ASCI/ALLIANCES CENTER FOR ASTROPHYSICAL THERMONUCLEAR FLASHES AT THE UNIVERSITY OF CHICAGO YEAR 4 ACTIVITIES REPORT

September 2001

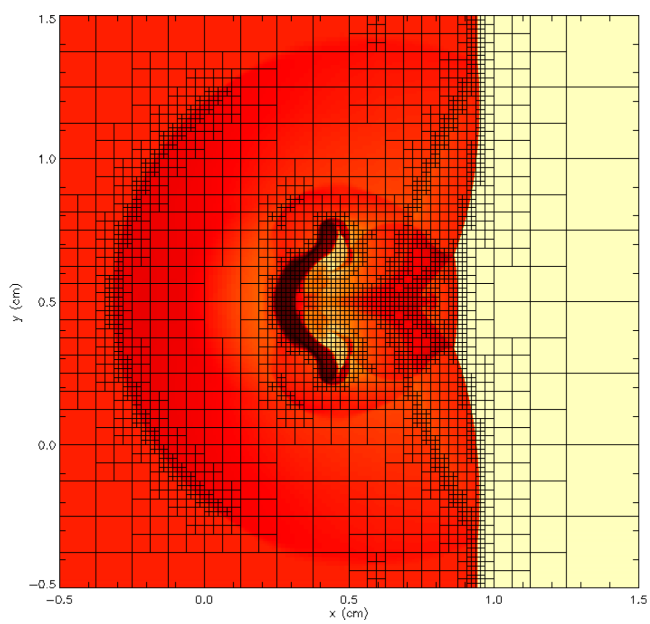

Figure 1: 3-D simulation of the impact of a shock on a magnetized interstellar medium cloud, using the new MHD module in `FLASH` v2.0; also shown is the adaptive mesh used in this calculation.

Abstract

We summarize the Year 4 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 v2.0; 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; computer science progress was made in libraries and tools, and applied to FLASH I/O and visualization challenges; and a variety of validation, verification, and basic physics studies relevant to the FLASH code.

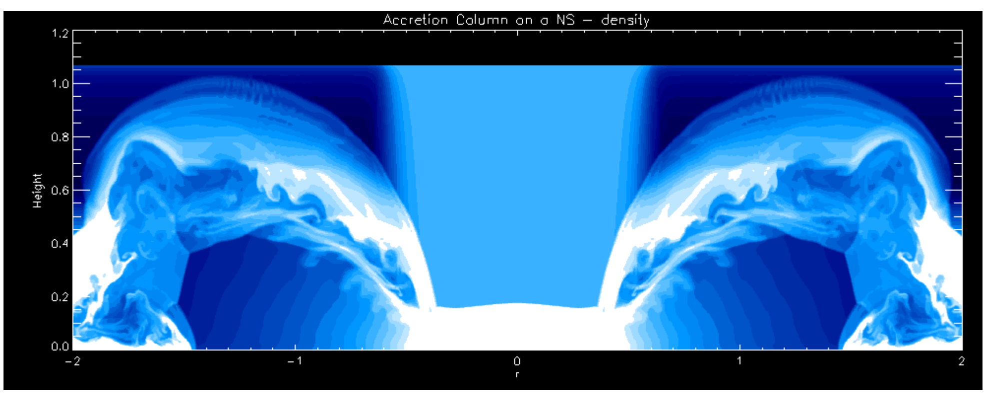

Figure 2: 2-D simulation of the impact of a relativistic accretion column onto the surface of a neutron star, using new special relativistic PPM solver.

Contents

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 has been composed of three disciplinary groups (Astrophysics, Computer Science, and Validation/Basic Science), as well as a cross-cutting group (the Code Group).

In Year 4, we completed the first modern architecture production version of the `FLASH` Code (now at revision level 2.0), which is capable of addressing many of our astrophysics problems on the largest existing parallel-architecture computers; we are now using this version of the code, and have also provided an early release version to several close external collaborators. Our scientific focus for the past year has been on microphysical processes: flame structure and propagation; and mixing instabilities driven by shear and by unfavorable stratification. Our computer science and code work has focused on architectural issues, as we are now well underway in planning the code's future development. The major highlights of this year's activities are described immediately following.

1.2 Major Year 4 Achievements

In Year 4 we have seen our Center begin to garner some of the external signatures of recognition for our efforts; these might be regarded as validation of the idea that a Center of the type funded by the ASCI/Alliance Program can – in a remarkably short time by the usual academic standards – produce substantive results that compare favorably with the best produced anywhere else.

1.2.1 `FLASH` v2.0

We have now completed v2.0 of the `FLASH` code, which represents our first instantiation of the application of modern CS code construction concepts to a fully-functional AMR astrophysics code. While much remains to be done, we now have a realized architectural framework which both serves as a production vehicle for astrophysics and physics calculations and as the test bed for extensive new code development efforts. This version is not only an architectural advance over previous versions; it also has substantially greater capabilities, including especially AMR-based magnetohydrodynamics. This version of our Center's key contribution will be distributed at our web site.

1.2.2 Gordon Bell Prize

A major success for our Center has been the garnering of the Supercomputing 2000 Gordon Bell Prize: the `FLASH` Code achieved 0.25 Tflops on 6420 processors of ASCI Red; and the paper describing the optimizations and performance of the code [12] was selected as the winner of the Gordon Bell prize at Supercomputing 2000 in the "Special" category for "... [utilizing] innovative techniques to produce new levels of performance on a real application". To the best of our knowledge, `FLASH` is the first AMR-based code to have won one of the Gordon Bell prizes. This is the second year in a row that our Center has won one of the Gordon Bells: in 1999, H. Tufo (then a postdoc in our Center) garnered the Gordon Bell by demonstrating outstanding scaling performance for a spectral element code running on ASCI Red. (This code is the core prototype for the anelastic solver P. Fischer is now building for the Center.)

1.2.3 Individual Recognition

We were also extremely pleased that Dr. Paul Ricker, the first `FLASH` code architect, was awarded both the 2001 DOE-Defense Programs Early Career Scientist award, as well as the 2001 Presidential Early Career Award for Scientists and Engineers (PECASE); these awards were presented in recognition of the quality of work done, and in our view validate our choices in the quality of the young scientists we were able to attract to our Center, and the approach we ultimately took in getting to where we are today.

2 The `FLASH` Code

Participants: A. Caceres[1], A. Calder, T. Dupont, J. Dursi[1], B. Fryxell (Group Leader), R. Kirby, T. Linde, A. Mignone[1], K. Olson, K. Ricker, P. Ricker, K. Riley, R. Rosner, F. Rubini (Univ. of Florence), A. Siegel (Code Architect), F. Timmes, H. Tufo, N. Vladimirova, G. Weirs, K. Young, M. Zingale

The Code Group is responsible for the architecture of the code framework, incorporating physics modules developed by other groups, maintaining the code (including code verification), and writing and maintaining the documentation. In addition, members of the Code Group are responsible for constructing new modules for hydrodynamics, MHD, radiative transfer, and other physics packages, as well as improving the adaptive mesh package (`Paramesh`). (Validation of the code has been a joint effort of the Code Group and the Validation & Basic Science Group.) Code optimization and scaling studies on the ASCI computers is performed in collaboration with the Computer Science Group. Visualization capabilities continue to be dramatically enhanced through interaction with the Futures Laboratory at Argonne National Laboratory. Finally, limited support

[1]Graduate student

is provided to help new customers in the astrophysics community to begin using the code; our principal external collaborators to date have been astrophysicists at Northwestern University, the University of Torino, and the University of Palermo.

2.1 FLASH architecture overview

The current version of the FLASH code is FLASH v2.0. This code is built around a number of significant core architectural changes aimed at simplifying the development, maintenance, and re-usability of the FLASH framework. These changes are aimed both at application developers (users who wish to customize the code by adding their own physics, numerical strategies, etc.) and our own in-house developers, who benefit greatly from a more modular design. Additionally, tools are provided to simplify the experience of the end-user who is interested only in running the current form of the code.

The FLASH v2.0 architecture makes a clear distinction between the FLASH "framework", which defines algorithmic interfaces and the main thread of execution, and the particular physics modules. As is typical in modern software architecture, the framework controls the thread of execution and makes calls to various abstract methods, which can easily be interchanged if they adhere to a common interface. When a single common interface is difficult to identify, various Design Patterns can be employed to allow some flexibility across different implementations and retain plug-and-play capabilities.

An important decision in developing FLASH v2.0 centered around choosing a language for the framework. The physics modules themselves should always be language-independent, requiring only the proper inter-language bindings on the platform in question. However, the choice of framework language brought a number of difficult issues to the forefront. Java, for example, has excellent support for object-oriented design concepts, but is very weak on performance, interoperability with FORTRAN, and usability with MPI (no official Java bindings to MPI have as of yet been defined). C++ offers good performance but is notoriously difficult to port. Furthermore, a certain degree of sophistication in C++ design, uncommon among scientific programmers, is required to avoid programming nightmares. Also, given the breadth and sophistication of FLASH, we strongly favored a strategy that allowed incremental testing and backward compatibility with all previous versions of the FLASH code. After weighing these and other issues, we ultimately chose to implement the architecture using Fortran 90 (F90).

After defining an incremental testing strategy, we developed a "database" as an F90 module that warehoused all common grid data and parameters that are not specific to an individual subroutine (the F90 module type mimics a singleton class in C++, and behaves similar to a class in Java with all static variables). The database is then the mechanism by which the framework shares data – each framework subroutine, program, or module contains a reference to the database and accesses its private variables through accessor and mutator methods. The database contains a rich set of overloaded methods which hide the details of repackaging the data for different modules (getDataXSlice, getDataTranspose, etc). Furthermore, F90 intent statements are used to clarify the purpose of each variable.

The physics modules themselves communicate only through interfaces, and may not access the database variables. This ensures that the physics modules know nothing of the framework in which they exist and facilitates the swapping of new modules or the incorporation of new framework services (such as an alternate AMR package). Our solution to the common interface problem was initially a simple one – to pass the maximum amount of data that could reasonably be expected to be needed by the corresponding physics module and to have each implementation choose what subset it needed. More sophisticated approaches are being considered for future versions of FLASH.

In choosing this approach, we retained the essentially polymorphic structure of previous versions of FLASH by using a pre-compile-time setup script to glue together the proper physics modules required for a specified application. However, since the setup script is such a complicated and important part of the code, we chose to implement it entirely in the Python language, rather than as a mixture of cshell, awk, and sed. This implementation has greatly increased the ability of the script to grow easily in proportion to the increasing complexity of the FLASH component hierarchy. Furthermore, by incorporating GNU's autoconf into the setup, we have improved the portability of the code onto clusters on which it has never been tested.

Finally, significant progress was made both in the automated testing and usability of the code. For the former, a Python-based testing utility (Flash_Test) was developed to allow automated job submission, ouput comparison, and fidelity testing. Regarding the latter, a Globus-based Java-Swig front end was developed that facilitates the setup and deployment of the code across a client-server architecture.

2.2 Overview of Year 4 accomplishments

Our overarching focus was to continue our transition to the new architecture (FLASH v2.0) as the production version of the FLASH Center code; this transition has now been completed. From where we started at the beginning of the year, this involved significant work in the following areas: testing, deployment, optimization, documentation, refinement of solver interfaces. While these base-level changes were being made to FLASH v2.0, plans were in place to take advantage of/support the new architecture by extending the code to include the following new/improved physics/solvers/tools: Flash_test, runtime visualization support, Lagrangian particle tracking, enhanced user interface features, code-maintenance tools, mhd, alternate hydro solvers, gravity, interactive visualization tools. Each of these issues is discussed in more detail below.

The principal accomplishment of the FLASH v2.0 architecture is the abstraction of the AMR mesh via the incorporation a new Database module. This implies the elimination of global-scope data, name hiding, and encapsulation more in line with a modern OO framework. Carrying out these changes required a complete overhaul of the code's data structures at the lowest level. By the time of last year's Site Review, there was some "anecdotal" evidence that an intermediate version of FLASH v2.0 was giving correct results on some of the ASCI machines. (We say "anectodal" because at the time we had no formal, operational definition of working vs. non-working code.) Thus, concurrent with our development of FLASH v2.0 was a significant effort to define a formal, general set of testing procedures that, if passed, allowed us to pronounce the code "correct". This resulted in the development of a full-fledged Flash Test Suite (`Flash_test`) as a principal focus in the adoption of v2.0.

At the same time we had good evidence that the new version of the code was performing with adequately small loss in performance to be a suitable production code. This also had to be studied in greater detail, which ultimately led to the inclusion of a standard set of performance tests in `Flash_test`. Furthermore, it showed us the need to make a number of important optimizations to our Database module to improve performance on some of the ASCI machines (details below).

While these base-level changes are complicated in and of themselves, by far our most difficult challenge was carrying them out at the same time that another set of programmers were preparing new physics and support modules to include in the code. Since v2.0 was still evolving in the low-level ways described above, we had to carefully define strategies to make the new modules compliant with a somewhat volatile and evolving architecture. Ultimately, we were able to accomplish this by defining a standard set of procedures for evolving a v1.6x module to v2.0.

FLASH v2.0 has been stable for over six months. It has been used by in-house developers for a number of significant simulations (e.g., our MHD simulations), and has been distributed to several of our ongoing external collaborators. We expect to make v2.0 our publicly released version (via the Web) by the end of this year. In the following, we sketch some of the significant new work that has gone into v2.0.

2.3 The physics of FLASH

In order to establish a baseline for all further discussions, we first summarize the current capabilities of the FLASH code:

- Compressible hydrodynamics. The current default hydrodynamic algorithm is an explicit higher–order Godunov method based on the Piecewise Parabolic Method (PPM) of Colella & Woodward [17], derived in its present form from the PROMETHEUS code [27]. Modules which make use of other algorithms will be described below.

- Arbitrary equations of state. Each problem – from astrophysics to verification or validation – requires its own equation of state. Typically, we use computationally-optimized equations of state based on table lookup and interpolation [82, 84], though in some circumstances far simpler equations of state, such as a gamma law, suffice and are available. New equation of state modules can be added easily when required.

- Arbitrary nuclear reaction network. Any number of nuclear species and reactions can be included up to the memory limits of current computers [80, 83]. The choice of network depends on the initial composition and thermodynamic state of the material and whether we are interested in detailed nucleosynthesis or just need a good approximation to the energy generation rate. For problems not involving nuclear burning, the reaction network module can be turned off.

- Gravity. An external gravitational acceleration can be specified *a priori*, or the gravitational field can be computed self-consistently via a Poisson solver, using either multigrid or multipole methods.

- Thermal conduction, in the diffusion approximation; we use explicit time integration, which suffices for the subset of astrophysics problems we have been considering to date.

The physics just described for `FLASH` leads to the following set of equations, which govern the motion of compressible matter undergoing nuclear burning in the presence of gravitational stratification: To begin with, we require a continuity equation

$$\frac{\partial \rho}{\partial t} + \bigtriangledown \cdot (\rho \mathbf{v}) = 0, \tag{1}$$

where ρ is the gas density, and $\mathbf{v}$ is the gas velocity. The motion of each nuclear species must be followed independently by solving the set of advection–diffusion equations

$$\frac{\partial \rho X_i}{\partial t} + \bigtriangledown \cdot (\rho X_i \mathbf{v}) = \bigtriangledown \cdot \rho D_i \bigtriangledown X_i + \rho \dot{X}_{i_{nuc}}, \tag{2}$$

where X_i is the mass fraction of the i'th species, D_i is the corresponding diffusion coefficient, and $\dot{X}_{i_{nuc}}$ is the change in composition of the i'th species due to nuclear burning. For most of our target astrophysics calculations, the species diffusion term can be ignored. The equation for conservation of momentum then takes the form

$$\frac{\partial \rho \mathbf{v}}{\partial t} + \bigtriangledown \cdot (\rho \mathbf{v}\mathbf{v}) = -\bigtriangledown P + \bigtriangledown \cdot \sigma - \rho \bigtriangledown \Phi, \tag{3}$$

where P is the gas pressure, σ is the viscous stress tensor, and Φ is the gravitational potential. For Type Ia supernova simulations, it is necessary to compute the self-gravity of the star; in this case, the gravitational potential is obtained by solving Poisson's equation

$$\bigtriangledown^2 \Phi = -4\pi G \rho \tag{4}$$

where G is the gravitational constant. Under more restricted conditions (e.g., studies of the evolution at small spatial scales, or X-ray bursts on a neutron star's surface), stellar expansion can be ignored, and one can assume that the last term in the momentum equation can be replaced by a static spherical gravitational acceleration. `FLASH` v2.0 can now deal with any of these cases.

Energy balance is computed by solving the corresponding equation for energy conservation,

$$\begin{aligned} \frac{\partial \rho E}{\partial t} + \bigtriangledown \cdot (\rho E + P)\mathbf{v} &= \bigtriangledown \cdot (\mathbf{v}\sigma - \mathbf{q}) \\ &\quad - \rho \mathbf{v} \cdot \bigtriangledown \Phi + \rho \dot{\epsilon}_{nuc}, \end{aligned} \tag{5}$$

where

$$E = \epsilon + \frac{1}{2}\mathbf{v}^2 \tag{6}$$

is the sum of the specific internal and kinetic energies and $\dot{\epsilon}_{nuc}$ is the specific rate of energy generation by nuclear burning. Due to the high density of the gas in compact objects, energy transport is entirely in the diffusive regime for much of their temporal evolution (for Type Ia supernovae, this is not true in the ejected envelope); in that case the diffusive energy transport flux, including both radiation and conduction, is given by

$$\mathbf{q} = \frac{-4acT^3}{3\rho} \left(\frac{1}{\kappa_{rad}} + \frac{1}{\kappa_{cond}} \right) \bigtriangledown T, \tag{7}$$

where a is the radiation constant, c is the speed of light, T is the temperature, κ_{rad} is the radiative conductivity, and κ_{cond} is the (electron) thermal conductivity [81]. The last term in the energy equations represents the heat generated by nuclear burning. At this point, the energy equation adopted by `FLASH` v2.0 assumes that radiation and conduction operate fully in the diffusive regime and is solved fully explicitly; these approximations suffice in cases in which the diffusion time scale is longer than the CFL time. Finally, the equations are closed by an equation of state

$$P = f(\rho, \epsilon) \tag{8}$$

which consists of a mixture of electron degeneracy pressure, radiation pressure, and ideal gas pressure. These are the equations that `FLASH` is designed to solve; an overview of additional physics that we plan to incorporate into the `FLASH` Code is discussed further below.

The current (`FLASH` v2.0) version of the `FLASH` code [28] thus represents a major advance along the road to the ultimate goal of a fully flexible code for solving general astrophysical fluid dynamics problems. `FLASH` v2.0 solves the equations described above, is modular and adaptive, and operates in parallel computing environments. It has been designed to allow users to configure initial and boundary conditions, change algorithms, and add new physical effects within certain limits. It uses `Paramesh` [56] to manage a block-structured adaptive grid, placing resolution elements only where they are needed most. Inter-processor communication is accomplished using the Message-Passing Interface (`MPI`) library to achieve portability and scalability on a variety of different message-passing parallel computers[31]. To date, it has been successfully tested on a variety of Unix-based platforms, including

- SGI systems, *e.g.,* the Nirvana Cluster at LANL
- SP-2 at ANL, ASCI Blue Pacific, ASCI White, and Frost at LLNL, and Blue Horizon at UCSD, all built by IBM
- ASCI Red at SNL, built by Intel
- Intel-based systems running Linux ("Beowulf" systems), such as Chiba City at ANL, and the Hive cluster at NASA/Goddard Space Flight Center
- Alpha-based clusters, such as CPlant at SNL
- SGI/Cray T3E (at PSC/Pittsburgh)

2.4 Code maintenance and testing

Code testing and maintenance is now a significant component of the `FLASH` v2.0 framework. In an effort to encourage its widespread use, we have added significant documentation and an intuitive, easy-to-use user interface (with both gui and scripting versions).

The main focus of this year's efforts in this area have however been in substantially enhancing the power of our testing program. First, the test suite has been enhanced by the addition of a number of new tests problems. Second, we have defined the concept of a "grid" of `Flash_test` deployers, which collects any individual run of `Flash_test` into a central, web-interfaced repository. Together with an increased frequency of tests (from one week to nightly), our testing procedures now allow any one of the FLASH Center scientists involved in code development to immediately establish the current status of the most current version of `FLASH`. We have also refined our strategy for handling failed tests by formalizing rollback and notification procedures. Furthermore, we have introduced the concept of "mini-tests", which are appropriate for individual developers before check-in of (for example) new modules. Finally, we have enhanced the report interface and error checking, and now generate forcheck logs on a monthly basis.

2.5 Deployment

Since an important focus of our code development process is to construct a code which is readily deployed by external users, we have paid considerably more attention to the user interfaces. First, we have enhanced `setup` by adding many options to the `setup` tool: there are now report files used for particular problems; one can preprocess the source code (in order, for example, to produce a formatted, documented list of parameters needed for a particular problem); one can "stamp" each checkout with a minor version number. Second, we now use `autoconf` so that the user now has the option to produce a system-dependent `Makefile.h` using a `Configure` script. This eases deployment on machines that we have yet to test on. Third, we have added many new features to the *Flash User Interface* (FUI), which is the `Java`-based GUI front-end to `FLASH`.

2.6 Code-maintenance tools

In addition to substantially revising and enhancing our user documentation (see below), we have also developed an internal documentation of both F90 coding standards and `FLASH` v2.0 coding rules. This documentation (which is primarily aimed at `FLASH` developers – as opposed to users – has been complemented by an added library of scripting tools based on Understand's `F90` parser to check new code for violation of our rules.

2.7 Runtime/remote visualization

We have now created a new visualization module in `FLASH` v2.0 built off of Parallel VTK. This module produces rendered image files at runtime when requested by the user. The programmer can build PVTK sub-modules directly in "native" `C++`, or at compile time, or can use a scripting interface at runtime via an embedded `Python` interpreter.

2.8 Local visualization

We have adopted the `Chombovis` three-dimensional visualization tool, and have developed routines to convert `FLASH` v2.0 output into `Chombovis` native format.

2.9 Particles module

We have added module which can perform Lagrangian particle tracking for an arbitrary distribution of particles (with AMR); this is an essential capability for both our basic physics and our validation efforts. Our plans are to enhance this module to include inter-particle and particle-fluid interactions in the near future; this capability will allow us to simulate more realistic fluid tracers used in validation experiments.

2.10 MHD

A major step forward for our physics capabilities has been the incorporation of an MHD module in `FLASH`; this module was extensively tested as a separate code in Year 3; and this year has been successfully adapted to the `FLASH` AMR-based code architecture. This effort, and some of the science that has been accomplished this year with this new module, is described separately in our discussion of this year's "integrated calculation" (§3).

2.11 Alternate hydro solvers

In conjunction with the testing of `FLASH` v2.0, work on several alternative numerical techniques for treating the Euler terms and solution advancement has progressed. Thus, several Runge-Kutta modules have been developed for time advancement and, in addition to the PPM method currently employed, TVD, weighted ENO, and high-resolution central shock-capturing schemes are now available, as well as a non-dissipative central differences scheme.

Alternative time advancement methods require a "delta-formulation", which entails substantial changes throughout `FLASH` v2.0; one of the most important capabilities which the delta-formulation allows is adaptive (local) time stepping, which we view as an important added future capability to `FLASH`. Consequently, we have now initiated an implementation study for the delta formulation in `FLASH` v2.0; while not trivial, an implementation of the delta-formulation appears tractable, without interference with the sections of the code already debugged, tested, and optimized.

2.12 Extensions to database module

We have made several major changes to the Database module, discussed above in our introductory section. There is now an enhanced interface, which includes a much greater range of AMR mesh services (see the User Documentation for details). We have included a pointer-returning version of accessor methods to give users maximum opportunity to optimize; have introduced the concept of integer keynumbers for lookups to replace strings; and have added variable registration and attribute-defining capabilities in `Config` files.

2.13 Documentation

A complete set of FLASH v2.0 documentation is now being distributed, and should be available by the time of the Site Visit. We have also continued the use of FAQ-based user feedback (started last year).

2.14 Performance and scaling

The FLASH code underwent a large optimization effort in preparation for last year's integrated calculations; these optimizations included both single processor tuning and parallel performance improvements, and were fully described in last year's Annual Report. These efforts were rewarded: FLASH Code achieved 0.25 Tflops on 6420 processors of ASCI Red; and the paper describing the optimizations and performance of the code [12] was selected as the winner of the Gordon Bell prize at Supercomputing 2000 in the "Special" category. To the best of our knowledge, FLASH is the first AMR-based code to have won one of the Gordon Bell prizes. The present version of FLASH, v2.0, largely shares the performance characteristics of this tuned code, as verified by runs we have performed on LLNL's Frost machine.

2.15 Future developments of the FLASH code

Evolution of FLASH from v1.0 to v1.61, and subsequently to v2.0, were the first major steps in our code development. The next steps in its development relate to refinement of its code architecture. FLASH v2.0 defines a new generation of the FLASH Code, which is designed to incorporate new object-oriented features as it evolves, ranging from architectural modifications to new physics modules. Some of this new work is listed below.

1. Flexible AMR. Although the present code is based entirely on the use of Paramesh to provide AMR capability, we are interested in exploring alternative patch-based AMR packages, such as AMRA [57]. In order to provide this capability, we are in the process of abstracting the existing mesh interface, and (in close consultation with the CCA), plan to implement a new mesh interface which will allow us to switch meshing packages.

2. Relativistic hydrodynamics. For some of our target astrophysics problems, special relativistic effects can become important. It is therefore important to have at least the capability to test for the consequences of such effects. We have developed a special relativistic version of the PPM hydro module, which has been tested on a relativistic jet problem, and will be incorporated into FLASH v2.0.

3. Radiation transport. A module for single-group flux-limited diffusion on an AMR grid has been under development. Because our initial collaboration with staff scientists as LLNL had to be terminated because the

relevant LLNL staff left LLNL, we have had to make a major change in our strategy for radiation hydrodynamics. As a consequence, we collaborated with D. Swesty (SUNY/Stony Brook) and P. Saylor (UIUC) on a NASA-funded proposal for radiation hydrodynamics, using as a base our `FLASH` code. This (3-year) proposal has now been funded, and we expect to be able to use the radiation hydrodynamics module developed by this collaboration in our `FLASH` code.

4. Discontinuous Galerkin techniques. For parallel codes, communication overhead can be reduced by using algorithms with a very compact stencil for spatial difference operators. We are conducting a comparative study of one such family of techniques, namely Discontinuous Galerkin (DG) methods using a wide variety of analytic test problems. This study also includes a comparison of DG results on structured meshes with those obtained earlier with `FLASH` v1.6 for Rayleigh-Taylor instabilities.

5. Subsonic hydrodynamic solvers. During the early phases of our target astrophysics simulations, fluid motions are very subsonic. In some cases, gravitational stratification may in addition be weak. An example is convection near or at the center of an evolved star. In such cases, one saves considerable computational effort by filtering out sound waves (the anelastic approximation) and, if permissible, additionally ignoring gravitational stratification (leading to the Boussinesq approximation). We have pursued two complementary avenues to address these simplifications: first, we have developed an anelastic spectral element hydro solver, which is described in more detail in §5; second, we have developed a semi-implicit compressible hydrodynamics module [72], which will be described in detail in a poster paper at this year's Site Visit (this solver has already been used in the thesis of one of our graduate students, J. Biello, in a study of [astrophysical] semi-convection). The next steps are to marry these solvers to the `FLASH` framework.

3 The Integrated Calculation: Mixing driven by Rayleigh-Taylor Instability

3.1 Background

Rayleigh-Taylor (R-T) instability is thought to be one of the primary physical mechanisms for modulating the speed of (initially laminar) nuclear flames within white dwarfs about to undergo Type Ia supernova explosions. As reported last year, we initiated a major study of mixing driven by R-T instability, in collaboration with both G. Dimonte and B. Remington at LLNL; this work was led at Chicago by A. Calder and B. Fryxell. Within the past year, we have continued this work, but enhanced it substantially by including magnetic field effects (which have been heretofore entirely neglected in the context of this problem). Our large calculations of this year have focused comparisons of hydrodynamic and magnetohydrodynamic R-T mixing.

The purely hydrodynamic simulations of R-T mixing have been carried out in the context of the so-called "α-group" collaboration (led by G. Dimonte) by A. Calder (in collaboration with B. Fryxell and R. Rosner). In addition to the specific calculations carried out as part of the α-group collaboration, we have also carried out a series of large single-mode calculations in order to understand the effects of varying resolution on the interpretation of the growth of the mixing zone width; results from these latter calculations will be discussed by A. Calder at the this year's (2001) Site Visit. These single mode calculations form the basis for the new MHD calculations (for the same problem, but with non-vanishing magnetic field) which we have also carried out this year (which are described in the following, and will also be discussed in detail by T. Linde at this year's Site Visit).

3.2 Validation of the MHD calculations

In the fourth year, we have successfully implemented and began careful validation of the magnetohydrodynamic (MHD) module in the `FLASH` Code. As a first step, we have carried out a series of detailed test calculations intended to verify and evaluate the reliability, convergence and physical accuracy of the MHD module, particularly in the context of astrophysical flows. To date, we have computed and analyzed solutions of Brio-Wu [9], Orszag-Tang [55] and MHD shock-plasma cloud interaction [23] test problems. Our results are in excellent agreement with published reference solutions. Given the importance of code testing, we plan to continue our MHD validation efforts as we begin production MHD simulations.

3.3 Magnetic Rayleigh-Taylor instability

We have also begun a systematic study of the R-T instability of compressible plasmas in the presence of magnetic fields. This fundamental problem plays a significant role both in astrophysical applications, for example determining properties of young supernova remnants or in the context of Type Ia supernovae (as described above), and in laboratory experiments such as the Z-pinch experiment conducted at Sandia National Laboratories. In this research project, we are extending our [12] ongoing investigation of purely hydrodynamic R-T instability to include magnetohydrodynamic effects. Since many of the detailed properties of the Rayleigh-Taylor instability are governed by the small-scale processes, we expect to find significant differences between purely hydrodynamic and magnetic cases even when the initial field is relatively weak, i.e., the high-β limit. (We note here that the high-β limit corresponds to what one would expect in the interior of a pre-supernova white dwarf star.)

We have completed two- and three-dimensional simulations of a single mode R-T instability. The fluid initial conditions for the instability are identical to those used in our hydrodynamic simulations. The magnetic field in the simulations is initially uniform and parallel to the interface separating heavy and light fluids, and the magnitude of the field is approximately one half of that of the critical field that linearly stabilizes the instability. Our findings are consistent with previous studies [35], which showed that the tangential field suppresses the growth of the single-mode instability, as predicted by linear theory. We also find that the field magnitude is amplified hundredfold, mostly on small scales, that the dominant field component is along the gravity vector, and that the locally strong field efficiently suppresses fluid mixing. In our ideal MHD simulations, the results are sensitive to grid resolution. In particular, we find that the nonlinear growth rate increases with the increase in grid resolution at low resolutions, but decreases at very high resolutions. We believe that locally very strong fields that develop at high resolutions suppress fluid motions and thereby reduce the growth of the instability. This must have considerable effect on the mixing of materials, and we plan to investigate this further during the coming year.

3.4 Results and performance

We used the `FLASH` code on Blue Horizon because of last year's restrictions on the use of the ASCI machines by foreign nationals. (The principal author of the MHD module is not a US national.)

The current version of the MHD-enabled `FLASH` code runs at $\approx$ 100 Mflop (single processor/Blue Horizon), with nearly perfect scaling up to 1024 processors for sufficiently large problems. More details will be presented during the Site Visit.

3.5 Further work

In the immediate future, we plan to continue improving our MHD solver to the point where it will become fully interchangeable with the `FLASH` code hydro solver. In parallel, we plan to revisit several of our purely hydrodynamic studies and investigate to what extent the addition of magnetic field effects will change the results. We will particularly try to understand the impact of magnetic field on surface gravity waves in nova ocean surface mixing calculations. We also intend to examine the stability of accretion columns on neutron stars and verify the analytic model of [48].

4 Astrophysics

Participants: E. Brown, A. Calder, J. Dursi[1], J. Chen[1], B. Fryxell, R. Krasnoplosky, D. Lamb, C. Litwin, A. Mignone[1], J. Niemeyer, T. Plewa, F. Peng[1], P. Ricker, F. Timmes, R. Rosner, J. Truran (Group Leader), N. Vlahakis, Y.-N. Young, M. Zingale, J. Zuhone[2]

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 work

The fourth 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 [80], Timmes & Arnett [82], Timmes & Swesty [84], and Timmes [81]) 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 discussed below.

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 begin preliminary calculations on all three of our target astrophysics problems, using all available ASCI platforms.

4.3 Fluid-flame interactions

4.3.1 Model flames

Following N. Vladimirova's work on KPP and incompressible flames, J. Dursi and R. Rosner have begun fundamental work aimed at understanding compressible astrophysical flames.

[1]Graduate student
[2]Undergraduate at UIUC, and summer intern at FLASH Center.

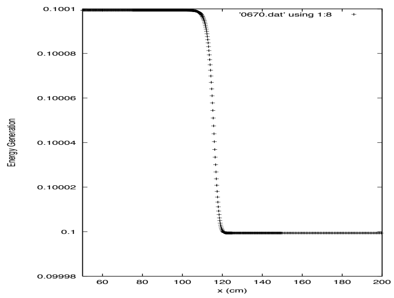

Figure 3: Sample one-dimensional flame profile

The work has begun with the creation of a "library" of KPP-like flames (see Figure 3) – e.g., those with a reaction rate ϵ of

$$\epsilon = \alpha \left(\frac{T - T_u}{T_b - T_u} \right)^a Y_{fuel}^b \tag{9}$$

using the `FLASH` Code, while varying

1. Ratio of flame speed to sound speed
2. Lewis number
3. Thickness of reaction zone
4. Density contrast across flame

Each of these four parameters affect the dynamics of flame combustion in different ways. Parameters 1 and 4 control the feedback of the flame into the hydrodynamics, with parameter 4 controlling the Landau-Darrieus instability and parameter 1 setting the minimum velocity where fluid motions can significantly curve the flames. Parameter 2 determines the behavior of the flame in regions of curvature (e.g., when wrinkled by a flow field), and parameter 3 sets the minimum relevant length scale for flow-flame interactions.

In the astrophysical case, all four parameters are in regimes which are basically impossible to capture numerically: The astrophysical flame is very slow compared to sound waves, making evolution costly, and relatively small fluid velocities important. The Lewis number is on the order of 10^7, making material diffusivity unresolvable (but hopefully unimportant). The reaction zone is extremely thin, meaning that only very small regions can be simulated, and the expansion caused by the flame is of order unity, limiting the scope of approximations that can be made.

Because of these complications, it is difficult to study astrophysical flames a priori. We are taking a flanking approach, attacking the problem from the

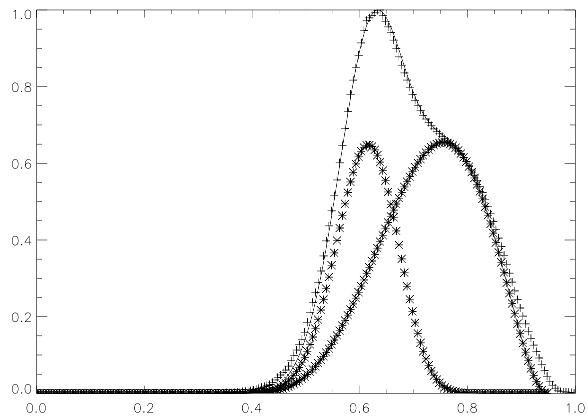

Figure 4: ^{12}C burning (temp plotted along x-axis, burn rate plotted along y-axis) plotted using '+'s, with two KPP flames adding up to the solid line shown.

side by understanding each of these aspects separately, and then approaching the more complex astrophysical regime.

We can take this approach with some confidence in its applicability to real astrophysical flames by noting that a flame of the sort we hope to understand, ^{12}C burning at a density of 5×10^8 g cm^{-3} can be modeled as two KPP-like flames with large exponents a and b (see Figure 4).

Now that the library of flames has been developed, the next step is to begin multidimensional runs using the 1-D flame as a starting point (see Figure 5) to study flame-flow interactions in simple configurations in both stratified and non-stratified atmospheres.

4.3.2 Flames-turbulence interactions

While modelling work exploring flame-turbulence interactions has 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 [chemical] cases makes flame feedback into fluid motions much stronger.

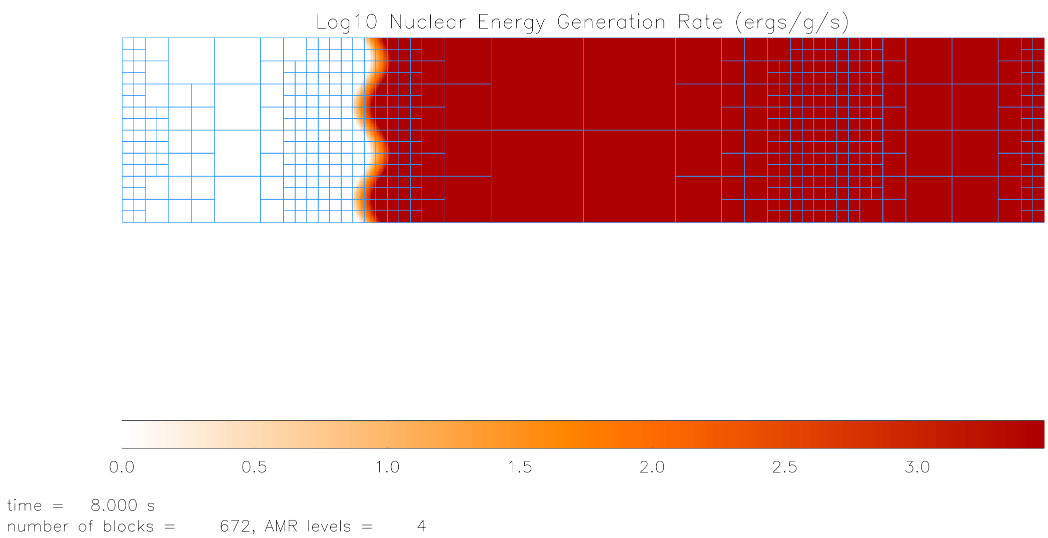

Figure 5: 2-D Wrinkled-flame simulation, starting with a perturbed 1-D flame model.

Thus, modelling work has begun to study this interaction, at first in 2-D, by J. Dursi. The turbulence is generated by adding a time-correlated, stochastic "stirring" term to the fluid equations, as per the prescription in Eswaran & Pope [25]. This stirring, which happens on small scales in 2-D and large scales in 3-D, 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 reached statistical equilibrium, as measured by examining the evolving power spectrum, a 1-D astrophysical flame from M. 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.

4.3.3 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 [39, 53]. For this to happen, the region must be free of any temperature fluctuations; any burning that was occurring in that region must be quenched.

In order to study this problem, our initial focus has been on validating the flames computed with `FLASH`: this year, we have demonstrated Galilean invariance, have shown that our flame speeds are consistent with those computed by earlier by Timmes & Woosley [85], and have demonstrated directional independence. These are important validation issues for our code, and an essential step on our way to a more realistic treatment of the supernova problem.

In our exploration of the quenching problem, 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 (e.g., 5×10^7 g cm^{-3}). At low densities, the flame speed is much slower, and a reasonable calculation takes 300,000 time steps, making them very expensive. (A full calculation can take over a month of wall clock time.)

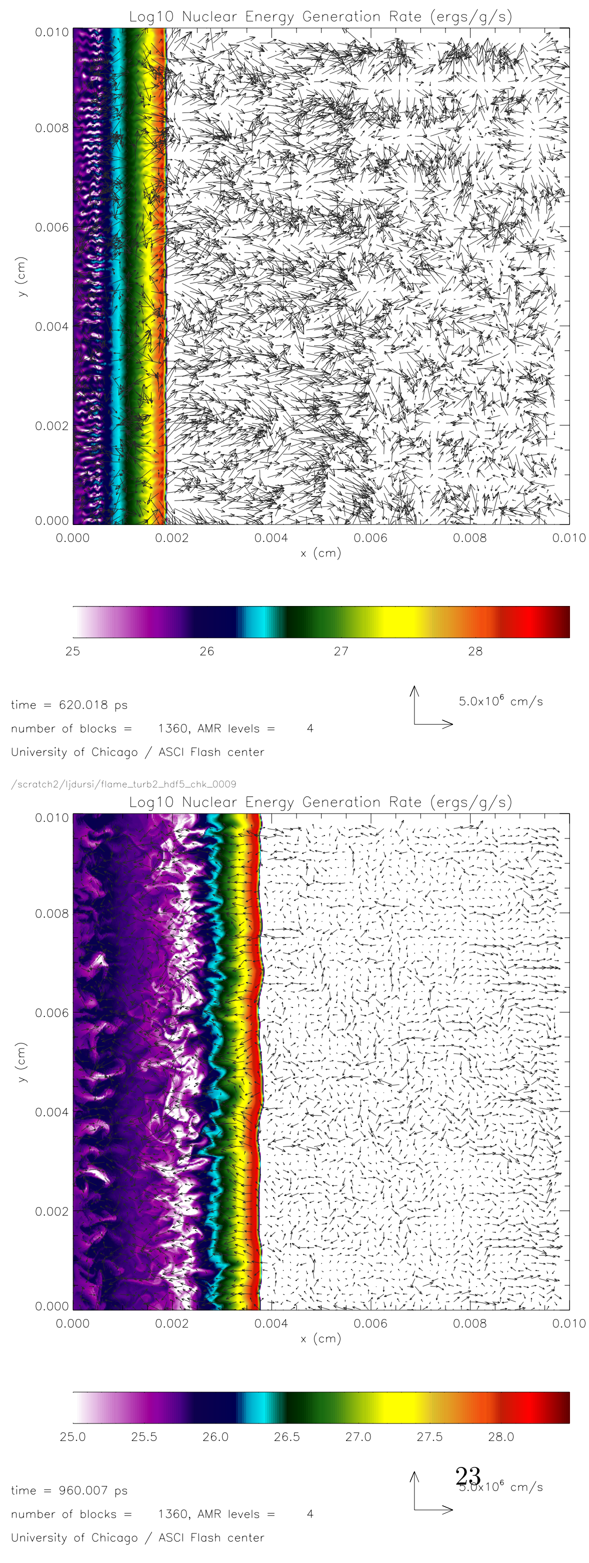

Figure 6: Evolution of flame-turbulence interaction. Note that the flame *strongly* suppresses wrinkling at the front.

4.3.4 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 isobarically, 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 towards 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^{-3}. 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 Codes

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 ∇p and the gravitational force ρg) calculated in separate modules by different methods are 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. Müller at the Max Plank 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 progress. In the meanwhile, using the non-HSE PPM solver, we have begun to evolve a pre-convective 1-D model from 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 Highly 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 Center member P. Fischer at Argonne National Labs has been continuing his work on an anelastic[1] code using a block-structured solver similar to the FLASH framework, and is doing Rayleigh-Bernard convective simulations as per Lantz & Sudan [**?**]; these calcula-

[1] Anelastic codes filter out sound waves, but allow for gravitational stratification of the background fluid.

tions 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 timescales. 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 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 (University 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 Finally, we are collaborating with former postdoc 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 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 early next 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.

- The TYCHO stellar evolution code An ancillary activity 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 a 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 (circa 1986) and Caughlan & Fowler[13]. The standard option uses Schwarzschild convection; a hydrodynamic treatment of convective overshooting is being developed. Mass loss is included and based on the theory of [44] for $T_{eff} \geq 7.5 \times 10^3$ 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 element 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.

4.5 X-ray burst studies

Previous reports have described the wide variety of X-ray burst calculations we have performed in order both 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 carry out.The next major step in this regard 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 is being studied. The accreted hydrogen and helium ignite where the gas pressure is somewhat less than the magnetic pressure, which motivates the question of how the fuel is actually distributed over the surface when ignition occurs (for an overview of the problem, see [10]). An analytical investigation of the stability of an accreted magnetized mound of material to short-wavelength ballooning modes has been completed [48]. For a realistic model atmosphere we demonstrate that the instability occurs when the overpressure exceeds the magnetic pressure by a factor (several) $\times\, a/h \gg 1$, 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.

An investigation of the role of the rp-process (defined by a sequence of (r)apid (p)roton captures onto seed nuclei provided by helium burning [14, 94, 93, 73]) in a Type I X-ray burst will also be done. For typical conditions, this nuclear processing can produce nuclei with $A > 56$ (as is the case for stable burning; see [74]), and might have implications for energy generation during the late phases of the burst event [64, 43], as well as on the amount of carbon produced to power further bursting, as described in the next paragraph. Preliminary calculations are underway in collaboration with A. Glasner (Hebrew University of Jerusalem).

Within the past two years several "super bursts" (X-ray energies $\sim 10^{42}$ erg and durations of several hours) have been observed from accreting neutron stars [20, 32, 77]. Preliminary calculations suggest that the unstable ignition of ^{12}C at large depths is the cause of these super bursts [22, 78]. At the high densities under which ignition occurs, thermal conduction of heat is efficient and sets the decay timescale of the burst ($\sim$ days). 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. The FLASH Center is well-poised to perform detailed investigations into these events.

4.5.1 rp-Process studies for `FLASH` simulations of X-ray bursts

As a component of `FLASH` research concerning type I X-ray bursts, we are currently studying the energy output and nucleosynthesis of the rp-process operating in the accreted H/He shells on neutron stars. The energy output from such burning is reflected in the light curves of these bursts. The makeup of the ashes of such burning has implications for the thermal and conductive properties of the crusts, and hence on such diverse topics as magnetic field evolution of, and gravitational wave emission from, accreting neutron stars. Using an extensive reaction network, Timmes has performed one-zone calculations of the consequences of rp-process synthesis that confirm earlier results of Rembges et al. [64] and more recently Schatz et al. (2001), for conditions appropriate to these environments. Brown, Peng, and Truran (in collaboration with A. Glasner) are developing a one-dimensional code to explore the nuclear consequences of rp-process nucleosynthesis in greater detail. Their code will clearly measure the viability of using truncated reaction networks to provide energetic and nucleosynthesis predictions. The use of such networks is essential to any realistic multidimensional study of X-ray bursts with Flash.

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 [88]. 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 ~ 30 % by mass of the envelope [50] 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 [51] that has previously been proposed is shear-induced mixing [40]. 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 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 [71, 1].

4.6.2 Wind-driven mixing

This summer, a UIUC undergraduate student, John 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. The key "next step" which they are pursuing is the extension of the simulation work to a realistic model of the white dwarf surface and accreted envelope. Much of the work done involved getting a compound initial 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 results were successful, and the next step is to perturb the interface and begin driving gravity waves with an externally imposed 'wind'.

4.6.3 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 [29, 37]. 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 towards our future two- and three-dimensional simulations, using different initial models which can help us to understand novae and their observed diversity. We also expect the convection calculations to provide the "background" velocity shear profile which the mixing calculations just described above require as an input.

4.6.4 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 Ia 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. [86] 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^{-3}. 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 [87] , 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 modeling

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. A key element in its implementation is the work carried out by the Basic Physics Group in its studies of flame speedup; our aim is to incorporate the results obtained in these studies in our flame model.

4.7.3 Type Ia supernovae

In pursuit of one of the Center's primary goals, P. Ricker has used FLASH v1.62 to carry out our first simulations of Type Ia supernovae. These calculations involve 3-D prompt detonations of a Chandrasekhar-mass ($1.38 M_{\odot}$) white dwarf. The density and pressure are initialized by interpolating a 1-D degenerate polytrope of the correct mass onto the 3-D adaptive mesh used by FLASH. The composition is initially 50oxygen everywhere. The detonation is initiated by setting a small spherical region to a temperature of 5×10^9 K. In some cases, we begin the detonation slightly off-center. This model produces a healthy explosion, but it converts all of the fuel to ^{56}Ni, in disagreement with observations, which indicate the presence of intermediate-mass isotopes. Nevertheless, it is an important precursor calculation to our forthcoming, more difficult calculations involving deflagration. We have also successfully carried out 3-D calculations of static white dwarfs, demonstrating that FLASH can maintain hydrostatic equilibrium in the absence of perturbations, even for highly degenerate material in a star which is close to the Chandrasekhar stability limit.

4.8 Further astrophysical studies with FLASH

4.8.1 Generally-applicable MHD effects

We have been working on physics studies of the circumstances under which accretion onto magnetized compact objects (neutron star or white dwarf) occurs. One central question is how the accreted material 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 [47] 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 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 [48] and have obtained estimates for the onset of instability (due to unstable ballooning modes).

4.8.2 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` (see below). Self-gravity will be included in the forthcoming version 2.0 public distribution of `FLASH`. Ricker has also been 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.

4.8.3 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 197th American Astronomical Society meeting.

4.8.4 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 magnetospheres of magnetically-linked disk-star systems; 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 [90], 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 [91], 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 4×10^{-13} M_{sun}.

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).

4.8.5 Formation of stars and planets

A. Königl 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, Königl and collaborators envision studying the effects of ambipolar diffusion; this would require additions and modifications to the present `FLASH` code. Königl 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, Königl 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 to be modified by magnetic effects. Königl 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 the nonlinear regime, requiring numerical simulations for their study. The spatial scales of this problem decrease as the instability progresses; Königl 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; astrophysics 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; previously at LLNL)
5. A. Ferrari (jets, accretion disks; Univ. of Torino)

6. A. Glasner (novae; Hebrew University of Jerusalem)
7. W. Hillebrandt (novae and supernovae; MPI Garching bei München)
8. R. Hoffman (reaction networks; LLNL)
9. D. Lin (novae and X-ray bursts; Northwestern University)
10. E. Marietta (supernovae; University of Arizona/Tucson)
11. E. Müller (relativistic astro; MPI Garching bei München)
12. T. Plewa (supernovae; previously MPI Garching bei München, now FLASH)
13. T. Strohmayer (X-ray bursts; NASA Goddard)
14. D. Swesty (radiative transfer; SUNY/Stony Brook)
15. R. Taam (novae and X-ray bursts; Northwestern University)
16. S. Woosley (supernovae and X-ray bursts; University of California at Santa Cruz)

5 Computer Science

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

5.1 Mission and goals

The Computer Science research component of the FLASH Center is carried out in multiple interrelated areas, including Numerical Algorithms and Methods, Software architecture and design, Scientific Visualization, Distributed Computing, and Scalable Performance and I/O. These are the fundamental research areas on whose results the `FLASH` code development effort is, and will be, based.

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

[1] Graduate student

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.

5.2 Numerical algorithms and methods

In this area we seek to develop scalable numerical methods, solvers, and libraries for scientific simulations. During the last year, we have been conducting a number of experiments on all of the ASCI machines and similar supercomputers. In particular, we have carried out two- and three-dimensional Rayleigh-Taylor simulations (on O2K, ASCI Red, ASCI Blue Mountain), two- and three-dimensional forced convective heat transfer in grooved and grooved-flat channel simulations (on O2K and Intel Paragon), buoyant convection in a rotating hemispherical shell simulations (on O2K, T3E), and hairpin vortex simulations (on O2K, ASCI Red).

5.2.1 Spectral Element calculations

Our code implementation milestones include a spectral element code for multimillion gridpoint simulations of incompressible flows in general two- and three-dimensional domains which now runs on all three ASCI platforms, as well as on (for example) the T3E, IBM SP-2, O2K, and NOW. We have achieved 319 Gigaflops on 2048 nodes of ASCI Red for one of the hairpin vortex simulations. This code uses MPI/NX for internode and OpenMP for intranode parallelism, thus exploring mixed-mode computations. Further advances along this line include extension to solving the anelastic equations (e.g., equations allowing for compressibility effects at very low Mach number), in collaboration with the Astrophysics and Code Groups (cf. §3-4).

One area of particular interest is development of scalable solvers for elliptic problems. Towards this goal, we have developed a parallel direct solver for solution of the coarse-grid problem that readily scales to thousands of processors [89].

We have interacted with all three of the ASCI labs in this area of research. In particular, we have worked with A. Cleary at LLNL to put our parallel direct solver into HYPRE, worked with R. Tuminaro at SNL to put our parallel direct solver into ML, and (as part of a collaboration with the Code and Validation/Basic Science Groups) worked with B. Benjamin at LANL this fall to simulate new gas curtain experiment with the `FLASH` Code.

5.2.2 Discontinuous Galerkin (DG) techniques on unstructured and structured meshes

Our goal is to determine, first, if the DG method offers any advantages over other high resolution methods on structured meshes, and second, if unstructured meshes can compete with structured meshes for the physics of interest (in this case Rayleigh-Taylor instability simulations).

The advantage that DG offers is a more compact stencil, which might result in more efficient use of refinement and better message passing efficiency; possible disadvantages are that the method may require a smaller time step to maintain stability compared to PPM, may require more memory, and may require more work/cell for the third order method due to a large number of required flux computations.

The DG work is largely carried out by our collaborators at RPI. The focus of the RPI efforts is on effective parallel adaptive analysis of fluids problems using these high-order discontinuous Galerkin (DG) techniques. In previous years, they carried out a number of simulations (of the canonical RT problem, using the same initial and boundary conditions used by our *Flash-1.x* simulations) using DG on both structured and unstructured meshes. Progress over the past year includes:

- Completion of a parallel version of the variable polynomial order DG method [60] 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 [26].
- Completion of an effective local time stepping algorithm [61].
- 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 [62, 63].

5.3 Scalability and I/O

5.3.1 Performance visualization (The `Jumpshot` Project)

Our activities in this area have focused on improvements in capability and performance of `Jumpshot`. Thus, we have

- Completed a new more efficient and scalable logfile format called SLOG-2.
- Designed a new display engine for logfiles in SLOG-2 format, and designed a `Java` interface for scalable display of various `Java` components. This work will allow great flexibility in the types of graphical displays possible for performance data.
- Incorporated a hierarchical-style display for scalability in numbers of processes and threads as well as in time and number of events.
- Prototyped a conversion sequence for old logfiles: clog − > clog2trace − > trace − > trace2slogII − > slogII.

5.3.2 Parallel I/O performance

Our focus has been on improving the performance of parallel I/O, a crucial issue for our FLASH Center simulation activities. The first step has been a series of performance studies of parallel I/O with `HDF5`. This has been carried out by studying the performance of a `FLASH`-based I/O benchmark, which uses `HDF5` over `MPI-IO`. As a result, we discovered a major bottleneck in the `HDF5` non-contiguous data-handling methods, and improved `FLASH` I/O performance and `HDF5` performance in general.

5.4 Numerical libraries

5.4.1 Spectral methods

A major milestone has been the completion of the anelastic spectral element code `NEK5000`. This code, based on the 1999 Gordon-Bell prize-winning code, has demonstrated the usefulness of the "MPI-everywhere" approach over multithreading; it is appropriate for low-Mach-number regimes, and (as described earlier in our discussions of astrophysical convection flows) can be used to compute initial conditions for `FLASH`.

5.4.2 Autopack

We have collaborated with J.-F. Remacle (Rensselear) on the `Autopack` package, which is actively being used in their adaptive codes; and discussions are underway about the use of `Autopack` in `Paramesh` and the main `FLASH` code.

5.4.3 Data reduction for visualization

An essential element of visualizations of FLASH Center simulation data is the ability to handle data on arbitrary meshes, and the ability to readily (down)sample mesh data. For these reasons, we have focused on providing improved usability of the data reduction tool by extending it to include uniform grid subsampling, and developing new preprocessing tools for HDF5 FLASH data files. Ongoing work includes parallel algorithm development for maintaining 2-1 level restrictions, filling cavities, and stitching nonconformal meshes together.

5.4.4 Adaptive mesh research

Our research in AMR methodology focused on the development of theoretical performance models for both uniform grid and adaptive multiresolution subsampling. We used these models to analyze a number of scenarios in which the hardware system configurations and task complexity change to determine the regimes for which each is most cost-effective. These models were verified using tools and infrastructure developed as part of the Globus project.

In addition, we are continuing our interaction with the Code Group in defining an appropriate mesh interface which will allow the FLASH Code to view the meshing package as a module.

5.4.5 Study of use of PETSc for implicit calculations

An important issue for us to to see to what extent the PETSc libraries can be used effectively within FLASH. With this motivation, we have demonstrated significant speedup using PETSc for the Poisson solver inside a single block for the FLASH code.

5.5 Distributed computing

The Globus project has continued work on high performance data transfer tools (GridFTP). This has been used to transfer data from ASCI labs to Argonne, and to enable high performance staging of visualization data. The FLASH Center is highly dependent upon efficient data transfers from the ASCI computing sites and Chicago; and therefore this type of work represents essential infrastructure for our Center computing activities. As part of our effort to hook Globus and FLASH together, we have developed a Globus-based FLASH remote job setup and use facility.

- The UofC/ANL Distributed Systems Laboratory has continued work on high performance data transfer tools (GridFTP). We have used GridFTP with numerous applications, improved performance considerably since last year, and have developed a flexible striped GridFTP server suitable for advanced data reduction/transformation needs using MPI-IO "plug-in" modules on the server side.

- We have used GridFTP tolls to transfer FLASH simulation data from ASCI labs to Argonne and to enable high performance staging of FLASH visualizations to ActiveMural displays.

- The UofC/ANL Distributed Systems Laboratory has 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. (Work on a demo is underway.)

- We have also begun collaborating with the DISCOM Distributed Data Management group to develop a large-scale ASCI data management system that integrates HPSS and GridFTP. This may provide a key piece of an improved ASCI− >ANL/UofC data movement solution.

- The `Globus` CoG Kit (`Java` version of `Globus` components) was used in the development of a remote configuration and startup utility for the `FLASH` code.

5.6 Visualization

Our core activity within the FLASH Center is the visualization of major FLASH datasets such as X-Ray bursts and cell detonations in large-scale and immersive display environments. In addition, we have carried out research in several areas relevant to FLASH, including the development of new methods for displaying vector-valued data, and the design of new software for parallel image processing.

5.6.1 Novel visualization methods

In an effort to assist in the visualization of FLASH Center data, we have pursued a novel method for displaying vector-valued data. This method – the Line-Integral Convolution (LIC) method – has been used for the display of velocity data in 2-D. Our new work has also entailed

- parallelization of LIC in 2-D;

- multi-resolution line integral convolution (LIC) run on Chiba with MPI (this work is still in progress);

- extension of LIC to 3-D;

- development of serial multi-resolution LIC in 3-D on SGI;

- Conversion of serial, multi-resolution 3-D LIC from SGI to Chiba (still in progress).

This method has been used on the newly produced FLASH Center data sets involving vector-valued results (e.g., the MHD calculations).

5.6.2 Cluster-based rendering

Because of the enormous size of the new FLASH Center data sets, the development of efficient and effective methods for displaying simulation results has become a major priority. With this motivation, we have designed new cluster-based rendering software.

5.7 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.

5.8 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. Some prototypical examples include:

- The Argonne scalability group is working with the ASCI Software Pathforward 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.
- 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.
- R. Lusk served on the review panel for ASCI level-2 proposals.

6 Validation and Basic Science

Participants: A. Alexakis[1], G. Bal, A. Calder, F. Cattaneo, P. Constantin, J. Curtis[1], A. Draganescu[1], T. Dupont (Group Leader), J. Dursi[1], J. Foo[3], B. Fryxell, D. Grier, C. Huepe, L. Kadanoff, A. Kiselev, T. Linde, C. Litwin, A. Malagoli, M. Medved[1], A. Oberman, R. Rosner, O. Ruchayskiy[1], L. Ryzhik, R. Scott, H. Tufo, N. Vladimirova, B. Winn[1], C. Yang[1], Y.-N. Young

[1]Graduate student
[3]NSF/REU Summer student, now at Brown Univ.

6.1 Mission and goals

Our Validation & 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.

6.2 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 [38, 39]. 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 National 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 two summers ago (one working on data analysis, the other working on simulations); last year, we again sent two students during the summer out to Sandia/Livermore (to work on mixing and flame models); and this year, B. Fryxell and A. Calder participated in a workshop on this topic at LLNL during January 2001. 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 earlier this year, in January 2001.

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 been accepted (and is now in press) on this work [98], 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.

During this past year, we have been carrying out a full grid of compressible calculations for both single-mode and multi-mode perturbations in both 2 and 3-D. 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 [**?**] 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`.

6.3 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. 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 [41, 18] 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: $L_c/l = const * U/v_0$. 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. Vadimirova and O. Ruchayskiy. It was also predicted and verified numerically that the same phenomenon occurs in a cellular flow that has closed streamlines. However, the critical characteristic width of a region quenched by such a flow with velocity amplitude U is significantly smaller: $L_c/l = const * (U/v_0)^{1/4}$ [19].

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, it is expected in this case as well also that the fluid advection will distort 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 [42].

More recently the study of active turbulent combustion models has been started. A simple such model has been proposed by A. Kerstein (private communication). It consists in a Boussinesq-like approximation in a spatially periodic gravitational potential. The model is physically somewhat artificial but it has the merit that it achieves with minimal complication a situation that has a stable configuration in the absence of chemistry and that becomes unstable under when the chemical reaction is turned on. Graduate student Brandy Winn has verified analytically that the system proposed has indeed different nonlinearly stable states in the presence of reaction and in the absence of reaction. (material in preparation). Numerical calculations of N. Vladimirova, show the surprising result that for a spatially uniform gravitational field the transition between the two states is obtained by a simple front-like motion, much as in the case of a shear, and without apparent instabilities. We plan to investigate this aspect analytically.

6.4 Thin flame model

Substantial progress was made in providing an interface propagation model for turbulent combustion. A new interface propagation model with numerical validations and a rigorous mathematical justification was provided. The results are in the PhD dissertation of Adam Oberman [54]; this work has been presented at the Pacific Institute for Mathematical Sciences conference on viscosity methods, and several derivative papers are in preparation.

To better understand how turbulent advection enhances combustion a simplified model was studied. The model uses a single progress variable, such as the temperature, which is

- advected by a given (turbulent) flow field,
- reacts, and
- diffuses.

There are four relevant spatial scales: L_0, the integral scale of turbulence, L_K, the Kolmogorov cutoff (smallest scale of the turbulence), L_F, the laminar flame thickness, and L_T the turbulent flame thickness (unknown). In the relevant astrophysical parameter regime, $L_0 >> L_K >> L_F$ and $L_T = L_F$. The relevant velocities are: V_A, a characteristic velocity of the turbulence, V_F, the laminar flame speed, and V_T, the (unknown) turbulent flame speed. Determining V_T is a major problem in turbulent combustion. Previous work [**?**], gave an upper bound $V_T < V_A$. Still, V_T is sensitively flow-dependent.

In stellar-scale computations, it is not possible to resolve L_F; hence the turbulent flame speed, V_T is poorly approximated. By replacing the very small L_F with an infinitely thin interface, one can use numerical front propagation methods. This gives an equation which is (1) advected by the flow and (2) self-propagates with a given speed (L_F). This model (the G-equation) has been investigated by Majda-Souganidis, and by Anne Bourlioux. The model has the disadvantage that it can give the wrong flame speed, as compared to a finite thickness flame.

A new interface propagation model was produced that includes propagation by the flow and by the given speed L_F in which the front shrinks by mean curvature. Numerical simulations with nonzero L_F on three systems: (1) the fully resolved reaction-diffusion advection equation, (2) the G-equation, and (3) the new model. The conclusions were that the G-equation gave an interface speed which could be too fast by an order of magnitude, and the new model gave the correct speed. Subsequently, the model was shown to have unique solutions, and it was proven that the interface moves at exactly the same speed as a particular level set of the reaction-diffusion advection equation.

This recent work provides a satisfactory model when the flame thickness, L_F, is not resolved, but the smallest scale of the velocity field, V_K, is. However, a model is needed for the case in which the smallest scales of the velocity field are not resolved. This very difficult problem modeling turbulence, and it may not be realistic to expect a full solution. However, a partial answer which provides dimensionally correct solutions may be in range.

6.5 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.

6.6 Radiation transport

To provide a better theoretical understanding of how one can effectively model transport of particles that stream through low density regions, two mathematicians, G. Bal and L. Ryzhik considered the problem of the free (linear) transport of particles in a tube with randomly reflecting boundary; the particles move in a straight line until a collision with the wall at which time the new velocity is randomly chosen. In the work so far the tube is two-dimensional and the velocity of the particles is on the unit circle. Assuming that the thickness of the tube is a small parameter ε, they studied the macroscopic limit of transport as $\varepsilon \to 0$. Since the boundary is randomly reflecting, one expects the macroscopic limit to be a mono-dimensional diffusion equation.

The result, however, is that for isotropic reflection at the boundary of a straight tube, particles move too fast to the left and right for the diffusive equilibrium to be reached. To obtain diffusion, grazing angles must be cut off. When particles are re-emitted isotropically in the directions v such that $|v \cdot n| \geq \eta$, where n is the normal to the tube, we obtain a diffusive regime with diffusion coefficient of size $\ln \eta^{-1}$. In other words, a diffusive regime is attained at times of order $\varepsilon^{-1} \ln \eta^{-1} << \varepsilon^{-1}$ instead of ε^{-1} as in classical diffusion. Moreover, the difference between transport and diffusion is of order $\eta^{-1}\varepsilon$.

When the tube is bent (a 2-d annulus of radii 1 and $1+\varepsilon$ was used), the cut-off of grazing angles is no longer necessary. We obtain that diffusion is attained at times of order $\varepsilon^{-1} \ln \varepsilon^{-1}$.

It seems that the above results have not appeared in the literature. These results are being extended to more general geometries, among which are the three-dimensional tubes (straight and bent). Bal and Ryzhik also plan to generalize the theory to the non-linear radiative transfer equations. They would like to address the problem of causality of the diffusive limit, and see whether the hyperbolic correction and the flux-limited diffusion equations behave as in the case without boundaries. These results should form the basis for a more rigorous testing of the radiative transport approximations now being incorporated into `FLASH`.

6.7 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 recently begun 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 approach 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 will study this both theoretically and numerically. 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.

Thus the efforts on this approach have been on simple one-space-dimensional model problems, including (1) scalar advection diffusion equations, (2) Burgers equation, (3) Buckley-Leverett equation. We are currently working on 1-d gas dynamics.

6.8 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.

6.9 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). 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. These contacts will become more important after our MHD module is integrated into *Flash-2*. Third, we submitted (and won) a DOE SciDAC grant for building an MHD addon 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.

6.10 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 α (subgrid) model; and development of a new subgrid model for MHD, based on the ideas underlying the α 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

7 Leveraging

A substantial number of our activities take advantage of other related (non-ASCI) projects carried out by scientists affiliated with our Center. Examples include

- The Argonne Mathematical and Computer Sciences group carries out a large number of non-ASCI supported activities directly related to our Center; outstanding examples include work on MPI, MPI-IO, mathematical libraries, and advanced visualization.
- Activities in the Chicago Material Research Sciences Center play an important role in our Validation and Basic Science program. Examples include the experimental and theoretical work on interfaces; studies of models for turbulence; experiments and theoretical work on double diffusing systems; and work on level set stretching.
- Computational physics work carried out as part of NASA-supported activities at Chicago, including work on pseudospectral codes and incompressible MHD, has played important roles in assisting studies carried out as part of our Center activities.
- The core adaptive mesh refinement package used by the present versions of `FLASH`, `Paramesh`, is a software project whose origins are at the Goddard Space Flight Center, where its development was initially supported by NASA; NASA in fact is continuing this support at an enhanced level.
- The University of Chicago is a partner in the National Partnership for Advanced Computational Infrastructure (NPACI), and this activity (which supports T. Clark) has provided additional expertise in parallel computing that has been useful to FLASH.
- Members of the FLASH Center have initiated new projects with direct connection to the FLASH Center code development effort, but supported by new funds outside the ASCI program. Thus, we have been funded to carry out further MHD code development by the DOE SciDAC program; and funded for the development of (relativistic) radiation hydrodynamics modules by NASA.

8 Center Management and Personnel

The fourth year has been rather stable from the management perspective. The personnel staffing level has been roughly constant, with most of the changes occurring in the code group (where we have added staff, as detailed below). We are however re-aligning the working groups slightly, in order to reflect much more naturally the evolution in our Center's scientific interests and direction; this is discussed in detail immediately following. A full listing of the scientists and support staff supported fully or in part by the Center is provided in the table shown in the Appendix below.

8.1 Management structure

Our current Center management structure – in place for the past year and a half – seems to be working well: 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, and J. Truran, as well as code architect A. Siegel and ex officio member R. Stevens); we meet weekly, on Friday afternoons, using the Access Grid (reducing the "overhead" for our Argonne colleagues). In addition, science issues and code issues are discussed weekly at Monday afternoon meetings, which see wide participation from Center members from all of the working groups.

In this coming year, we are making two further changes to our management structure: First, with the off-site relocation of B. Fryxell, A. Siegel will take on leadership of the Code Group. With this change, all staff whose primary responsibility is coding will report directly to Siegel; and the Code Group will primarily consist of such staff. (We of course expect others – especially from the Astrophysics Group – to continue their contributions to the `FLASH` Code coding effort; however, with this change, we aim to give the astrophysicists more opportunities to <u>use</u> `FLASH`, and to focus their code development efforts on physics modules, as opposed to the `FLASH` Code architecture/framework.) Second, we are splitting the Basic Physics & Validation Group into two distinct groups: the first (Validation) will be led by B. Fryxell, and will focus on our collaboration efforts with the National Laboratories; the second (Basic Physics) will be led by T. Dupont, and will continue our focus on the fundamental physics program.

8.2 New staff hires and departures

In FY01, we have hired one additional young computational scientist, T. Plewa (who comes to us from the Copernicus Center in Warsaw, via the Max Planck Institut fr̈ Astrophysik in Garching bei München, Germany); and one new MHD theorist/simulator, L. Malyshkin (who comes to us from Princeton University). Malyshkin is starting in early October 2001. By late October, we will also have on board two additional young programmers, who will report to the Code group leader/code architect, A. Siegel.

We also sustained a serious (and sad) loss in early October, due to the untimely death of Christof Litwin. He has played an important role on the MHD theory end of our Center's activities. It will not be easy to find a replacement for him, but in the short term (i.e., over the next year), this should not prove to be a major problem for our already planned MHD activities.

8.3 Faculty

The fourth year has seen the addition of one new (junior) faculty member, namely the appointment of Andrey Kravtsov to the Dept. of Astronomy & Astrophysics (from Ohio State University). He now joins the other faculty additions resulting from the creation of the FLASH Center at Chicago – F. Cattaneo (assist. professor, Dept. of Mathematics), R. Kirby (L.E. Dickson Instructor, Depts. of Computer Science and Mathematics), A. Kiselev (assist. professor, Dept. of Mathematics), L. Ryzhik (L.E. Dickson Instructor, Dept. of Mathematics), and R. Stevens (professor, Dept. of Computer Science). The build-up of computational science at Chicago also led to the arrival of Ridgway Scott from Houston; Scott is now a member of the FLASH Center, and co-director of the Computations Institute.

9 Specific Actions Resulting from the Year 3 Site Review

Here we specifically focus on three issues identified by last year's Site Review:

9.0.1 Enlarging the "community of coders".

The code group has been substantially strengthened in several ways, as discussed immediately above in the management section. First, we have added experienced staff with specific expertise in building large AMR-based hydrodynamic application codes (T. Plewa); second, we have initiated new collaborations in several areas of code module development (radiative hydrodynamics, magnetohydrodynamics, and time-dependent ionization); third, we are adding staff whose primary (and only) responsibility is coding, thus relieving code group members who are also part of the astrophysics group of their past considerable responsibilities for assisting in the development of the core `FLASH` code. These various issues are discussed in more detail above.

9.0.2 Anelastic solver.

We identified the strong need (discussed in the Astrophysics section) for a hydrodynamic solver which is capable of attacking problems in which sound waves play little if any dynamical role but for which (gravitational) stratification is essential; such problems commonly arise in constructing the initial conditions for a variety of Flash-related problems, and are not appropriately attacked by using the existing fully explicit, fully compressible FLASH code. We were urged by the Review Team to remedy this need. In response, we initiated two different routes: first, we have collaborated with P. Fischer (ANL), who has led the development of a new anelastic solver based on spectral element techniques. This new development was discussed in more detail in the Computer Science section. In addition, we are collaborating with former postdoc F. Rubini (now Professor of Physics at the University of Florence, Italy) on the incorporation of a semi-implicit hydro solver in FLASH. We expect to carry out comparisons of these two approaches over the next year.

9.0.3 Documentation.

Following the development of FLASH v2.0, the previous documentation is no longer sufficient to describe our code accurately. We have therefore made a significant effort to revamp our documentation, including (as recommended by the Review Team) hiring a staff member whose primary responsibility is the development and maintenance of our documentation. This documentation is now online at our web site.

9.0.4 Code distribution and export controls.

An essential point identified by us has been the importance of allowing free, wide distribution of the FLASH Code. We have viewed this step as essential because, first, this is the most powerful means of pushing the further development of FLASH (viz., increasing the number of users exercising the code, encouraging development of new physics modules); second, it is an important tradition of astrophysics code development efforts that such codes become "community codes", thus assisting in the more rapid development of computational astrophysics as a discipline; third, because members of the FLASH Center who depart for other research institutions (including research institutions abroad) are placed at a terrific disadvantage if their access to the FLASH code is predicated on the geographic location of their new home institution. The key obstacle to such free distribution has been export control of possibly sensitive codes. This past year, we have (with the kind assistance of security staff members at both Argonne National Laboratory and Lawrence Livermore National Laboratory) obtained a clear statement that the FLASH code is not subject to export control; and that this should continue to be the case as long as we exercise "due diligence" in the code distribution process, especially as the `FLASH` code evolves and attains new capabilities.

10 Education and Computational Science at Chicago

The University of Chicago at the highest levels is involved in a broad study of the role of computation in education and research. In his recent annual report on The State of the University, the Provost listed computation as his first focus area under new initiatives. A committee, chaired by Vice President for Research and for Argonne, Robert Zimmer, with Rick Stevens as Associate Chair, has been formed and will report to the administration shortly. Our new administration has indicated a willingness to entertain bold proposals in this area. This is a cause for considerable optimism about the future of computation here.

In the meanwhile, we have not waited for committee reports, and simply proceeded in two major directions: first, an enhancement of teaching activities in the computational sciences, and second, the creation of a new research institute which serves as a "home" for computationally-related research activities, and directly bridges such activities at the University and at Argonne National Laboratory.

10.1 Students

There are now a total of 17 graduate students who have actively worked on the FLASH Center problems from four departments (Astrophysics, Computer Science, Mathematics, and Physics); seven have graduated within the past 18 months.

Four graduate students are currently working on the astrophysics portion of the Center's research: A. Alexakis (supervisor R. Rosner), J. Dursi (supervisor R. Rosner), A. Mignone (supervisor R. Rosner), and F. Peng (supervisor J. Truran). Two of the students (Dursi and Mignone) are also closely associated with the Code Group. A Computer Science student is focusing on visualization (M. Papka; supervisor R. Stevens). The mathematicians are focusing on flame theory (B. Winn, supervisor P. Constantin), multiscale physics (C. Yang, supervisor L. Kadanoff) and adjoint methods (A. Drageanescu, supervisor T. Dupont); the students in Physics are working on interface instabilities and mixing (M. Medved, supervisor H. Jaeger), code physics (A. Caceres, no supervisor as yet), flame modeling (O. Ruchayskiy, supervisor R. Rosner), and multiply-diffusive instabilities (J. Curtis, supervisor D. Grier).

Seven former students completed their thesis research and have received their PhD degrees during this past year: J. Biello (supervisor R. Rosner), on *Semiconvection*, now an instructor in applied mathematics at RPI; Yingjie Liu (supervisor T. Dupont), on *Symmetric Error Estimates for Moving Mesh Finite Element Methods*, now in Jim Glimm's group at Stony Brook; R. Loy (supervisor J. Flaherty, RPI), now a postdoctoral fellow in MCS/ANL, and a member of the FLASH Center; A. Oberman (supervisor P. Constantin), on *Flame modelling*, now a postdoctoral fellow in applied mathematics at UT/Austin; Y.-N. Young (supervisor R. Rosner), on *Mixing Instabilities in Astrophysics*, now a postdoctoral fellow in the Applied Mathematics Dept. of Northwestern University; S. Zhan (supervisor D.Q. Lamb), on *Thermal Structure and Thermonuclear Flashes in Accreting Neutron Star Envelopes*, now in private industry; M. Zingale (supervisor J. Truran), on *Helium Detonations on Neutron Stars*, a postdoctoral fellow within the FLASH Center here in Chicago until mid-September, and a postdoctoral fellow at UC Santa Cruz (supervisor S. Woosley) thereafter.

This past summer, we have also started to participate in the NSF-funded Research Experience for Undergraduates (REU) program within the Physics Department. Thus, R. Rosner has worked with J. Foo (Brown University) on analytical studies of flame propagation in stratified fluids.

10.2 Teaching

The Computer Science Department has substantially increased its course offerings relevant to FLASH Center activities, and FLASH Center-related scientists are teaching in its program. Last autumn I. Foster taught a course (CS347) on Scalable Internet Services; this is closely related to the GLOBUS work that is finding its way into various ASCI efforts. H. Tufo gave a course (CS103) on parallel computing using MPI, the Beowulf course. Winter quarter had R. Scott teaching Scientific Parallel Computing (CS340). In the spring T. Dupont taught a course (CS342) on Numerical Hydrodynamics, and R. Stevens gave Introduction to Collaborative Environments (CS361). Finally, outside the CS Department, R. Rosner taught a course on computational astrophysics (A330) in the Dept. of Astronomy & Astrophysics during the Spring Quarter.

This coming year will have Computer Architecture (CS322) taught by R. Stevens, Software Development in ANSI C (CS533) taught by A. Siegel, Scientific Parallel Computing (CS340) taught by R. Scott, Introduction to Numerical Computation (CS285), and Optimal Control of Systems Governed by Partial Differential Equations (CS3XX) taught by T. Dupont, and (again outside the CS Department) Computational Physics and Astrophysics will be taught during Winter Quarter by R. Rosner.

The CS Department has also generally increased its course offerings in areas of direct relevance to our Center, such as courses on Networks and Distributed Systems (D. Beazley) and Matrix Computation (CS378; Y. Amit). The Department will also offered a new course sequence starting in the winter for computer graphics and visualization that is directly relevant to the development of visualization tools needed by the Center; this will be taught every other year. Finally, the Department of Mathematics is expanded its offerings in applied mathematics, with courses on computation taught by F. Cattaneo.

10.3 Computation Institute

The University of Chicago and Argonne National Laboratory jointly founded a new institute, the Computation Institute (CI) in the autumn of 1999. Co-directed by R. Scott and R. Stevens, the aim of this institute is to play a major role in facilitating the interactions between computer scientists, applied mathematicians, and applications scientists at both the University and at Argonne. The Institute will focus on leveraging the more obvious and well-developed computational science activities that currently exist such as the FLASH Center and computational astrophysics to emerging areas like computational biology and computational archaeology.

The CI also plays a major role in catalyzing the development of a formal computational science curriculum at the University in the next year or so. This initiative had among its multiple roots the Computational and Applied Mathematics program (CAMP; http://www.math.uchicago.edu/camp) at Chicago as well as the extensive interactions between Chicago computationally-oriented scientists and scientists within the Argonne MCS. The current plan is to establish a Committee on Computational Science. At The University of Chicago, this is called a "Committee with a capital C" and is almost like a department. This is to be a program that will grant Ph.D.'s in Computational Science. The details of this program, which have been worked out by members of the CI, including several FLASH Center members, include degree requirements, course descriptions, and Committee membership; this plan is to be submitted for approval to the appropriate University faculty oversight committees by Winter quarter.

What makes the CI unique among the existing institutes at the University is its relationship with Argonne National Laboratory. The other institutes are all "creatures" of the University alone, while the CI is truly a joint enterprise of the two institutions. The Institute is currently in the midst of organizing and fundraising. A first retreat was held at the University's Gleacher Center in late September 1999, and attracted 70 senior scientists from the University and from Argonne. Issues that the Institute leadership is addressing in the near term include: the types of activities supported by the CI, the nature and number of appointments to the CI, and the issue of space and infrastructure resources. We believe that the CI is a very important outcome, not only because it was strongly influenced by the success of the FLASH Center as a computational science project, but also as an example of University and Argonne cooperative activity. More information can be obtained at the CI's web site http://www-fp.mcs.anl.gov/ci.

Since its start in 1999, CI members have garnered a substantial number of grants in the computational sciences, including two grants (in radiation hydrodynamics, funded by NASA; and in magnetohydrodynamics, funded by the DOE SCIDAC program)) of direct relevance to the FLASH Center which have been funded within the past year. In another development relevant to the FLASH Center, the University has proposed moving the CI to the southern end of the

4th floor of the Research Building, i.e., just down the hallway from the FLASH Center. As can be imagined, this proposal is most welcome from our perspective.

11 Workshops

As in previous years, FLASH Center staff has been involved in scientific workshops directly relevant to the Center: The FLASH Center sees among its important roles to be a supporter of national and international workshops in areas related to computational science. Thus, during this past year, we have been involved in two workshops relevant to our Center activities.

During this past year, the FLASH Center, in cooperation with the NSF-funded Materials Research Science and Engineering Center of the University of Chicago, supported a workshop on the dynamics of materials over the period July 24 - August 1, 2001. This brought together engineers and scientists interested in the basic science of continuous media and in the applications of that science to engineering problems. The main workshop activity was intensive and extensive discussion of theory, experiment, simulation and design issues related to the mechanics of solids and liquids. There were lectures by participants from industry and several universities on topics of current research, in addition to a set of tutorial lectures. The organizers were Michael Brenner (MIT), Thomas Halsey (ExxonMobil), Leo Kadanoff (Chicago), and L. Mahadevan (MIT, Cambridge).

The FLASH Center has also played a significant role in supporting the "Neutron Stars Workshop" at the Institute for Nuclear Theory (University of Washington, Seattle, Washington), organized by H.-Thomas Janka (Max Planck Institut for Astrophysik, Garching, Germany), Don Lamb (ASCI FLASH Center, University of Chicago), and Chris Pethick (NORDITA, Copenhagen, Denmark); the workshop ran from 18 June to 24 August 2001.

The scientific program of the workshop covered a broad variety of topics connected with the formation, evolution and internal state of neutron stars. Neutron stars are born in supernova explosions of massive stars. Their evolution proceeds from the initially hot and proton-rich state of the collapsed stellar iron core to the cold and more compact final configuration, in which the composition is not well known.

During the workshop we had lectures on a regular basis (typically every Tuesday, Wednesday and Thursday mornings) as well as several more informal sessions with a larger number of shorter seminars, usually filling the whole afternoons. Meetings over lunch, in which there was generally rather wide participation, were valuable for encouraging information transfer between people with different backgrounds. The talks discussed problems and questions associated with

- the dynamics of supernova explosions, including the role of the nuclear equation of state, neutrino-matter interactions in the dense core, and neutrino oscillations;

- the cooling of nascent as well as young neutron stars;
- the internal and surface physical properties of neutron stars, and how observations can be used to determine these;
- the potential importance of neutron star binaries for cosmic gamma-ray bursts; and
- events around neutron stars, such as X-ray bursts and the nucleosynthesis of heavy elements (r-process) in supernova explosions.

Both theoretical and observational aspects were addressed, and the lectures were generally extremely good. Because of an interesting mix of people with different backgrounds being around at any time, the seminars became very interactive events. This was therefore a particularly good chance for the younger participants of the meeting to look behind the surface of sometimes polished presentations. In fact, many of the younger people participated very actively in the question and discussion parts of the seminars. We heard from some of the students that they definitely enjoyed the workshop, and that it gave them an educational experience very different from that at most conferences.

During the first few weeks of the workshop a large number of younger people, PhD students as well as postdocs, attended the program. We took care to give these people a chance to present their own work in a talk, and asked the more senior speakers to start their lectures with a suitable introduction. This worked amazingly well, particularly if one considers the broad range of subjects discussed.

Halfway through the program we had the pleasure of hosting a collaboration meeting of the supernova group led by Tony Mezzacappa. This brought a large fraction of the U.S. supernova community to the INT, and there was a correspondingly lively and productive atmosphere during these two weeks. The promise of Tera- and Petaflop computing of supernova models within the next five years provided much stimulus to come up with innovative ways of exploiting these possibilities.

One of the most important results of this meeting for many people was the realization of how crucially Jim Wilson's simulations of successful supernova explosions depend on the assumption of very specific properties of the nuclear equation of state in the nascent neutron star. Only by allowing pions to form in the medium (which in fact leads to higher temperatures and therefore larger neutrino fluxes and stronger heating behind the shock), in addition to the assumption of accelerated energy transport on large scales by neutron-finger instabilities inside the neutron star, was he able to obtain explosions powerful enough to explain the energetics of observed supernovae.

Another important result was the appreciation of the fact that there is still room for improving the calculations of neutrino properties to allow for correlations in the nuclear medium. During the past decade, much progress has been made in techniques for solving hydrodynamical and transport problems, and now it is time to direct attention again to aspects of micro-physics of dense matter. The meeting helped to revive the interest of nuclear physicists in developing equations of state which cover the range of physical conditions appropriate for stellar collapse, and which are in a form suitable for implementation in large numerical calculations. There were also many examples of collaborations beginning between participants who had not worked together in the past.

12 Infrastructure

12.1 Space

In the past year, very modest changes were made to our office space. The major changes entail the addition of a large laboratory-type space which will allow us to separate the AccessGrid node activities from our computing/visualization work; and a new large office which is intended to house the additional staff coming to Chicago for our enhanced activities in radiation hydrodynamics and magnetohydrodynamics.

12.2 High Performance Storage System (HPSS)

The work at ANL on IBM's HPSS system has been essentially completed; and we are presently awaiting word as to whether we will receive a no-cost licence for HPSS. As a consequence, we are presently planning not to renew our current licence for HPSS.

12.3 Center web site

Our Center web site (http://flash.uchicago.edu/) is continuously updated, including a gallery of computational results, full descriptions of the activities of the various research groups and teams within the Center, and the documentation for the `FLASH` code. The web site is also the locus for our code distribution efforts.

13 Bibliography

References

[1] Alexakis, A., Young, Y.-N., & Rosner, R. 2001, *On the shear instability of fluid interfaces: Stability analysis*, Phys. Rev. E, submitted.

[2] Andersen, J. 1991, *Accurate masses and radii of normal stars*, A&A Reviews, 3, 91.

[3] Angulo, C. 1999, Nuclear Phys. A, 656, 3.

[4] Arnett, D. 1977, *Neutrino trapping during gravitational collapse of stars*, ApJ, 218, 815.

[5] Arnett, D. 1996, *Supernovae and Nucleosynthesis* (Princeton University Press).

[6] Asida, S.M., & Arnett, D. 2000, *Further Adventures: Oxygen Burning in a Convective Shell*, ApJ, 545, 435-443.

[7] Bazan, G., & Arnett, D. 1998, *Two-dimensional Hydrodynamics of Pre–Core Collapse: Oxygen Shell Burning*, ApJ, 494, 316

[8] Brackbill, J., & Barnes, D.C. 1980, J. Comp. Phys., 35, 426.

[9] Brio, M., & Wu, C.C. 1988, *An upwind differencing scheme for the equations of ideal magnetohydrodynamics*, *J. Comput. Phys.*, 75:400–422, 1988.

[10] 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.

[11] Calder, A., Curtis, B.C., Dursi, L.J., Fryxell, B., Henry, G., MacNeice, P., Olson, K., Ricker, P., Rosner, R., Timmes, F.X., Tufo, H.M., Truran, J.W., & Zingale, M. 2000, *High-Performance Reactive Fluid Flow Simulations Using Adaptive Mesh Refinement on Thousands of Processors*, Supercomputing 2000, in press.

[12] Calder, A., et al. 2001, ApJ, submitted.

[13] Caughlan, G., & Fowler, W.A. 1988, Atomic and Nuclear Data Tables, 40, 283

[14] Champagne, A. E., & Wiescher, M. 1992, *Explosive hydrogen burning*, Ann. Rev. Nucl. Part. Sci., 42, 39.

[15] Chan, A., Gropp, W., & Lusk, E. 2000, *Scalable Log Files for Parallel Program Trace Data*, ANL preprint

[16] Christensen-Dalsgaard, J. 2000, private communication

[17] Colella, P., & Woodward, P.R. 1984, JCP, 54, 174-201.

[18] Constantin, P., Kiselev, A., Oberman, A., & Ryzhik, L. 2000, *Bulk Burning Rate in Passive - Reactive Diffusion*, Arch. Rational Mechanics, **154**, 53-91.

[19] Constantin, P., Kiselev, A., & Ryzhik, L., *Quenching of flames by fluid advection*, 2001, Commun. Pure Appl. Math. 54, no. 11, 1320–1342.

[20] Cornelisse, R., Heise, J., Kuulkers, E., Verbunt, F., & in't Zand, J.J.M. 2000, ApJ, 357, L21

[21] Couchman, H.M.P. 1991, *Mesh-refined P3M - A fast adaptive N-body algorithm*, ApJ, 368, 23.

[22] Cumming, A., & Bildsten, L. 2001, ApJ, submitted

[23] Dai, W., & Woodward, P.R. 1994, *Interactions between magnetohydrodynamical shocks and denser clouds*, ApJ, 436, 776–783, 1994.

[24] de Jager, C., Nieuwenhuijzen, H., & van der Hucht, K.A. 1988, *Mass loss rates in the Hertzsprung-Russell diagram*, A&AS, 72, 259.

[25] Eswaran, V., & Pope, S.B. 1988, Computers & Fluids, 16, 257–278.

[26] Flaherty, J.E., Krivodonova, L., Remacle, J.-F., & Shephard, M.S. 2002, *Aspects of discontinuous Galerkin methods for hypwerpoloc conservation laws*, Finite Elements in Analysis and Design, in press.

[27] Fryxell, B., Müller, E., & Arnett, W.D. 1989, *Hydrodynamics and Nuclear Burning*, Max–Planck–Institut für Astrophysik Report 449.

[28] Fryxell, B., Olson, K., Ricker, P., Timmes, F.X., Zingale, M., Lamb, D.Q., MacNeice, P., Rosner, R., Truran, J., & Tufo, H. 2000, *FLASH: An Adaptive Mesh Hydrodynamics Code for Modeling Astrophysical Thermonuclear Flashes*, ApJ, in press.

[29] Glasner, S.A., Livne, E., & Truran, J.W. 1997, *Reactive Flow in Nova Outbursts*, ApJ, 475, 754.

[30] Gomez, E., & Scott, L.R. 1998, *Overlapping and Short-Cutting Techniques in Loosely Synchronous Irregular Problems*, LNCS No. 1457, Ferreira, Rolim, Simon & Teng, eds. Springer-Verlag) pp. 116-127.

[31] Gropp, W., Lusk, E.R., & Skjellum, A. 1999, *Using MPI: Portable Parallel Programming with the Message-Passing Interface*, 2nd edition (Cambridge: MIT Press).

[32] Heise, J., in't Zand, J.J.M., & Kuulkers, E. 2000, AAS/High Energy Astrophysics Division, 32, 2803

[33] Iglesias, C., & Rogers, F.J. 1996, *Updated Opal Opacities*, ApJ, 464, 943

[34] James, R.A. 1977, JCP, 25, 71.

[35] Jun, B.-I., & Norman, M.L. 1995, *A numerical study of Rayleigh-Taylor instability in magnetic fields*, ApJ, 453, 332–349.

[36] Karonis, N.T., de Supinski, B.R., Foster, I., Gropp, W., Lusk, E., & Bresnahan, J. 2000, *Exploiting Hierarchy in Parallel Computer Networks to Optimize Collective Operation Performance*, Proceedings of IPDPS2000, to appear.

[37] Kercek, A., Hillebrandt, W., & Truran, J.W. 1998, *Two-dimensional simulations of the thermonuclear runaway in an accreted atmosphere of a C+O White Dwarf*, A&A, 337, 379.

[38] Khokhlov, A.M. 1995, *Propagation of Turbulent Flames in Supernovae*, ApJ, 449, 695.

[39] Khokhlov, A.M., Oran, E.S., & Wheeler, J.C. 1997, *Deflagration-to-Detonation Transition in Thermonuclear Supernovae*, ApJ, 478, 678.

[40] Kippenhahn, R. & Thomas, H.-C. 1978, *Accretion belts on white dwarfs*, A&A, 63, 625.

[41] Kiselev, A., & Ryzhik, L. 2000, *Enhancement of the Traveling Front Speeds in Reaction-Diffusion Equations with Advection*, 2001, Annales l'Institut Henri Poincaré Anal. Non Linéaire, **18**.

[42] Kiselev, A., & Ryzhik, L. 2001, *An upper bound for the bulk burning rate for systems*, Nonlinearity, to appear.

[43] Koike, O., Hashimoto, M., Arai, K., & Wanajo, S. 1999, *Rapid proton capture on accreting neutron stars—effects of uncertainty in the nuclear process*, AAP, 342, 464-73.

[44] Kudritzki, R.P., Pauldrach, A., Puls, J., & Abbott, D.C. 1989, *Radiation-driven winds of hot stars. VI - Analytical solutions for wind models including the finite cone angle effect*, A&A, 219, 205

[45] Kurucz, R.L. 1991, in *Stellar Atmospheres: Beyond Classical Models*, NATO ASI Series C, vol. 341

[46] Lantz, S.R., & Sudan, R.N. 1995, *Magnetoconvection dynamics in a stratified layer. 1: Two-dimensional simulations and visualization*, ApJ, 441, 903

[47] Litwin, C., Rosner, R., & Lamb, D.Q. 1999a, MNRAS, *On accretion flow penetration of magnetospheres*, 310, 324-30; Litwin, C., Rosner, R., & Lamb, D.Q. 1999b, Plasma Phys. Control. Fusion, 41, B343-B350.

[48] Litwin, C., Brown, E.F., & Rosner, R. 2000, *Ballooning instability in polar caps of accreting neutron stars*, ApJ, 553, 788-795.

[49] Litwin, C., & Rosner, R. 2001, *Plasmoid Impacts on Neutron Stars and Highest Energy Cosmic Rays*, Phys. Rev. Lett., in press.

[50] Livio, M. & Truran, J.W. 1994, *On the interpretation and implications of nova abundances: an abundance of riches or an overabundance of enrichments*, ApJ, 425, 797.

[51] 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.

[52] Marder, B. 1987, J. Comp. Phys., 68, 48.

[53] Niemeyer, J. & Woosley, S.A. 1997, *The Thermonuclear Explosion of Chandrasekhar Mass White Dwarfs*, ApJ, 475, 740.

[54] Oberman, A. 2001, *Motion of level sets by advection, growth and mean curvature as a model for combustion*, thesis, University of Chicaogo, http://www.math.uchicago.edu/~oberman/research.html.

[55] Orszag, S.A., & Tang, C.-M. 1979, *Small-scale structure of two-dimensional magnetohydrodynamic turbulence*, J. Fluid Mech., 90, 129–143.

[56] PARAMESH 1999, see web site at http://esdcd.gsfc.nasa.gov/ESS/macneice/paramesh/paramesh.html

[57] Plewa, T. 2000, private communication.

[58] Powell, K.G., Roe, P.L., Linde, T.J., Gombosi, T.I., & DeZeeuw, D.L. 1999, J. Comp. Phys., 154, 284.

[59] Rauscher, T., & Thielemann, K.-F. 2000, Atomic Data Nuclear Data Tables, 75, 1

[60] Remacle, J.-F., Flaherty, J.E., & Shephard, M.S. 2002, *An adaptive discontinuous Galerkin technique with orthogonal basis applied to Rayleigh-Taylor instabilities*, SIAM Review, in press.

[61] Remacle, J.-F., Flaherty, J.E., & Shephard, M.S. 2001,*An efficient local time stepping scheme for transient adaptive calculations*, in preparation.

[62] Remacle, J.-F., Shephard, M.S., Flaherty, J.E., & Klaas, O. 2001, *Parallel Algorithm oriented mesh database*, to appear 10th International Meshing Roundtable.

[63] Remacle, J.-F., Karamete, B.K., & Shephard, M.S. 2000, *Algorithm oriented mesh database*, Proc. 9th Int. Meshing Roundtable, SAND2000-2207, pp. 349-359.

[64] Rembges, J.F., Liebendörfer, M., Rauscher, T., Thielemann, F.K., & Schatz, H. 1998, *Hydrogen consumption in x-ray bursts*, in *Proceedings of the 9th workshop on Nuclear Astrophysics, eds. W. Hillebrandt & E. Muller (Garching bei München: Max-Planck-Institut fur Astrophysik*), p. 71.

[65] 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. 2000, *Large-Scale Simulations of Clusters of Galaxies.*, 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)

[66] 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. 2001, *The Structure of Self-Gravitating Hydrodynamic Turbulence*, BAAS, 197.

[67] 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. 2001, *Self-Gravitating Hydrodynamic Simulation using FLASH*, in preparation.

[68] Ricker, P.M., & Sarazin, C.L. 2000, *Off-Axis Cluster Mergers*, 2001, to appear in Proceedings of the 20th Texas Symposium on Relativistic Astrophysics, Austin, TX, December 10-15, 2000.

[69] Ricker, P.M., & Sarazin, C.L. 2001, *Off-Axis Cluster Mergers: Effects of a Strongly Peaked Dark Matter Profile*, ApJ, in press.

[70] 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. 2001, *A Framework for High-Performance Astrophysical Simulation*, in preparation.

[71] Rosner, R., Alexakis, A., Young, Y.-N., Truran, J.W., & Hillebrandt, W. 2001, *On the C/O Enrichment of Novae Ejecta*, ApJ submitted.

[72] Rubini, F., & Taverne, V. 1999, private communication.

[73] 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.

[74] Schatz, H., Bildsten, L., Cumming, A., & Wiescher, M. 1999, *The rapid proton process ashes from stable nuclear burning on an accreting neutron star*, ApJ, 524, 1014-29.

[75] Sedov, L.I. 1959, *Similarity and Dimensional Methods in Mechanics* (New York: Academic).

[76] Sod, G. 1978, JCP, 27, 1.

[77] Strohmayer, T.E. 2000, AAS/High Energy Astrophysics Division, 32, 2410.

[78] Strohmayer, T.E. & Brown, E.F. 2001, *A Remarkable Three Hour Thermonuclear Burst from 4U 1820-30*, ApJ, submitted

[79] SUMAA3d 1999, see web site at http://www-unix.mcs.anl.gov/sumaa3d

[80] Timmes, F.X. 1999, *Integration of Nuclear Reaction Networks for Stellar Hydrodynamics*, ApJ Suppl., 124, 241.

[81] Timmes, F.X. 2000, *Physical Properties of Laminar Helium Deflagrations*, ApJ, 528, 913.

[82] Timmes, F.X., & Arnett, W.D. 1999, *The Accuracy, Consistency, and Speed of Five Equations of State for Stellar Hydrodynamics*, ApJS, 125, 277.

[83] Timmes, F.X., Hoffman, R.D., & Woosley, S.E. 2000, *An Inexpensive Nuclear Energy Generation Network for Stellar Hydrodynamics*, ApJ Suppl., 129, 377.

[84] Timmes, F.X., & Swesty, F.D. 2000, *The Accuracy, Consistency, and Speed of an Electron-Positron Equation of State Based on Table Interpolation of the Helmholtz Free Energy*, ApJS, 126, 501.

[85] Timmes, F.X., & Woosley, S.E. 1992, *The conductive propagation of nuclear flames. I - Degenerate C + O and O + NE + MG white dwarfs*, ApJ, 396, 649.

[86] 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, 543, 938-54.

[87] 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*, ApJ, to be submitted.

[88] Truran, J.W. 1982, in *Essays in Nuclear Astrophysics*, Barnes, C.A., Clayton, D.D., & Schramm, D.N. (Eds.), Cambridge University Press, p. 467.

[89] Tufo, H.M., & Fischer, P.F. 1999, in *Fast Parallel Direct Solvers for Coarse Grid Problems*, J. Par. & Dist. Comput., in press.

[90] Uzdensky, D., Konigl, A., & Litwin, C. 2001, *Magnetically Linked Star-Disk Systems: I. Force-free Magnetospheres and Effects of Disk Resistivity*, ApJ, in press.

[91] Uzdensky, D., Konigl, A., & Litwin, C. 2001, *Magnetically Linked Star-Disk Systems: II. Effects of Plasma Inertia and Reconnection in the Magnetosphere*, ApJ, in press.

[92] van Leer, B. 1979, J. Comp. Phys., 32, 101.

[93] 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.

[94] Weaver, T.A., & Woosley, S.E. 1993, *Nucleosynthesis in massive stars and the 12C(alpha,gamma)16O reaction rate*, Phys. Rep., 227, 65.

[95] Woodward, P., & Colella, P. 1984, JCP, 54, 115.

[96] Wu, E.E., Bolmarcich, A., Snir, M., Wootton, D., Parpia, F., Chan, A., Lusk, E., & Gropp, W. 2000, *From Trace Generation to Visualization: A Performance Framework for Distributed Parallel Systems*, Proceedings of SC'00 (November, 2000),to appear (refereed conference proceedings).

[97] Young, P., Mamacek, E., Arnett, D., & Liebert, J. 2001, in preparation

[98] Young, Y.-N., Tufo, H., Rosner, R., & Dubey, A. 2001, *On the Miscible Rayleigh-Taylor Instability: 2-D and 3-D*, JFM, in press.

[99] Vladimirova, N., Malagoli, A., Cattaneo, F., & Ruchayskiy, O. 2000, PRL, submitted.

[100] 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. 2000, *Helium Detonations on Neutron Stars*, ApJS, 133, 195-220.

14 Appendices

14.1 Center members and affiliates (Sept. 1, 2001)

The following table includes all scientists and support staff who receive full or partial support from the FLASH Center, as of Sept. 1, 2001.

Name	Position	Center Affiliation	Institutional Unit(s)	Institution
Robert Rosner	Faculty	Director Astro/Code/V&P	A&A/Physics/EFI	UChicago
Alex Alexakis	Graduate student	V&P	Physics	UChicago
Guillaume Bal	Research scientist	V&P	Math	UChicago
Edward Brown	Research scientist	Astro	A&A/EFI	UChicago
Alvero Caceres	Graduate student	Code	Physics	UChicago
Alan Calder	Research scientist	Astro/Code	A&A	UChicago
Fausto Cattaneo	Faculty	V&P	Math	UChicago
Anthony Chan	Comput. staff	CS	MCS	UChicago/ANL
Jackie Chen	Graduate student	Astro	A&A	UChicago
Peter Constantin	Faculty	V&P	Math	UChicago
Lois Curfman-McInnes	Research scientist	CS	MCS	ANL
Jennifer Curtis	Graduate student	V&P	Physics	UChicago
Andrei Draganescu	Graduate student	V&P	Math	UChicago
Todd F. Dupont	Faculty	V&P	CS/Math/JFI	UChicago
Jonathan Dursi	Graduate student	Astro/Code	A&A	UChicago
Carrie Eder	Admin. staff	-	-	UChicago
Joseph E. Flaherty	Faculty	CS	CS	RPI
Paul Fischer	Senior Researcher	CS/V&P	MCS	ANL
Jasmine Foo	Undergraduate	Physics	Physics	Brown Univ.
Ian T. Foster	Senior researcher	CS	MCS	ANL
	Faculty		CS	UChicago
Lori A. Freitag	Senior Researcher	CS	MCS	ANL
Bruce Fryxell	Senior researcher	Astro/Code/V&P	EFI	UChicago
William D. Gropp	Senior researcher	CS	MCS	ANL
Randy Hudson	Comput. staff	CS	MCS	UChicago/ANL
Christophe Josserand	Research scientist	V&P	JFI	UChicago
Leo Kadanoff	Faculty	V&P	Phys./Math/EFI/JFI	UChicago
Alexander Kiselev	Faculty	V&P	Math	UChicago
Andrey Kravtsov	Faculty	Astro	A&A	UChicago
Mila Kuntu	Admin. staff	-	-	UChicago
Don Q. Lamb	Faculty	Astro/EFI	A&A	UChicago
Timur Linde	Research scientist	Code/V&P	A&A	UChicago
Christof Litwin	Senior researcher	Astro/V&P	A&A	UChicago

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Name	Position	Center Affiliation	Institutional Unit(s)	Institution
Ray Loy	Research scientist	CS	MCS	ANL
Ewing L. Lusk	Senior researcher	CS	MCS	ANL
Andrei Kravtsov	Assist. Professor Astro	A&A	UChicago	
Ruben Krasnopolsky	Research scientist	Astro/V&P	A&A	UChicago
Andrea Malagoli	Senior researcher	V&P	A&A	UChicago
Samuel Meder	Staff scientist	CS	CS	UChicago
Milica Medved	Graduate student	V&P	Physics	UChicago
Andrea Mignone	Graduate student	Astro/Code	A&A	UChicago
Adam Oberman	Postdoctoral Fellow	V&P	Math	UTexas/Austin
Kevin Olson	Senior researcher	Astro/Code	EFI	UChicago
Michael Papka	Graduate student/Staff scientist	CS	CS/MCS	UChicago/ANL
Fang Peng	Graduate student	Astro	A&A	UChicago
Tomek Plewa	Research scientist	Astro/Code	EFI	UChicago
Ray Pierehumbert	Faculty	V&P	Geosci.	UChicago
Paul E. Plassmann	Faculty	CS	CS	PSU
J.-P. Remacle	Research scientist	CS	Applied Math	RPI
Kathleen Ricker	Staff/Documentation	Code	A&A	UChicago
Paul Ricker	Research scientist	Astro/Code	A&A	UChicago
Katherine Riley	Comput. staff	Code	-	UChicago
Francesco Rubini	Faculty	Code	Physics	Univ. of Florence
Oleg Ruchayksiy	Graduate student	V&P	Physics	UChicago
Lenya Ryzhik	Faculty	V&P	Math	UChicago
Ridgway Scott	Faculty	CS	CS/Math	UChicago
Mark S. Shephard	Faculty	CS	CS	RPI
Andrew Siegel	Comput. staff	Code	-	UChicago
Barry F. Smith	Senior researcher	CS	MCS	ANL
Rick Stevens	Senior researcher	CS	MCS	ANL
	Faculty		CS	UChicago
Frank X. Timmes	Research scientist	Astro/Code	A&A	UChicago
James W. Truran	Faculty	Astro	A&A/EFI	UChicago
Natasha Vladimirova	Research scientist	Code/V&P	A&A	UChicago
Greg Weirs	Research scientist	Code/V&P	A&A	UChicago
Brandy Winn	Graduate student	Basic Physics	Math	UChicago
Yuan-nan Young	Postdoctoral fellow	V&P	Applied Math	NWU
Michael Zingale	Postdoctoral fellow	Astro/Code	A&A	UCSC
John Zuhone	Undergraduate	Astro	Physics	UIUC

Table acronym definitions:

- Center Affiliation: Astro: Astrophysics group; CS: Computer Science group; Code: Flash Code group; V&P: Validation/Basic Science group.

- Institutional Unit: A&A: Dept. of Astronomy & Astrophysics; CS: Dept. of Computer Science; EFI: Enrico Fermi Institute; Geosci.: Dept. of Geophysical Sciences; JFI: James Frank Institute; MCS: Mathematics and Computer Science Division; Phys.: Dept. of Physics
- Institution: ANL: Argonne National Laboratory; NWU: Northwestern University; PSU: Pennsylvania State University; RPI: Rensselear Polytechnic Institute; UChicago: The University of Chicago; UIUC: University of Illinois at Urbana/Champaign

14.2 Publications

A continuously updated publications list is provided at our website, at http://flash.uchicago.edu/publications/ . The publication list, as of Sept. 1, 2001, is given below.

1. 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.
2. 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.
3. A. Alexakis, Y.N. Young, & R. Rosner, *On the shear instability of fluid interfaces: Stability analysis*, Phys. Rev. E (2001), submitted.
4. B. 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.
5. B. Ayata & T.F. Dupont, *Convergence of a Step-Doubling Galerkin Method for Parabolic Problems*, to be submitted.
6. 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.
7. K.E. Belle, C.E. Woodward, A. Evans, S. Eyres, R.D. Gehrz, M. Schuster, M.A. Greenhouse, J. Krautter, S.G. Starrfield, & J. Truran, *Nicmos Imagery of Nova Shells*, American Astronomical Society Meeting, vol. 194, May 1999, p. 8611.
8. J. Bresnahan, J. Insley, & M.E. Papka, *Interacting with Scientific Visualizations: User-Interface Tools within Spatially Immersive Displays*,

Argonne National Laboratory, Argonne ANL/MCS-P789-0100, January 2000.

9. A.C. Calder, B. 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*, SC 2000 (2000), Gordon Bell submission.

10. 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.

11. 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).

12. A. Chervenak, I. Foster, C. Kesselman, & S. Tuecke, *Protocols and Services for Distributed Data-Intensive Science*, Proc. ACAT2000 (2001).

13. 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.

14. P. Constantin, A. Kiselev, A. Oberman, & L. Ryzhik, *Bulk Burning Rate in Passive - Reactive Diffusion*, Arch. Rational Mechanics, **154**, 53-91 (2000).

15. P. Constantin, A. Kiselev, & L. Ryzhik, *Quenching of flames by fluid advection*, Commun. Pure Appl. Math., **54**, no. 11, 1320–1342 (2001).

16. T.F. Dupont & Y. Liu, *Symmetric Error Estimates for Moving Mesh Galerkin Methods for Advection Diffusion Equations*, SIAM J. Num. Anal. (2000), submitted.

17. 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.

18. L. Freitag & R. Loy, *Comparison of Remote Visualization Strategies for Interactive Exploration of Large Data Sets*, in *Proc. 15th International Parallel and Distributed Processing Symposium* (2001), in press.

19. L. Freitag & R. Loy, *Data Reduction Techniques for Interactive Visualization on Computational Grids*, ANL/MCS Tech Report, May 2001.

20. 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).

21. B. Fryxell, K. Olson, P.M. Ricker, F.X. Timmes, M. Zingale, D.Q. Lamb, P. MacNeice, R. Rosner, J.W. Truran, & H.M. Tufo, *Flash: a Multidimensional Hydrodynamics Program for Modeling Astrophysical Fluids and Thermonuclear Flashes*, ApJ (2000), 131, 273-334.

22. 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.

23. 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, in press (2000).

24. 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.

25. 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.

26. M. Hereld, I.R. Judson, & R.L. Stevens, *Tutorial: Introduction to Building Projection-based Tiled Display Systems*, IEEE Computer Graphics & Applications, vol. 20, 2000.

27. M. Hereld, I.R. Judson, J. Paris, & R.L. Stevens, *Immersive Projection Technology*, in Immersive Projection Technology, Ames, Iowa, 2000.

28. J. Kane, D. Arnett, B.A. Remington, S.G. Glendinning, G. Bazán, R.P. Drake, & B.A. Fryxell, *Supernova Experiments on the Nova Laser*, ApJS **127** (2000), 365.

29. J. Kane, D. Arnett, B.A. Remington, S.G. Glendinning, G. Bazán, E. Muller, B.A. Fryxell, & R. Teyssier, *Two-Dimensional versus Three-Dimensional Supernova Hydrodynamic Instability Growth*, ApJ **528** (2000), 989.

30. J.O. 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).

31. A. Kercek, W. Hillebrandt, & J.W. Truran, *Two- and Three-Dimensional Simulations of the Thermonuclear Runaway in an Accreted Atmosphere of a C+O White Dwarf*, LNP Vol. 287: Proceedings of the 9th workshop on Nuclaear Astrophysics, 1998, p. 56.

32. 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.

33. 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 **337** (1998), 379.

34. 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 Müller, E. (Eds.), Publications of the Max-Planck-Institute for Astrophysics (1998), p. 56.

35. A. Kercek, W. Hillebrandt, & J. W. Truran, *Three-Dimensional Simulations of Classical Novae*, A&A **345** (1999), 831.

36. A. Kiselev & L. Ryzhik, *An upper bound for the bulk burning rate for systems*, Nonlinearity, in press (2001).

37. 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)

38. 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.

39. D.Q. Lamb, *Some Startling Discoveries about X-Ray Bursts*, ApJS **127** (2000), 395.

40. T. Linde & A. Malagoli, *On Local Div B Control in Ideal MHD Simulations*, JCP (2001), submitted.

41. C. Litwin, E.F. Brown & R. Rosner, *Ballooning instability in polar caps of accreting neutron stars*, *ApJ*, **553** (2001), 788-795.

42. C. Litwin & R. Rosner, *Plasmoid Impacts on Neutron Stars and Highest Energy Cosmic Rays*, Phys. Rev. Let. (2001), in press.

43. C. Litwin & R. Rosner, *Relativistic Space-Charge Limited Bipolar Flow*, Phys. Rev. E **58** (2000), 1163.

44. C. Litwin, R. Rosner, & D.Q. Lamb, *On Accretion Flow Penetration of Magnetospheres*, MNRAS **310** (1999), 324.

45. C. Litwin, R. Rosner, & D.Q. Lamb, *On Stream Accretion onto Magnetized Compact Objects*, American Astronomical Society Meeting, vol. 194, May 1999, pp. 2909.

46. 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.

47. M. Micono, G. Bodo, S. Massaglia, P. Rossi, A. Ferriai, & R. Rosner, *Kelvin-Helmholtz Instability in Three Dimensional Radiative Jets*, A&A **360** (2000), 795-808.

48. J.C. Niemeyer & J.W. Truran (eds.), *Type Ia Supernovae: Theory and Cosmology* (2000).

49. A. Oberman, *Motion of level sets by advection, growth and mean curvature as a model for combustion*, thesis, University of Chicaogo (2001), http://www.math.uchicago.edu/~oberman/research.html .

50. 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.

51. R. Olson & M.E. Papka, *Remote Visualization with Vic / Vtk*, Visualization 2000 Hot Topics, Salt Lake City, Utah, 2000.

52. P.M. Ricker, S. Dodelson, & D.Q. Lamb, *Cosmos: a Hybrid N-Body /Hydrodynamics Code for Cosmological Problems*, ApJ **536** (2000), 122.

53. P.M. Ricker, B. Fryxell, K. Olson, F.X. Timmes, M. Zingale, D.Q. Lamb, P. MacNeice, R. Rosner, & H. Tufo, *Flash: a Multidimensional Hydrodynamics Code for Modeling Astrophysical Thermonuclear Flashes*, American Astronomical Society Meeting, vol. 195, December 1999, p. 4205.

54. 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*, 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).

55. 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.

56. 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*, 2001, in preparation.

57. P.M. Ricker, & C.L. Sarazin, *Off-Axis Cluster Mergers*, to appear in Proceedings of the 20th Texas Symposium on Relativistic Astrophysics, Austin, TX, December 10-15, 2000.

58. P.M. Ricker, & C.L. Sarazin *Off-Axis Cluster Mergers: Effects of a Strongly Peaked Dark Matter Profile*, 2001, ApJ, in press.

59. 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*, 2001, in preparation

60. 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.

61. R. Rosner, A. Alexakis, Y.-N. Young, J.W. Truran, & W. Hillebrandt, *On the C/O Enrichment of Novae Ejecta*, ApJ(2001), submitted.

62. 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. Schiffer, R.E. Segel, D. Seweryniak, R.H. Siemssen, J.W. Truran, J. Uusitalo, I. Wiedenhoever, & B. Zabransky, *The* $^{44}Ti(\alpha,p)$ *Reaction and its Implication on the* ^{44}Ti *Yield*, Physical Review Letters **84** (2000), 1651-4.

63. 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.

64. 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.

65. 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.

66. 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, Howell, S., Kuulkers, E., & Woodward, C. (Eds.), Cambridge University Press, Cambridge (1998), 352-367.

67. S. Starrfield, J.W. Truran, & W.M. Sparks, *The Nova Outburst: Thermonuclear Runaways on Degenerate Dwarfs*, New Astronomy Review **44** (2000), 81.

68. 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.

69. T.E. Strohmayer, & E.F. Brown, E.F. 2001, ApJ, submitted

70. 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.

71. F.X. Timmes, *Integration of Nuclear Reaction Networks for Stellar Hydrodynamics*, ApJS **124** (1999), 241.

72. F.X. Timmes, *Physical Properties of Laminar Helium Deflagrations*, ApJ **528** (2000), 913.

73. F.X. Timmes & D. Arnett, *The Accuracy, Consistency, and Speed of Five Equations of State for Stellar Hydrodynamics*, ApJS **125** (1999), 277.

74. F.X. Timmes, R. Hoffman, & S.E. Woosley, *An Inexpensive Nuclear Energy Generation Network for Stellar Hydrodynamics*, ApJ (2000), in press.

75. F.X. Timmes & J.C. Niemeyer, *Regimes of Helium Burning*, ApJ **537** (2000), 993.

76. 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.

77. 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), in press.

78. F.X. Timmes, M. Zingale, K. Olson, P. Ricker, B. Fryxell, A.C. Calder, L.J. Dursi, J.W. Truran, & R. Rosner, *On the Cellular Structure of 3-Dimensional Carbon Detonations*, ApJ (2000), 543, 938-54.

79. J.W. Truran, *The Early Stages of a Nova Outburst*, Stellar Evolution, Stellar Explosions and Galactic Chemical Evolution, 1998, p. 425.

80. J.W. Truran, *Nova Explosions: Abundances and Light Curves*, LNP Vol. 287: Proceedings of the 9th workshop on Nuclear Astrophysics (1998), p. 107.

81. J.W. Truran, *Nova Explosions: Abundances and Light Curves*, in *Nuclear Astrophysics*, Hillebrandt, W. & Müller, E. (Eds.), Publications of the Max-Planck-Institute for Astrophysics (1998), p. 107.

82. 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.

83. 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.

84. 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.

85. H.M. Tufo & P.F. Fischer, *Fast Parallel Direct Solvers for Coarse Grid Problems*, J. Par. & Dist. Computing (2001), in press.

86. T. Udhesi, R. Hudson, & M.E. Papka, *Seamless Multiresolution Isosurfaces using Wavelets," Argonne National Laboratory*, Argonne ANL/MCS-P801-0300, March 2000.

87. D. Uzdensky, A. Konigl, & C. Litwin, *Magnetically Linked Star-Disk Systems: I. Force-free Magnetospheres and Effects of Disk Resistivity*, ApJ (2001), in press.

88. D. Uzdensky, A. Konigl, & C. Litwin, *Magnetically Linked Star-Disk Systems: II. Effects of Plasma Inertia and Reconnection in the Magnetosphere*, ApJ (2001), in press.

89. 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.

90. S. Vainshtein, Z. Mikic, R. Rosner, & J. Linker, *Evidence for Topological Nonequilibrium in Magnetic Configurations*, Phys. Rev. E, **62** (2000), 1245-51.

91. A. Venkatesan, A.V. Olinto, & J.W. Truran, *Neutron Stars and Black Holes as Machos*, ApJ **516** (1999), 863.

92. P.A. Young, E.E. Mamajek, D. Arnett, & J. Liebert, *Observational Tests and Predictive Stellar Evolution*, ApJ, in press (2001).

93. Y.N. Young, & R. Rosner, *Linear and Weakly Non-linear Analysis of Doubly Diffusive Vertical Slot Convection*, Phys. Rev. E, **57** (1998), 5554-63.

94. Y.N. Young, & R. Rosner, *Numerical Simulation of Double-Diffusive Convection in a Rectangular Box*, Phys. Rev. E, **61(3)** (2000), 2676-2694.

95. 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.

96. 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 (2001), in press.

97. Y.N. Young & S. Wunsch, *Universality of Scalar Statistics in Stably Stratified Turbulence*, Phys. Rev. Let. (2001), in press.

98. 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.

99. 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.

100. M. Zingale, F.X. Timmes, B. Fryxell, D.Q. Lamb, K. Olson, A.C. Calder, L.J. Dursi, P.M. Ricker, R. Rosner, P. MacNeice, & H.M. Tufo, *Helium Detonations on Neutron Stars*, ApJS (2000), 133, 195-220.

101. 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.