

---

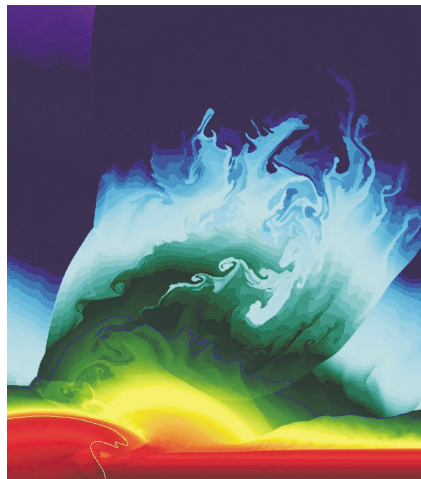
ASCI/ALLIANCES CENTER FOR  
ASTROPHYSICAL THERMONUCLEAR  
FLASHES  
AT THE UNIVERSITY OF CHICAGO

---

YEAR 5 ACTIVITIES REPORT

May 2002

**PHYSICS TODAY**  
FEBRUARY 2002



THE POWER OF GRID COMPUTING

### **Abstract**

We summarize the Year 5 activities at the University of Chicago Center for Astrophysical Thermonuclear Flashes. Major achieved milestones include completion of the first modern architecture version of our production code, *Flash-2.0*; a number of new astrophysics and validation calculations using the production Flash code; performance and scaling studies on the ASCI platforms; optimization of existing physics modules, and the development of new physics modules (including modules for self-consistent gravity and magnetohydrodynamics); further investigations of code architectures and advanced code engineering; and a variety of validation, verification, and basic physics studies relevant to the Flash code.

The work of the FLASH Center is beginning to gain some prominence, as the cover image of our first “integrated calculation” of a surface detonation on a neutron star (from the February 2002 cover of *Physics Today*) illustrates.

# Contents

<b>1</b>	<b>Introduction</b>	<b>3</b>
1.1	Overview . . . . .	3
1.2	Management structure . . . . .	3
<b>2</b>	<b>Code Development</b>	<b>3</b>
2.1	Mission and goals . . . . .	4
2.2	Progress to date . . . . .	4
<b>3</b>	<b>Computer Science</b>	<b>6</b>
3.1	Mission and goals . . . . .	6
3.2	Scalability and I/O . . . . .	6
3.2.1	Performance Visualization (The <b>Jumpshot</b> Project) . . . . .	6
3.2.2	Parallel I/O Performance . . . . .	7
3.3	Numerical algorithms and methods . . . . .	7
3.4	Numerical Libraries . . . . .	7
3.4.1	Autopack . . . . .	7
3.4.2	Data Reduction for Visualization . . . . .	8
3.4.3	Discontinuous Galerkin (DG) Methods (at RPI) . . . . .	8
3.5	Distributed Computing . . . . .	8
3.6	Visualization . . . . .	10
3.7	Software Architecture for Scientific Computing . . . . .	10
3.8	ASCI Lab and other Interactions . . . . .	10
3.9	Efforts of the Rensselaer team . . . . .	11
<b>4</b>	<b>Astrophysics</b>	<b>11</b>
4.1	Mission and goals . . . . .	12
4.2	Overview of activities . . . . .	12
4.3	Fluid-Flame Interactions . . . . .	12
4.3.1	Model Flames: Flame-Shear Interactions . . . . .	12
4.3.2	Effects of Curvature on Nuclear Flames . . . . .	14
4.3.3	Flames-Turbulence Interactions . . . . .	14
4.3.4	Quenching of thermonuclear flames . . . . .	15
4.3.5	Matchhead Calculations . . . . .	17
4.4	Hydrostatic Modeling and Anelastic Code . . . . .	17
4.4.1	Hydrostatics with current FLASH solvers . . . . .	18
4.4.2	HSE version of PPM . . . . .	18
4.4.3	High subsonic flows . . . . .	18
4.5	X-ray burst studies . . . . .	21
4.5.1	Rp-process studies for FLASH simulations of X-ray bursts . . . . .	21
4.6	Nova Explosions . . . . .	24
4.6.1	Exploring the mixing process . . . . .	24
4.6.2	Multidimensional Initiation of Convection . . . . .	25
4.6.3	Gravity-Wave Driven Mixing . . . . .	26
4.6.4	Anelastic code . . . . .	31

4.6.5	Nova simulations with ODT . . . . .	31
4.7	Supernova explosions . . . . .	31
4.7.1	Cellular structure of carbon detonations in three dimensions	32
4.7.2	Subgrid models . . . . .	32
4.7.3	Self-gravity and N-body in FLASH . . . . .	33
4.7.4	Self-gravitating turbulence . . . . .	33
4.7.5	Type Ia supernovae . . . . .	33
4.7.6	Massive star evolution . . . . .	34
4.7.7	Evolution of the first stars and galactochemical evolution	34
4.7.8	Very massive primordial stars . . . . .	36
4.8	Further astrophysical studies with FLASH . . . . .	39
4.8.1	Generally-applicable MHD effects . . . . .	39
4.8.2	Self-gravitating turbulence . . . . .	39
4.8.3	Accretion physics . . . . .	39
4.8.4	Formation of stars and planets . . . . .	40
4.9	ASCI Lab and other interactions . . . . .	41
4.10	Students . . . . .	42
<b>5</b>	<b>Basic Science and Validation</b>	<b>42</b>
5.1	Mission and goals . . . . .	42
5.2	Rayleigh-Taylor and Richtmyer-Meshkov instabilities . . . . .	43
5.3	Speed-up and Quenching of Flames in Fluids . . . . .	44
5.4	Multi-scale modeling . . . . .	46
5.5	Adjoint methods . . . . .	47
5.6	Spatially variable time steps . . . . .	48
5.7	MHD . . . . .	48
5.8	Subgrid Modeling for MHD . . . . .	49
5.9	ASCI Lab and other interactions . . . . .	51
<b>6</b>	<b>Publications</b>	<b>56</b>

# 1 Introduction

## 1.1 Overview

The “FLASH” problem is centered on simulating the accretion of matter onto a compact star and the subsequent stellar evolution, including nuclear burning either on the surface of the compact star, or in its interior. Our activities 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. Our Center is composed of four disciplinary groups (Astrophysics, Computer Science, Basic Science, and Validation/), as well as a cross-cutting group (the Code Group).

In Year 5, we are finishing the first revision of our modern architecture production version of the FLASH Code (now at released revision level 2.0), which is capable of addressing many of our astrophysics problems on the largest existing parallel-architecture computers. Our scientific focus during the current year has been on microphysical processes (flame structure and propagation; mixing instabilities driven by shear and by unfavorable stratification) and on developing the roadmaps (and laying the ground work) for attacking the core astrophysics problems in the next five year period.

## 1.2 Management structure

Our current Center management structure has been slightly altered: Overall Center management is led by the Director (R. Rosner), in close consultation with the Management Group (composed of the Working Group leaders T. Dupont, B. Fryxell, E. Lusk, A. Siegel, and J. Truran, as well as ex officio members D. Lamb and R. Stevens); this reflects the fact that the code group is now a regular Working Group, and the fact that we have separated the Basic Physics and Validation efforts into two groups, led by T. Dupont and B. Fryxell, respectively. The management group meets weekly, on Friday afternoons, using the Access Grid (reducing the “overhead” for our Argonne colleagues). In addition, science issues are discussed weekly at Monday afternoon meetings; and code issues are discussed at weekly Tuesday afternoon meetings. Both meetings see wide participation from Center members from all of the working groups.

# 2 Code Development

Participants: A. Siegel (Group leader), A. Caceres<sup>1</sup>, A. Calder, J. Dursi<sup>1</sup>, W. Freis, B. Fryxell, R. Krasnoplosky, T. Linde, A. Mignone<sup>1</sup>, J. Morgan<sup>1</sup>, K. Olson, T. Plewa, K. Riley, P. Ricker, D. Sheeler, N. Vladimirova, G. Weirs, M. Zingale (UCSC)

## 2.1 Mission and goals

The Code Group's responsibility is to develop and maintain the FLASH code. Activities range from long-range code architecture studies to the nitty gritty of code implementation, testing, maintenance, debugging, and user-interface design to user interactions.

## 2.2 Progress to date

After an extensive in-house testing period followed by an early Fall pre-release, FLASH2.0 underwent final public release in January 2002. This was the successful culmination of a crucial transitional period for the future of FLASH. FLASH2.0 represents a significant paradigm shift from earlier versions of the software, incorporating a number of important modern software design strategies necessary to move the code into a new regime of size and scope.

From the beginning, the FLASH software design plan has always emphasized four core principles: ease of use, portability, efficiency, accuracy. We believe that identifying these four qualities is not a trivial observation and gets to the heart of the difference between large-scale scientific computing and typical business software. When any scientific code fails to meet these criteria, it will typically be rejected in favor of more efficient, ad hoc problem-specific scripts developed by individuals or small groups and not widely supported for distribution. This does not promote software reuse and is contrary to the goal of a community code project such as FLASH.

With FLASH2.0, we have focused on improvements to the underlying framework without compromising these core principles. This has not been a trivial step. The improved framework design has aimed to enhance the developer's ability to comprehend, test, debug, and extend FLASH, with the ultimate goal of facilitating the incorporation of functionality from "external" developers (and streamlining our own in-house software efforts). However, achieving buy-in from scientific programmers is still challenging. Performance, ease of use, and fidelity of results often preclude architectural sophistication. Over-design which substantially erodes performance or renders it more difficult to use or comprehend is unacceptable. Framework improvements must also be phased in incrementally, with a working version of the code always available from the repository capable of producing meaningful scientific results. Meeting these constraints while still introducing radical improvements to the core of the code was the major accomplishment of FLASH2.0.

Since its release, FLASH2.0 has proven to be stable, efficient (< 10% loss in performance), and highly portable (tested regularly on 5 platforms with 8 different compilers). It has complete buy-in from our developer and user-base and is the sole platform for the future of FLASH. We have also kept the code simple to use at the client level as well as for the non-expert application programmer. We believe that new FLASH2.0 architecture will facilitate rapid future growth of the code in several ways:

- modular structure reduces time for new in-house developers to learn code

and become productive contributors.

- built-in testing strategies reduce time spend debugging, fixing problems.
- easier for external contributors to add modules with limited understanding of code internals.
- interfaces more easily with tools provided by other development groups.

The next minor release of FLASH, version 2.1, is on-target for release in late May. FLASH2.1 in part represents a major effort to further enhance the end-user experience by simplifying the setup and build process, improving documentation, identifying and removing non-portable language features, and dramatically improving error-checking. These changes have gone hand in hand with improved functionality, which includes:

- new version of PARAMESH (PARAMESH3.0) w/o permanent guard-cell storage
- optimized uniform grid implementation
- "universal" mesh abstraction to facilitate interoperability
- automated tool to generate portable C bindings for database.
- new externally contributed EOS modules
- Parallel hdf5.0 for i/o
- pvtk-based remote visualization module
- fully tested MHD solver
- fully tested relativistic hydro solver
- enhanced testing strategies
- rebuilt local visualization tool (fidlr)
- parallel FFT package

Internally, we continue to enhance and refine the software process as that allow us to maintain, develop, and support our product. This includes tools such as an enhanced feature tracking database, a tool for developers to update and define new testing benchmarks, new classes of tests for minor repository check-ins, more complete performance tests, tools for checking adherence to coding standards, improvements to internal documentation (beginning of FLASH developers guide), scheduling of meetings and refinement of information flow, etc.

Finally, a "FLASH Future" workgroup has been organized, with the goal of designing a blueprint for the next major version of FLASH. This group, headed by Greg Weirs, has produced a proposal outlining a set of core architectural and algorithmic improvements that will allow the FLASH framework to accommodate a wider range of numerical solvers.

## 3 Computer Science

Participants: E. Lusk (Group Leader), A. Chan, T. Clark, P. Fischer, J. Flaherty, I. Foster, L. Freitag, W. Gropp, R. Hudson, J. Hensley, R. Loy, S. Meder, M. Papka<sup>1</sup>, J.-F. Remacle, P. Ricker, R. Ross, R. Scott, M.S. Shephard, M. Singer, R. Stevens, R. Thakur, H. Tufo, T. Udeshi

### 3.1 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.

We note that because the interactions between Center computer scientists and computer scientists at the DOE National Laboratories are so extensive, we have not called out these interactions in a separate section; instead, we mention these interactions as part of the following discussion of our studies and results.

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 Libraries
3. Distributed Computing
4. Advanced Scientific Visualization
5. Software Architecture for Scientific Computing

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

### 3.2 Scalability and I/O

#### 3.2.1 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 parallel program. In particular, we have

1. Completed an JNI implementation of TRACE-API (Part of SLOG-2 specification) which can be used by other TRACE-API implementors, e.g. IBM's PE product, to create SLOG-2 files. IBM is now able to generate SLOG-2 files through their own implementation of TRACE-API.



2. Enhanced SLOG-2 file format to allow for “thread” based drawable objects requested by IBM. Plus implementation of “shadow” drawables in SLOG-2 to allow for a more higher level description/visualization of logfile.
3. Verified that SLOG-2 logfile format is more robust than SLOG-1 format for FLASH generated logfiles.
4. Completed the core display engine for SLOG-2 format with a hierarchical-style display in the number of processes and threads as well as in time, i.e., a working new Jumpshot to display SLOG-2 files.

### 3.2.2 Parallel I/O Performance

We have been working on improving the performance of parallel I/O, not only in FLASH but also in the ASCI Labs in general. We have been collaborating with Gary Grider of LANL on I/O hints for specifying aggregation nodes. This is a way to tune parallel I/O for a particular machine while staying within the MPI standard for I/O. We added this capability to the ROMIO implementation of MPI-I/O, which is used by multiple vendor MPI libraries and is also available within MPICH. Other enhancements include the “delayed open”, which improves scalability when not all processes participate in I/O. We have been working with James Nunez of LANL on buffer alignments, which improves performance on the Blue Mountain machine.

Rob Ross of Argonne is now a member of the SAF Performance Optimization Team (SPOT), which is seeking to tune performance for the Sets And Fields libraries.

### 3.3 Numerical algorithms and methods

We have developed a high-order anelastic code and tested it on model problems. In addition, we have developed stabilization techniques appropriate for high-order simulations of turbulent flows.

### 3.4 Numerical Libraries

#### 3.4.1 Autopack

We are currently incorporating use of Autopack into several communications routines of Flash 2.1 / Paramesh 3. Jumpshot has been invaluable in providing information to guide this effort. The Autopack library has been extended to allow direct replacement of select MPI routines, to provide enhanced functionality with minimal change of existing code. We plan to compare efficiency and ease of implementation for hand-optimized code vs. code using Autopack.

Collaboration with J.-F. Remacle (Rensselaer) continues with active use of Autopack in their adaptive codes. for visualization. Computation of octant face-neighbor links allows cavities in the reduced data set to be easily interpolated. We have also studied the effects of Quality-of-service reservations on network communication and overall performance.

Currently we are developing additional parallel algorithms to enforce neighbor size restrictions in the mesh of the reduced data set. Discussions are underway with Joy and Hamann of UC Davis on stitching nonconformal meshes. An improved user interface will make the tool more accessible. Preliminary work has been done to make Flash data sets available during a production run; the goal is to connect the Datavise tool directly to Flash instead of postprocessing from its data files. Ongoing participation in the CCA will lead to a standard mesh interface.

### 3.4.2 Data Reduction for Visualization

We have added new functionality to the Datavise data reduction tool.

### 3.4.3 Discontinuous Galerkin (DG) Methods (at RPI)

The focus of the RPI efforts is 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 a formulation for including viscous terms in the DG discretization of NS equations. The formulation developed is in its initial stage of testing.
- Development of flexible domain discretization data structures and of a parallel control mechanism for parallel adaptive analyses [? ?].

## 3.5 Distributed Computing

The UofC/ANL Distributed Systems Laboratory has continued work on components needed in the long term of the FLASH project to facilitate more interactive simulation/visualization/validation cycles. Our view of this cycle is depicted in the following figure.

Note that remote execution and high-performance data transfer are key elements in making interactive simulations of this type possible, as the resources used for executing large-scale simulations, for rendering visualizations, and for

displaying these visualizations are not co-located, nor are they likely to be co-located in the future.

Our past work in these areas is being used in the FLASH project now as follows.

1. We are currently using Globus GRAM tools from the Java CoG Kit in a remote configuration and startup utility for the FLASH code.
2. We have used GridFTP tools to transfer FLASH simulation data from ASCI labs to Argonne (the top piece of Figure 1) and to enable high performance staging of FLASH visualizations to ActiveMural displays (the right side and bottom pieces of Figure 1). The DSL's contributions since the last project report (September 2001) have included the following.
3. Improving on existing GRAM tools, we have added support for reliability checking and failure handling. This work is important for securely submitting jobs to remote resources (e.g., the ASCI centers) and for gracefully recovering from job failures of several types. We have continued support of the ASCI DISCOM group in the Distributed Resource Management area, assisting in the creation of their distributed computing environment, which we believe can be used to improve the FLASH project's use of the ASCI center computing resources.
4. Based on use of GridFTP in numerous scientific projects (e.g., DOE SciDAC and NSF ITR projects) we have made a number of feature improvements to the GridFTP libraries and carried these through to GridFTP tools including those used in FLASH simulation data transfers. We have made performance improvements that have enabled sustained data transfers in excess of 2.0 Gb/s into a single compute cluster (connected via a 3.0 Gb/s network) from multiple points across North America. We have released this software to the public, so there is now a very broad user base for this software.
5. The integration of GridFTP with the Visualization team's ActiveMural display software has proceeded. We are currently adding scaling features to enable display on devices of varying resolutions, continuing performance testing with new PVFS software, and are beginning to design and develop an integrated movie player application for ActiveMural that will use a striped GridFTP server as an input source for movie data.
6. In our new work with the DISCOM Distributed Data Management group (LANL), we have begun developing a large-scale ASCI data management system that integrates HPSS and GridFTP. Recent work here has included improving Kerberos support in the current GridFTP implementation, a key requirement for the ASCI centers.
7. Note that while we have done some modest work toward integrating these technologies into the mainstream FLASH work (some are being used today), there is considerably more that could be done. Integrating these

technologies into the mainstream FLASH activities requires the involvement of several people central to the FLASH project. Given the reduction in current funding, and the relative ranking of importance of this project relative to the other key CS areas in the FLASH project, the rate of progress of making FLASH more “Grid-aware” will be paced primarily by the progress made by S. Meder, the key CS person interfacing between the Distributed Computing group and FLASH.

### 3.6 Visualization

Our core activity within the FLASH Center is the visualization of major FLASH datasets such as the white dwarf simulations, X-ray bursts, and cellular detonations in large-scale and immersive display environments. We have carried out research in several areas relevant to FLASH, including the development of new methods for displaying vector data and development of scalable desktop visualization tools. We have continued our work in the visualization of vector data, extending the use of 2D Line Integral Convolution (LIC) to the 3-D setting. We have continued the exploration of the desktop tool to work with MPD system daemons for fast secure start up of remote MPI based visualization from the users desktop. Cluster based visualization work has continued for the real-time interaction of users with data on large format displays.

### 3.7 Software Architecture for Scientific Computing

We have continued to work with the Common Component Architecture forum to develop abstract common interfaces for mesh and field data on adaptive meshes (as will be needed in future *Flash* code architectures). Prototypical interfaces for dense arrays (both local and distributed) and for basic unstructured mesh access have been defined and are being tested in simple applications.

### 3.8 ASCI Lab and other Interactions

There are a large number of interactions between the computer science component of the FLASH project and ASCI laboratory personnel. Prototypical examples include:

- The Globus group is interacting heavily with the ASCI DRM group on an integrated computing grid for the ASCI labs. This is also not funded by FLASH directly but represents a connection between FLASH participants and the ASCI labs.
- The Argonne scalability group is working with the ASCI Software Path-forward Project, focusing this year on additions to the ROMIO implementation of MPI-IO and a new design for a portable MPI-2 implementation. This work is not funded by FLASH, but was partly initiated through the FLASH project.

### 3.9 Efforts of the Rensselaer team

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

- A more effective parallel version of the DG method that can support a variety of spatial discretizations ranging from totally unstructured meshes to highly efficient octree type decompositions. The software is capable of handling adaptive mesh (h-) refinement, method-order variation (p-refinement), or combinations of the two (hp- refinement).
- Execution of test cases to form a comparative basis with the FLASH results and progress toward structuring a version for integration to flash.
- Effective error estimation procedures for DG methods in one and multiple dimensions. One-dimensional DG solutions of hyperbolic problems with piecewise polynomials of degree  $p$  display superconvergence at the roots of the Radau polynomial of degree  $p + 1$  where solutions converge at an  $O(h^{p+2})$  rate instead of the global  $O(h^{p+1})$  rate for a mesh with spacing  $h$ . Solutions at the downwind ends of elements converge at an even higher  $O(h^{2p+1})$ . Recently, we have shown that the superconvergence applies in multiple dimensions, where solutions at outflow boundaries of elements converge at the  $O(h^{2p+1})$  rate. These superconvergence results have enabled us to get asymptotically correct estimates of discretization errors at very low costs.
- Extension of the local time stepping algorithm.
- Flexible domain discretization data structures and parallel control mechanism for parallel adaptive analyses.
- Solution limiting and the automatic detection of discontinuities by using error estimates. Error estimates, as described, can be used to detect the presence of discontinuities and apply limiting procedures or order-reduction algorithms only in these regions. This greatly reduces spurious dissipation in regions of smooth flow.

## 4 Astrophysics

Participants: J. Truran (Group Leader), A. Alexakis<sup>1</sup>, E. Brown, A. Calder, J. Dursi<sup>1</sup>, B. Fryxell, A. Heger, R. Krasnoplosky, D. Lamb, A. Mignone<sup>1</sup>, J. Morgan<sup>1</sup>, J. Niemeyer, K. Olson, F. Peng<sup>1</sup>, T. Plewa, P. Ricker, F. Timmes, R. Rosner, N. Vlahakis, Y.-N. Young, M. Zingale, J. Zuhone<sup>1</sup>

---

<sup>1</sup>Graduate student

## 4.1 Mission and goals

The astrophysics group has the responsibility to develop the astrophysically-relevant physics modules for the *Flash* code; 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 activities

The fifth 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 [45], Timmes & Arnett [47], Timmes & Swesty [48], and Timmes [46]) 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 (for isolated boundaries), and are currently being utilized for our calculations of the detonation of a Chandrasekhar mass white dwarf.

Significant progress has occurred over the past year in understanding of flame physics, essential to future studies of x-ray bursts, novae, and Type Ia supernovae.

The modifications and improvements to the *Flash* code described in §2 above have allowed us to continue exploratory calculations on all three of our target astrophysics problems, using all available ASCI platforms.

## 4.3 Fluid-Flame Interactions

### 4.3.1 Model Flames: Flame-Shear Interactions

Following Natalia Vladimirova's work on KPP and incompressible flames, Bob Rosner and Jonathan Dursi have begun fundamental work aimed at understanding compressible astrophysical flames.

Because flames are inherently subsonic phenomena, much work on flame-flow interactions has worked in the incompressible limit. However, flames in astrophysical environments may well be traveling through highly compressible flows due to, eg, strong turbulence.

While models exploring such interactions have been performed in the terrestrial chemical combustion regime, relatively little fundamental work has been done in this area with astrophysical flames. There are reasons to imagine that there will be different results in our case:

- Very small Prandtl number means turbulent velocities extend to all scales, and thus the range of length scales over which interactions may play a role is extended.

## Nuclear Energy Generation Rate (ergs/g/s)

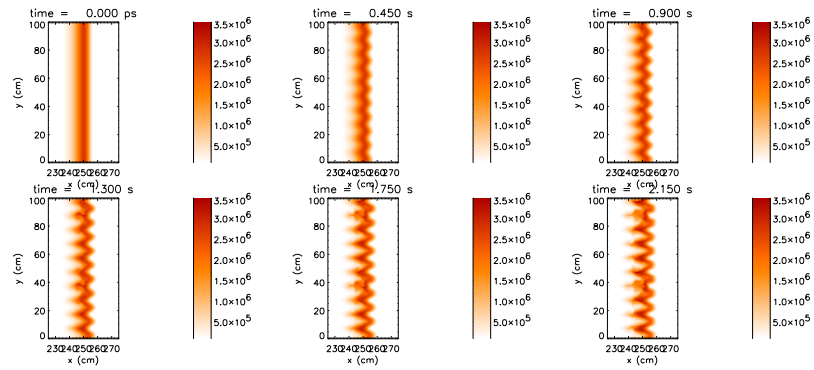


Figure 1: Evolution of a KPP flame with  $Le=1$  undergoing a periodic shear with wavelength  $\sim 10$  flame thicknesses and a velocity of order the flame velocity.

- Very high reaction rates and no intermediate radicals make local quenching difficult or impossible, as well as greatly simplifying the interactions between the flame structure and the flow.
- High Lewis number changes flame behavior under curvature.
- Higher energy release than in typical terrestrial cases makes flame feedback into fluid motions much stronger.
- The nearly-degenerate high density material alters the interaction between energy release and fluid reactions.

As a first step to understanding the interactions of flame and flow in astrophysical flames, Jonathan Dursi is performing a large parameter study of the interactions of compressible KPP-like flames and a low- and moderate-speed periodic shear (see, *e.g.*, Fig. 1). By varying the compressibility of both the flow and the flame, and such parameters as the Lewis number, we can hope to understand the physical effects involved when a nuclear flame undergoes shearing in a supernovae precursor.

#### 4.3.2 Effects of Curvature on Nuclear Flames

One model of Type Ia Supernovae consists of an initial deflagration that accelerates, either to a detonation or to an extremely fast deflagration. Any such acceleration mechanism will involve a wrinkling of the flame, which in terrestrial flames can locally enhance or reduce burning rates. The behavior of the local burning under stretch is often parameterized by a Markstein number,  $Mr$ .

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 are developing numerical experiments measuring the Markstein number for relevant astrophysical thermonuclear flames using a one-step burning, which has a simplified flame structure, and using a fuller network; also, parallel work is being 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.

#### 4.3.3 Flames-Turbulence Interactions

While studies exploring flame-turbulence interactions have been performed in the terrestrial chemical combustion regime, relatively little work has been done in this area with astrophysical flames. There are reasons to imagine that there will be different results in our case:

- Absence of walls means a cooling mechanism is gone.
- Very small Prandtl number means turbulent velocities extend to all scales



- Very high reaction rates and no intermediate radicals make local quenching difficult or impossible
- High Lewis Number changes flame behavior under curvature
- Higher energy release than in typical terrestrial case makes flame feedback into fluid motions much stronger.

Thus, modelling work has begun to study this interaction, at first in 2D, by Jonathan Dursi. The turbulence is generated by adding a time-correlated, stochastic “stirring” term to the fluid equations, as per the prescription in Eswaran and Pope [14]. This stirring, which happens on small scales in 2D and large scales in 3D, generates more realistic structures than simple white-noise forcing, which cancels itself out too readily for much coherent structure of the sort seen in real turbulence to form.

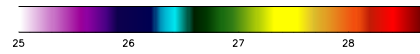
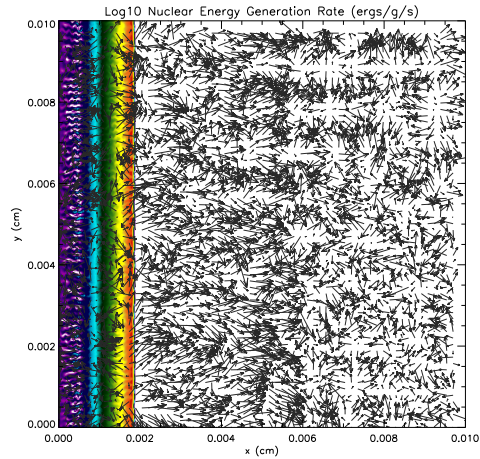
Once the turbulence has developed and hit a statistical equilibrium, measured by examining the evolving power spectrum, a 1D astrophysical flame from Mike Zingale’s work was mapped into the simulation domain and allowed to propagate. By evolving both the burning domain and the “rundown experiment” of the non-burning domain, detailed measurements can be made of the feedback onto the turbulent flow from the combustion; similarly, measurements can be made of the enhanced burning rate of the flame.

#### 4.3.4 Quenching of thermonuclear flames

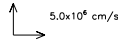
Work on understanding quenching of thermonuclear flames continued with a series of flame-vortex interaction calculations. Thermonuclear burning in a Type Ia supernova begins as a flame, deep in the interior of a white dwarf. Scrutiny of supernova spectra suggests that, at some point, the burning may undergo a transition from a deflagration to a detonation. Some mechanisms for this transition require a preconditioned region in the star. As the flame propagates down the temperature gradient, the speed increases, and the transition to a detonation may occur [22; 33]. For this to happen, the region must be free of any temperature fluctuations. Any burning that was occurring in that region must be quenched.

Flames computed with *FLASH* have been further validated this year, demonstrating Galilean invariance, speeds which are consistent with those computed by Timmes & Woosley [49], and directional independence. This is an important validation of our code, and an essential step on our way to a more realistic treatment of the supernova problem.

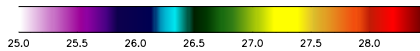
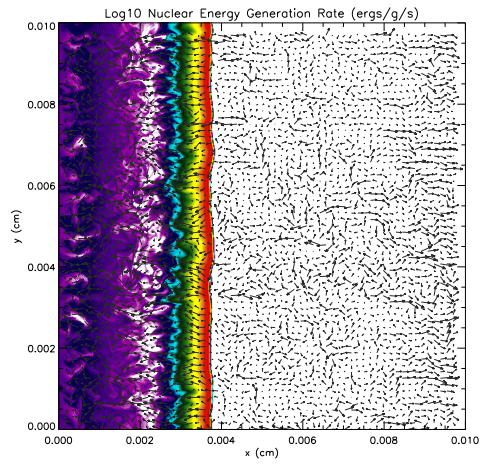
In our simulations, we pass a steady-state laminar flame through a vortex pair. The vortex pair represents the most severe strain the flame front will encounter inside the white dwarf. We vary the speed and size of the vortex pair in order to explore the characteristics of the quenching process as a function of stellar properties. This year, we completed the flame-vortex calculations at high densities, and begun work on similar calculations at lower densities ( $5 \times 10^7 \text{ g cm}^{-3}$ ). At low densities, the flame speed is much slower, and a



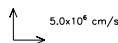
time = 620.018 ps  
 number of blocks = 1360, AMR levels = 4  
 University of Chicago / ASCI Flash center



/scratch2/jjgursi/flame\_turb2\_half5\_chk\_0009



time = 960.007 ps  
 number of blocks = 1360, AMR levels = 4  
 University of Chicago / ASCI Flash center



/scratch2/jjgursi/flame\_turb2\_half5\_chk\_0028

Figure 2: Evolution of flame-turbulence<sup>16</sup> interaction. Note that the flame *strongly* suppresses wrinkling at the front.

reasonable calculation takes 300,000 timesteps, making them very expensive. A full calculation can take over a month of wall clock time.

#### 4.3.5 Matchhead Calculations

A series of small calculations designed to systematically study explosive burning in pure helium environments is underway. The goal is to understand the conditions under which a helium detonation can persist. When a region of pure helium is perturbed isobarrically, the energy deposition will raise the temperature locally. This will result in a large increase in the nuclear energy generation rate, which further increases the temperature and raises the pressure. If a large enough region was perturbed (the matchhead), enough overpressure can be generated to sustain the detonation front.

These calculations are a next step toward a large scale simulation of an X-ray burst. Our previous calculation followed a detonation front through a deep helium layer on a neutron star. More realistic initial models would have shallower helium layers, whose base densities reach  $\sim 10^6$  g cm<sup>-3</sup>. At these densities it is unlikely that a detonation can be sustained. These matchhead calculations will map out the conditions where we can expect to find detonations.

Currently these calculations are in progress. At densities just on the transition between deflagrating and detonating, numerical difficulties have stalled the calculations. These are slowly being fixed, through the introduction of a temperature based timestep limiter, a new shock detection algorithm that prevents burning inside the shock front, and a new conservative variable based interpolation method that provides increased accuracy when filling guard cells.

### 4.4 Hydrostatic Modeling and Anelastic Code

Many simulations we wish to do with the FLASH code involve maintaining hydrostatic atmospheres for long periods of time. This is difficult for two reasons – operator splitting and explicit hydrodynamics: FLASH ‘operator splits’ gravity from hydrodynamics, so that two fairly large terms (the pressure gradient force and the gravitational force) calculated in separate modules by different methods required to cancel to high accuracy in hydrostatic equilibrium (HSE). Any error in the cancellation can generate spurious accelerations.

Further, long-time highly subsonic simulations are difficult to carry out with explicit hydrodynamical codes, as traditional explicit codes must follow along at the Courant-Friedrichs-Lewy (CFL) timestep. This means that simulations that evolve over times very long compared to sound-crossing times require extremely many timesteps to compute, which is both costly and error-prone.

Work on these two problems is progressing on a number of fronts. The first is to maintain hydrostatic equilibrium in the FLASH code with the current solvers; the next, to eliminate the operator split approach to the hydro solver, and solve the hydrodynamics in a way that is consistent with the gravity; the last three approaches focus on the removal of sound waves from the problem,

to allow stepping at much larger times, making long-time evolution for highly subsonic problems both less expensive and more accurate.

#### 4.4.1 Hydrostatics with current FLASH solvers

This past summer, a UIUC undergraduate student, J. Zuhone, worked with M. Zingale and J. Dursi to continue work done in the previous year by Y.-N. Young on numerical studies of wind-driven mixing. Much of the work done involved getting a compound initial vertical density profile stable to high accuracy in the FLASH code. Work was done developing boundary conditions, interpolation methods, and optimal interface smoothing techniques for bringing a hydrostatic model with a density discontinuity to stability in the FLASH code.

The improvements made to the code in the interpolation of a hydrostatic equilibrium initial model are being collected into a single, generic, ‘HSE’ initialization routine for FLASH.

#### 4.4.2 HSE version of PPM

Another approach was started this spring by B. Fryxell and J. Dursi, working with E. Muller at the Max Planck Institut für Astrophysik, in creating a ‘HSE PPM’ solver which would evolve only deviations from a hydrostatic background, thus ensuring good stability at near-equilibria. This work is still in process. In the meanwhile, using the non-HSE PPM solver, we have begun to evolve a pre-convective 1-D model (provided by A. Glasner) in the FLASH code, using techniques developed with J. Zuhone to keep the model stable. We hope to be able to evolve the simmering atmosphere to the point of convective turn-on, which will help to explain how convection sets in on white dwarf atmospheres and the resulting velocity patterns.

#### 4.4.3 High subsonic flows

It is well known from terrestrial combustion studies that the evolution of a deflagration (or flame) often is not significantly affected by acoustic waves, and it is reasonable to assume that this applies to certain aspects of the astrophysical situation as well. For the applications we consider here, the hydrodynamic field is therefore nearly in hydrostatic equilibrium, but with strong vertical stratification; and the flows tend to have very small Mach numbers. As a consequence, the CFL condition for fully explicit codes (such as the PPM module in FLASH) tends to make the long-term computation of such flows extremely laborious (and potentially inaccurate). There are however a variety of ways of resolving this difficulty, and we are pursuing three of them.

- Anelastic code (ANL): ANL Center member P. Fischer at Argonne National Labs has been continuing his work on an anelastic code using a block structured solver similar to the FLASH framework, and is doing Rayleigh-Bernard convective simulations as per Lantz & Sudan [27]; these calculations are then compared with simulations done by J. Dursi with

the FLASH code. This solver uses spectral techniques, and is based in part on the code which garnered the 1999 Gordon Bell prize.

- Anelastic code (NWU): In the area of the interaction of combustion and convection, A. Bayliss and R. Taam (Northwestern university ) have developed a model to follow the evolution of deflagration waves over long time scales. For the reasons discussed above, their model is also designed to filter out sound waves. Thus, assuming that only the hydrostatic pressure appears in the equation of state and the energy equation, sound waves are filtered out and timesteps can be used based on the vastly slower convective motions induced by nuclear burning and gravity. This is justified in their treatment by an expansion in terms of the Mach number, the ratio of a characteristic convection or flame velocity to the sound speed, which is (as already mentioned) often very small ( $< 0.01$ ) for the applications that we consider. This model is an extension and generalization to astrophysical problems of models employed in the study of terrestrial fires. Bayliss and Taam, in collaboration with J. Truran (Univ. of Chicago), plan to implement this method within the FLASH architecture to carry out numerical computations of the classical nova phenomenon.
- A semi-implicit solver: We are collaborating with former post-doc F. Rubini (now Professor of Physics at the University of Florence, Italy) on the incorporation of a semi-implicit hydro solver in FLASH. This solver has already been used as an independent code to attack the problem of “semi-convection” (in which the thermal stratification is unstable, but the compositional stratification is stable – a situation sometimes encountered in the interiors of highly evolved stars), leading to the PhD thesis work of former student J. Biello (now at RPI ). This solver uses compact finite differences; and offers the possibility of “tuning” the solver as the Mach number of the flow varies between very subsonic and sonic. Prof. Rubini will be visiting us later on during this calendar year, and insert this module in FLASH; we then expect to carry out comparisons of the various approaches to the highly subsonic flow problem over the next year.

In addition, we are working on a number of issues related to exploring the parameter space of initial models, and on improvements in the computational efficiency of our physics modules. Examples include:

- The TYCHO stellar evolution code (U. Arizona): An ancillary to the above is the provision of initial models, as already discussed earlier. In some cases, we require fairly extensive models for the entire star, as is provided by full stellar evolution codes. As part of our collaboration with D. Arnett at U. of Arizona, the TYCHO stellar evolution code is being completely rewritten as general purpose community code for stellar evolution and hydrodynamics. This code was originally developed for one-dimensional (1-D) hydrodynamics of the late stages of stellar evolution and core collapse [5]. A library of analysis programs is being built ( modules for apsidal

motion, pulsational instability, reaction network links, and history of mass loss are now available ). TYCHO uses an adaptable set of reaction networks; for these calculations, two networks were used. The reaction rates now used are from F.K. Thielemann and Caughlan & Fowler (1978). The standard option used Schwarzschild convention; a hydrodynamic treatment of convective overshooting is being developed. Mass loss is included, and is based on the theory of [44] for  $T_{\text{eff}} > 7.5 \times 10^3$  °K. For lower effective temperatures, the empirical approach of [24] is used. Opacities are from [33] and [45], and a comparison with the Los Alamos astrophysical opacities is in preparation. We use the Helmholtz EOS developed for FLASH [82], plus solution of the ionization equilibrium equations for ionization of H, He, and a set of heavier elements scaled from the solar abundance pattern. Options for rotational mixing and elements settling are being implemented.

Mapping even an acceptable one-dimensional model onto a different grid can be a problem [4,7,6]. Initially hydrostatic configurations will have a balance between pressure gradient forces and gravity, and any mismatch will generate spurious sound waves, as discussed earlier. It is desirable to construct the mapping to represent the physics implied by the differencing and zoning of the 1-D model accurately. Success has been demonstrated in mapping a TYCHO initial model onto a multidimensional hydrodynamics code grid.

- F. Timmes is investigating how to implicitly integrate the internal energy equation and the nuclear reaction networks together in a fully coupled fashion (no operator splitting). The results indicate a more robust transition into and out of NSE situations. this should be implemented in FLASH within the next year.
- As an off-shoot of the above, F. Timmes is seeking a way to implicitly integrate the entire 1-D set of hydrodynamic equations and the nuclear reaction networks together, in a fully coupled fashion. Implementation on uniform grids reproduces previously obtained results on laminar deflagrations. He is presently implementing a PPM-like Riemann solver, so shocks may be handled in an implicit manner. This implicit solver may be put into FLASH in about a year.
- A further consequence of these studies is an investigation into direct solutions (e.g., Gaussian elimination) of linear systems on parallel machines. The parallel solution nuclear reaction networks is about 5 times faster than the best serial solvers for 1000 isotope networks. For 2000 isotopes, the solution by parallel solvers is about an order of magnitude faster than serial solvers. The installation of one promising parallel solver, MUMPS (Multifrontal Massively Parallel Solver), into FLASH should occur within the next year.

## 4.5 X-ray burst studies

Previous reports have described the wide variety of X-ray burst calculations we performed in order to understand better the proper use of FLASH, especially its adaptive mesh refinement strategy, and to explore the basic physics underlying nuclear burning on the surface of a neutron star; these basic studies are all preliminary to the eventual full-scale simulation of a neutron star X-ray burst we intend to do. The next major step on this topic will be the numerical simulation of a helium deflagration on the surface of a neutron star.

In work related to X-ray bursts, the spreading of accreted fuel (hydrogen and helium) away from the polar cap of a strongly magnetized ( $B \geq 10^{12}$  G) accreting neutron star has been studied. The accreted hydrogen and helium burn where  $8\pi P_{\text{gas}}/B^2 < 1$ , which motivates the question of how the fuel is actually distributed over the surface when ignition occurs. An analytical investigation of the stability of an accreted magnetized mound of material to short-wavelength ballooning modes has been completed. For a realistic model atmosphere, Litwin, Brown, & Rosner [28] demonstrated that the instability occurs when the overpressure exceeds the magnetic pressure by a factor  $\approx 8a/h \gg 1$ , where  $a$  is the lateral length scale and  $h$  is the vertical length scale. This instability is expected to produce an enhanced transport of matter across the magnetic field. With the development of a MHD module for FLASH v2, it will be possible to numerically simulate this spreading, as well as study the spreading at much weaker magnetic fields relevant to bursting sources.

Within the past two years several “super bursts” (X-ray energies  $> 10^{42}$  ergs and durations of several hours—see Figure 3) have been observed from accreting neutron stars [11; 12; 25; 26; 44]. Preliminary calculations [13; 44] suggest that the unstable ignition of  $^{12}\text{C}$  at large depths is the cause of these super bursts. At the high densities under which ignition occurs, thermal conduction of heat is efficient and sets the decay timescale of the burst (of order days). For the most energetic bursts, neutrino cooling may actually remove most of the released nuclear energy [44]. These bursts offer insight into burning at high densities and temperatures, and could constrain the properties of the outermost layers of an accreting neutron star. More detailed calculations of the cooling of the burning layer are underway.

### 4.5.1 Rp-process studies for FLASH simulations of X-ray bursts

We are currently investigating the energy output and nucleosynthesis of the rp-process (defined by a sequence of rapid  $p$  proton captures onto seed nuclei provided by helium burning) in a type I X-ray burst. For typical conditions, this nuclear processing can produce massive nuclei with  $A \approx 100$  (as is the case for stable burning; see [40]), and might have implications for energy generation during the late phases of the burst event, as well as on the amount of carbon produced to power further bursting, as described above. Using an extensive reaction network, F. Peng has performed one-zone calculations of the rp-process nucleosynthesis under relevant conditions; these calculations (Figures 4 and 5)

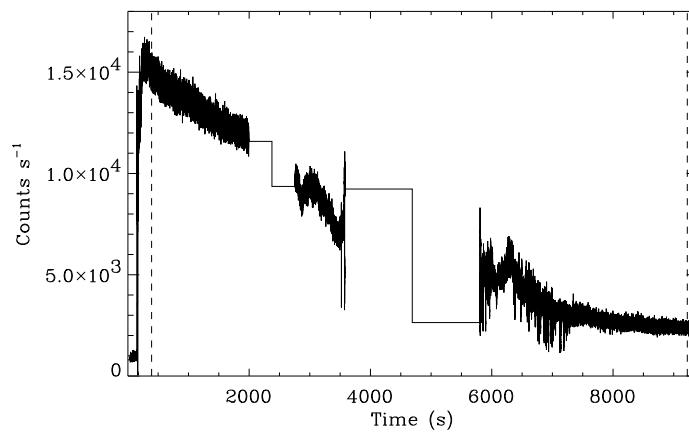


Figure 3: A superburst observed by *RXTE*/PCA from 4U 1820–30. The peak count rate corresponds roughly to the Eddington luminosity,  $\sim 10^{38}$  ergs  $s^{-1}$ . Figure reproduced from Strohmayer & Brown (2002).



compare favorably with published results [36; 24; 41]. Brown, Peng, and Truran (in collaboration with A. Glasner, Hebrew University of Jerusalem) are developing a one-dimensional evolution code to explore rp-process nucleosynthesis in greater detail, including the effects of convective heat transport and mixing. We have begun a collaboration with H. Schatz (MSU) and M. Wiescher (Notre Dame) on the development of the nuclear reaction networks for this calculation. The code will also explore the viability of using truncated reaction networks to provide energetic and nucleosynthetic predictions. The use of such networks is essential to any realistic multidimensional study of X-ray bursts with FLASH.

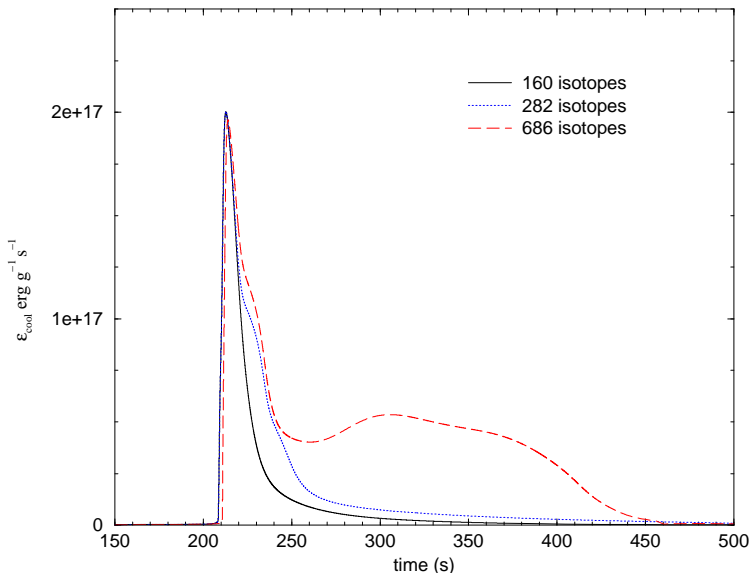


Figure 4: Effective cooling rate (a finite-difference approximation to  $\rho^{-1}\nabla \cdot \vec{F}$ ) for a one-zone burst nucleosynthesis calculation. The bump at late times is a signature of the rp-process.

One effect of the rp-process is to lower the thermal conductivity of the outer envelope of the neutron star (due to the larger  $Z^2/A$  of the ions) relative to previous estimates for a pure iron crust. A recent study by Brown, Bildsten & Chang [7] extended the calculations of Potekhin et al. [34] and surveyed the effect of different compositions on the emergent thermal luminosity observable after accretion halts (as happens regularly for neutron stars in soft X-ray transients). For a given core temperature, the thermal luminosity can vary by a factor of 2 to 3 and depends on the mass of residual H/He on the surface. The lower thermal conductivity of the rp-process ashes also implies a higher interior temperature and suggests that neutrino cooling is significant for transient accreting neutron stars.

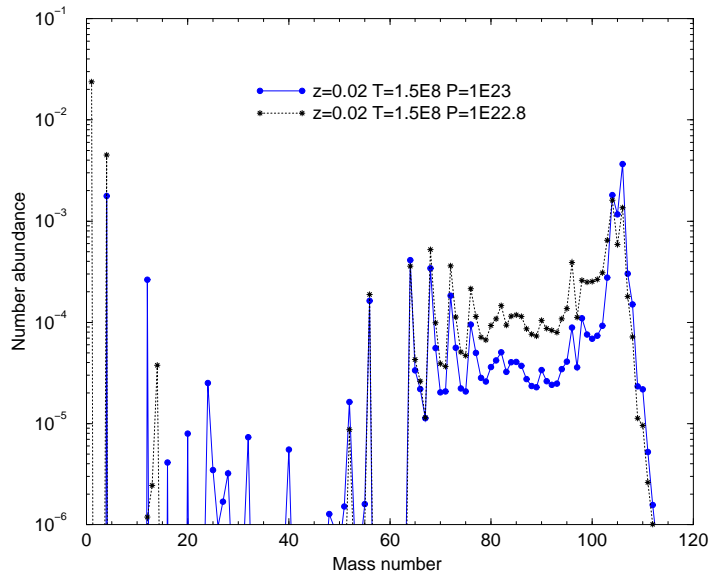


Figure 5: Final abundances following rp-process nucleosynthesis. Two different pressures were used. The distribution agrees in gross detail with the calculations of Schatz et al. (2001), which used a pressure intermediate between the two cases used here.

## 4.6 Nova Explosions

This year’s FLASH Center activities included a concerted effort to understand the physics underlying hydrodynamic thermonuclear runaways on white dwarfs, leading to nova explosions. The most critical question in this regard involves the identification of the mechanism by which carbon, oxygen, and neon enriched matter is dredged up from the underlying white dwarf into the active burning regions of the envelope [53]. One dimensional numerical simulations have confirmed that the detailed features of a nova explosion – e.g., the light curve, the energetics, and the composition of the ejected shell – are strongly dependent upon both the time history and the magnitude of such envelope enrichment. The dredge up of carbon, oxygen, and neon to levels  $\sim 30\%$  by mass of the envelope [30] allows more explosive hydrogen burning and concomitant energy input on a dynamical timescale. We have begun to address this problem on several fronts.

### 4.6.1 Exploring the mixing process

A core issue for understanding nova is the extensive observed mixing of stellar material (such as carbon and oxygen) into the burned envelope ejecta; since this material cannot be the result of nuclear burning of the accreted hydrogen/helium envelope, some process of “dredge up” of stellar matter must operate. One of the

several possible mechanisms of dredge up [31] that has previously been proposed is shear-induced mixing [23]. The results of this early work unfortunately were inconclusive, and subsequent ideas for mixing by other mechanisms (such as convective overshoot or turbulent erosion) were similarly unsuccessful. We have reexamined this problem with the use of the FLASH code, based on ideas derived from oceanographic research.

R. Rosner, together with postdoctoral fellow Y.-N. Young and student A. Alexakis, have reconsidered the problem of shear mixing at (density) interfaces in stratified media. In oceanographic work, it has been long recognized that Kelvin-Helmholtz instabilities cannot account for the observed mixing at ocean or lake surfaces; the focus there has been on resonant instabilities of surface gravity waves driven by an overlying wind. We have now successfully reproduced this work using the FLASH code, verifying the linear instability, and extending the work into the previously unexplored highly nonlinear regime. In this regime, the unstable surface waves are shown to break, leading to a mixing layer substantially thicker than previously obtained from Kelvin-Helmholtz studies. Our ongoing work is now to incorporate these new results into a model for interface mixing that can be inserted into our full nova calculations.

Papers describing much of this early work have now been prepared for publication [2; 38].

#### 4.6.2 Multidimensional Initiation of Convection

Two-dimensional simulations are currently being run with the FLASH code, using a 1-D initial model that has been used for two different sets of multidimensional simulations [16; 21]. These two earlier simulations have given differing answers about dredge up from the white dwarf into the accreted layer. As a first step in our nova studies, we would like to be able to identify and understand the source of this discrepancy. Our simulations, being carried out by J. Dursi, will not only shed light on the difference in results from these two groups, but also serve as a first step toward our future two- and three-dimensional simulations, using different initial models which can help us to understand novae and their observed diversity.

To explain observed abundances from classical nova outbursts, and to help explain their energetics, nova models must incorporate a mechanism that will dredge up the heavier white dwarf material into the lighter accreted atmosphere. One proposed mechanism relies on the fluid motions from an early convective phase to do the mixing. This year, we have made progress investigating two aspects of this mechanism.

Using techniques developed by J. Dursi and M. Zingale, we have begun to evolve a pre-convective 1-D model from A. Glasner in the FLASH code. We evolve the simmering atmosphere to the point of convective turn-on, which will help us to explain how convection sets in on white dwarf atmospheres and the resulting velocity patterns. In Fig. 6 we see the results of attempting this simulation without taking care to maintain hydrostatic equilibrium; in Fig. 7 we see the same simulation results with improved boundary conditions, initialization,

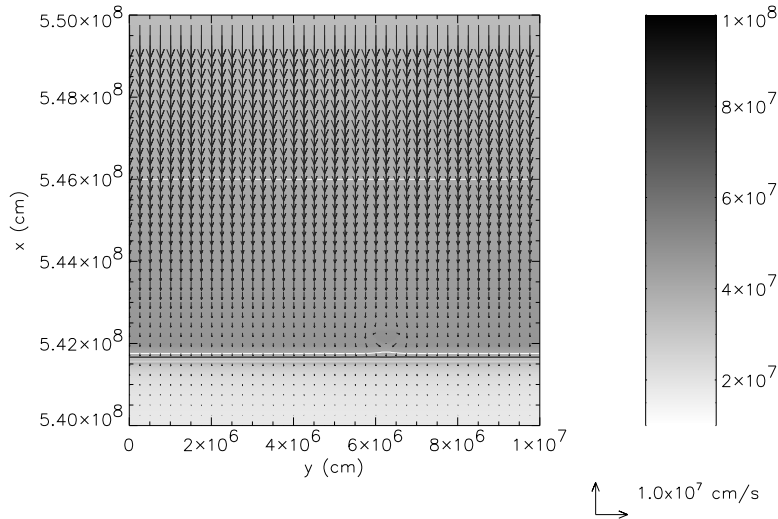


Figure 6: A perturbed nova atmosphere after 0.2 seconds of evolution. Small deviations from hydrostatic equilibrium resulted in a settling downward, resulting in compressional heating which wipes out the original perturbation.

and hydro solver.

A realization of the evolution of the convection is shown in Fig. 8. The 5% temperature perturbation applied to the hottest part of the atmosphere causes convective rolls to form in the already convectively-unstable atmosphere. Beside the large-scale velocity field, the downward motion from these rolls also induces an interface wave on the C/O interface, which could be important for the mixing process.

### 4.6.3 Gravity-Wave Driven Mixing

Classical Novae result from the explosive thermonuclear burning of material accreted from a companion star onto the surface of a white dwarf. Observed abundances and explosion energies estimated from observations indicate that there must be significant mixing of the heavier material of the C/O or O/Ne white dwarf into the lighter accreted material (H/He). This mixing is critical because otherwise hydrogen burning would be too slow to reproduce observed nova characteristics in outburst. Further, without this mixing it is difficult to understand the observed abundances of intermediate-mass nuclei in the ejecta. Accordingly, nova models must incorporate a mechanism that will dredge up the heavier white dwarf material [38, and references therein].

A recently proposed mixing mechanism is the breaking of nonlinear resonant gravity waves at the C-O surface [37; 2; 38]. The gravity waves, driven by the “wind” of accreted material can break, forming a layer of well-mixed material. This mixed layer can then be transported upward by convection, thereby

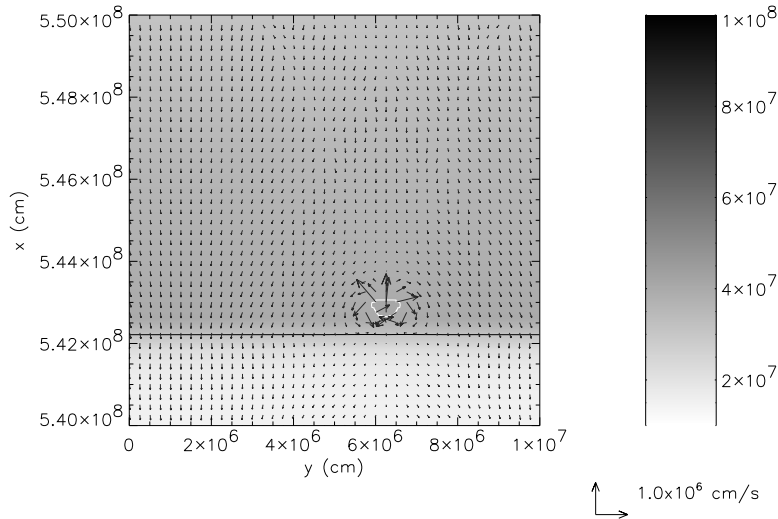


Figure 7: The same simulation as Fig. 6, but with new techniques applied to the evolution so that the desired physical phenomenon can be observed.

enriching the accreted material. Because the length scale of this mixed layer may be very small (much smaller than the length scale of convection), previous precursor simulations have not captured this effect.

We present preliminary two dimensional calculations of linear gravity waves in a flat, periodic domain driven by two different winds – a step-function wind, and a more realistic boundary-layer profile. The simulations were performed with FLASH, a parallel, adaptive-mesh simulation code for the compressible, reactive flows found in many astrophysical environments [15]. Both winds have the same maximum velocity of  $2 \times 10^8 \text{ cm s}^{-1}$ . Hydrostatic boundary conditions were used at the lower boundary, periodic conditions on the sides, and an outflow condition was used at the upper boundary.

The theory of gravity waves assumes an incompressible medium (originally air over water) [10], which may not be assumed for a white dwarf. The simulations began with the similar initial conditions consisting of a simple  $\gamma = 5/3$  gas. The density and pressure profiles were obtained by integrating the equation of hydrostatic equilibrium,

$$\frac{dp}{dy} = -\rho g \hat{\mathbf{k}}, \quad (1)$$

which for the case of a compressible, gamma-law gas gives

$$\rho = \rho_i \left[ 1 - (\gamma - 1) \frac{g \rho_i y}{P_0 \gamma} \right]^{\frac{1}{\gamma-1}} \quad (2)$$

and

$$P = P_0 \left[ 1 - (\gamma - 1) \frac{g \rho_i y}{P_0 \gamma} \right]^{\frac{\gamma}{\gamma-1}}. \quad (3)$$

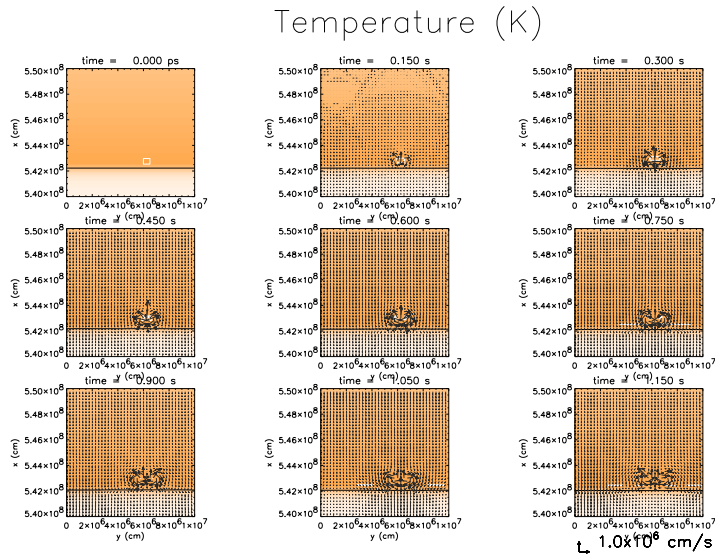


Figure 8: Beginning of convective roll formation in A. Glasner’s initial nova atmosphere. The white contour represents a temperature peak of  $T = 4.01 \times 10^7 \text{K}$ , and the black contour represents the interface between the C/O white dwarf and the accreted stellar material.

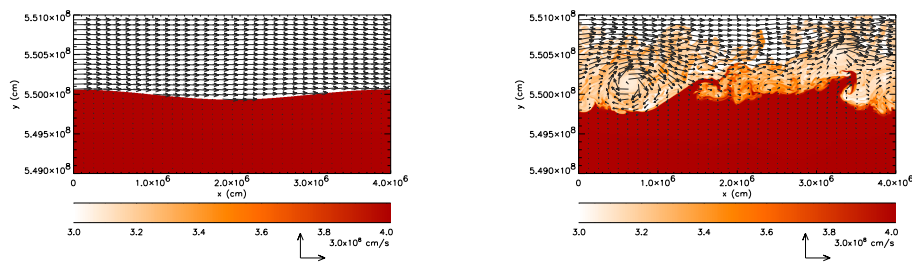


Figure 9: Preliminary simulation results showing a gravitational wave on the interface between a C/O white dwarf and a H/He atmosphere. Plotted is density, with velocity vectors. These figures represent evolution of a wave driven by a ‘step-function’ wind, which immediately drives a Kelvin-Helmholtz instability. The left figure is the initial condition; the right figure shows the state after 59 ms of evolution.

Here  $P_0$  is the pressure at the interface and  $\rho_i$  is the density immediately above or below the interface. The density discontinuity was a factor of 10, gravity was constant, and periodic boundary conditions were used on the horizontal boundaries. The wave was created by forcing the interface to be sinusoidal, perturbing the pressure, and adding a velocity.

The simulations shown here demonstrate that the step-function wind profile immediately induces a Kelvin-Helmholtz instability. This immediately introduces mixing; however, because the Kelvin-Helmholtz instability is driven by the velocity shear between the layers [10], there may be a limit to how much material can be dredged up by the wind.

The second sets of simulation results show that a wind which goes to zero velocity at the interface can interact with a gravity wave, driving the wave toward breaking. Current sets of simulations, up to our longest run (several wave crossing times), have shown a linear increase with time of the amount of C/O that has been mixed in the accreted wind. The aim of our work is to determine the dependence of the mixing rate (amount of C/O /time /cm<sup>2</sup>) on the wind velocity and wind profile. Although the mixing rate is expected to be

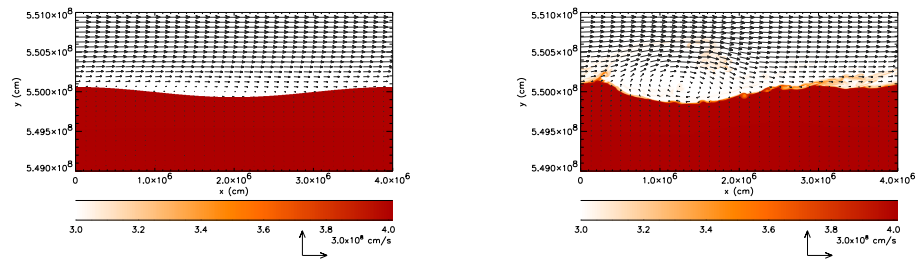


Figure 10: Same as Figure (9), but with a boundary-layer wind profile. The left figure is the initial condition, while the right figure shows the computational domain at 197 ms.



a dominantly two-dimensional effect, the height of the “mixed layer” is going to be dominated by three-dimensional turbulent advection, and this will need further study with three dimensional simulations.

While the details of operation of this mixing mechanism in nova environments remain to be explored, we interpret our results to date as indicating that such “wind” driven gravity wave instabilities may play a significant role.

#### **4.6.4 Anelastic code**

Doing convective calculations with an explicit code like the PPM module in FLASH is computationally very expensive. P. Fischer at Argonne National Labs has been continuing his work on an anelastic code using a block-structured solver similar to the FLASH framework, and is doing Rayleigh-Bernard convective simulations as per Lantz & Sudan [27] and comparing them with simulations done by Jonathan Dursi with the FLASH code. Some of this work is described further in the computer science section of this Report.

#### **4.6.5 Nova simulations with ODT**

The “One Dimensional Turbulence” (ODT) model, developed by A. Kerstein at Sandia National Labs in California, has been successfully used to model mixing in many physical systems. Pre-runaway mixing in a nova can serve to dredge up material from the white dwarf, which will crucially affect the runaway evolution; since examining large numbers of different mixing scenarios with FLASH code simulations is prohibitively expensive, we have chosen to use ODT as a method for exploring the dependencies on our initial model assumptions.

ODT, as originally formulated, does not include gravity as a dynamic effect, nor multiple species nor energy source terms. This summer, these effects were added to a version of a code which implements ODT, and initial experiments were undertaken with modeling dredge-up from the white dwarf’s surface. These calculations complement the direct numerical simulations of gravity wave breaking discussed just above.

### **4.7 Supernova explosions**

Progress has also been made in our efforts to understand the physics of Type Ia supernova explosions. We have chosen to focus our attention on the manner in which the burning regimes of the nuclear flame can provide a clear and consistent picture of the stages of the explosion. It is an understanding of the evolution from the early flamelet regime to the distributed burning regime and, ultimately, to a possible deflagration-detonation transition - the microphysics of flames - that is essential to the formulation of realistic sub-grid models for the behavior on small scales. We have studied several aspects of this problem.

#### 4.7.1 Cellular structure of carbon detonations in three dimensions

While there have been a number of experiments and numerical studies for detonations occurring in terrestrial materials, the role of the cellular structure of detonations in astrophysical applications to Type Ia supernovae has not yet been fully explored. Issues of interest include: (i) the degree to which the resolution required to reveal the cellular structure can act to define the minimum resolution required for multidimensional simulations of detonations in Type Ia supernova models and (ii) the implications of such structures for the spectra and nucleosynthesis contributions of supernovae. In the context of our ASCI studies and goals, we were concerned with whether the resulting cellular structure might give rise to levels of chemical inhomogeneity in the detonated matter that could provide constraints upon the character of the burning history.

Timmes et al. [50] have performed two-dimensional simulations of carbon detonations for conditions that are compatible with the results of one-dimensional models of Type Ia supernova events, with an initial (upstream) density of  $10^7$  g cm<sup>-3</sup>. These studies were described in detail at last year's site visit. This work has continued with a three-dimensional simulation of a carbon detonation [51], for the same initial conditions as described above for the two-dimensional case. This was a large integrated calculation, carried out on 1000 processors on ASCI Blue Mountain, at LLNL. (Details of the simulation are described in §3 above.) An obvious question here is whether there might be significant differences between the 2D and 3D cellular structures of carbon detonations. As for the 2D case, we found strong dependences upon the spatial resolution (and dimensionality) of the calculation. The strong symmetries that are present in the two-dimensional simulations are weakened or entirely absent in three dimensions. The distribution of the silicon ashes produced behind a detonation front formed by a supernova explosion is displayed in Figure 4. The three-dimensional structure of the front results in pockets of unburned material and a slight reduction in the propagation velocity of the detonation. As with the 2-D simulation, the scales of what features persist are small with respect to a pressure scale height, it would appear unlikely that variations in composition between under-reacted and over-reacted regions will impact either the nucleosynthesis yields or spectral features of supernova explosions.

#### 4.7.2 Subgrid models

For the FLASH code to be able to use a subgrid model for the evolution of a flamelet through a supernova Type Ia progenitor, it must know accurately where the flame is; however, we will never be able to have enough resolution to evolve the flame itself. Thus, we must use some sort of interface-tracking method to follow the flame's progress. This is greatly complicated by the parallel, adaptive, multidimensional nature of the code, and the fact that we expect the flame front to go through complex changes in topology during its evolution.

A variant of the Level Set Method algorithm which overcomes these difficulties has been developed for the FLASH code, and is being implemented.

### 4.7.3 Self-gravity and N-body in FLASH

P. Ricker has been working with K. Olson (NASA/GSFC) to add self-gravity capabilities to FLASH using adaptive multilevel refinement and multipole expansion algorithms. He has used these solvers to perform several large calculations involving self-gravity with FLASH. Self-gravity will be included in the forthcoming version 2.0 public distribution of FLASH. Ricker is also collaborating with K. Riley and with F. Miniati (MPI für Astrophysik) to enable the FLASH framework to include a particle-tracking module. This module will be used to follow the motion of flow-tracer particles and to simulate dark matter, stars, cosmic rays, and other collisionless matter components.

### 4.7.4 Self-gravitating turbulence

P. Ricker, R. Rosner, and J. Dursi are studying the development of turbulence in the nonlinear phase of the Jeans instability. Recent cosmological simulations have begun to resolve the mass scales of the first molecular clouds but have not been able to determine the initial mass function (IMF) of the resulting stars. This primordial IMF determines the metallicity of the intergalactic medium at high redshift and influences the reionization of the intergalactic medium. Using FLASH they are studying the gravitational stability of both stirred and unstirred turbulent gas to determine how the structure of Jeans turbulence affects the fragmentation of the first molecular clouds. Preliminary results from these calculations were presented at the 197<sup>th</sup> American Astronomical Society meeting.

### 4.7.5 Type Ia supernovae

P. Ricker is currently using FLASH 2.1 to carry out two types of full-scale Type Ia supernova simulations. Both calculations take place within the context of a Chandrasekhar-mass ( $1.38M_{\odot}$ ) white dwarf initially composed of 50% carbon and 50% oxygen, and the simulations are carried out on 2-D and 3-D adaptive meshes.

The first type of calculation is intended to study the observational effects of cellular structure in delayed detonation models. Using a spherically symmetric initial white dwarf model corresponding to the (assumed isotropic) input of nuclear energy during the deflagration phase of the model, we begin these calculations with a detonation initiated ‘by hand’ at a finite, parametrized radius. The detonation is then followed past the point at which it escapes from the star. Simulated observations of the resulting explosions will be carried out using the radiation transport code of P. Höflich (U. Texas). We expect the cellular structure present at late times in the model to provide a lower bound on observable anisotropy in the explosion.

The second type of calculation will study the convective ignition models proposed by Höflich & Stein (2001). In these calculations, we follow the evolution of the white dwarf in the hours immediately preceding the thermonuclear runaway. In the Höflich and Stein picture, convective motions combine with the relatively

long nuclear burning timescales during this period to produce an inhomogeneous carbon/oxygen ratio. The resulting entropy and composition gradients modify the speed of the burning front once ignition takes place. Thus convective motions provide a mechanism for producing the diversity observed among Type Ia supernovae. Our FLASH calculations improve on those of Höflich & Stein by incorporating a more realistic treatment of nuclear burning and more realistic boundary conditions (Höflich & Stein use a reflecting exterior boundary), and by using adaptive mesh refinement to obtain a factor of 10 better spatial resolution in two dimensions.

#### 4.7.6 Massive star evolution

A. Heger has been working on nucleosynthesis in massive stars in collaboration with R.D. Hoffman (LLNL), T. Rauscher (U Basel) and S.E. Woosley (UCSC) [35]. They followed the entire evolution and nucleosynthesis of massive stars from central hydrogen ignition till onset of core collapse, and then through the supernova explosion, simulated by a parametrized “piston” model that reproduced a typical explosion energy for core collapse supernovae of  $1.2 \times 10^{51}$  erg. Figure 11 shows the result for  $21 M_{\odot}$  of initial solar composition. These are the first calculations to follow all isotopes consistently through the whole evolution of the star. They employ an adaptive network nuclear reaction network that adds and removes isotopes as needed, based on a nuclear reaction rate database for each element up to bismuth from proton drip line to neutron drip line.

One of the question of special interest was the production of the proton-rich heavy isotopes: some of them they saw see being easily made in the massive stars (mass number ranges around 130 and around 180), while we find deficiencies in production around mass numbers 150 and 100. In particular, the light isotopes of molybdenum and ruthenium, for which the production site is not yet clearly identified, are not made in these models.

#### 4.7.7 Evolution of the first stars and galactochemical evolution

A. Heger and F.X. Timmes, in collaboration with S.E. Woosley (UCSC), study the chemical evolution of the galaxy with particular emphasis on the early chemical evolution of the universe. They compute an extended grid of massive primordial (metal-free) stars with a fine spacing of initial stellar masses of  $1 M_{\odot}$  from 11 to  $40 M_{\odot}$  and a spacing of  $5 M_{\odot}$  up to stellar masses of  $100 M_{\odot}$ . The nucleosynthesis results from these calculations will be used in a galactochemical evolution code similar to the work by [52]. The abundances will then used as input for the next generation of stellar models in order to step by step build up the chemical composition in the galaxy. Whether the present galactic element and isotope abundances can be reproduced places constraint on the production sites – stars, stellar explosions and astrophysical flashes.

A critical question in these models mixing of the helium core and the hydrogen envelope. In contrast to later stellar generation, in metal-free stars the entropy difference between the core and the envelope is only very small. If

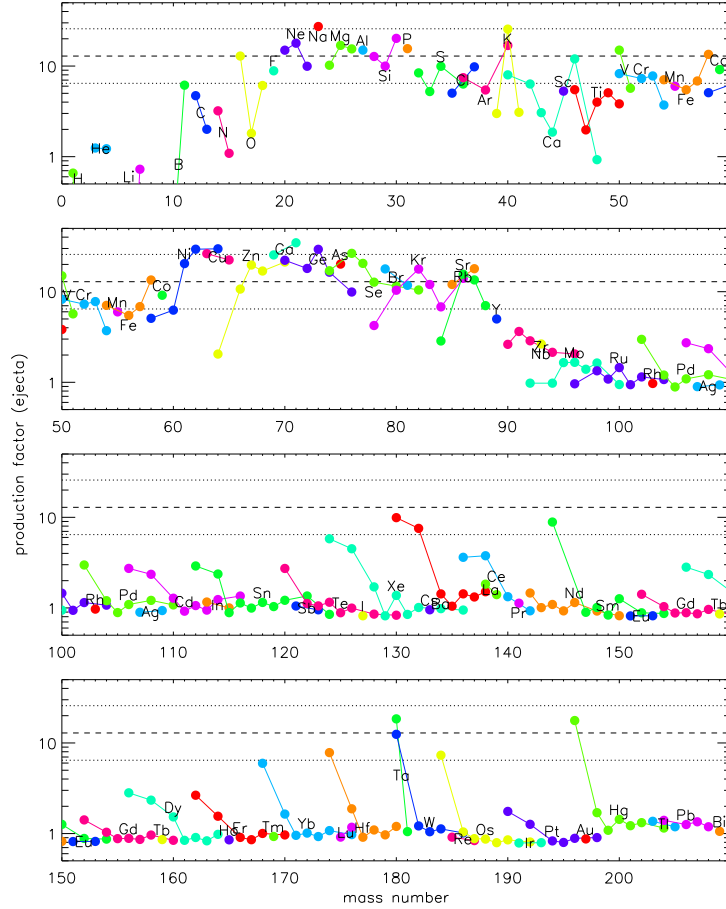


Figure 11: Production factor of isotopes (dots) in a  $21 M_{\odot}$  star of initial solar composition as a function of isotope mass number. Colors, connected by lines, indicate the different elements. Shown is the abundance of all stable isotopes in the ejecta of the supernova, after radioactive isotopes have decayed, divided by their respective solar abundances. The dashed line indicates the production factor of  $^{16}\text{O}$ , the most abundant species produced by massive stars (besides helium, which is made in all stars), and the dotted lines give a range of “acceptable” co-production of a factor 2.

this mixing occurs, carbon from the helium burning in the center of the star is converted into nitrogen, then primarily produced from the initial hydrogen and helium, while otherwise it can only be made in a subsequent stellar generation when the ejecta are mixed with the interstellar medium – in stars the carbon produced typically remains well separated from the hydrogen.

#### 4.7.8 Very massive primordial stars

A problem that has been only little studied in the recent decade are the pair instability supernovae, the fate of stars that die with helium cores of  $\sim 65 - 130 M_{\odot}$ . However, they now regained considerable interest, since current cosmological simulations indicate, that the first stars to form in the universe were likely very massive, with masses around  $100 M_{\odot}$  (e.g., [1; 5; 32] and references therein). It has been recently shown that, unlike assumed before, such primordial massive stars can indeed retain almost all of their mass [3] and thus reach the regime of pair instability [4]. These stars then entirely disrupt, powered by explosive oxygen and silicon burning with explosion energies of up to 100 times that of “normal” supernovae and produce radioactive  $^{56}\text{Ni}$  yields of up to 100 times that of Type Ia supernovae (e.g., [18], see Figure 13). These explosions should be visible out to the edge of the universe where such stars are formed (i.e., redshifts of  $\sim 20$ ; [19]) with the next generation of space telescope (NGST).

Due to their tremendous importance for cosmology, A. Heger, P. Ricker, and R. Rosner plan to study the explosion of these objects in multi-dimensional simulations using FLASH. The critical issues are mixing processes during the explosion – the classical mixing time-scale according to mixing length theory becomes comparable to the collapse/explosion time scale – and rotation, which at least requires two dimensions for a credible simulation. Indeed, rotation can make a most important difference in these stars. As show by [17; 42] rotation can significantly increase the critical mass above which pair-unstable helium cores collapse into black hole rather than explode. Of particular interest are the consequences of both, a detailed description of the mixing processes and rotation on the nucleosynthesis of the star, which they plan to follow in detail with an extended network (thousand isotopes or more) using trace particles. Constituting the first generation of stars (Pop III stars), the chemical yields from these objects sets the stage for all chemical evolution to follow later in the universe. It is also planned to follow the mixing in these explosions for longer time and use this for computing more detailed light curves from these first lighthouses in the universe to predict constraints on their observability.

The typical time-scale for the collapse and explosion (till the nuclear reactions have mostly ceased) is about a minute. Different from Type Ia supernovae, the star is non-degenerate and the burning occurs over extended regimes; different from core collapse supernovae, the densities are much lower – a peak of density on only  $10^7 \text{ g cm}^{-3}$  is reached. Being less challenging than the core astrophysics projects of the FLASH center, this should make this an interesting test problem for the FLASH code.

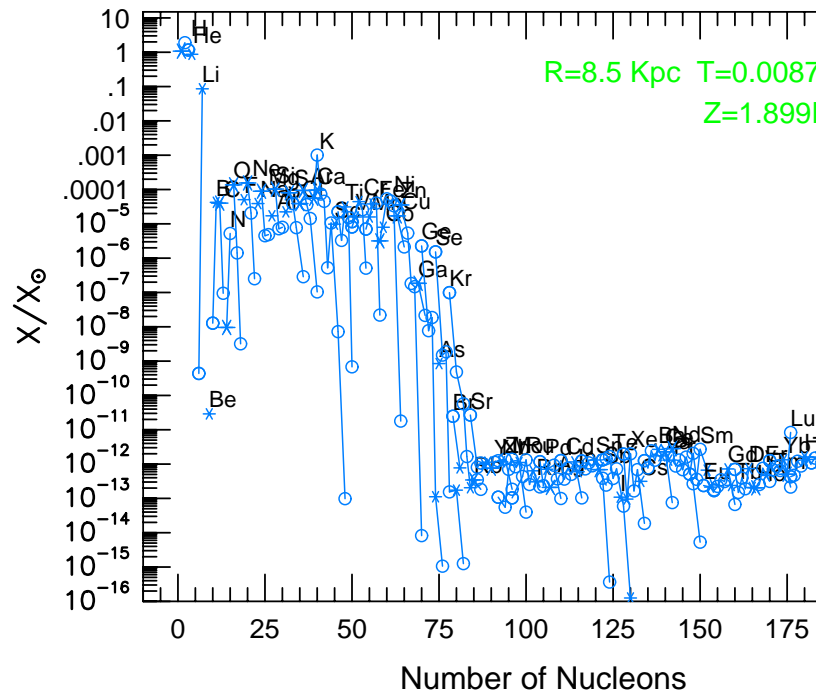


Figure 12: Isotope production factors in a galactochemical evolution model based on preliminary yield of primordial stars from 11 to 40  $M_{\odot}$  when an enrichment of 0.0001 solar is reached.

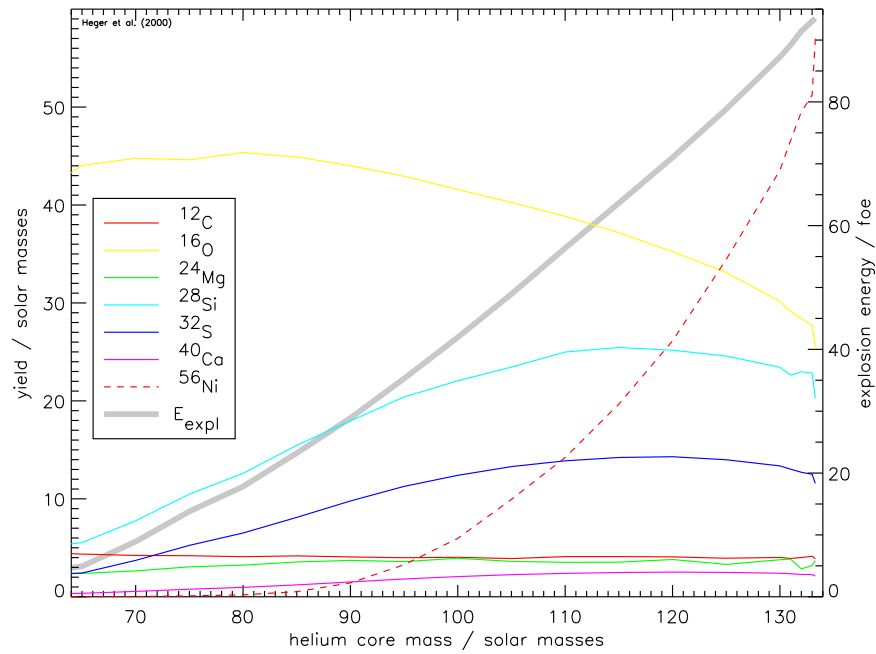


Figure 13: Production of bulk elements and explosion energy in pair instability supernovae as a function of helium core mass at time of explosion. The right scale gives the mass of ejecta of carbon (*red*), oxygen (*yellow*), magnesium (*green*), silicon (*cyan*), sulfur (*blue*), calcium (*magenta*) and  $^{56}\text{Ni}$  (*red, dashed*). The left scale gives the explosion energy in “foe”,  $1 \text{ foe} = 10^{51} \text{ erg}$ . For metal free stars without mass loss the depicted mass range of helium cores corresponds to initial stellar masses of  $\sim 140 - 260 M_{\odot}$ . Stars on either side of this range collapse to black holes rather than exploding.



## 4.8 Further astrophysical studies with FLASH

### 4.8.1 Generally-applicable MHD effects

We have been working on studies of the circumstances under which accretion onto magnetized compact objects (neutron star or white dwarf) occurs. One central question is how the accreted materials is “placed” on the stellar surface: does the accretion occur primarily at the poles, or is the material more uniformly spread over the surface? Work by C. Litwin, R. Rosner, and D.Q. Lamb [29] has shown that the answer seems to depend on the geometry of the accreting stream: If the stream is well-collimated, then it is possible that accretion occurs only over a small portion of the stellar surface, which may not even be at the poles. In more recent work, C. Litwin, E. Brown, and R. Rosner [28] have examined the stability of accretion columns on neutron stars, asking under what circumstances magnetic fields may prevent the spreading of material over the stellar surface and have obtained estimates for the onset of instability (due to unstable ballooning modes).

### 4.8.2 Self-gravitating turbulence

P. Ricker, R. Rosner, and J. Dursi are studying the development of turbulence in the nonlinear phase of the Jeans instability. Recent cosmological simulations have begun to resolve the mass scales of the first molecular clouds, but have not been able to determine the initial mass function (IMF) of the resulting stars. This primordial IMF determines the metallicity of the intergalactic medium at high redshift and influences the reionization of the intergalactic medium. Using FLASH they are studying the gravitational stability of both stirred and unstirred turbulent gas to determine how the structure of Jean turbulence affects the fragmentation of the first molecular clouds. Preliminary results from these calculations were presented at the 197<sup>th</sup> American Astronomical Society meeting.

### 4.8.3 Accretion physics

Since many accreting systems possess magnetospheres with strong magnetic fields (with strength on the stellar as much as  $10^8$  G in the case of white dwarfs and  $10^{15}$  G in the case of neutron stars), it is an important question how such magnetic fields affect the accretion of ionized matter. We have addressed this question by analytical and semi-analytical methods. In particular, we studied the evolution of the MHD stability of accreted matter in the polar caps; and of particle acceleration processes associated with accretion of magnetized plasmoids.

In the first investigation, we studied force-free, axisymmetric magnetic fields twisted by the relative disk-star rotation, in linked disk-star systems. We found that both analytic self-similar equilibria, for a uniform relative rotation, and numerical equilibria for a Keplerian disk, are similar; both exhibit a “finite

time ” (i.e, twist) singularity when the field effectively opens. The disk surface resistivity required for a steady state was determined, and was found to be far higher than what could unrealistically be expected. We also studied the mass redistribution in the magnetosphere caused by the field evolution; a density enhancement near the rotation axis found. We also addressed the question whether magnetic field twisting by relative rotation may lead to magnetic reconnection in the magnetosphere; we found that this appears impossible, for realistic parameters, in the axisymmetric configuration.

In the next investigation, we have addressed the question whether the accreted matter, which is commonly presumed to be accreted in the vicinity of magnetic poles, is confined to the polar caps or whether it can spread along the surface of a neutron star. Because the density scale height  $h$  is much smaller than the lateral pressure gradient length scale  $a$ , magnetic tension can confine an overpressure much greater than the magnetic pressure. The question is, however, whether such equilibria are stable. As an initial step, we have performed a stability analysis of magnetohydrodynamic Rayleigh-Taylor-like ballooning modes. For strong fields ( $B > 10^{12}$  G), we found that these modes stabilized by line tying in the neutron star crust until the overpressure exceeds  $8(a/h)B^2/8\pi$ ; the instability occurs within one scale height from the crust. This instability limits the amount of accreted matter that can be confined in a polar cap to  $4 \times 10^{-13} M_{\odot}$ .

Finally, we have addressed the question of particle acceleration associated with accretion of plasmoids in magnetospheres. This work was a byproduct of our earlier work [48] on stream accretion onto magnetic white dwarfs. In the present work [49] we addressed the question of the spectrum of relativistic particles generated during plasmoid accretion by magnetic neutron stars. In particular, we considered the accretion of plasmoids resulting from ionization of iron planetesimals, originating, e.g., in the matter captured by the neutron star during a supernova explosion, such as discussed previously in the context of gamma ray bursts. We have found that during the accretion of such plasmoids, polarization electric fields can accelerate nuclei to energies in the range in the ultra-high energy cosmic rays (UHECR), as high as  $10^{20}$  eV and higher. The calculated energy spectrum has the power-law form, with the exponent agreeing, within experimental uncertainties, with observations of Akeno Ground Air Shower Array (AGASA).

#### 4.8.4 Formation of stars and planets

A. Konigl and collaborators at the University of Chicago are initiating research projects that will require numerical MHD simulation. They plan to use the FLASH code, especially for those flows whose study can benefit the most from adaptive mesh refinement (AMR). Specific problems to be addressed include the following:

Fragmentation during the collapse phase of a magnetized, rotating protostellar cloud core. Some existent numerical work indicates the possibility of fragmentation during this phase, producing perhaps a multiple system instead

of a single star. The intention of this project is to perform simulations of the process, using a fully 3-D, fully MHD code. The first phase of this project will be concerned with the study the ideal MHD effects. In a later phase, Konigl and collaborators envision studying the effects of ambipolar diffusion; this would require additions and modifications to the present FLASH code. Konigl and collaborators anticipate working closely with the FLASH code developers for this; this kind of code would also be beneficial for many other applications.

Gravitational instability of a protostellar accretion disk. In this project, Konigl and collaborators plan to study numerically the non-linear development of a self-gravitational instability in a magnetized accretion disk. The Toomre criterion, valid in the linear regime for a non-magnetized system, has be modified by magnetic effects. Konigl and collaborators have found both stabilizing and destabilizing magnetic effects in the linear regime. However, the most interesting effects, such as formation of giant planets, appear in the nonlinear regime, requiring numerical simulations for their study. The spatial scales of this problem decrease as the instability progresses; Konigl and collaborators expect that AMR can be very helpful in this kind of problem, and therefore they expect that FLASH will be their tool of choice.

Planet growth and migration. Problems associated with planet growth and migration will be studied using both semianalytical techniques, and 2-D hydrodynamic and hydromagnetic simulations. The FLASH code is particularly well suited to this kind of study.

#### 4.9 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. R. Eastman (radiative transfer, supernovae; LLNL)
5. A. Glasner (novae; Hebrew University of Jerusalem)
6. W. Hillebrandt (novae and supernovae; MPI Garching bei München)
7. R. Hoffman (reaction networks; LLNL)
8. D. Lin (novae and X-ray bursts; Northwestern University)
9. E. Marietta (supernovae; University of Arizona/Tucson)
10. E. Müller (relativistic astro; MPI Garching bei München)
11. T. Strohmayer (X-ray bursts; NASA Goddard)

12. D. Swesty (radiative transfer; SUNY at Stony Brook)
13. R. Taam (novae and X-ray bursts; Northwestern University)
14. S. Woosley (supernovae and X-ray bursts; University of California at Santa Cruz)

#### 4.10 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 J. Truran), A. Mignone (supervisor R. Rosner), F. Peng (supervisor J. Truran), and J. Zuhone (supervisor J. Truran). Two of the students (Dursi and Mignone) are also closely associated with the Code Group, while one student (Alexakis) is also very heavily involved with the activities of the Basic Physics and Validation groups.

## 5 Basic Science and Validation

Participants: T. Dupont and B. Fryxell (Group Leaders), A. Alexakis<sup>1</sup>, A. Calder, F. Cattaneo, P. Constantin, J. Curtis<sup>1</sup>, A. Draganescu<sup>1</sup>, D. Grier, L. Kadanoff, R. Kirby, A. Kiselev, T. Linde, A. Malagoli, M. Medved<sup>1</sup>, A. Oberman, R. Rosner, O. Ruchayskiy<sup>1</sup>, L. Ryzhik, R. Scott, N. Vladimirova, B. Winn<sup>1</sup>, C. Yang<sup>1</sup>, Y.-N. Young

### 5.1 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. The aim is two-fold: first, we seek to understand basic physical processes relevant to the FLASH Center problems in order to construct reliable computational models (for example, of unresolved flames); second, our computational and modeling tools must be validated by comparisons with laboratory experiments, and in order to carry out such comparisons, we need substantial understanding of the underlying basic physics. It is noteworthy here that a number of the issues we have identified as central to the FLASH Center are also of considerable interest to the larger ASCI program as a whole.

The Validation Group has taken advantage of the particular interests of the Basic Science Group, and has focused its validation program on experiments which relate closely to the physical processes we need to understand as part of the FLASH project, viz., a variety of mixing instabilities at interfaces. Because of the close connection between the Basic Science and the Validation, we discuss them here together.

---

<sup>1</sup>Graduate student

## 5.2 Rayleigh-Taylor and Richtmyer-Meshkov instabilities

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

We therefore started out by aiming at a variety of mixing problems, including convective mixing, mixing in a flame front, and Rayleigh-Taylor and Richtmyer-Meshkov mixing. The latter two problems provide an especially good opportunity to use both historical and newly-generated data. The experimental program has a strong collaborative component with the NNSA Laboratories, including work with G. Dimonte (LLNL; Rayleigh-Taylor), B. Remington (LLNL; Rayleigh-Taylor, Richtmyer-Meshkov), and B. Benjamin (LANL; Richtmyer-Meshkov). As part of this program, we sent two graduate students to LLNL summer 1999 (one working on data analysis, the other working on simulations); in 2000, we again sent two students during the summer out to Sandia/Livermore (to work on mixing and flame models); last year, B. Fryxell and A. Calder participated in a workshop on this topic at LLNL during January 2001; and this summer A. Calder will visit LLNL for a summer school on high energy density physics, which plays directly into the Richtmyer-Meshkov problems we are studying. These studies of mixing are part of a broad collaboration between Chicago experimentalists, theorists, and computational physicists, including a dozen or so students and postdocs together with S. Wunch and A. Kerstein (Sandia/Livermore) and people in the CNLS at LANL. One particular success is that a simplified mixing model, pioneered by Kerstein, was further developed and tested at Chicago with good agreement between results at Chicago and Livermore. In collaboration with G. Dimonte, we are participating in a consortium of experimentalists, theorists/modelers, and computational physicists to focus on the Rayleigh-Taylor problem; the first consortium meeting took place Oct. 30, 1998; the second took place Oct. 11-12, 1999; and (as already mentioned) a third took place this past year.

In order to carry out this program, one of our foci has been the (nonlinear) development of the Rayleigh-Taylor instability. There are two specific questions we seek to understand:

*Does the nonlinear evolution of the Rayleigh-Taylor instability lead to significant flame front stretching?*

*Does Rayleigh-Taylor mixing lead to a significantly enhanced effective heat and mass diffusivity?*

Our “stable” of distinct types of hydrodynamic codes we can use to answer these questions include a pseudospectral code, a spectral element code (both of which are useful for solving weakly compressible problems) and the fully-compressible FLASH code. Thus, what we do is:

1. Carry out direct numerical simulations for well-defined weakly compressible problems that have available experimental data, using the two distinct spectral codes; a JFM paper has appeared on this work [56], which (among other things) shows that we obtain the same results for the integral scales of the flow to within 1-2%.
2. Carry out direct numerical simulations of both the weakly compressible problem and the more compressible (larger Atwood number) problem using the FLASH code and compare the results with both experimental data and results obtained from other (compressible) codes.

We have carried out a full grid of compressible calculations for both single-mode and multi-mode perturbations in both 2 and 3-D. These results will be part of a publication that describes the work of the consortium working on the RT problem. We have also (in collaboration with B. Remington and J. Kane of LLNL) carried out RT and RM calculations for a multiple-layer laser target and have been comparing the results of our calculations both with experimental data obtained at the Omega laser and with simulation results obtained by other codes. This validation work has now been written up by A. Calder [8] and submitted for publication.

Finally, we have initiated a collaboration with the Benjamin group at LANL, who operate a Richtmyer-Meshkov instability experiment using a “gas curtain” flowing within a shock tube. We have obtained preliminary results for this problem with FLASH.

### 5.3 Speed-up and Quenching of Flames in Fluids

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. Until recently, most of this work has been done in the context of passive advection, i.e., the flow is given and not influenced by the combustion. In previous work [? ? ] P. Constantin and colleagues have 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. This result holds for a variety of flows and chemical reactions, but the front geometry assumes an idealized unbounded region of burning gases. On the other hand, for certain chemical reactions (for instance for ignition-type ones) simple molecular diffusion is capable of quenching small enough burning regions surrounded by cold material. A natural question in this context is: how can one describe the influence that a turbulent flow has on a combustion process that originates in a finite blob of hot material? For ignition type reactions they have proved that

evolution depends qualitatively on the relative strength of the advecting flow and the size of the initial hot region. More precisely, if the characteristic width  $L$  of the initial hot region is sufficiently large compared to the laminar front width  $l$ , then the hot region grows and its boundary decomposes into front-like structures that propagate with the same asymptotic speed as a single front in the given flow. Turbulent flow enhances thus the rate of growth of a large enough hot region. However, if the initial hot region has a characteristic width  $L$  that is smaller than a critical width  $L_c$  then the same enhanced mixing leads, generically, to flame extinction (quenching). It was rigorously established that in a shear flow the critical size of the initial hot region is a linear function of the advection amplitude:  $L_c/l = \text{const} * U/v_0$ . Here  $v_0$  is the laminar front speed, and  $U$  is the amplitude of the turbulent shear flow. The constant of proportionality depends on the geometry of the streamlines of the shear flow. In particular, a hot region of arbitrarily large characteristic width can be quenched by a strong enough shear flow, provided the flow is not degenerate. The quantitative prediction for  $L_c/l$  has been confirmed numerically, in calculations by N. Vladimirova and O. Ruchayskiy; a manuscript is in preparation.

Almost all of the mathematical studies of combustion in the presence of advection were restricted to the cases where material and temperature diffusivities are equal (Lewis number equal to one) and the reaction-diffusion system may be reduced to one equation. Recently a study was undertaken of a system of reaction-diffusion equations with passive advection term and Lewis number  $L_e$  not equal to one. As in the  $L_e = 1$  case, in this as well the fluid advection distorts the reaction front, increasing the area available for reaction and thus speeding up the reaction process. While a variety of estimates on the influence of the flow on reaction are available for a single reaction-diffusion equation (that is, if Lewis number is equal to one), the case of the system is largely open. A general upper bound on the reaction rate in such systems was found in terms of the reaction rate for a single reaction-diffusion equation, showing that the long time average of reaction rate with  $L_e \neq 1$  does not exceed the  $L_e = 1$  case for chemical reactions of KPP type. Thus the upper estimates derived for  $L_e = 1$  apply to the systems. Both front-like and compact initial data (hot blob) were considered [? ].

Our main focus this year was on active combustion models. Encouraged by the numerical work of Vladimirova we set out to investigate analytically the Boussinesq active combustion model. In the simplest model and geometry one deals with a two dimensional Navier Stokes equation coupled to a nonlinear advection-diffusion equation. The domain is an infinite strip, of width  $L$  and infinite extension in the direction of gravity. The results are as follows. When the nonlinearity is of KPP type one can prove that for  $L$  small enough (small compared to the laminar front width and so that a Rayleigh number based on it is small) one has global nonlinear asymptotic stability of the (slowest) KPP traveling wave, and exponential decay of cross-channel gradients. This is quite remarkable, because the exponential stability is a by-product of the fluid interacting with the flame. If the width  $L$  is large then we can prove that the bulk burning rate (which is defined even if the solutions are not traveling

waves) is bounded in time average. The bound implies that this model cannot produce a transition to detonation. The technique of the proof uses an aspect of KPP nonlinearity (concavity), which is crucial for the proof (see previous work) of the non-quenching property of passively advected KPP. This is a curious link between upper bounds and lower bounds. We plan to investigate the non-quenching issue for the KPP nonlinearity in the future. The results about KPP-Boussinesq will be written up very shortly. (Constantin, Kiselev, Ryzhik, Winn). The constraint of small Rayleigh number across a thin flame front is a natural condition for stability. The condition of a narrow channel is peculiar, and has to do with the degenerate nature of the KPP nonlinearity. We are rather confident that for ignition-type nonlinearity this condition can be removed (Winn, work in progress).

A natural immediate problems to investigate is quenching in Boussinesq-ignition type nonlinearity: what characteristics determine extinction? Another problem is whether uniform upper bounds can be obtained in the ignition nonlinearity case, and in Lewis number different than one cases. (Is there a connection between quenching and transition to detonation?) We will also look at other geometries, and at self-gravitating rotating active combustion models.

## 5.4 Multi-scale modeling

Recent ASCI efforts here at Chicago and at the Alliance Laboratories have been aimed at performing multi-scale simulations in which knowledge from several length-scales is brought together in order to do a meaningful simulation of larger-scale phenomena. We have a considerable interest in doing the basic research which will enable the construction of meaningful and accurate multi-scale simulations.

We have three threads of effort aimed at this problem area:

1. We have been looking at the phenomenology of multi-scale hydro simulation using as our example problem the Rayleigh Benard system. This system has a behavior which can illuminate the analogous Rayleigh-Taylor problem. Our integration effort has resulted in a review and assessment paper by Leo Kadanoff published in *Physics Today* in August, 2001. This paper shows how the many individual structures of Rayleigh-Benard flow work together to produce the overall heat transfer in that system. We hope that this convective turbulence situation can serve as a prototype from which we can learn how to integrate structures into larger calculations.
2. Cristian Huepe is doing a simple adaptive mesh calculation aimed at illustrating how to predict and control the production of singularities in an aggregation problem, somewhat like that of stellar accretion. His goal is to predict the singularities before they form, and then excise them from his calculation so that other effects can be computed without an excessive slow-down from the singularities.
3. Cheng Yang is computing the interface singularities which occur for a pair of dielectric fluids in an electric field. He is particularly interested in jet formation mechanisms. His jets are simpler than astrophysical jets, but we expect that



they will offer insight into jet-formation and free-surface problems in the astrophysical context. His simulations have successfully produced both point-like and jet-like singularities.

## 5.5 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, R. Kirby, 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.

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. These are both very big, long-term areas of research within the FLASH project.

To illustrate the questions that one may consider in studying how the experimental measurements constrain the model one can think about having discrete points at which some things are frequently measured; the locations can be fixed in time or moving. We then want to know whether there is a simulation within the range of plausible ones, that matches the measurements within the accuracy we attribute to them. In a hydrodynamic experiment one can have both “weather stations” (fixed measurement locations) and “weather balloons” (passive tracers), and for a simulation of the experiment to be consistent it must match the information provided by both. A measurement need not be a local quantity; sometimes it is an average over a local area, and other times it involves projecting out an entire dimension.

We usually have much qualitative information about quantities in the models of experiments and it is known that in some simple cases this is very important in assessing the value of measurements. For example, the fact that a concentration can never be negative constrains the solutions of advection diffusion equations, and increases the value of discrete measurements. However, the value of such information is poorly understood in complex situations.

The range of questions that can be practically addressed will depend heavily on the efficiency of the computational processes that are used. If one must simulate an event thousands of times to determine whether a plausible set of adjustments to the simulation will make it match the experiment, then this ap-

proach will be constrained to very simple situations. For FLASH the efficiency will need to be very good, since some of the experiments we want to match are challenging computations to do even once. There are many well-understood techniques in optimal control that will be of value to us. However, substantial extensions to what is current practice will be needed to achieve the efficiency we aim for. We expect it will be useful to exploit multigrid ideas in several ways and we have studying this on some model problems. The use of qualitative information is expected to be important; this, however, complicates the computational questions, since inequality constrained optimization is much less developed than unconstrained, or equality constrained, optimization.

In the next year we expect to extend the multigrid work, to run a series of numerical experiments on systems of equations that model simple hydrodynamical situations, and to evaluate the strengths of various software tools for automating parts of the process of gradient formation.

## 5.6 Spatially variable time steps

R. Kirby, an instructor in CS and Math, joined the FLASH project this year and has looked at questions related to using time steps that vary in space. This is natural for the FLASH code since the adaptive mesh refinement results in highly variable CFL conditions, but may also be of value in situations in which the speed of propagation varies strongly in the computational domain.

Kirby has developed some rather flexible code for testing spatially varying time steps (SVTS), and has used it on scalar equations and systems in 1-D. He has also experimented with a scalar equation in 2-D.

Putting SVTS into FLASH at this time would be a very major effort. However, as further abstraction is added to the code (something the Code group is actively engaged in), this may change. The next step in evaluating SVTS techniques will involve using T. Linde's uniform grid MHD code to test SVTS which would allow experimentation on Euler and MHD problems.

## 5.7 MHD

Validation of MHD effects remains extremely challenging. The problem is that most laboratory experiments on conducting gases or fluids do not operate in astrophysically-relevant regimes: for example, most hot plasma experiments generally do not even operate in regimes which are fully collisional, so that the applicability of single-fluid theory (and related equations) is highly suspect. This problem is particularly acute for problems in which dissipative effects may be important, since it is usually the case that these effects dominate at small spatial scales (on which the plasma is most likely to be collisionless).

With these concerns in mind, we have adopted a multi-pronged approach. First, we are planning to use the MHD module in FLASH (developed principally by T. Linde) for validation simulations in collaboration with scientists at SNL (e.g., associated with the Sandia Z-pinch). Specifically, a graduate student who is principally trained at SNL will spend the summer of 2002 developing a

comprehensive set of validation test problems for SNL and the FLASH Center. Second, we have discussed a variety of possible validation comparisons with experiments at the Princeton Plasma Physics Laboratory (with M. Yamada, H. Ji, W. Tang, and N. Fisch), based on both plasma and conducting fluid (liquid metal) experiments. This includes a collisional reconnection experiment, a surface wave experiment using conducting fluids, and a Hall thruster experiment. To formalize this and other similar interactions we and PPPL participate in a multi-institution NSF proposal (led by U. of Wisconsin) to create the Center for Magnetic Self-Organization in Laboratory and Astrophysical Plasmas. Third, we submitted and won a DOE SciDAC grant for building a Hall MHD add-on to FLASH, which will be used to extend *Flash* to the two-fluid regime; this should allow us to attack laboratory problems which are not fully in the collisional regime. As a result of this effort the FLASH code will become the baseline computational platform for the Center of Magnetic Reconnection Studies at the University of Iowa (directed by A. Bhattacharjee).

## 5.8 Subgrid Modeling for MHD

The long term objective is to develop robust sub-grid-scale (SGS) models for astrophysical magnetohydrodynamics (MHD) simulations. The short term objective, a necessary first step, is to measure the “memory” or decorrelation time in a variety of MHD turbulence situations.

SGS modeling is needed when it is impossible to capture numerically the full dynamical range of the physical problem. The unresolved scales are described by an SGS model. SGS models are built from two basic ingredients: an averaging procedure, and a closure scheme. The averaging is used to replace the dynamics over the many unresolved degrees of freedom by their net effect on the resolved scales. The closure scheme gives a relation between the evolution of the resolved scales and the evolution of the averaged quantities. Both averaging and closure must be chosen carefully to develop a SGS model that represents the unresolved dynamics. For reasons given below, we are favoring Lagrangian averaging schemes.

Averages for fluid equations come in two basic flavors: Eulerian and Lagrangian. The choice of technique depends on the nature of the problem. Eulerian averages are the ones most commonly used; they are taken at a fixed spatial location and commute with both time and space derivatives. They are easy to implement, and give rise to averaged terms with straightforward physical interpretations; however, they do not preserve the geometrical structure of the original un-averaged equations. For example, the conservation of circulation along a co-moving closed curve is not preserved by Eulerian averaging, i.e., Kelvin’s circulation theorem fails. Similarly, in MHD Eulerian averaging does not preserve the conservation of magnetic flux threading a co-moving closed curve, i.e., Cowling’s theorem fails. Lagrangian averages are taken following a fluid trajectory and do not commute with either time or space derivatives separately, but they do commute with the advective derivative. Their implementation is mathematically more involved than that for Eulerian averages and often give

rise to terms that are more difficult to interpret physically. Their great advantage is that they can generate averaged equations that preserve the geometrical structure of the original equations. In particular many of the important conservation laws of the original equations, like Kelvin's and Cowling's theorems, remain valid in the averaged equations. Because the turbulent transport of angular momentum and magnetic flux play such crucial roles in many astrophysical situations, and because a non-negligible fraction of this transport is mediated by unresolved scales we have chosen to develop Lagrangian based SGS schemes. This choice requires substantial effort in mathematical and numerical development. Recently, Holm and collaborators have developed an elegant, powerful formalism to generate Lagrangian averaged equations. Their method can be used with any system whose dynamics can be written in terms of a Lagrangian, and the MHD equations fall into this general category. To give a flavor of the type of work that is required to implement these schemes as workable SGS models we present a simple illustrative example based on the incompressible Euler equations. After (Lagrangian) averaging the Euler equation is replaced by the averaged equation

$$\partial_t \mathbf{u} + \mathbf{v} \cdot \nabla \mathbf{u} = -\nabla p, \quad \nabla \cdot \mathbf{v} = 0 \quad (4)$$

where

$$(1 - \hat{\Delta})\mathbf{v} = \mathbf{u}, \quad \hat{\Delta} = \nabla \cdot \langle \xi \xi \rangle \cdot \nabla. \quad (5)$$

Here  $\mathbf{u}$  is the *averaged* velocity, and  $\mathbf{v}$  is the averaged *advective* velocity. The two are not the same in general, but are related by the elliptic equation (5) whose structure depends on the tensor quantity  $\langle \xi \xi \rangle$ , where  $\xi$  is the displacement of a fluid particle relative to its average Lagrangian position. The displacement covariance tensor  $\langle \xi \xi \rangle$  plays a central role in these Lagrangian models by encoding the statistical information required to close the scheme. In the simple case of stationary, homogeneous, isotropic, turbulence closure can be achieved by assuming that  $\langle \xi_i \xi_j \rangle = \alpha^2 \delta_{ij}$  where the constant has dimensions of length, and physically corresponds to the coherence length of the small scale turbulent fluctuations. Under these assumptions (5) becomes

$$\mathbf{v} = (1 - \alpha^2 \nabla^2)^{-1} \mathbf{u} \quad (6)$$

The resulting averaged equations, like the original unaveraged ones, conserve energy and preserve Kelvin's circulation theorem. We recognize (6) as a smoothing operation. Thus, within this model, the effect of the small scale fluctuations is to generate an advective velocity that is smoother than the velocity being advected; this last property, in particular, being characteristic of Lagrangian models. The assumptions of homogeneity and isotropy are unrealistic in most astrophysically relevant situations, and more general closure schemes must be sought. A possibility could for instance be provided by an evolution equation for  $\langle \xi \xi \rangle$  of the form

$$\partial_t \langle \xi \xi \rangle + \mathbf{v} \cdot \nabla \langle \xi \xi \rangle = \langle \xi \xi \rangle \cdot \nabla \mathbf{u} + \alpha^2 / \tau \nabla^2 \langle \xi \xi \rangle, \quad (7)$$

where  $\alpha$  once again measures the magnitude of the random displacements, and  $\tau$  is the characteristic “memory” time of the unresolved turbulence. In conventional hydrodynamic turbulence,  $\tau$  is known from laboratory and numerical experiments to be comparable to the turnover time. In other words, hydrodynamic turbulence has a short memory. The corresponding result for MHD turbulence is not known. So one of the central tasks for the development of workable SGS models for MHD is to determine, through targeted numerical simulations, the behavior of  $\tau$  in a variety of MHD turbulence situations.

The above considerations naturally suggest a sequence of steps for the development and implementation of SGS models

- **Derivation of the Lagrangian averaged equations.** The derivation of the Lagrangian averaged equations must be extended to the case of a magnetofluid. This involves recasting the ideal equations in terms of a Lagrangian, averaging the Lagrangian, and then taking a variational derivative of the Lagrangian to obtain the averaged (ideal) equations of motions. Dissipative processes are then included phenomenologically to regularize the equations.
- **Check for mathematical consistency.** This step is necessary to verify that the averaged equations preserve the transport properties of the original equations. In particular that Kelvin’s circulation theorem and Cowling’s theorem hold for the averaged equations. Also the conservation of invariant properties like energy, momentum, kinetic, magnetic and cross helicities in the ideal limit must be verified.
- **Formulate closure schemes.** In order to close the schemes the evolution of the statistical properties of two quantities must be provided as functions of the averaged variables. For MHD the two quantities are the displacement covariance tensor, as illustrated above, and the correlation tensor between the displacement and its Lagrangian curl, which arises in the expression for the averaged Lorentz force.
- **Test and calibrate closure schemes.** The first part of this task is to determine the decorrelation time for MHD turbulence as a function of mean field strength and magnetic Reynolds number (the dimensionless inverse diffusivity). This can be accomplished by integrating the Eulerian equations for MHD turbulence together with a Lagrangian solver to evolve a statistically significant population of particle trajectories (between  $10^4$  and  $10^6$ ). Numerical simulation of this type are currently under way.

## 5.9 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 by meeting here twice and twice in Livermore. One important bridge to his group continues to be Dr. S. Wunsch, who obtained his PhD with Kadanoff at Chicago, and has been working in Kerstein's group ever since.

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 we also visited extensively at the DP labs.

The particular collaborations are as follows:

LLNL:

- G. Dimonte, A. Cook et al.: LEM experiments, Rayleigh-Taylor instabilities, "Alpha Group"
- B. Remington's group: Rayleigh-Taylor and Richtmyer-Meshkov instability experiments on Nova, Omega, and NIF lasers; calculations of instabilities in supernovae

LANL:

- D. Holm: Application and testing of  $\alpha$  (subgrid) model; and development of a new subgrid model for MHD, based on the ideas underlying the  $\alpha$  model
- M. Gittings, R. Holmes, and B. Weaver: Comparison of Rayleigh-Taylor and Richtmyer-Meshkov simulations to laser experiments, using RAGE
- B. Benjamin's group: gas curtain experiments
- J. Kamm and B. Rider: simulations of gas curtain experiments

LANL:

- Graduate student Brandy Winn visited Sandia/Livermore, in a collaboration with A. Kerstein.

## References

- [1] T. Abel, G.L. Bryan, M.L. Norman, *The Formation of the First Star in the Universe*, Science, Vol. 295, Iss. 5552 (2002), 93-98.
- [2] A. Alexakis, Y.-N. Young, & R. Rosner Phys. Rev. E **65** (2002) 026313.
- [3] I. Baraffe, A. Heger, S.E. Woosley, *On the Stability of Very Massive Primordial Stars*, ApJ **550**, 890-896.
- [4] J.R. Bond, W.D. Arnett, B.J. Carr, *The evolution and fate of Very Massive Objects*, ApJ **280** (1984) 825-847.

- [5] V. Bromm, P.S. Coppi, R.B. Larson, *The Formation of the First Stars. I. The Primordial Star-forming Cloud*, ApJ **564**, 23-51.
- [6] Brown, E.F., & Bildsten, L. 1998, *The ocean and crust of a rapidly accreting neutron star: Implications for magnetic field evolution and thermonuclear flashes*, ApJ, 496, 915.
- [7] E. F. Brown, L. Bildsten & P. Chang, *Variability in the Thermal Emission from Accreting Neutron Star Transients*, ApJ in press (2002)
- [8] Calder, A., et al. 2001, ApJ, submitted.
- [9] Champagne, A. E., & Wiescher, M. 1992, *Explosive hydrogen burning*, Ann. Rev. Nucl. Part. Sci., 42, 39.
- [10] S. Chandrasekhar, *Hydrodynamic and Hydromagnetic Stability* (New York: Dover) 1981.
- [11] R. Cornelisse, J. Heise, E. Kuulkers, F. Verbunt & J. J. M. in't Zand, *The longest thermonuclear X-ray burst ever observed?. A BeppoSAX Wide Field Camera observation of 4U 1735-44*, ApJ **357** (2000), L21
- [12] R. Cornelisse, E. Kuulkers, J. J. M. in't Zand, F. Verbunt & J. Heise, *A four-hours long burst from Serpens X-1*, A&A **382** (2002), 174
- [13] A. Cumming & L. Bildsten, *Carbon Flashes in the Heavy Element Ocean on Accreting Neutron Stars*, ApJ **559** (2001), L127
- [14] Eswaran, V. and Pope, S. B. 1988. *Computers & Fluids*, 16, 257-278
- [15] B. Fryxell, et al., ApJS **131** (2000) 273.
- [16] Glasner, S.A., Livne, E., & Truran, J.W. 1997, ApJ, 475, 754.
- [17] W. Glatzel, K.J. Fricke, M.F. El Eid, *The fate of rotating pair-unstable carbon-oxygen cores*, A&A **149**, (1985) 413-422.
- [18] A. Heger, S.E. Woosley, *The Nucleosynthetic Signature of Population III*, ApJ **567** (2002), 532-543.
- [19] A. Heger, S.E. Woosley, I. Baraffe, & T. Abel: *Evolution and Explosion of Very Massive Primordial Stars*, to appear in Proc. Lighthouses in the Universe, "ESO Astrophysics Symposia", Springer-Verlag (2002).
- [20] Heise, J., in't Zand, J. J. M., & Kuulkers, E. 2000, AAS/High Energy Astrophysics Division, 32, 2803
- [21] Kercek, A., Hillebrandt, W., & Truran, J.W. 1998, A&A, 337, 379.
- [22] Khokhlov, A.M., Oran, E.S., & Wheeler, J.C. 1997, ApJ, 478, 678.
- [23] Kippenhahn, R. & Thomas, H.-C. 1978, A&A, 63, 625.

- [24] O. Koike, M. Hashimoto, K. Arai & S. Wanajo, *Rapid Proton Capture on Accreting Neutron Stars—Effects of Uncertainty in the Nuclear Process*, A&A **342** (1999), 464
- [25] E. Kuulkers, *A Superburst from GX 3+1*, A&A **383** (2002), L5
- [26] E. Kuulkers, et al., *A Half-A-Day Long Thermonuclear X-Ray Burst from KS 1731–260*, A&A **382** (2002), 503
- [27] Lantz, Steven R. and Sudan, R. N. 1995. ApJ, 441, 903
- [28] C. Litwin, E. F. Brown & R. Rosner, *Ballooning Instability in Polar Caps of Accreting Neutron Stars*, ApJ **533** (2001), 788
- [29] Litwin, C., Rosner, R., & Lamb, D.Q. 1999a, MNRAS, 310, 324-30; Litwin, C., Rosner, R., & Lamb, D.Q. 1999b, Plasma Phys. Control. Fusion, 41, B343-B350.
- [30] Livio, M. & Truran, J.W. 1994, ApJ, 425, 797.
- [31] Livio, M. & Truran, J.W. 1990, in *Nonlinear Astrophysical Fluid Dynamics*, Buchler, J.-R. & Gottesman, S.T. (Eds.), New York Academy of Sciences, 617, 126.
- [32] Nakamura, F., & Umemura, M., 2001, *On the Initial Mass Function of Population III Stars*, ApJ, **548** (2001), 19-32.
- [33] Niemeyer, J. & Woosley, S.A. 1997, ApJ, 475, 740.
- [34] A. Y. Potekhin, G. Chabrier & D. G. Yakovlev, *Internal temperatures and cooling of neutron stars with accreted envelopes*, A&A **323** (1997), 415
- [35] T. Rauscher, A. Heger, R.D. Hoffman, S.E. Woosley, *Nucleosynthesis in Massive Stars with Improved Nuclear and Stellar Physics*, ApJ (2002), in press.
- [36] J. F. Rembges, M. Liebendörfer, M., T. Rauscher F.-K. Thielemann, & H. Schatz, *Hydrogen Consumption in X-Ray Bursts*, in PROCEEDINGS OF THE 9TH WORKSHOP ON NUCLEAR ASTROPHYSICS, ed. W. Hillebrandt and E. Muller (1998, Garching bei München: Max-Planck-Institut für Astrophysik), 71
- [37] R. Rosner, et al., Bull. AAS **32** (2000) 1538.
- [38] R. Rosner, A. Alexakis, Y.-N. Young, J.W. Truran, & W. Hillebrandt, ApJ **562** (2001) L177.
- [39] Schatz, H., Aprahamian, A., Goerres, J., Wiescher, M., Rauscher, T., Rembges, J.F., Thielemann, F.K., Pfeiffer, B., Moller, P., Kratz, K.L., Herndl, H., Brown, B.A., & Rebel, H. 1998, *rp-process nucleosynthesis at extreme temperature and density conditions*, Phys. Rep., 294(4), 167.



- [40] H. Schatz, L. Bildsten, A. Cumming, & M. Wiescher, *The Rapid Proton Process Ashes from Stable Nuclear Burning on an Accreting Neutron Star*, ApJ **524** (1999), 1014
- [41] H. Schatz, et al., *The Endpoint of the Rp Process on Accreting Neutron Stars*, PRL **86** (2001), 3471
- [42] G.S. Stringfellow, S.E. Woosley, *Dynamics and Nucleosynthesis in Rotating Pair-Instability Supernovae*, in “The Origin and Distribution of the Elements”, ed. G.J. Mathews, World Scientific Press, Singapore, (1988), 467.
- [43] Strohmayer, T. E. 2000, AAS/High Energy Astrophysics Division, 32, 2410.
- [44] T. E. Strohmayer & E. F. Brown, *A Remarkable Three Hour Thermonuclear Burst from 4U 1820–30*, ApJ **566** (2001), 1045
- [45] Timmes, F.X. 1999, ApJ Suppl., 124, 241.
- [46] Timmes, F.X. 2000, ApJ, 528, 913.
- [47] Timmes, F.X., & Arnett, W.D. 1999, ApJS, 125, 277.
- [48] Timmes, F.X., & Swesty, F.D. 2000, ApJS, 126, 501.
- [49] Timmes, F.X., & Woosley, S.E. 1992, ApJ, 396, 649.
- [50] Timmes, F.X., Zingale, M., Olson, K., Fryxell, B., Ricker, P., Calder, A.C., Dursi, L.J., Truran, J.W., & Rosner, R. 2000, *On the Cellular Structure of Carbon Detonations*, ApJ, in press.
- [51] Timmes, F.X., Zingale, M., Dursi, L.J., Fryxell, B., Ricker, P., Olson, K., Calder, A.C., Tufo, H.M., MacNeice, P., Truran, J.W., & Rosner, R. 2000, *Similarities and Differences Between the 2D and 3D Cellular Structure of Carbon Detonations*, to be submitted to ApJ.
- [52] F.X. Timmes, S.E. Woosley, T.A. Weaver, *Galactic chemical evolution: Hydrogen through zinc*, ApJS **98** (1995), 617-658.
- [53] Truran, J.W. 1982, in *Essays in Nuclear Astrophysics*, Barnes, C.A., Clayton, D.D., & Schramm, D.N. (Eds.), Cambridge University Press, p. 467.
- [54] Van Wormer, L., Görres, J., Iliadis, C., Wiescher, M., & Thielemann, F.K. 1994, *Reaction rates and reaction sequences in the rp-process*, ApJ, 432, 326.
- [55] Weaver, T.A., & Woosley, S.E. 1993, *Nucleosynthesis in massive stars and the  $^{12}\text{C}(\alpha, \gamma)^{16}\text{O}$  reaction rate*, Phys. Rep., 227, 65.
- [56] Young, Y.-N., Tufo, H., Dubey, A., & Rosner, R. 2001, JFM, 447, 377.

## 6 Publications

1. Brown, E. F., Bildsten, L., & Chang, P., *Variability in the Thermal Emission from Accreting Neutron Star Transients*, 2002, ApJ, in press
2. Ciecielag, P., Plewa, T., & Rozycka, M., *Mass transfer in the vicinity of a protoplanet's orbit*, 2001, R.E. Schielicke, ed, Astronomische Gesellschaft Abstract Series, Vol. 18. Abstracts of Contributed Talks and Posters presented at the Annual Scientific Meeting of the Astronomische Gesellschaft at the Joint European and National Meeting JENAM 2001 of the European Astronomical Society and the Astronomische Gesellschaft at Munich, September 10-15, 2001, abstract #P41
3. Fryxell, B., Zingale, M., Timmes, F.X., Lamb, D.Q., Olson, K., Calder, A.C., Dursi, L.J., Ricker, P., Rosner, R., Truran, J.W., MacNeice, P., & Tufo, H., *Numerical Simulations of Thermonuclear Flashes on Neutron Stars*, 2001, Nuclear Phys., A688, 172-176.
4. Kane, J.O., Robey, H.F., Remington, B.A., Drake, R.P., Knauer, J., Ryutov, D.D., Louis, H., Teyssier, R., Hurricane, O., Arnett, D., Rosner, R., & Calder, A., *Interface imprinting by a rippled shock using an intense laser*, 2001, Phys. Rev. E, 63, 055401 (Rapid Communications).
5. Kempner, J. C., Sarazin, C. L., and Ricker, P. M. "*Chandra Observations of Abell 85: Merger of the South Subcluster.*", 2002, ApJ, submitted
6. Kempner, J. C., Sarazin, C. L., and Ricker, P. M., *Dynamics of the Multiple Merger Cluster of Galaxies Abell 85*, 2001, in X-rays at Sharp Focus: Proceedings of the Chandra Science Symposium, S. Vrtilek, E. M. Schlegel, and L. Kuhi, eds., July 16-18, 2001,
7. Litwin, C., Brown, E. F., & Rosner, R. *Ballooning Instability in Polar Caps of Accreting Neutron Stars* 2001, ApJ, 533, 788
8. Litwin, C., & Rosner, R., *Plasmoid Impacts on Neutron Stars and Highest Energy Cosmic Rays*, 2001, PRL, 86, 4745-8.
9. Plewa, T., & Rozycka, M., 2001, Sgr A\* and Sgr A East: intimate life in the Galactic center, to appear in M. Rosado, L. Binette and L. Arias, eds, ASP Conf. Series, Proceedings of the Conference Galaxies: the Third Dimension, Cozumel, Mexico, December 3-7, 2001 (astro-ph/0202470)
10. Randall, S. W., Sarazin, C. L., & Ricker, P. M., *The Effect of Merger Boosts on the Luminosity, Temperature, and Inferred Mass Functions of Clusters of Galaxies*, 2002, ApJ, submitted
11. Ricker, P. M. & Sarazin, C. L., *Off-Axis Cluster Mergers: Effects of a Strongly Peaked Dark Matter Profile*, 2001, ApJ, 561, 621

12. Ricker, P. M. & Sarazin, C. L. *Off-Axis Cluster Mergers*, 2001, in Proceedings of the 20th Texas Symposium on Relativistic Astrophysics, J. C. Wheeler and H. Martel, eds. (Melville, NY: AIP Press, 2001), 152
13. Ricker, P. M., Calder, A. C., Dursi, L. J., Fryxell, B., Lamb, D. Q., MacNeice, P., Olson, K., Rosner, R., Timmes, F. X., Truran, J. W., Tufo, H. M., and Zingale, M., *Large-Scale Simulations of Clusters of Galaxies*, 2001, in Proceedings of the VII International Workshop on Advanced Computing and Analysis Techniques in Physics Research (ACAT 2000), P. C. Bhat and M. Kasemann, eds. (Melville, NY: AIP Press, 2001), 316
14. Ricker, P.M., Olson, K., Calder, A.C., Dursi, L.J., Fryxell, B., Lamb, D.Q., MacNeice, P., Rosner, R., Timmes, F.X., Truran, J.W., Tufo, H.M., & Zingale, M., *Self-Gravitating Hydrodynamic Simulation using FLASH*, 2002, in preparation.
15. Ricker, P. M., Calder, A. C., Dursi, L. J., Fryxell, B., Lamb, D. Q., MacNeice, P., Olson, K., Rosner, R., Timmes, F. X., Truran, J. W., Tufo, H. M., & Zingale, M., *Large-Scale Simulations of Clusters of Galaxies*, 2001, to appear in Proceedings of the VII International Workshop on Advanced Computing and Analysis Techniques in Physics Research (ACAT 2000), Fermilab, October 16-20, 2000 (astro-ph/0011502)
16. Ricker, P. M., Dursi, L. J., Rosner, R., Calder, A. C., Fryxell, B., Olson, K., Timmes, F. X., Truran, J., Tufo, H., Zingale, M., & MacNeice, P., *The Structure of Self-Gravitating Hydrodynamic Turbulence*, 2001, BAAS, 197
17. Ricker, P. M., Olson, K., Calder, A. C., Dursi, L. J., Fryxell, B., Lamb, D. Q., MacNeice, P., Rosner, R., Timmes, F. X., Truran, J. W., Tufo, H. M., & Zingale, M., *Self-Gravitating Hydrodynamic Simulation using FLASH*, 2001, in preparation
18. Ricker, P. M., & Sarazin, C. L., *Off-Axis Cluster Mergers*, 2001, to appear in Proceedings of the 20th Texas Symposium on Relativistic Astrophysics, Austin, TX, December 10-15, 2000
19. Ricker, P. M., & Sarazin, C. L., *Off-Axis Cluster Mergers: Effects of a Strongly Peaked Dark Matter Profile*, 2001, ApJ, in press
20. Ricker, P. M., Siegel, A., Calder, A. C., Dursi, L. J., Fryxell, B., Lamb, D. Q., MacNeice, P., Olson, K., Riley, K., Rosner, R., Timmes, F. X., Truran, J. W., Vladimirova, N., Weirs, G., & Zingale, M., *A Framework for High-Performance Astrophysical Simulation*, 2001, in preparation
21. Rosner, R., Alexakis, A., Young, Y.-N., Truran, J.W., & Hillebrandt, W., *On the C/O Enrichment of Novae Ejecta*, 2001, ApJ Letters, 562, L177-9.
22. Strohmayer, T. E., & Brown, E. F., *A Remarkable Three Hour Thermonuclear Burst from 4U 1820–30*, 2001, ApJ, 566, 1045

23. Young, Y.-N., Tufo, H., Dubey, A., & Rosner, R., *On the Miscible Rayleigh-Taylor Instability: 2-D and 3-D*, 2001, JFM, 447, 377.
24. Zingale, M., Timmes, F.X., Fryxell, B., Lamb, D.Q., Olson, K., Calder, A.C., Dursi, L.J., Ricker, P., Rosner, R., MacNeice, P., & Tufo, H., *Helium Detonations on Neutron Stars*, 2001, ApJS, 133, 195-220.
25. S. Adjerid, K.D. Devine, J.E Flaherty, & L. Krivodonova, A Posteriori Error Estimation for Discontinuous Galerkin Solution of Hyperbolic Problems, *Comp. Meth. Appl. Mech. Engng.*, 191, 466- 473, (2002).
26. J. Ahrens, K. Brislawn, K. Martin, B. Geveci, C.C. Law, & M.E. Papka, Large Scale Data Visualization Using Parallel Data Streaming, *IEEE Computer Graphics & Applications*, (2001).
27. J. Ahrens, C. Law, W. Schroeder, K. Martin, & M. Papka, A Parallel Approach for Efficiently Visualizing Extremely Large Time-Varying Datasets, Los Alamos National Laboratory, Los Alamos, Technical Report LAUR-00-1620, (2000).
28. A. Alexakis, Y. N. Young, & R. Rosner, Shear Instability of Fluid Interfaces: Stability Analysis, *PRE*, 65, 026313, (2002).
29. A. Alexakis, Y. N. Young, & R. Rosner, Weakly Non-Linear Analysis of Wind-Driven Gravity Waves, *JFM*, March (2002), submitted.
30. W. Allcock, J. Bester, J. Bresnahan, A. Chervenak, I. Foster, C. Kesselman, S. Meder, V. Nefedova, D. Quesnel, & S. Tuecke, Data Management and Transfer in High Performance Computational Grid Environments, *Parallel Computing.*, (2002).
31. W. Allcock, J. Bresnahan, I. Foster, L. Liming, J. Link, & P. Plaszczac, GridFTP Update January 2002, Technical Report.
32. W. Allcock, J. Bester, J. Bresnahan, A. Chervenak, I. Foster, C. Kesselman, S. Meder, V. Nefedova, D. Quesnel, & S. Tuecke, Secure, Efficient Data Transport and Replica Management for High- Performance Data-Intensive Computing, in *IEEE Mass Storage Conference*, April, (2001).
33. B. Ayata & T.F. Dupont, Convergence of a Step-Doubling Galerkin Method for Parabolic Problems, (2002) to be submitted.
34. R. Bank, T.F. Dupont, S. Garcia, Y. Liu, & R. Santos, Symmetric Error Estimates for Moving Mesh Mixed Methods for Advection Diffusion Equations, *SIAM J. Num. Anal.* (2000), submitted. 11. K.E. Belle, C.E. Woodward, A. Evans, S. Eyres, R.D. Gehrz, M. Schuster, M.A. Greenhouse, J. Krautter, S.G. Starrfield, & J. W. Truran, *Nicmos Imagery of Nova Shells*, American Astronomical Society Meeting, vol. 194, May 1999, p. 8611.

35. J. Bresnahan, J. Insley, & M.E. Papka, Interacting with Scientific Visualizations: User-Interface Tools within Spatially Immersive Displays, 71 Argonne National Laboratory, Argonne ANL/MCS-P789-0100, January (2000).
36. A. C. Calder, B.C. Curtis, L.J. Dursi, B. Fryxell, G. Henry, P. MacNeice, K. Olson, P. Ricker, R. Rosner, F.X. Timmes, H. M. Tufo, J.W. Truran, & M. Zingale, High-Performance Reactive Fluid Flow Simulations Using Adaptive Mesh Refinement on Thousands of Processors, in Proc. Supercomputing 2000, IEEE Computer Soc. (2000), <http://sc2000.org/proceedings/>
37. A. C. Calder, B. Fryxell, T. Plewa, R. Rosner, L. J. Dursi, V. G. Weirs, T. Dupont, H. F. Robey, J. O. Kane, B. A. Remington, R. P. Drake, G. Dimonte, M. Zingale, F. X. Timmes, K. Olson, P. Ricker, P. MacNeice & H. M. Tufo, On Validating an Astrophysical Simulation Code, *ApJ*, (2002) submitted.
38. A.C. Calder, B. Fryxell, R. Rosner, J. Kane, B.A. Remington, L.J. Dursi, K. Olson, P.M. Ricker, F.X. Timmes, M. Zingale, P. MacNeice, & H. Tufo, Flash Simulations of Multi-Layer Targets, American Astronomical Society Meeting, vol. 196, May (2000), p. 2203.
39. A. Chan, W. Gropp, & E. Lusk, Scalable Log Ffiles for Parallel Program Trace Data, ANL preprint.
40. A. Chervenak, I. Foster, C. Kesselman, C. Salisbury, & S. Tuecke, The Data Grid: Towards an Architecture for the Distributed Management and Analysis of Large Scientific Datasets., *Journal of Network and Computer Applications* (2000).
41. A. Chervenak, I. Foster, C. Kesselman, & S. Tuecke, Protocols and Services for Distributed Data-Intensive Science, *Proc. ACAT 2000* (2001).
42. H. Chevaugeron, P. Hu, J.-F. Remacle, J.E. Flaherty & M.S. Shephard, Application of DG method to suite of test problems, (2002), in preparation.
43. L. Childers, T. Disz, R. Olson, M.E. Papka, R. Stevens, & T. Udeshi, Access Grid: Immersive Group-to-Group Collaborative Visualization, in *Immersive Projection Technology*, Ames, Iowa, (2000).
44. P. Constantin, A. Kiselev, A. Oberman, & L. Ryzhik, Bulk Burning Rate In Passive - Reactive Diffusion, *Arch. Rational Mechanics*, 154, 53-91 (2000).
45. P. Constantin, A. Kiselev & L. Ryzhik, Quenching of Flames by Fluid Advection, *Commun. Pure Appl. Math.* 54, no.11, 13201342, (2001).
46. P. Constantin, A. Kiselev & L. Ryzhik & B. Winn, Stability and Speed of Reaction Fronts in Boussinesq Active Combustion, in preparation.

47. P. Constantin, A. Kiselev & L. Ryzhik, Area of Level Sets in Combustion Advected by Turbulent Flows, in preparation
48. T.F. Dupont & Y. Liu, Symmetric Error Estimates for Moving Mesh Galerkin Methods for Advection Diffusion Equations, *SIAM Jour. Numer. Anal.*, (2002), to appear.
49. L.J. Dursi, J. Niemeyer, A. Calder, B. Fryxell, D. Lamb, K. Olson, P. Ricker, R. Rosner, F. Timmes, H. Tufo, & M. Zingale, Compressed Reactive Turbulence and Supernovae Ia Recollapse Using the Flash Code, *American Astronomical Society Meeting*, vol. 195, December (1999), p. 4202.
50. P.F. Fischer, N.I. Miller, & H.M. Tufo, An Overlapping Schwarz Method for Spectral Element Simulation of Three-Dimensional Incompressible Flows, *Parallel Solution of Partial Differential Equations* (2000).
51. J. E. Flaherty, L. Krivodonova, J. F. Remacle & M.S. Shephard, Aspects of Discontinuous Galerkin Methods for Hyperbolic Conservation Laws, *Finite Elements in Analysis and Design*, (2002), to appear.
52. I. Foster, The Grid: A New Infrastructure for 21st Century Science, *Physics Today*, Feb., (2002).
53. L. Freitag & R. Loy, Theoretical Cost Comparison of Remote Visualization Strategies, Technical Report, Argonne National Laboratory, March, 2002, *International Journal of Information*, (2002), to appear.
54. L. Freitag & R. Loy & M. Nandwani, Comparison of Subsampling Approaches for Remote, Interactive Exploration of Large Data Sets, Poster, SC2001, Denver, November, (2001).
55. L. Freitag & R. Loy, Data Reduction Techniques for Interactive Visualization on Computational Grids, Technical Report ANL/MCS- P906-0901, Argonne National Laboratory, May, (2001).
56. L. Freitag & R. Loy, Comparison of Remote Visualization Strategies for Interactive Exploration of Large Data Sets, *Proceedings of the 15th International Parallel and Distributed Processing Symposium*, San Francisco, April 23, (2001).
57. B. Fryxell, K. Olson, P. Ricker, F.X. Timmes, M. Zingale, D.Q. Lamb, P. MacNeice, R. Rosner, J. Truran & H. Tufo, FLASH: An Adaptive Mesh Hydrodynamics Code for Modeling Astrophysical Thermonuclear Flashes, *ApJS*, 131, (2000), 273-334.
58. B. Fryxell, F.X. Timmes, M. Zingale, L.J. Dursi, P. Ricker, K. Olson, A.C. Calder, H. Tufo, P. MacNeice, J.W. Truran, & R. Rosner, The Cellular Structure of Carbon Detonations, *American Astronomical Society Meeting*, vol. 196, May (2000), p. 3902.

59. B. Fryxell, M. Zingale, F.X. Timmes, D.Q. Lamb, K. Olson, A.C. Calder, L.J. Dursi, P. Ricker, R. Rosner, J.W. Truran, P. MacNeice, & H. Tufo, Numerical Simulations of Thermonuclear Flashes on Neutron Stars, Nuclear Physics A, (2000) in press.
60. B. Fryxell, M. Zingale, F.X. Timmes, K. Olson, D. Lamb, A. Calder, J. Dursi, P. Ricker, R. Rosner, & H. Tufo, Helium Burning on Neutron Stars: 2-Dimensional Results, American Astronomical Society Meeting, vol. 195, December (1999), p. 4204.
61. R.D. Gehrz, J.W. Truran, R.E. Williams, & S. Starrfield, Nucleosynthesis in Classical Novae and its Contribution to the Interstellar Medium, PASP 110 (1998), 3.
62. V. Girault & L.R. Scott, Stability of Dispersive Model Equations for Fluid Flow. In conference proceedings, Estep, D. and S. J. Tavener, eds., SIAM, (2002).
63. V. Girault & L.R. Scott, Analysis of a Two-Dimensional of a Grade-Two Fluid Model with a Tangential Boundary Condition, J. Math. Pures Appl., 78: 981-1011, (1999).
64. V. Girault & L.R. Scott, Finite Element Discretizations of a Two-Dimensional Grade-Two Fluid Model, MMAN, 35:1007-1053, (2001).
65. V. Girault & L.R. Scott, Hermite Interpolation of Non-Smooth Functions Preserving Boundary Conditions, Mathematics of Computation, 71:1043-1074, (2002).
66. V. Girault & L.R. Scott, A Quasi-Local Interpolation Operator Preserving the Discrete Divergence. *Calcolo*, :1-20, (2002), to be submitted.
67. M. Greiner, P.F. Fischer & H. M. Tufo, Two Dimensional Simulations of Enhanced Heat Transfer in an Intermittently Grooved Channel, J. Heat Transfer, to appear.
68. M. Greiner, P.F. Fischer, H. M. Tufo & R.A. Wirtz, Three Dimensional Simulations of Enhanced Heat Transfer in a Flat Passage Downstream from a Grooved Channel, J. Heat Transfer, to appear.
69. J. Hensley, R. Hudson, K. Hwang, J. Insley, I. Nadjakova, M.E. Papka M. E. & R. Stevens, Case Study: Visualizing Astrophysical Thermonuclear Flashes, Visualization, (2002), submitted.
70. M. Hereld, I.R. Judson, & R.L. Stevens, Tutorial: Introduction to Building Projection-based Tiled Display Systems, IEEE Computer Graphics & Applications, vol. 20, (2000).
71. M. Hereld, I.R. Judson, J. Paris, & R.L. Stevens, Immersive Projection Technology, in Immersive Projection Technology, Ames, Iowa, (2000).

72. J. Kane, D. Arnett, B.A. Remington, S.G. Glendinning, G. Bazan, R.P. Drake, & B.A. Fryxell, Supernova Experiments on the Nova Laser, *ApJS* 127, (2000), 365.
73. J. Kane, D. Arnett, B.A. Remington, S.G. Glendinning, G. Bazan, E. Muller, B.A. Fryxell, & R. Teyssier, Two-Dimensional Versus Three-Dimensional Supernova Hydrodynamic Instability Growth, *ApJ* 528 (2000), 989.
74. J. Kane, H.F. Robey, B.A. Remington, R.P. Drake, J. Knauer, D.D. Ryutov, H. Louis, R. Teyssier, O. Hurricane, D. Arnett, R. Rosner, & A. Calder, Interface Imprinting by a Rippled Shock Using an Intense Laser, *Phys. Rev. E*, 63 (2001), 055401 (Rapid Communications).
75. A. Kercek, W. Hillebrandt & J. W. Truran, Two-Dimensional Simulations of the Thermonuclear Runaway in an Accreted Atmosphere of a C+O White Dwarf, *A&A* (1998), 337, 379.
- 5
76. A. Kercek, W. Hillebrandt, & J.W. Truran, Two- and Three-Dimensional Simulations of Classical Novae, *Astronomische Gesellschaft Meeting Abstracts*, Abstracts of Contributed Talks and Posters presented at the Annual Scientific Meeting of the *Astronomische Gesellschaft* at Heidelberg, September 14-19, 1998, talk #C10 14 (1998), 10.
77. A. Kercek, W. Hillebrandt, & J.W. Truran, Two and Three Dimensional Simulations of Thermonuclear Runaways in Accreted Atmospheres on White Dwarfs, in *Nuclear Astrophysics*, Hillebrandt, W. and Miller, E. (Eds.), *Publications of the Max-Planck-Institute for Astrophysics* (1998), p. 56.
78. A. Kercek, W. Hillebrandt, & J.W. Truran, Three-Dimensional Simulations of Classical Novae, *A&A* 345 (1999), 831.
79. Kirby, R. On the Convergence of High Resolution Methods with Multiple Time Scales for Hyperbolic Conservation Laws, *Math Comp.*, (2002), to appear.
80. A. Kiselev & L. Ryzhik, Enhancement of the Traveling Front Speeds in Reaction-Diffusion Equations with Advection, *Ann. Inst. H. Poincaré Anal. Non Linéaire* 18 (2001).
81. A. Kiselev & L. Ryzhik, An Upper Bound for the Bulk Burning Rate for Systems, *Nonlinearity* 14, (2001), 1297-1310.
82. J. Krautter, J.W. Truran, et al., X-Ray Pulsations and a “Burst” in the X-Ray Light Curve of Classical Nova V1494 Aql (1999 #2) in Outburst, *Astronomische Gesellschaft Abstract Series*, 18 (2001), 101.



83. L. Krivodonova & J.E. Flaherty, Error Estimation for Discontinuous Galerkin Solution of Multidimensional Hyperbolic Problems, *Advances in Computational Mathematics*, (2002), to appear.
  84. D.Q. Lamb, Some Startling Discoveries about X-Ray Bursts, *ApJS* 127 (2000), 395.
  85. T. Linde & A. Malagoli, On Local Div B Control in Ideal MHD Simulations, *JCP* (2001), submitted.
  86. C. Litwin, E.F. Brown & R. Rosner, Ballooning Instability in Polar Caps of Accreting Neutron Stars, *ApJ*, 553 (2001), 788-795.
  87. C. Litwin & R. Rosner, Plasmoid Impacts on Neutron Stars and Highest Energy Cosmic Rays, *Phys. Rev. Let.* (2001), in press.
  88. C. Litwin & R. Rosner, Relativistic Space-Charge Limited Bipolar Flow, *Phys. Rev. E* 58 (2000), 1163.
  89. C. Litwin, R. Rosner, & D.Q. Lamb, On Accretion Flow Penetration of Magnetospheres, *MNRAS* 310 (1999), 324.
  90. C. Litwin, R. Rosner, & D.Q. Lamb, On Stream Accretion onto Magnetized Compact Objects, *American Astronomical Society Meeting*, vol. 194, May (1999), pp. 2909.
  91. Y. Liu, R. Bank, T.F. Dupont, S. Garcia, Y. Liu & R. Santos, Symmetric Error Estimates for Moving Mesh Mixed Methods for Advection Diffusion Equations, submitted.
- 6
92. E. Marietta, A. Burrows, & B. Fryxell, Type Ia Supernova Explosions in Binary Systems: the Impact on the Secondary Star and its Consequences, *ApJS* 128 (2000), 615.
  93. M. Miccono, G. Bodo, S. Massaglia, P. Rossi, A. Ferrari, & R. Rosner, Kelvin-Helmholtz Instability in Three Dimensional Radiative Jets, *A&A* 360 (2000), 795-808.
  94. J.C. Niemeyer & J.W. Truran (eds.), *Type Ia Supernovae: Theory and Cosmology* (2000).
  95. A. Oberman, Motion of Level Sets by Advection, Growth and Mean Curvature as a Model for Combustion, thesis, University of Chicago (2001), <http://www.math.uchicago.edu/~oberman/research.html> .
  96. K.M. Olson, P. MacNeice, B. Fryxell, P. Ricker, F.X. Timmes, & M. Zingale, Paramesh: a Parallel, Adaptive Mesh Refinement Toolkit and Performance of the ASCI/Flash Code, *American Astronomical Society Meeting*, vol. 195, December (1999), p. 4203.

97. R. Olson & M.E. Papka, Remote Visualization with Vic / Vtk, Visualization 2000 Hot Topics, Salt Lake City, Utah, (2000).
98. M. E. Papka, Development and Analysis of a Movie Playback Tool for Use in Tiled Display Environments, University of Chicago Computer Science Master's Thesis, (2002).
99. J.-F. Remacle, J.E., Flaherty & M.S. Shephard, An Adaptive Discontinuous Galerkin Technique with Orthogonal Basis Applied to Rayleigh-Taylor Instabilities, SIAM Review, to appear.
100. J.-F. Remacle, O. Klass, J.E., Flaherty & M.S. Shephard, A Parallel Algorithm Oriented Mesh Database, Engineering with Computers (2002), to appear.
101. J.-F. Remacle & M.S. Shephard, An Algorithm Oriented Mesh Database, International Journal for Numerical Methods in Engineering, (2002), to appear.
102. J.-F. Remacle & M.S. Shephard, & J.E. Flaherty, Some Issues on Distributed Mesh Representations, 8th International Conference on Numerical Grid Generation in Computational Field Simulations, (2002).
103. J.-F. Remacle, K. Pinchedez, J.E., Flaherty & M.S. Shephard, An Efficient Local Time Stepping Scheme for Transient Adaptive Calculations, Comp. Meth. Appl. Mech. Engng. (2001), submitted.
104. J.-F. Remacle, J.E., Flaherty, M.S. Shephard & O. Klass, Parallel Algorithm Oriented Mesh Database, Proc. 10th International Meshing Roundtable, Report No. SAND 2001-2976C, pp. 341-349, (2001).
105. P.M. Ricker, A. Siegel, A.C. Calder, L.J. Dursi, B. Fryxell, D.Q. Lamb, P. MacNeice, K. Olson, K. Riley, R. Rosner, F.X. Timmes, J.W. Truran, N.Vladimirova, G. Weirs, & M. Zingale, A Framework for High-Performance Astrophysical Simulation, (2002), in preparation.
106. P.M. Ricker, K. Olson, A.C. Calder, L.J. Dursi, B. Fryxell, D.Q. Lamb, P. MacNeice, R. Rosner, F.X. Timmes, J.W. Truran, H.M. Tufo, & M. Zingale, Self-Gravitating Hydrodynamic Simulation using FLASH, (2002), in preparation.
107. Ricker, P.M., and Sarazin, C.L. 2001, Off-Axis Cluster Mergers: Effects of a Strongly Peaked Dark Matter Profile, ApJ, 561, (2001) 621.
108. P.M. Ricker, L.J. Dursi, R. Rosner, A.C. Calder, B. Fryxell, K. Olson, F.X. Timmes, J.W. Truran, H. Tufo, M. Zingale, & P. MacNeice, The Structure of Self-Gravitating Hydrodynamic Turbulence, BAAS, (2001), 197.

109. P.M. Ricker, S. Dodelson, & D.Q. Lamb, *Cosmos: a Hybrid N-Body /Hydrodynamics Code for Cosmological Problems*, *ApJ* 536 (2000), 122.
110. P. M. Ricker, A.C. Calder, L.J. Dursi, B. Fryxell, D.Q. Lamb, P. MacNeice, K. Olson, R. Rosner, F.X. Timmes, J.W. Truran, H.M. Tufo, & M. Zingale *Large-Scale Simulations of Clusters of Galaxies*, in *Proceedings of the VII International Workshop on Advanced Computing and Analysis Techniques in Physics Research (ACAT 2000)*, P. C. Bhat and M. Kasemann, eds. (Melville, NY: AIP Press, 2001), 316
111. P.M. Ricker, & C.L. Sarazin, *Off-Axis Cluster Mergers*, *Proceedings of the 20th Texas Symposium on Relativistic Astrophysics*, Austin, TX, December 10-15, (2000) to appear.
112. P.M. Ricker, B. Fryxell, K. Olson, F.X. Timmes, M. Zingale, D.Q. Lamb, P. MacNeice, R. Rosner, & H. Tufo, *Flash: a Multi- dimensional Hydrodynamics Code for Modeling Astrophysical Thermonuclear Flashes*, *American Astronomical Society Meeting*, vol. 195, December (1999), p. 4205.
113. R. Rosner, A. Alexakis, Y.N. Young, J.W. Truran, & W. Hilderbrandt. *On the C/O Enrichment of Nova Ejecta*, *ApJ Letters*, 562, L177, (2001).
114. R. Rosner, A.C. Calder, L.J. Dursi, B. Fryxell, D.Q. Lamb, J.C. Niemeyer, K. Olson, P.M. Ricker, F.X. Timmes, J.W. Truran, H.M. Tufo, Y.N. Young, M. Zingale, E. Lusk, & R. Stevens, *Astrophysical Thermonuclear Flashes*, *CiSE*, 2 (2000), no. 5.
115. A.A. Sonzogni, K.E. Rehm, I. Ahmad, F. Borasi, D.L. Bowers, F. Brumwell, J. Caggiano, C.N. Davids, J.P. Greene, B. Harss, A. Heinz, D. Henderson, R.V.F. Janssens, C.L. Jiang, G. McMichael, J. Nolen, R.C. Pardo, M. Paul, J.P. Schier, R.E. Segel, D. Seweryniak, R.H. Siemssen, J.W. Truran, J. Uusitalo, I. Wiedenhoever, & B. Zabransky, *The  $^{44}\text{Ti}(p)$  Reaction and its Implication on the  $^{44}\text{Ti}$  Yield*, *Physical Review Letters* 84 (2000), 1651-4.
116. S. Starrfield, G.J. Schwarz, J.W. Truran, & W.M. Sparks, *Hydrodynamic Studies of the Evolution of the Extraordinary Nova LMC 1991*, *American Astronomical Society Meeting*, vol. 193, December (1998), p. 10106.
117. S. Starrfield, G.J. Schwarz, J.W. Truran, & W.M. Sparks, *The Effects of Metallicity on Hydrodynamic Studies of the Nova Outburst*, *American Astronomical Society Meeting*, vol. 194, May (1999), p. 8609.
118. S. Starrfield, W.M. Sparks, J.W. Truran, & M.C. Wiescher, *The Effects of New Nuclear Reaction Rates and Opacities on Hydrodynamic Simulations of the Nova Outburst*, *ApJS* 127 (2000), 485.

119. S. Starrfield, J.W. Truran, W.M. Sparks, P. Hauschildt, S.N. Shore, & J. Krautter, *Observational and Theoretical Studies of the Nova Outburst, in Wild Stars in the Old West*, S. Howell, E. Kuulkers, & C. Woodward. (Eds.), Cambridge University Press, Cambridge (1998), 352-367.
120. S. Starrfield, J.W. Truran, & W.M. Sparks, *The Nova Outburst: Thermonuclear Runaways on Degenerate Dwarfs*, *New Astronomy Review* 44 (2000), 81.
121. S. Starrfield, J.W. Truran, M.C. Wiescher, & W.M. Sparks, *Evolutionary Sequences for Nova V1974 Cygni using New Nuclear Reaction Rates and Opacities*, *MNRAS* 296 (1998), 502.
122. T.E. Strohmayer & E.F. Brown, *A Remarkable Three Hour Thermonuclear Burst from 4U 1820-30*, *ApJ*, (2001), submitted
123. D. Swesty, E.Y.M. Wang, & A.C. Calder, *Numerical Models of Binary Neutron Star System Mergers. I.: Numerical Methods and Equilibrium Data for Newtonian Models*, *ApJ* 541 (2000), 937.
124. F.X. Timmes, *Integration of Nuclear Reaction Networks for Stellar Hydrodynamics*, *ApJS* 124 (1999), 241.
125. F.X. Timmes, *Physical Properties of Laminar Helium Deflagrations*, *ApJ* 528 (2000), 913.
126. F.X. Timmes & D. Arnett, *The Accuracy, Consistency, and Speed of Five Equations of State for Stellar Hydrodynamics*, *ApJS* 125 (1999), 277.
127. F.X. Timmes, R. Hoffman, & S.E. Woosley, *An Inexpensive Nuclear Energy Generation Network for Stellar Hydrodynamics*, *ApJ* (2000), in press.
128. F.X. Timmes & J.C. Niemeyer, *Regimes of Helium Burning*, *ApJ* 537 (2000), 993.
129. F.X. Timmes & F.D. Swesty, *The Accuracy, Consistency, and Speed of an Electron-Positron Equation of State Based on Table Interpolation of the Helmholtz Free Energy*, *ApJS* 126 (2000), 501.
130. F.X. Timmes, M. Zingale, K. Olson, B. Fryxell, P.M. Ricker, A.C. Calder, L.J. Dursi, H.M. Tufo, P. MacNeice, J.W. Truran, & R. Rosner, *On the Cellular Structure of Carbon Detonations*, *ApJ*, (2000), 543, 938-54.
131. F.X. Timmes, M. Zingale, L.J. Dursi, B. Fryxell, P. Ricker, K. Olson, A.C. Calder, H.M. Tufo, P. MacNeice, J.W. Truran & R. Rosner, *Similarities and differences between the 2D and 3D cellular structure of carbon detonations*, (*ApJ*, 2000), to be submitted.
132. J.W. Truran, *The Early Stages of a Nova Outburst*, *Stellar Evolution, Stellar Explosions and Galactic Chemical Evolution*, (1998), p. 425.

133. J.W. Truran, Nova Explosions: Abundances and Light Curves, LNP Vol. 287: Proceedings of the 9th workshop on Nuclear Astrophysics (1998), p.107.
134. J.W. Truran, Nova Explosions: Abundances and Light Curves, in Nuclear Astrophysics, Hillebrandt, W. & Muller, E. (Eds.), Publications of the Max-Planck-Institute for Astrophysics (1998), p. 107.
135. J.W. Truran, The Early Stages of a Nova Outburst, in Proceedings of the Second Oak Ridge Symposium on Atomic and Nuclear Astrophysics, Mezzacappa, A. (Ed.), IOP Publishing Ltd (1998), pp. 425-431.
136. J.W. Truran & J.J. Cowan, The Helium R-Process and Neutron- Capture Element Abundances in Low Metallicity Stars, American Astronomical Society Meeting, vol. 196, May (2000), p. 0513.
137. Y. Tuchman & J.W. Truran, Composition Influence upon the Core Mass-Luminosity Relation and Possible Implications for the Extinction Timescales of Classical Novae, ApJ 503 (1998), 381.
138. H.M. Tufo & P.F. Fischer, Fast Parallel Direct Solvers for Coarse Grid Problems, J. Par. & Dist. Comput., 61 p. 151-177 (2001).
139. T. Udhesi, R. Hudson, & M.E. Papka, Seamless Multiresolution Isosurfaces using Wavelets, Argonne National Laboratory, Argonne ANL/MCSP801-0300, March (2000).
140. D. Uzdensky, A. Konigl, & C. Litwin, Magnetically Linked Star-Disk Systems:I. Force-free Magnetospheres and Effects of Disk Resistivity, ApJ, 565, p. 1191 (2002).
141. D. Uzdensky, A. Konigl, & C. Litwin, Magnetically Linked Star-Disk Systems:II. Effects of Plasma Inertia and Reconnection in the Magnetosphere, ApJ, 565, p. 1205 (2002).
142. S. Vazhkudai, J.M. Schopf, & I. Foster, Predicting the Performance of Wide Area Data Transfers, Proceedings of the 16th International Parallel and Distributed Processing Symposium (IPDPS 2002), April, (2002).
143. S. Vazhkudai, S. Tuecke, & I. Foster, Replica Selection in the Globus Data Grid in Proceedings of the First IEEE/ACM International Conference on Cluster Computing and the Grid (CCGRID 2001), Pages 106-113, IEEE Computer Society Press, May (2001).
144. S. Vainshtein, Z. Mikic, R. Rosner, & J. Linker, Evidence for Topological Nonequilibrium in Magnetic Configurations, Phys. Rev. E, 62 (2000), 1245-51.
145. A. Venkatesan, A.V. Olinto, & J.W. Truran, Neutron Stars and Black Holes as Machos, ApJ 516 (1999), 863.

146. N. Vladimirova, P. Constantin, A. Kiselev, O. Ruchayskiy, & L Ryzhik, Enhancement and Quenching of Combustion by Fluid Flow, (2002), in preparation.
147. S. Wunsch, & Y.N. Young, Universality of Scalar Statistics in Stably Stratified Turbulence, PRE, (2002), to appear.
148. Y.N. Young, H.M. Tufo, A. Dubey, & R. Rosner, On the Miscible Rayleigh-Taylor Instability: Mixing Layer Width Scaling in 2- and 3- D, JFM 447, pp 377-408 (2001).
149. Y.N. Young, & R. Rosner, Numerical Simulation of Double-Diffusive Convection in a Rectangular Box, Phys. Rev. E, 61(3) (2000), 2676- 2694.
150. Y. N. Young, H. Tufo, A. Dubey, & R. Rosner, Miscible Rayleigh- Taylor Instability: 2D versus 3D, American Astronomical Society Meeting, vol. 196, May (2000), p. 2206.
151. Y.N. Young, & R. Rosner, Linear and Weakly Non-linear Analysis of Doubly Diffusive Vertical Slot Convection, Phys. Rev. E, 57 (1998), 5554-63.
152. M. Zingale, F.X. Timmes, B. Fryxell, D.Q. Lamb, K. Olson, A.C. Calder, L.J. Dursi, P. Ricker, R. Rosner, J.W. Truran, P. MacNeice, & H. Tufo., 2000, Helium Detonations on Neutron Stars, ApJS 133, (2000), 195-220.
153. M. Zingale, F.X. Timmes, B. Fryxell, D.Q. Lamb, K. Olson, A.C. Calder, L.J. Dursi, P. Ricker, R. Rosner, J.W. Truran, P. MacNeice, & H. Tufo, Helium Detonations on Neutron Stars, American Astronomical Society Meeting, vol. 196, May (2000), p. 1703.
154. M. Zingale, F.X. Timmes, B. Fryxell, D.Q. Lamb, K. Olson, P. Ricker, A.C. Calder, L.J. Dursi, R. Rosner, & J.W. Truran, 2- Dimensional Helium Detonations on the Surface of Neutron Stars, Rossi2000: Astrophysics with the Rossi X-ray Timing Explorer, (2000), p. E67.
155. M. Zingale, F.X. Timmes, A. Calder, J. Dursi, B. Fryxell, D. Lamb, K. Olson, P. Ricker, R. Rosner, J. Truran, & H. Tufo, Direct Simulations of Thermonuclear Flames with the Flash Code, American Astronomical Society Meeting, vol. 195, December (1999), p. 4201.