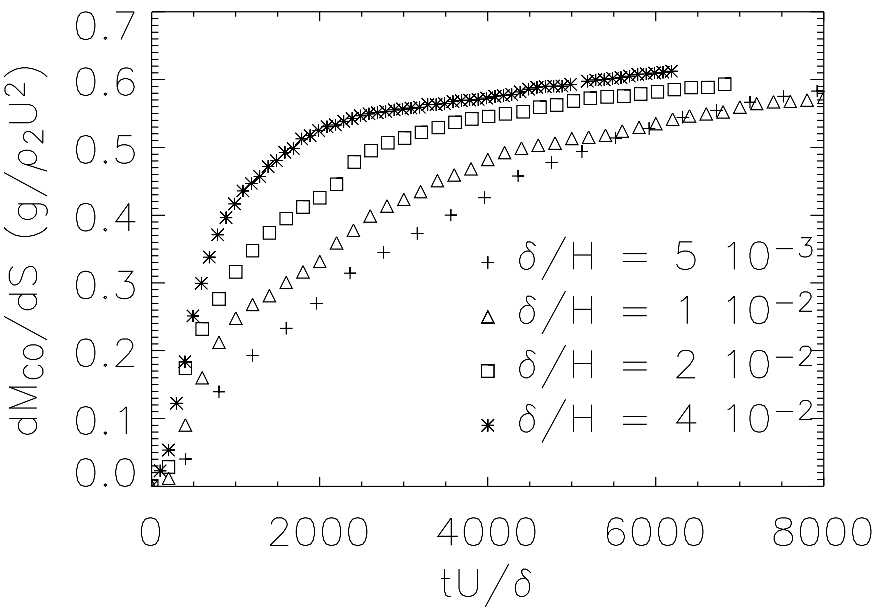
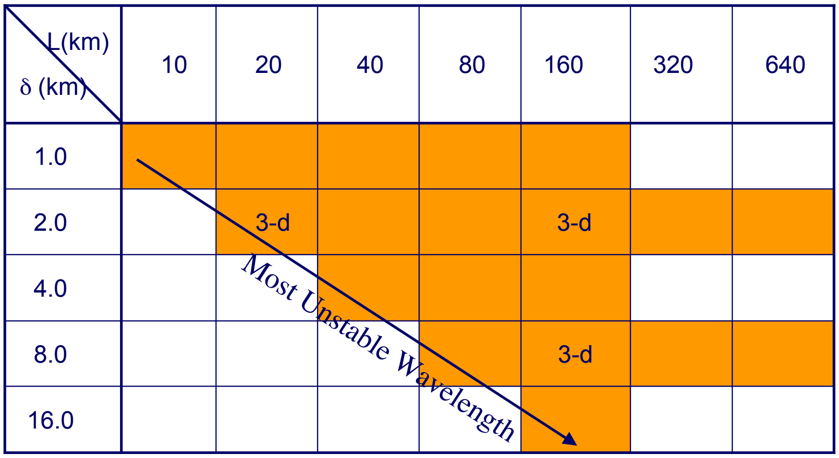


Figure 7: The mixed mass of C/O, per unit area, as a function of time. This was computed by averaging over the horizontal direction in the simulations. Time is scaled to $\delta/U_{\rm max}$ and $M_{\rm CO}$ is scaled to $\rho_2 U_{\rm max}^2/g$. Four different values of $g\delta/U_{\rm max}^2$ were used: 0.01, 0.02, 0.04, and 0.09.



L(km) δ (km)	10	20	40	80	160	320	640
1.0	▨	▨	▨	▨	▨		
2.0		▨ 3-d	▨	▨	▨ 3-d	▨	▨
4.0			▨	▨	▨		
8.0				▨	▨ 3-d	▨	▨
16.0					▨		

Figure 8: The parameter space explored in our two dimensional and three dimensional simulations of wind-driven gravity-wave mixing of C/O substrate into the accreted H/He-rich envelopes of white dwarf stars in nova binary systems. The arrow indicates the trend of the most stable wavelength predicted by the linear theory.

breaking was observed. The reason for this is that, due to the direct cascade, the energy of the wind was dissipated before amplifying the wave to a large enough amplitude for the cusp to break. Thus very little mixing was observed. Further simulations with a wind that is forced might be needed to observe mixing in this case.

4.3.3 One-dimensional nova models

Having identified critical features of the wave breaking and mixing mechanism, we then incorporated our findings into a “global” nova simulation. In order to explore the global properties and implications of this local mixing mechanism, we computed several one-dimensional models of a novae with a modified version of the KEPLER stellar evolution code [31]. For the underlying white dwarf, we used a mass of 1.0 $M_\odot$, a radius of 5000 km, and a luminosity of 10^{31} ergs s^{-1}. The white dwarf was composed of a 50%/50% carbon/oxygen mixture. The accreted material was assumed to be of solar composition, and the accretion rate was 10^{-9} $M_\odot$. Convection was modeled using the Ledoux criterion for stability and mixing length theory, and possible effects of convective overshooting were not considered.

Two scenarios were investigated for generating the gravity wave induced mixed layer.

1. In the first case, we considered the possibility that the shear arises when, during the early stages of the runaway and heating of the envelope, the convective cells drive a wind at the interface between the H-rich atmosphere and the C/O substrate. If mixing were to occur at this stages, convection would be able to

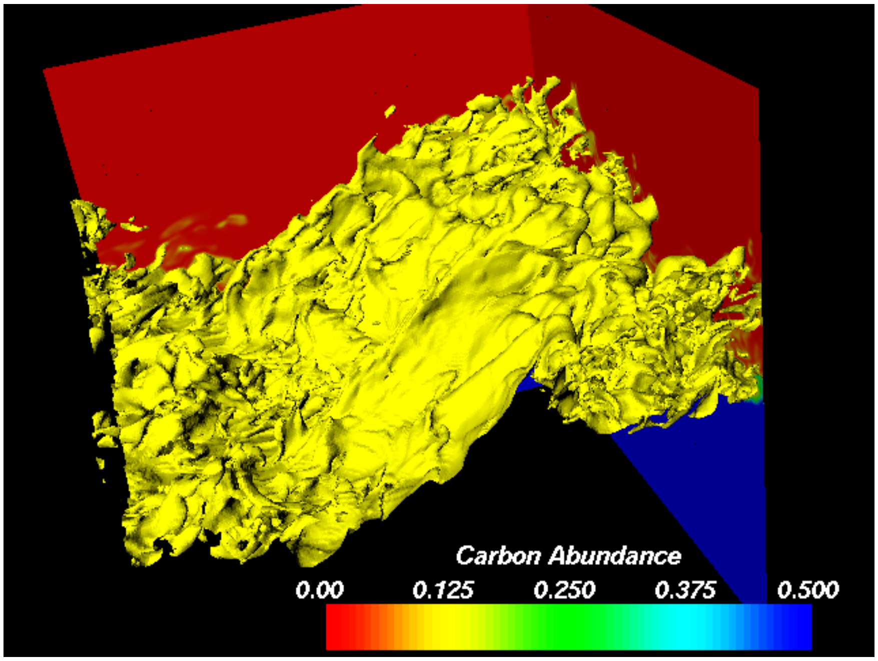


Figure 9: Illustration of the level of mixing of carbon (and oxygen) into the accreted hydrogen/helium-rich envelope on the white dwarf component of a classical nova binary system. For our case A identified above, this shows the isosurface corresponding to a carbon admixture at a level 0.125 mass fraction in the envelope.

distribute the material throughout the convective zone. In fact, as evidenced in Figure 10, the convective region encounters the interface only well after the peak of the runaway and thus no significant enrichment occurs.

2. In the second scenario, we assume rather that the shearing action originates from an accretion-driven wind blowing across the surface of the white dwarf during the early stages of accretion. We assume that the wind persists throughout the H/he layer with velocity sufficient to drive mixing on a timescale much less than that required to accrete a critical mass of fuel. In this case, the mixed layer is generated prior to runaway.

The results for these two cases are summarized, respectively, in the "Kippenhahn" diagrams shown in Figures 10 and 11. We find that if no enrichment occurs prior to the onset of convection, then the convective zone does not reach downward and contact the C/O interface, and no additional mixing occurs (in the one dimensional model) in the absence of convective overshoot. In contrast, an envelope with a (pre) mixed layer at the C/O interface, consistent with the scalings from our high resolution simulations, provides an enrichment level $\approx 25\%$ by mass in C/O (consistent with observations) and yields a significantly more violent (e.g."fast") nova event. These results emphasize the importance of a more sophisticated treatment of the early phases of accretion and the shearing that may be expected to be associated with these phases.

4.4 Type Ia supernova explosions

The observed brightnesses of distant supernovae—together with the assumption that their behaviors precisely mimic those of their nearby counterparts—provide evidence that the expansion of the Universe is accelerating. The tools of choice for these recent explorations of the rate at which the Universe is expanding include, specifically, supernova explosions of Type Ia. Observational studies have identified a correlation between the peak brightness of a SNe Ia and the rate of decline from maximum. Theoretical considerations point toward a "standard model" for Type Ia SNe consisting of a C/O white dwarf which grows to the Chandrasekhar limit as a consequence of mass accretion in a binary system. As the Chandrasekhar limit is approached, contraction yields compression of the core and ignition occurs under highly degenerate conditions. It is the response of the star to this ignition - and the ensuing progress of the flame outward through the white dwarf star - that we wish to establish with our numerical simulations.

4.4.1 Three-dimensional simulations of the deflagration stage

Over the past year, there has been significant progress at the Flash Center toward modeling Type Ia supernovae. Progress has been made on three distinct fronts: (1) the generation of stable initial models of self-gravitating white dwarfs; (2) the development of a flame model; and (3) the integration of these two for application to our multi-physics global simulations of Type Ia explosions.

We have developed a flame model based on the "thick flame" flame model of Alexi Khokhlov. This development was carried out principally by Natasha Vladimirova. The

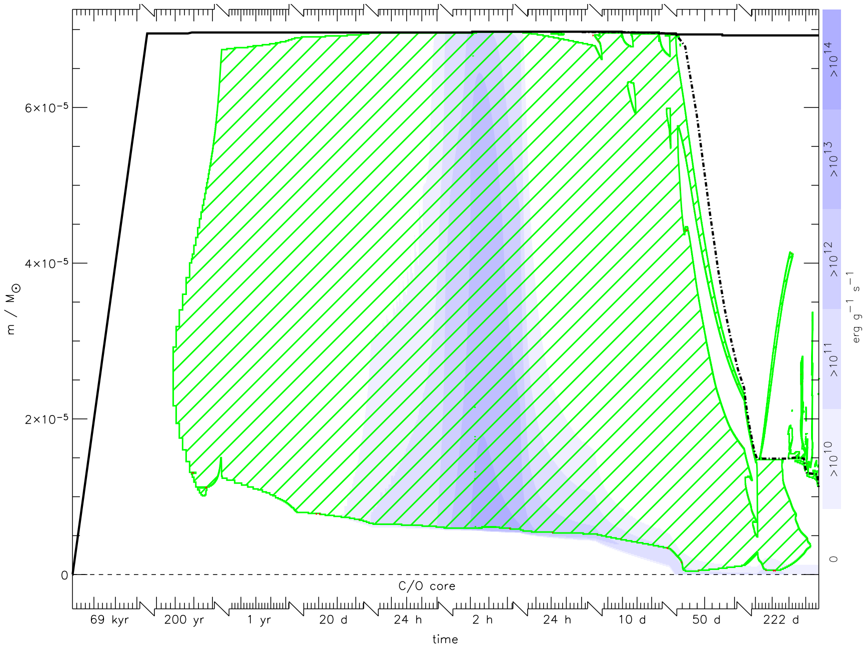


Figure 10: Kippenhahn diagram of a nova without enrichment. The x-axis indicates time intervals for the different evolutionary stages, and the y-axis gives the mass above the C/O substrate. Green hatching (framed by a green line) indicates convection, blue shading indicates nuclear energy generation for which each level of darker blue denotes an increase by one order of magnitude, starting at 10^{10} ergs $\mathrm{g}^{-1}\,\mathrm{s}^{-1}$. The thick black line shows the total mass of the stellar envelope (including ejecta), increasing because of accretion; the dash-dotted line indicates the mass outside of 10^{12} cm; and the dashed line marks the interface between the white dwarf C/O substrate and the accreted layers.

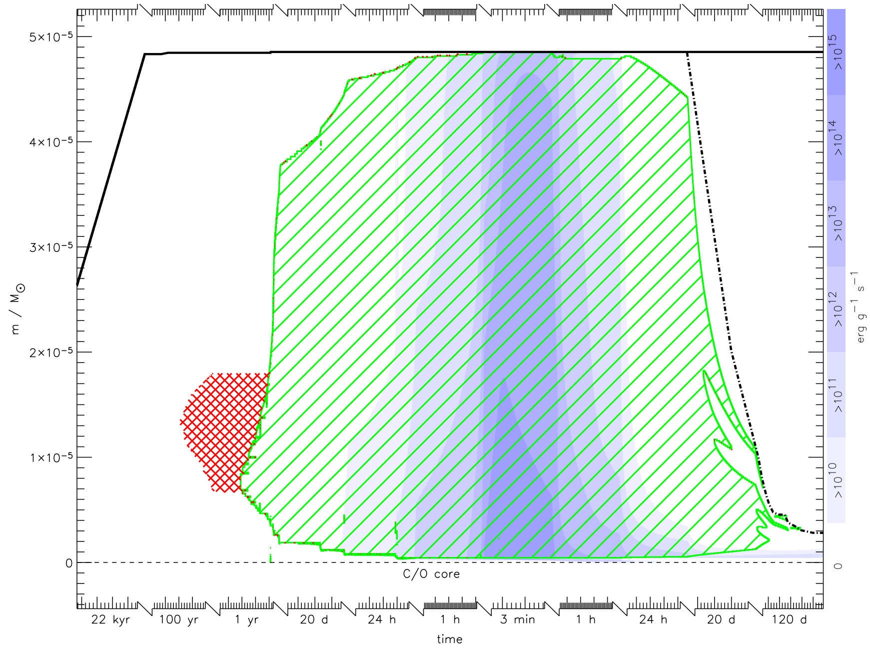


Figure 11: This is the same as in the previous figure, but for a model in which the inner $M_{\rm mix}$ = 4.6 x 10^{28} g are enriched in C/O with a linear composition gradient (with respect to the Lagrangian mass coordinate) between the WD composition (C/O) at the base and the accreted composition (solar) at the upper edge. Note that the convective zone does not reach the interface with the WD substrate, and that a significant semi-convective region, indicated by red hatching, develops prior to the onset of convection.

method allows flame propagation with a specified flame speed. Such a model is necessary for simulating Type Ia supernovae because the disparate length scales between the actual nuclear flame and the white dwarf star make simulations which resolve both prohibitively expensive. The model solves an advection-reaction-diffusion equation for the evolution of a scale variable that determines the position of the flame.

Concurrently, Tomek Plewa obtained realistic Type Ia precursor models from Peter Höflich. The models were adjusted as needed and damped to maintain hydrostatic equilibrium on the multidimensional Flash simulation domain.

Finally, we have made progress in integrating these into multi-physics simulations of carbon deflagrations in white dwarfs. Alan Calder worked with Natasha Vladimirova and Tomek Plewa to perform the first generation of self-gravitating hydrodynamics+flame capturing simulations of deflagrating C/O white dwarfs. These simulations were among the largest Flash simulations performed to date, and investigated multidimensional effects in the carbon deflagrations.

Simulations of a deflagrating white dwarf have been completed in both two and three dimensions. Representative behaviors are shown in the following three figures. The three dimensional runs, which involved the deflagration of complete Chandrasekhar mass white dwarf stars reveal particularly interesting features of such events.

1. The first run consisted of a complete 2000 km Chandrasekhar-mass white dwarf of composition 50%/50% C/O, with a 50 km ignition region at the very center of the star. The effective resolution of the simulation was 10 km. The simulation ran for 1.5 s of time. The results showed that bubbles of hot magnesium ash rose symmetrically along each of the axes. The simulation ran for 86 hours on 1024 processors of ASCI Frost for a total of 88,000 node-hours.

2. The second run consisted of a complete 2000 km Chandrasekhar-mass white dwarf of composition 50%/50% C/O, with a 50 km ignition region offset from the center of the star by 12 km. The effective resolution of the simulation was 5 km. The simulation has revealed the response of the white dwarf over an interval of 1.4 sfollowing ignition. The results show that bubble of hot magnesium ash rises asymmetrically. The first run of this simulation utilized 58 hours of continuous execution on 1024 processors of ASCI Frost for a total of 59,000 node hours. The second run utilized 62 hours of continuous execution on 1024 processors of ASCI Frost for a total of 63,000 node hours.

The results of our simulations were found to be consistent with those of other researchers, for studies of the same resolution. They are distinguished by the fact that we have utilized the entire star - rather than a quadrant or octant. For the case of central ignition, and our chosen resolution, the outgoing bubbles proceeded along the coordinate axes, maintaining symmetry for the remainder of the simulation as would be expected. In contrast, the simulation we ran with the match-head located just slightly off center yielded an extremely non-spherical behavior, with a rising bubble in the direction of the initial displacement (see Figures 13 and 14). This non-symmetric burning holds potentially important implications for models of Type Ia supernovae because it indicates that an off-center ignition may not incinerate the entire star.

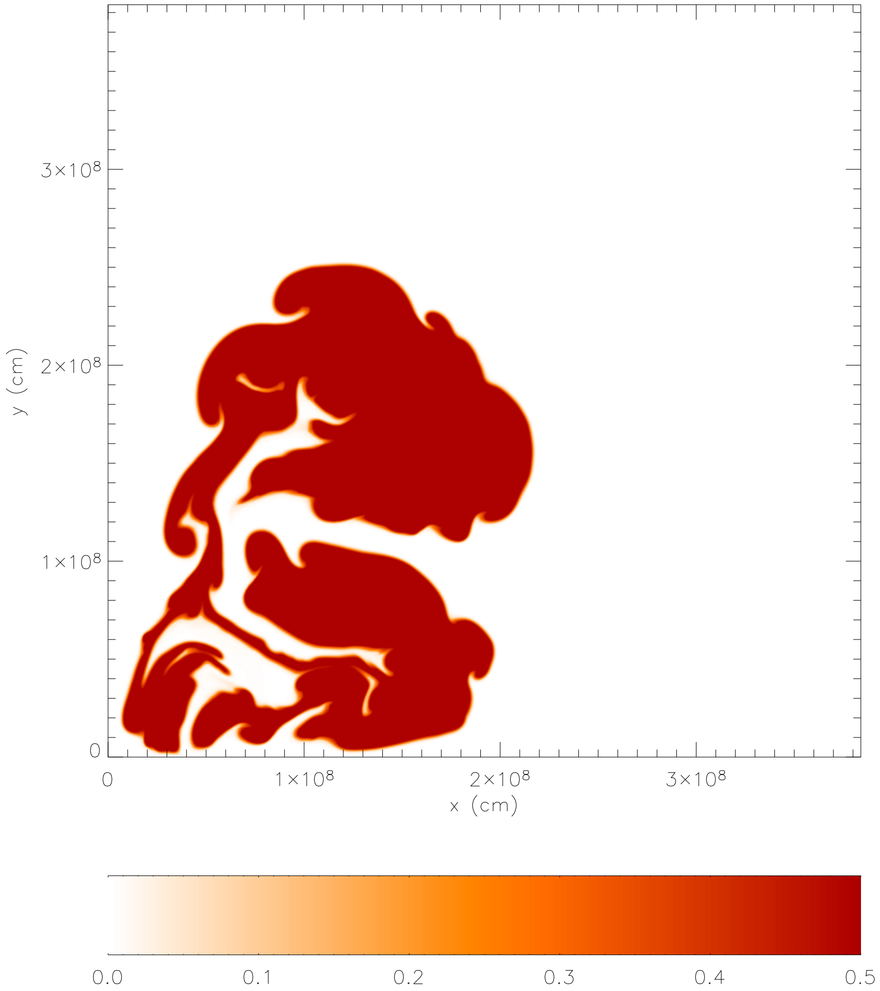


Figure 12: Image of ^{24}Mg abundance resulting from a 2-d cylindrically symmetric simulation of a deflagrating white dwarf. The simulation domain represents one quadrant of the star, and the effective mesh resolution is 5 km. The image shows the rising ‘bubble’ of hot magnesium at 2.75 s after the start of the simulation. The initial conditions consisted of a 50%/50% carbon/oxygen Chandrasekhar mass white dwarf of radius approximately 2000 km, with a 50 km ignition region of burned magnesium at the center.

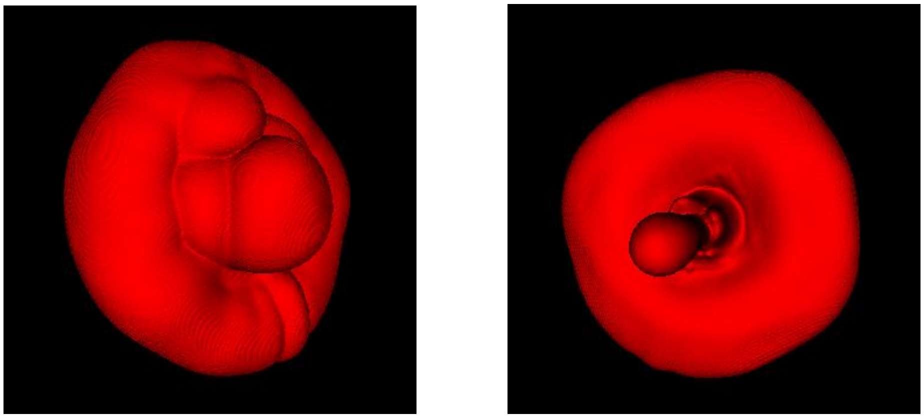


Figure 13: An isosurface of the magnesium abundance viewed from two different directions from a three dimensional simulation of a deflagrating white dwarf. The simulation domain includes the entire star, and the effective mesh resolution is 5 km. The images show the rising “bubble” of hot magnesium at 1.07 safter the start of the simulation. The initial conditions consisted of a 50%/50% carbon/oxygen white dwarf of radius approximately 2000 km, with a 50 km ignition region of burned magnesium non-axially offset from the center by 12 km.

4.4.2 Metallicity dependence of Type Ia luminosities

A critical question with regard to the use of Type Ia supernovae as standard candles is whether there might exist a metallicity dependence that could influence observations of events at high red shift (lower metallicity populations). Frank Timmes, Ed Brown, and Jim Truran [29] have explored the idea that the observed variations in the peak luminosities of Type Ia supernovae originate in part from a scatter in metallicity of the main-sequence stars that become white dwarfs. Previous numerical studies have not self-consistently explored metallicities greater than solar. One-dimensional Chandrasekhar mass models of SNeIa produce most of their ^{56}Ni in a burn to nuclear statistical equilibrium between the mass shells $0.2\ M_\odot$ and $0.8\ M_\odot$, for which the electron to nucleon ratio Y_e is constant during the burn. We were able to demonstrate analytically that, under these conditions, charge and mass conservation constrain the mass of ^{56}Ni produced to depend *linearly* on the original metallicity of the white dwarf progenitor. Detailed post-processing of W7-like models confirmed this linear dependence. The effect that we have identified is most evident at metallicities larger than solar, and is in agreement with previous self-consistent calculations over the metallicity range common to both calculations. The observed scatter in the metallicity (approximately $1/3Z_\odot$–$3Z_\odot$) of the solar neighborhood is enough to induce a 25% variation in the mass of ^{56}Ni ejected by Type Ia supernova. This is sufficient to vary the peak V-band brightness by $|\Delta M_V| \approx 0.2$. This scatter in metallicity is present out to the limiting redshifts of current observations ($z \lesssim 1$). Sedimentation of neon can possibly amplify the variation in ^{56}Ni mass to $\lesssim 50\%$. Further numerical studies can determine if other

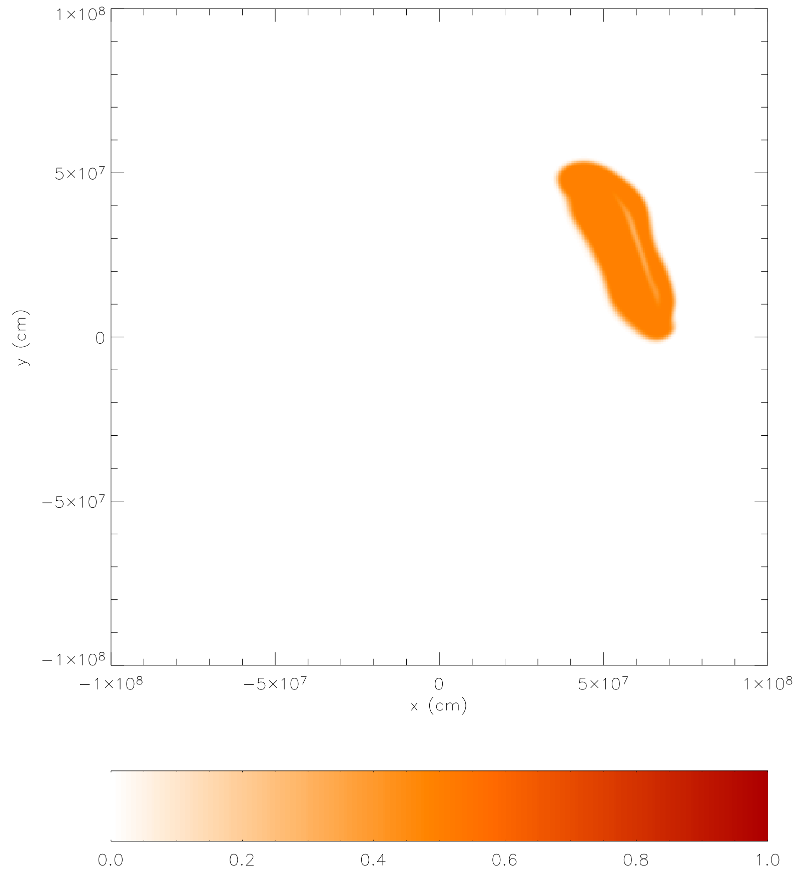


Figure 14: An isosurface of the magnesium abundance in the coordinate system centered on the initial white dwarf configuration.

metallicity-induced effects, such as a change in the mass of the ^{56}Ni-producing region, offset or enhance the variation we identify.

4.4.3 Energetics of C/O deflagrations

Ed Brown and undergraduate student Nathalie Boittin are studying the explosive burning of ^{12}C/^{16}O mixtures under conditions appropriate for a Type Ia supernova. Specifically, they are seeking to understand and perhaps improve the simplified nuclear kinetic scheme of Khokhlov [12; 13; 14; 6] used in simulations of a white dwarf deflagration. N. Boittin has completed calculations of the nucleosynthesis for varying T, ρ and Y_e and is comparing her findings of the dominant reaction flows and heating rate $\dot{S}$ with those of Hix & Thielemann [9; 10]. These studies will not only inform the flame model used in the Flash simulations, but also are preparatory work for a detailed self-consistent 1-D calculation to confirm the dependence of the ^{56}Ni mass on Y_e [29].

4.5 X-ray bursts

Studies of X-ray bursts have been concerned with several aspects of the problems associated with accretion and thermonuclear burning on the surfaces of neutron stars.

4.5.1 Superburst ignition

Ed Brown is investigating the conditions for thermally unstable ignition of ^{12}C on the surface of an accreting neutron star. This ignition occurs at $\rho \gtrsim 10^8\ \mathrm{g\,cm^{-3}}$; at these densities, the large electronic thermal conductivity couples the crust to the core, which acts as a heat sink. Preliminary calculations show that the superburst recurrence time is sensitive both to the level of impurities in the crust and to the neutrino emissivity of the core. The short recurrence time $\lesssim 10$ yr suggests that the crust thermal conductivity is substantially reduced below that of a simple lattice, and that enhanced neutrino cooling is not important. Improved knowledge of superburst recurrence times with observations of the quiescent thermal emission from soft X-ray transients and improved calculations of X-ray burst nucleosynthesis will open a new vista on studying the properties of matter at super-nuclear densities.

Ed Brown is working with J. Fisker (Universität Basel) on a calculation of type I X-ray burst and superburst ignition with a self-consistent determination of the luminosity emanating from the deep crust.

4.5.2 Crustal evolution of accreting neutron stars

Ed Brown and graduate student Fang Peng are exploring conditions appropriate to nuclear burning on neutron stars for a range of accretion rates. Fang Peng performed a one-dimensional calculation of unstable H/He burning and rp-process nucleosynthesis under conditions appropriate for an accreting neutron star. Single-zone calculations compared well with the calculations of Schatz et al. [25]. This work is being extended to study the effects of heavy element sedimentation and diffusion on the unstable ignition of H/He for slower accreting ($\dot{M} \lesssim 10^{-10}\ M_\odot\,\mathrm{yr}^{-1}$) neutron stars. This project is motivated by recent discoveries of such type I X-ray bursts observed from sources at low persistent luminosities ($\lesssim 10^{36}\ \mathrm{ergs\,s^{-1}}$).

Ed Brown is also collaborating with M. Ouellette, a graduate student, and Prof. H. Schatz (both of Michigan State University) to calculate the sequence of electron captures and pycnonuclear reactions in the crust of an accreting neutron star, starting from the distribution of isotopes produced during unstable H/He burning. These results can be used as input to time-dependent simulations of the crust thermal relaxation, and provide a physical basis for estimating the nuclear heating in, and the mechanical properties of the crust.

4.6 Astrophysical flame microphysics

Large-scale simulations of supernovae of Type Ia, which are essential for the ultimate understanding of the supernovae mechanism, need flame physics input at three stages:

- Ignition and early flame propagation
- Large scale burning in a turbulent medium
- A transition to detonation (should one occur)

The current state of the art in multidimensional calculations is to ignore the first point by simply imposing some already-ignited regions in the domain, and to treat large-scale burning by using a flame speed model which is based on scaling arguments. Very little rigorous work has been done on the third point, on discovering an astrophysically relevant mechanism for deflagration-to-detonation transitions (DDT).

On the other hand, the terrestrial combustion literature has a large body of work on ignition, flames in turbulence, and transitions. An excellent review on turbulent flame velocity, for instance, is [19], where it is made clear that the problem is greatly more complicated than the simple scalings used in the current generation of large-scale simulations. The state of terrestrial flame-turbulence research is greatly more sophisticated than the current astrophysical corpus, and we would like to begin placing astrophysical combustion research on the same rigorous footing as terrestrial combustion research.

Beside turbulent burning, small-scale flame physics will also certainly be very important during the early ignition phase, before the flame has yet grown to the size of large turbulent eddies. Should there be a deflagration-to-detonation transition, this too will certainly depend on the small-scale flame behavior. Thus, one important aspect of research at the Flash center is understanding the microphysics of astrophysical flames.

One aspect of our investigation of flame physics has been to examine the behavior of well-known flame instabilities such as Landau-Darrieus in the context of astrophysical flames and degenerate matter. These instabilities can distort and wrinkle the flame surface, increasing the amount of burning and thus the rate of energy input.

4.6.1 Effects of curvature on nuclear flames

Any wrinkling or distorting of the flame surface will curve or strain the flame surface, which can in turn affect the flame speed, and thus the growth of further wrinkling. The

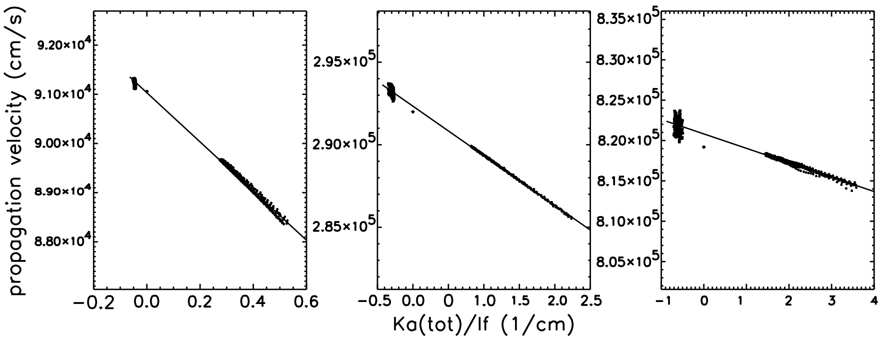


Figure 15: Flame speed versus dimensional strain rate for an astrophysical flame in a 50% Carbon, 50% Oxygen medium at a density of 5×10^7 g cm^{-3} (*left*), 1×10^8 g cm^{-3} (*center*) and 2×10^8 g cm^{-3} (*right*). Data points for positive strain are from simulations of a spherically expanding flame, data points for zero strain are for a planar flame, and those for negative strain are for a spherical flame propagating inwards. The slope of these lines are the Markstein lengths for these flames.

behavior of the local burning under stretch is often parameterized by a dimensionless Markstein number, Ma. This quantity is known to be related to the ratio of diffusivities, or Lewis number (Le) in the flame; in terrestrial flames, this number is of order unity, whereas in astrophysical flames in degenerate material, this number is of order 10^9.

The effect of curvature on local burning rate is often measured experimentally by observing the propagation of outwardly propagating spherical flames. As the radius of the flame increases, the local curvature decreases, and the flame's burning rate can be measured as a result of the curvature.

Jonathan Dursi and Mike Zingale (at UC Santa Cruz) have numerically measured the Markstein number [4] for relevant astrophysical thermonuclear flames using one-step burning. (See for instance Figure 15). Parallel work was done with a model flame where important flame parameters can be adjusted, so that the behavior we see in the astrophysical flame can be understood. It was found that the fact that astrophysical flames propagate solely by thermal (rather than species) diffusion means that the flames of interest resist being wrinkled on small scales. It was also found that certain types of model flames, such as artificially 'broad' flames using KPP-like reaction networks, do not behave like 'real' flames under strain and curvature, as shown in Figure 16.

4.6.2 The effect of magnetic fields on flame instabilities

The progenitors of Type Ia supernovae are not are thought to be white dwarfs. Many such objects have significant magnetic fields (of up to 10^9 G on their surface). Magnetic fields of this magnitude can certainly affect essentially hydrodynamic instabilities such as the Landau-Darrieus instability.

In this work in progress, Jonathan Dursi is examining the linear stability of flames under such a magnetic field. It is found that the magnetic field can greatly suppress

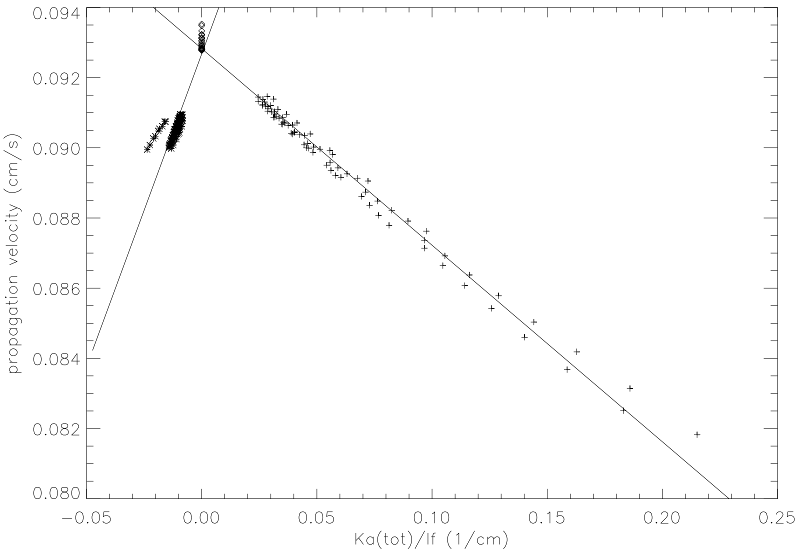


Figure 16: Flame speed versus dimension-full strain rate for a KPP flame with large Le, as in the previous figure. Note the odd 'kinked' behavior of these flames.

the instability but only if the magnetic field is strong enough that the Alfvén speed ($v_A = B/\sqrt{4\pi\rho}$) is greater than the flame speed S_l. An example of this is shown in Figure 17, where the growth of the instability becomes greatly different from the zero magnetic-field case only when $\bar{a}_u = v_A/S_l$ is significantly larger than one.

This effect, then, is likely to be relatively small in a white dwarf; however, it may play a larger role in burning dynamics on the surface of a neutron star.

4.7 ASCI lab and other interactions

The Astrophysics group has collaborated with scientists both at the Labs and at other universities; collaborators include:

1. D. Arnett (supernovae, validation; University of Arizona/Tucson)
2. A. Bayliss (novae and X-ray bursts; Northwestern University)
3. A. Burrows (supernovae; University of Arizona/Tucson)
4. A. Glasner (novae; Hebrew University of Jerusalem)
5. W. Hillebrandt (novae and supernovae; MPI Garching bei München)
6. R. Hoffman (reaction networks; LLNL)
7. E. Müller (relativistic astro; MPI Garching bei München)

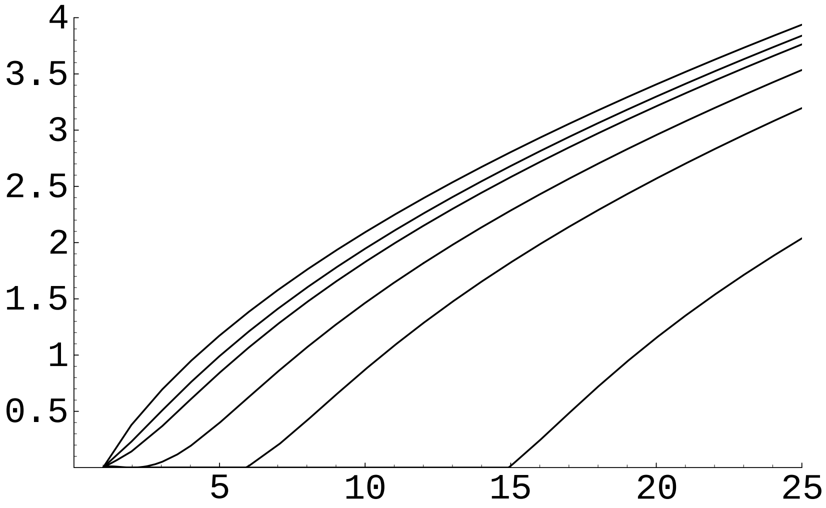


Figure 17: The scaled growth rate ($\bar{n}$) as a function of density jump across the flame $\alpha = \rho_u/\rho_b$, in the absence of gravity. Lines are plotted for, top to bottom, $\bar{a}_u$ = 0, 1,4/3, 2, 8/3, 4 where $\bar{a}_u$ is Alfvén speed in the unburned material in units of the flame speed, and $\bar{a}_u = 0$ corresponds to the zero magnetic field case.

8. T. Strohmayer (X-ray bursts; NASA Goddard)
9. D. Swesty (radiative transfer; SUNY at Stony Brook)
10. R. Taam (novae and X-ray bursts; Northwestern University)
11. S. Woosley (supernovae and X-ray bursts; University of California at Santa Cruz)

4.8 Students

Six graduate students are currently working on the astrophysics portion of the Center's research: A. Alexakis (supervisor R. Rosner), J. Dursi (supervisor R. Rosner), J. Morgan (supervisor D. Lamb), A. Mignone (supervisor R. Rosner), F. Peng (supervisor J. Truran), and J. Zuhone (supervisor D. Lamb).

5 Computer Science

Participants: A. Chan, J. Flaherty, I. Foster, W. Gropp, R. Hudson, R. Loy, E. Lusk (Group Leader), S. Meder, M. Papka, J.-F. Remacle, R. Ross, M.S. Shephard, R. Stevens, R. Thakur

5.1 Mission and goals

The Computer Science research component of the Flash Center is carried out in multiple interrelated areas, including Numerical Algorithms and Methods, Software architecture and design, Scientific Visualization, Distributed Computing, and Scalable Performance and I/O. These are the fundamental research areas on whose results the FLASH code development effort is, and will be, based. Most of the computer science research is carried out by Flash Center members employed by the University of Chicago but located at Argonne National Laboratory.

Our goals are to conduct computer science research in certain areas relevant to the ASCI program in general, and the Flash Center in particular. Our focus is in several broad areas:

1. Scalability and I/O
2. Numerical Mehtods
3. Advanced Scientific Visualization
4. Software Architecture for Scientific Computing

In the following, we describe our activities in these various areas in more detail.

5.2 Scalability and I/O

5.2.1 Performance visualization (The JUMPSHOT Project)

Activities in this area have been focused on the improvements in performance and ease of use of the new Scalable Log file format, SLOG-2, as well as the accompanied visualization tool, JUMPSHOT, for the performance visualization of a parallel program.

All work in the last year has been on JUMPSHOT-4 and SLOG-2, i.e. SLOG2SDK. The last major release of SLOG2SDK was on 09/19/2003. As of now, JUMPSHOT-4 is a full featured and very robust viewer for SLOG-2 log files.

Details are as follows:

1. Added ”join” method support in JUMPSHOT to support AIX’s UTE converted SLOG-2 file to support connected and disconnect thread view.
2. Improvement of the graphics code in JUMPSHOT: multiple layer of drawing canvas to minimize repeated drawing.
3. Allowed zoomable window to be fully adjustable vertically.
4. Improvement of the user interface of JUMPSHOT: using mouse clicking as a basic control all zoomable window. This allows for dragged zoom, instant zoom in/out and scrolling with mouse(similar to acrobat reader).
5. Addition of new data type to SLOG-2’s preview data to emphasize the innermost nested state so to allow for the estimation of MPI overhead graphically.

6. Addition of a search and scan facility to locate hard to find drawable in Timeline module.
7. Addition of new histogram module which collects statistics based on user selected duration and display the data graphics through a zoomable and scrollable window.
8. A centralized legend table that allows changes of color, legend name, different sort orders, visibility and searchablity. The legend table controls what are being displayed in both Timeline and Histogram modules.
9. A GUI logfile converter that allows JUMPSHOT to ”read” clog, rlog and UTE files.
10. A 50-page JUMPSHOT-4 user’s guide and website update.

Some other activities have been:

- Integration of SLOG2SDK into the MPE environment distributed both with MPICH and separately.
- Working with the Flash Center to ensure FLASH code can benefit from SLOG2SDK project.
- Continuation of work with IBM to make sure their UTE TRACE-API implementation produces viewable SLOG-2 files.

5.2.2 Parallel I/O performance

The most notable work this year has been on the implementation of a parallel version of NetCDF. NetCDFis a high-level application I/O library, comparable in functionality to HDF. HDF-5 is a parallel version of HDF, built on MPI-IO. In previous years we have helped with the tuning of HDF-5.

This year we focused on NetCDFbecause its semantics, particularly in regard to metadata, lend themselves to a scalable parallel implementation better than HDF-5. Because FLASH is architected in such a way that it is easy to use different parallel I/O libraries, we were able to test our implementation both on the FLASH I/O benchmark and on actual FLASH science runs. In some cases the I/O time improved by a factor of seven and total application elapsed time improved by a factor of three. We regard this as a very promising step forward for FLASH and ASCI applications in general.

5.3 Numerical algorithms and methods

We have held two “Flash Numerics Workshops” at Argonne in order to focus some of the applied mathematics expertise available at Argonne on specific algorithmic issues of significance to FLASH, particularly in the area of multigrid solvers. These were considered useful by both sides.

5.3.1 AUTOPACK

Development of AUTOPACK has continued and it has been further utilized in FLASH. In the library itself, the set of MPI-compatibility functions has been expanded. These provide for the ”drop-in” replacement of selected MPI functions to achieve message packing with minimal effort in existing codes. Internal improvements have made management of resources more dynamic. A new release (v 1.4) will be made before the site review.

AUTOPACK has been successfully combined with the FLASH multigrid (gravity) solver. A 3-D problem is currently being studied to improve its message-passing performance.

As a larger variety of solvers in FLASH has been deployed, more flexible load balancing has been needed. A new topologically-based algorithm has been developed to produce a workload-weighted Morton Ordering without computation of Morton numbers or requiring expensive parallel sorting.

For closer collaboration, the PARAMESH development team has granted direct access to their ”Sourcemotel” system. Code changes driven by FLASH will be rolled back into PARAMASH, and AUTOPACK will be used in current PARAMESH development.

5.4 Visualization

Visualization research this year focused on the development of FLASHVIZ, a desktop visualization tool that can couple remote clusters for high-performance parallel rendering. Such a tool gives Flash scientists a way to experiment with visualization of their data with multiple variables, isosurfaces, and views.

Visualization service work for FLASH this year consisted in close collaborations with Flash application scientists on the presentation of several large-scale computations carried out this year, namely gravity-waves on the surface of a white dwarf, a shock wave interacting with a flame vortex, and a Type Ia supernova.

5.5 Software architecture for scientific computing

Flash Center computer scientists participated in the CCA Forum and its Data Component working group. Also, we participated in the SciDAC TSTT (Terascale Simulation Tools and Technologies) Center resulted in a draft model for meshes (http://www.tstt-scidac.org/software/software.html). This activity keeps the Flash Center involved in community-wide efforts to standardize on scalable component interfaces for components of relevance to large-scale simulation.

5.6 ASCI lab and other Interactions

We are currently working with IBM and Livermore to make FLASH a viable “Marquee” application for BG/L, providing insight into how to utilize very large numbers of processors. This is the Flash contribution to pushing the envelope of scientific simulation on petaflops-scale machines.

5.7 RPI Work for the Flash Group

The focus of the RPI efforts have been on effective parallel adaptive analysis of fluids problems using high-order discontinuous Galerkin (DG) techniques. Progress over the past year includes:

- Completion of a parallel version of the variable polynomial order DG method that can effectively support a variety of spatial discretizations ranging from totally unstructured meshes to highly efficient octree type decompositions.
- Execution of test cases on a variety of parallel computers including runs using large numbers of CPU's on Blue Horizon. Progress on the development of effective error estimation procedures for DG discretizations.
- Completion of an effective local time stepping algorithm.
- Development of flexible domain discretization data structures and of a parallel control mechanism for parallel adaptive analysis.

5.7.1 New developments for this year

The work on the Discontinuous Galerkin (DG) code progressed in the following directions this year:

- Axisymmetric and spherical geometry capability were added to the code.
- New Riemann solvers were developed and integrated to the code, including HLL, HLLC and HLLE solvers.
- A new discontinuity detection procedure was developed and added to the code, using results from error analysis. This discontinuity detector detects shocks and contacts in the flow, and use this information to drive the adaptive process.
- An adaptive anisotropic mesh adaptation procedure for conforming mesh, developed by RPI were integrated to the code. The procedure enhances the adaptive process by further reducing the number of cells as compared to isotropic mesh adaptation.

5.7.2 Assessing the accuracy of the DG method

We are further assessing the accuracy of the DG method by a set of test problems. 1D and 2d test problems were solved using DG and compared to FLASH results. Problems were selected to test limits of the solver in some pathological cases. The results enabled us to detect some problems with our solver for difficult cases. The correction of these problems lead to new developments in the code that greatly improved performance on the test cases, as described below.

Corrected weakness of the DG code Two main problems were spotted. The first one was poor resolution near sonic points; the second one was the appearance of the carbuncle and odd-even decoupling phenomenon.

The first problem was solved by changing the limiting strategy. A new limiting strategy had been implemented in our code. After each time step, a limiting process is applied to each cell in the mesh to get ride of spurious solution. Our strategy is based on slope or moment limiting, for higher order. This strategy has been changed: instead of limiting the state variables, the limiting can now be done in the characteristic space. This greatly improved results and no sonic glitch appears in our results any more. The curves presented in Figure 18 show this improvement on a shock tube problem.

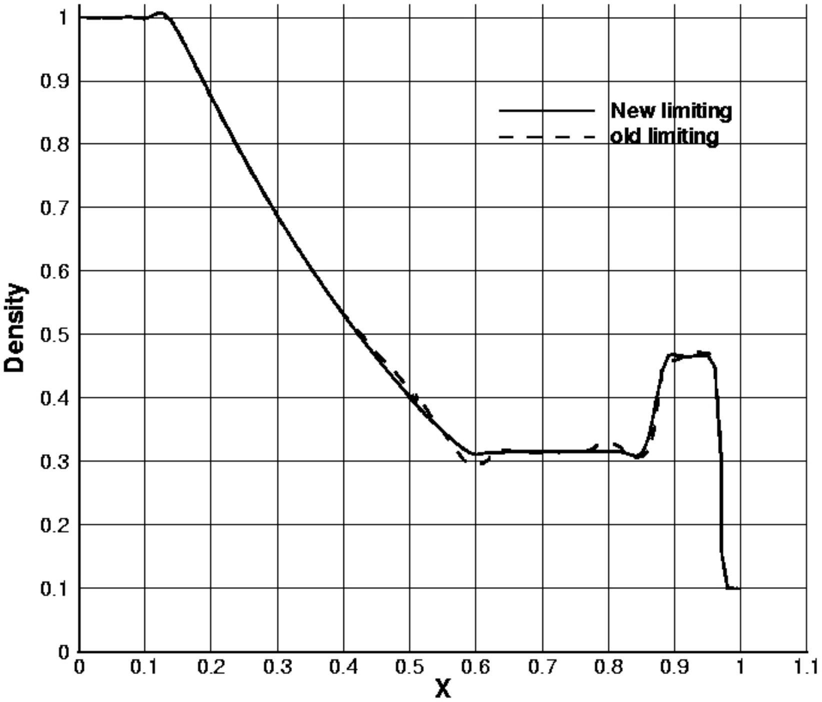


Figure 18: Sonic glitch shown on the solution of a shock tube problem. Previous limiting and new limiting results.

The second problem is related to the carbuncle phenomenon, where an entropy solution can be reached which has no physical meaning. This problem is known to be related to the Riemann solver, and one has to choose carefully this solver, such that the method converges to a meaningful entropy solution. The test case used to detect this problem is a stream collision perturbed by a small density increase in one cell where the two stream collide. The result with our initial strategy, using an exact Riemann solver, exhibits the carbuncle phenomenon, as shown in Figure 19, which displays a map of the velocity field in the direction orthogonal to the stream. This map shows some odd-even decoupling that depends only on the mesh. This problem was corrected by implementing a specific Riemann solver of the HLLE type. The corrected result exhibited in the figure shows the new results that are essentially the same has the one provided by the FLASH Code. The velocity field now shows some reflections of the initial perturbation that are linearly dependent on the size of the initial perturbation.

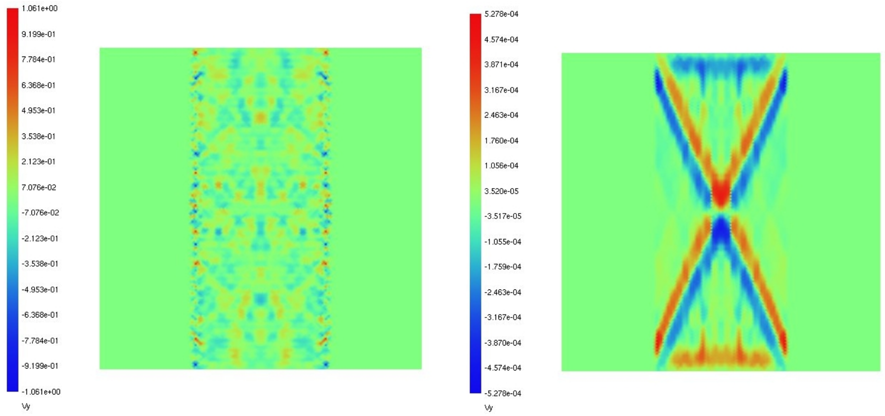


Figure 19: Carbuncle phenomenon. Left previous result, right corrected result with new solver

Strength of the DG code The other tests were made to assess other aspects of the method. One set of tests were selected to measure the amount of dissipation of the scheme. Very good results were found. The other point tested was the behavior of the code where a near-vacuum- or a vacuum-forming situation appears. Again, very good results were produced, which demonstrate the robustness of the method. The code was also tested against strong shocks, strong colliding shocks, Woodward-Collela and Shu-Osher problems. Good results were obtained for each of them. Two dimensional Riemann problems were also tested and the results compare well with results in the literature.

The accuracy of adaptive computation was also tested, both for space adaptivity (mesh refinement) and time adaptivity (local time stepping), and showed a great speed up without loss of accuracy.

5.7.3 Termination of the RPI effort on the DG method

The collaboration with RPI will terminate at the end of calendar year 2003 due to budgetary constraints.

6 Basic Science

Participants: A. Alexakis[1], A. Caceres[1], A. Calder, F. Cattaneo, P. Constantin, T. Dupont (Group Leader), J. Dursi[1], V. Dwarkadas, A. Draganescu[1], P. Gordon, L. Kadanoff, E. Kirr, M. Lewicka, T. Linde, R. Rosner, L. Ryzhik, N. Vladimirova, B. Winn[1]

6.1 Mission and goals

The Basic Science Group has focused on a variety of fundamental physics problems, including mixing, combustion, turbulence, the motion of interfaces, and multi-scale modeling. We seek to understand basic physical processes relevant to the Flash Center problems in order to construct reliable computational models.

Some of the questions that we consider are the following:

- Do we really understand nonlinear Rayleigh-Taylor? This is relevant to flame models in which R-T dynamics may figure.
- How do (nuclear) flame propagate in stratified media? Can we go beyond ad hoc conjecture for modeling effective flame speeds? This is relevant to all three Flash problems; flame speed up matters.
- Are generalized subgrid models possible? Such models are needed for essentially all astrophysical calculations, not just Flash.
- How does interface mixing work? Can computations reliably compute the "saturated state"? This is relevant for the Nova problem, both in the energetics and composition.
- How much physics is needed to capture "fast reconnection"? This is a key question for understanding dissipation and topological restructuring of fields in magnetospheres. Will this supply a cutoff in non-MHD models?
- Can one formalize the process of validation? A question of importance in many areas where we need to build confidence in our codes and modeling.

6.2 Flame/combustion modeling

A key problem for our astrophysics applications is that we do not understand how chaotic flows within the star affect the propagation of deflagration fronts. Convective instabilities in the burning region and Rayleigh-Taylor and Kelvin-Helmholtz instabilities along the burning front can all affect the propagation speed by stretching the flame front and by introducing small-scale turbulent mixing and energy transport, which may dominate molecular diffusion processes [15]. However, there is no hope that the deflagration front for a Type Ia supernova calculation can be resolved on a grid which simulates the behavior of the entire star. One reasonable approach is to do a high-resolution simulation of a small section of the burning front, in order to obtain its speed, and

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[1] Graduate student

then to use the result as a parameter in the full model, combined with a front tracking method.

There has been much recent work here and at several national labs on several mixing problems, especially Rayleigh-Taylor and Richtmyer-Meshkov mixing, both in the fully nonlinear regime. This has been a strong collaboration among several groups and the work is not yet finished. However during the last year, most of those involved have focused on other areas.

To understand how to model combustion in turbulent flows several studies have been carried out that investigate the effect of advection on reacting fluids using rigorous mathematical techniques as well as computational experiments.

The earlier work here on flame speed up was all in the context of passive advection: the flow is given and not influenced by the combustion. P. Constantin and colleagues studied the effect that strong turbulent advection has on flame front propagation. They established that a speed up occurs generically, and the rate of enhancement depends on the geometry of the flow. These mathematical results were confirmed in a quantitative way using computations with FLASH and other codes. The more recent work has been on active advection in the context of a Boussinesq model. The computations of Vladimirova motivated a lively set of theoretical investigations which are described next.

6.2.1 Active reactive advective diffusion

(a) Rayleigh-Taylor instability. Constantin and colleagues found sufficient conditions for linear instability of fronts, in special geometries.

They studied a simplified active combustion model in which the reaction influences the flow. The feedback of the flame on the fluid is taken in a Boussinesq approximation. The model thus couples an advection-diffusion-reaction equation for the temperature with an incompressible Navier-Stokes system driven by temperature differences. This problem was studied in a two dimensional strip of infinite vertical height and finite horizontal width. The vertical direction is the direction of gravity. The system admits planar fronts as particular solutions. These fronts correspond to traveling solutions of the one dimensional reaction-diffusion system without horizontal variation. We studied them in the context of the larger reactive Boussinesq system. Coupling with the Boussinesq system introduces at least two new interesting effects. One is symmetry breaking: gravity breaks the vertical symmetry of the reaction diffusion systems. This has a dynamical effect: fronts connecting low regions of hot fluid to high regions of cold fluid are susceptible to the Rayleigh-Taylor instability. The second effect is due to the introduction of new horizontal degrees of freedom: new length scales are introduced. When one ignores the fluid advection, the planar fronts have a characteristic thickness δ which is determined by the thermal diffusivity and the characteristic reaction time t_c. Using δ and t_c as length and time units, three significant nondimensional parameters emerge. One is the aspect ratio λ, the ratio of the horizontal width of the strip to the thickness of the planar front. The second parameter is the Prandtl number σ, the ratio of kinematic viscosity to thermal diffusivity. The third important parameter is the Rayleigh number ρ which measures the relative strength of the buoyancy force on the scale of the front thickness. For any Rayleigh number, if the aspect ratio

λ is small, then the only traveling solutions are planar fronts, and all solutions become eventually planar. This is a consequence of the fact that diffusion acts rapidly across a narrow strip. This stability mechanism is quite robust and operates for all kinds of nonlinearities. If the Rayleigh number is large enough, then the planar front loses stability to longwave perturbations, which are present if the aspect ratio is large enough. The instability is of Rayleigh-Taylor type and is also expected to be quite robust. Our results on planar front instability agree qualitatively with recent numerical results. The proof is based on the intuitive idea that, in the presence of gravity, the neutral mode - corresponding to the broken vertical translation symmetry - misaligns over long horizontal distances, and gives rise to a longwave unstable mode.

The instability results are linear: they plan to investigate the nonlinear counterparts. Important questions related to these would be the existence and stability of curved fronts, and estimates of their effective width (projection in the direction of propagation).

(b) Acceleration in open geometries. It was shown that fronts have bounded speeds when they are confined to cylinders. The bounds are quite general, and apply to turbulent situations in which the transport is not done by a uniformly propagating fronts. But the bounds diverge with the cross-section of the cylinder. There are claims (by physicists, such as Joulin and applied math people like Sivashinsky) that in open space the fronts move with unbounded speeds (more precisely that position is a power of time with exponent larger than one.) A next step is to try to see if one can (a) produce lower bounds in the whole space or (b) give an upper bound and disprove the claims. The question is widely open.

Two related areas the the mathematicians expect to investing in the coming year are the following:

- Stability issues in compressible flows for simple geometry. The group of mathematicians have begun a “junior seminar” on Evans function techniques that work somewhat in simple detonation front models. The hope is to apply these techniques to establish instability for large aspect ratios.
- Different geometries in the Rayleigh-Bernard problem, The emphasis will be on the effects of anisotropy and shear.

6.2.2 Heat-loss effects

In many combustion experiments the effects of finite domain size are important, so investigation of the theory in these areas will help us understand how such experiments can help us validate our code.

Constantin has begun to investigate the effects of heat-loss at the boundary on the qualitative behavior of solutions of reacting systems, both in the presence and absence of a flow. Mathematically, this is a genuine reaction-diffusion system even at Lewis number equal to one which makes the problem quite difficult. There are very few known rigorous results, for instance, existence of traveling waves has not been established even at $\mathrm{Le} = 1$. He have studied the problem with KPP type nonlinearity in an infinite cylinder of finite cross-section width L with a heat loss parameter q and in a shear flow. It turns out that in the absence of flow, and for a given q two scenarios are possible: the flame propagates if $L > L_0(q)$ is sufficiently large, or, the flame is extinguished, in the sense that $T(t) \leq Ce^{-\gamma t}$, if the channel is narrow, $L < L_0(q)$. This confirms previous numerical results of Matalon et. al. However, the presence of a shear flow $Au(y)$ introduces an additional possibility of flame blow-out by a flow, that is, the flame propagates from left to right if the flow amplitude $A = 0$ but there exists a critical flow amplitude A_0 so that the flame is blown-out: it starts to go from right to left if $A > A_0$, and its speed is linear in A: $V(A) \geq CA$. Moreover, if blow-out does not occur, then the flame propagates from left to right with the speed $V \geq CA$, that is, the propagation speed is linear in the flow amplitude. The speed turns out to be independent of the Lewis number. Finally, he establish existence of traveling fronts in the case $\mathrm{Le} = 1$ in the presence of the flow and non-zero heat-loss parameter.

6.2.3 Two-phase flow

Mathematical investigation of flame propagation is proceeding in a two-phase model, when the gaseous fuel is provided by the evaporation of the heated solid material. The goal is to show that pulsating traveling fronts exist. These are also known as “spinning modes” in the combustion literature. It has been recently shown that these modes exist provided that there is a sufficient amount of gaseous fuel ahead of the front, and there is current work on the extension of this result to the case when all fuel ahead is in the solid phase.

6.2.4 Cellular flows

Cellular flows provide a case in which the acceleration of the flame front is much slower than shear flows. This problem, in which the advection is passive, has been studied both theoretically and computationally here in the Flash center by several people.

We have revisited the problem of advection-diffusion problem in cellular flows. The main interest is understanding the interaction between the small diffusivity ε and the flow. We have studied the Dirichlet problem in a bounded domain with a prescribed temperature distribution on the boundary and in a cellular flow. This is known as the Zeldovich problem. We have rigorously shown that outside a boundary layer of width $\sqrt{\varepsilon}$ temperature is uniform inside each flow cell. This already makes the computational complexity of the problem be independent of ε. We have also obtained a formal asymptotic model inside the boundary layer, and are currently working on the rigorous approximation of the problem with a finite ε by the asymptotic problem.

6.2.5 Related projects

There are several related mathematical investigations that have been undertaken by members of the center. Peter Gordon has been studying combustion in the context in which the flows are friction dominated. In particular he and his collaborators have established an upper bound for the rate of combustion in porous media. Eduard Kirr has been studying problems with contact discontinues with the aim of improving the modeling of these with situations with control-volume-like schemes. In addition he has been looking at the effect of very small scale structure on the propagation of waves.

Marta Lewicka has been studying the stability of systems of conservation laws with large initial data; most of the general, rigorous theory has been developed in the context of initial data that are sufficiently small.

6.3 Multi-scale modeling

Leo Kadanoff worked with his graduate student Cheng Yang on the formation of a jet at the interface between two dielectric fluids in an electric field. This is a part of a long term program aimed at studying singularities in interfaces. As explained in a forthcoming paper [11], this program has considerable importance for the design of effective and correct computer code for e.g. Rayleigh Taylor instabilities. This particular effort showed how a interface could almost come to a conical point and then go unstable and head toward jet formation. Later work with another student, Marko Kleine Berkenbusch, was aimed at describing the charge distributions in this situation. They did the two dimensional case, and expect soon to attack the really interesting three dimensional situation.

6.4 Adjoint methods

A big question for large scale simulation is how can we gain confidence that our computed results are faithful reflections of physical reality? One important way is to use our mathematical models and our programs to simulate experiments and compare the computational and experimental results. However there are many things about most experiments about which we only have approximate knowledge. Errors in our estimates of initial conditions, boundary conditions, or parameters in our models will lead to computational results that differ from the experiment, even if we have included all the relevant physics and have done an excellent job of numerical modeling. While we may have information about the uncertainties, it is difficult to say how much the computed results will be influenced by this. T. Dupont and A. Draganescu have been studying the use of optimal control techniques in trying to determine when experimental and computational results are consistent or inconsistent. By the time of the last site visit several computational examples were available to show that this technique has promise for a range of problems. During the last year additional work has been done.

There are two broad areas of inquiry in comparing experimental and computational results. The first is improving our understanding of how partial knowledge constrains the solution of the model. The task is try to quantify the information content of experimental results. The second addresses the computational difficulties associated with this effort.

Since A. Draganescu is a graduate student in mathematics we have focused this last year on things that can be proved about the methods that we would like to use; he has to write a thesis. In particular he has looked at the use of multigrid methods for solving an initial-value-control / final-value-measurement problem related to a heat equation. He has established convergence results that show for this problem the fine grid problem needs only be approximated one time, i.e., one iteration on the fine grid suffices. This was done in the context of a linear problem but with an eye to extending it to a nonlinear advection diffusion reaction problem; this extension is underway. Solving control problem without doing many iterations on the fine grid is a very encouraging development since it means that the amount of work involved may well be reasonable even on very large problems. Although this theory only applies for the particular type of control/measurement system studied, there is reason to believe that it is valid more generally.

The gradients that are used in the optimal control problem are computed using an adjoint problem that is built from the linearized problem for the usual forward in time simulation. A topic that will be studied soon is the use of approximate linearized problems to compute approximate gradients. For 3-d time-dependent nonlinear problems being able to construct the linearized problem requires storing the solution at all times and all points of space; this can be a lot of storage. One can swap work for storage by recursive checkpoint strategies, but in optimization it is often the case that approximate gradients suffice. A linearized problem built from a coarse grid approximation of the simulated solution could be much more manageable.

6.5 Systematic subgrid modeling

The need for subgrid models is very wide spread. Constantin plans to develop an approach that provides some insight into how such models can be developed.

Solutions of the Navier - Stokes equations can be represented in terms of a diffusive Lagrangian map A and a virtual velocity v. In the ideal fluid case the virtual velocity is a time-independent function of A. The Navier-Stokes velocity u is computed from the impulse variable $w = (\nabla A)^T v$ by projecting on divergence-free vector-fields $u = \mathbf{P}w$. Some interesting subgrid models (the -alpha models), derived using ad-hoc Lagrangian perturbation arguments, can be in fact described effectively by simply replacing the projector $\mathbf{P}$ by a smoothing operator $\mathbf{P}_\alpha$.

The formal similarity between the exact diffusive Lagrangian representation of the Navier-Stokes equations and some of the subgrid models (alpha models) can be exploited in two ways. The first is to understand the errors introduced in the alpha models and devise systematic corrections. The second is to derive systematically models for active-reactive flow, with tests for the regions of their validity.

6.6 ASCI lab and other interactions

We have a regular program of exchange with LLNL, LANL, and Sandia/Livermore in the area of Validation and Basic Science.

Leo Kadanoff has for some time had a working relationship with A. Kerstein, of Sandia National Laboratory. In the last year, we have kept this relation ongoing.

Another form of interaction is via seminars. The Computations in Science seminar (co-sponsored with the Computations Institute) regularly invites speakers from DP labs and features topics of interest to the labs. For example, two recent seminars are

- Misha Chertkov, Los Alamos National Laboratory, Phenomenology of Rayleigh-Taylor Turbulence.
- Amitava Bhattacharjee, University of New Hampshire, Vortex and Current Singularities: Drivers of Impulsive Reconnection.

P. Constantin has lectured at summer schools in Edinburgh (Scotland) and Martina Franca (Italy) on diffusive Lagrangian transformations for the Navier-Stokes equations and at the Abdus Salam International Centre for Theoretical Physics in Trieste (Italy) on Passive and Active Reactive Diffusion.

Some particular collaborations are as follows:

- H. Berestycki, E.H.E.S.S. Paris. Pulsating waves, propagation of fronts in reaction diffusion systems.
- A. Kiselev, U. Wisconsin Madison, Quenching of flows in complex geometries, nonlinear feedback mechanisms in reactive convection.
- F. Hamel, Universite d'Aix-Marseille III, France, Pulsating fronts in periodic media, reduction of complex chemical kinetic schemes.
- K. Ohkitani, RIMS Kyoto, Japan, Computational Fluid Dynamics, MHD
- J-M. Roquejoffre, Director MIP (Industrial and Physical Mathematics), Universite Paul Sabatier, Toulouse, France. Solid and two phase combustion, propagation, Geometric models (Hamilton Jacobi - or G equation).

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