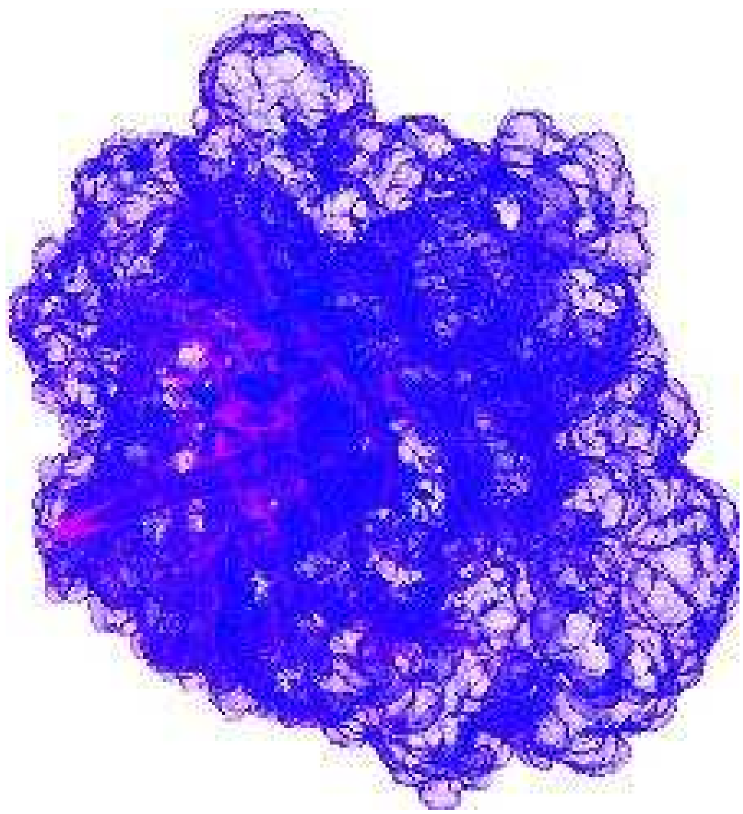
ASC/ALLIANCES CENTER FOR ASTROPHYSICAL THERMONUCLEAR FLASHES AT THE UNIVERSITY OF CHICAGO

YEAR 7 ACTIVITIES REPORT



October 2004

Abstract

We summarize the Year 7 activities at the University of Chicago Center for Astrophysical Thermonuclear Flashes. A detailed strategic plan for the next two years was developed and adopted early in the year.

Major milestones achieved by the Code Group include: (1) substantial progress in developing FLASH 3.0, a significantly more powerful code that will enable developers in the community to contribute modules to FLASH with relative ease; (2) optimization of an adaptive mesh multi-grid solver; and (3) provision of crucial support for the large-scale simulations carried out by the astrophysics group.

Major milestones achieved by the computational physics and validation group include: (1) substantial progress in developing a low Mach number solver; (2) substantial progress in developing a level set method for interface tracking; and (3) important validation work.

Major milestones achieved by the astrophysics group include: (1) achievement of the ability to determine the nucleosynthetic yield of the burning through the use of Lagrangian tracer particles and post-processing using a large nuclear reaction network; (2) completion of a series of high resolution large-scale 3-d simulations of the deflagration-phase of Type Ia supernovae involving a Chandrasekhar-mass white dwarf; and (3) parameter studies of a new subgrid model of the early deflagration phase and the convergence of flame burning properties with resolution. Progress was also made in studying the physics of X-ray bursts.

Major milestones achieved by the computer science group include (1) achievement of scalable performance visualization; and (2) development of new algorithms for data distribution on massively parallel platforms.

Major milestones achieved by the visualization group include (1) substantial progress in production visualization through further development of FlashView based on ParaView, and (2) significant advances in system integration and volume rendering through visualization research.

Credits for Title Page Picture: Calder et al. 2004

Contents

1 Introduction

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

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

2 Code

Participants: K. Antypas, A. Calder, A. Dubey (Group Leader), W. Freis, J.B. Gallagher, J. Joshi, K. Olson, P. Ricker, K. Riley, D. Sheeler, N. Taylor A. Siegel, T. Plewa

2.1 Mission and Goals

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

This year, the Code Group work included ongoing design and development of FLASH 3, getting ready for the final release of FLASH 2, development and enhancement of support tools, external collaborations and organization of a tutorial.

2.2 FLASH2 and FLASH 3

FLASH2 continues to be the production code for the Center. The enhancements to FLASH 2 were mostly related to optimization of the multigrid solver. A few minor modifications and bug fixes were done elsewhere in the code. The final release of FLASH 2 is expected in early 2005.

The primary design principals and software process for the development of FLASH 3 are in place. The framework, the Grid unit and Hydro unit have been imported from FLASH 2. The ideal gas gamma implementation has also been imported along with a couple of basic setups. The testing of all the imported units is underway.

2.3 Collaborations

Two new external collaborations were initiated which involved members of the Code Group. One is with the group at Catania, Italy to interface FLASH with FLY, their tree code. Initial evaluations of the possible gains are very encouraging. Dan Sheeler is the contact person from the Flash Center for this project. The second effort is to implement a Hybrid Characteristics based radiation module in FLASH,in collaboration with Erik-Jan Rijkhorst and Garrelt Mellema at University of Leiden. Anshu is the Code Group representative in this project. A new parallel algorithm has been designed to facilitate this implementation since the radiation module has its own characteristic interprocessor communication pattern.

In addition to the new collaborations mentioned above, Katherine Riley has worked extensively with IBM during the development of compilers and other systems software development for their BG/L machine. The FLASH code was instrumental in uncovering several issues in IBM software.

2.4 Tools

The tools supported in FLASH 2 have been successfully transferred to FLASH 3. These include fidlr, the idl tools for 2d visualization, and sfocu, the utility for comparison of two checkpoint files. Both of the tools are further enhanced to give meaningful results when comparing checkpoint files of FLASH 3 against those of FLASH 2.

FLASH 3 is under nightly regression testing, using the test suite. A new and improved version of the testsuite that will include unit test framework is under development by Noel Taylor. It will be a very flexible tool with a user friendly interface, and will be eventually released as an open source tool. There is an effort underway to make the on-line documentation clean and consistent.

2.5 Workshop/Tutorial

The Flash Center organized a well attended tutorial in May 2004. The audience was a mix of people new to the code, and some fairly sophisticated users. The tutorial was a combination of presentations, and hands-on and breakout sessions. The presentations included basic concepts such as MPI and AMR, solvers included in the distribution of the FLASH code, and some examples of applications that can be simulated using the code. During the hands-on sessions the users could work with standard FLASH supplied application setup, or they could use their own application of interest. The break-out sessions in science domains were found to be most useful by the more advanced users, and some interesting collaborations were initiated during those discussions.

3 Computational Physics and Validation

Participants: A. Haque, P. Hua, T. Linde, T. Plewa (Group Leader), G. Weirs, D. Yu

3.1 Mission and Goals

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

3.2 Low Mach Number Solver

Pan Hua has been working on the low Mach number hydro solver for simulation of the smoldering phases of novae and supernovae.

3.3 Level Set Solver

Dahai Yu is developing a level set technology to use in Flash. The intent is to be able to use these sets to model flame fronts, fluid interfaces, and rigid boundaries.

3.4 Enhanced Multigrid Solver

The multigrid task force made up of Pan Hua, Ju Zhang, Tomek Plewa, Todd Dupont, Anshu Dubey, and Dan Sheeler, made substantial progress in verifying the code and in some cases improved its performance substantially. This work is continuing.

3.5 Validation Studies

Ju Zhang has developed a set of diagnostics and is analyzing turbulent flame modeling data with the goals of better understanding turbulent flame dynamics and developing an area-enhancement-based subgrid flame speed model.

Aamer Haque is verifying FLASH using the Noh and Guderley problems. He has begun setting up FLASH for the converging shock wedge experiments, conducted at Cal Tech, for validation studies.

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

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

4 Astrophysics

Participants: A. Alexakis[1], E. Brown, A. Calder, A. Heger, J. Johnson[1], A. Khokhlov, D. Lamb, T. Linde, B. Messer (Deputy Group Leader), J. Morgan[1], H. Pan, F. Peng[1], T. Plewa, A. Poludnenko, K. Robinson[2], R. Rosner, F. Rubini, J. Zhang, A. Zhiglo [1], J. Zuhone[1]

4.1 Mission and Goals

The astrophysics group has the responsibility to carry out the large-scale astrophysics simulations which are the heart of the Flash Center and to carry out the

[1]Graduate student
[2]Undergraduate student

analysis and interpretation of the computational results in light of astrophysical observations.

4.2 Overview of Astrophysics Activities

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

The focus of Flash astrophysics activities over this period has been on Type Ia supernovae. The prime objective of the Center has been to identify and incorporate into the FLASH code the necessary physics to quantify the flame model, and to utilize this to carry out large scale, integrated, multi-physics simulations of these events. This work will be reviewed in the following discussions. Analytic and numerical studies of both nova explosions and X-ray bursts are also continuing, but large scale, integrated, multi-physics simulations of these events have not been a priority.

The seventh year of astrophysics research has witnessed significant activity on several fronts.

4.3 Type Ia Supernova Explosions

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

Over the past year much astrophysics research at the Flash Center has continued on the Type Ia supernova problem. The principal research effort has been in bettering our understanding of modeling the deflagration phase of a Type Ia supernova. To this end we have further refined the energetics of our model flame in FLASH, developed tracer particle technology tracking density and temperature histories of Lagrangian fluid elements, and with Edward Brown (now at Michigan State University) developed the technology for post-processing the particle trajectories with an advanced nuclear reaction network to calculate detailed abundances.

Preparatory to our continuation of large scale simulations of the deflagration phase of SNe Ia, our emphasis over the past year has been on two critical aspects of the underlying physics: (1) the achievement of an accurate determination both of the flame energetics and of the level of energy production and of neutronization associated with the post-flame-front phase of distributed burning; and (2) convergence of flame burning properties with resolution.

4.3.1 Flame Energetics and Ensuing Distributive Burning

A key ingredient in numerical simulations of the deflagration phase of Type Ia supernovae is the nuclear flame model. A realistic model must accurately describe the nuclear energy that is released, the timescale on which this energy release occurs, and the composition changes that accompany the burning. We have developed a three stage burning model that addresses thermonuclear burning in a C/O white dwarf by considering first ^{12}C burning (to ^{16}O and ^{24}Mg, then oxygen burning to silicon-group elements in a quasi-equilibrium ("NQSE") distribution, and then finally "silicon burning" to nuclear statistical equilibrium ("NSE"). We quantify the effects of the inclusion of detailed nuclear partition function information and electron screening. Self-heating calculations of thermonuclear burning then provide accurate measures of the timescales appropriate to the three stages of burning that define our flame.

The improvements to the Flame energetics arose from our re-thinking the treatment of the third stage of burning. A flame passing through a C/O white dwarf burns the C/O first to a quasi-equilibrium state of Si-group nuclei and then to nuclear statistical equilibrium (NSE) consisting of Fe-group nuclei. Our first approximation to NSE assumed that the material was principally Ni, which has the effect of liberating too much binding energy in the flame. We now utilize NSE distributions calculated as a function of temperature, density, and Y_e to provide measures of both the energy release and and the composition changes. Our NSE distributions are calculated with the inclusion of Coulomb effects, in a manner that is consistent with the screening factors by which the thermonuclear rates are enhanced.

As the flame passes through a piece of material, it changes the state from a degenerate and relatively cool mix of ^{12}**C** and ^{16}**O** to a mix of relatively hot NSE material, which is dominated by the **Fe**-peak elements. Both the increased temperature and the shift of the composition to close to self conjugate **Fe**-peak elements, which have much larger electron capture rates than ^{12}**C** and ^{16}**O**, result in a significant neutronization rate of the bulk material. The effect of the weak interactions on the hydrodynamic evolution can be divided into 3 parts.

1. Energy loss due to neutrino emission.

2. Change of the ionic contribution to the heat capacity due to a shift in the NSE composition caused by a lower Y_e.

3. Decrease of the contribution of the electron to the total pressure due to a decrease in degeneracy pressure of the electrons caused by a lower Y_e.

Previous supernova 1a simulations (e.g. Reinecke et al. 2002) have often ignored the effects of weak interactions on the hydrodynamic evolution of the supernova event. We estimate the combined effects to be possibly significant and are actively working implementing the effects of neutronization in the code. The implementation is based on the smallness of the nuclear timescale when compared to the hydrodynamic timescale, allowing us to treat the ashes as an instantaneously adjusting NSE state, only a function of ρ, T and Y_e. To this avail we have developed out own NSE-solver, which calculates the abundance distribution of 200 nuclei in nuclear statistical equilibrium, taking into account the effects of plasma screening corrections on the free energy and the appropriate temperature dependent nuclear partition functions. The resulting abundance distribution is then convolved with an interpolation of a table of weak rates from Langanke & Martinez-Pinedo (2000,2001) to give the neutrino energy loss rate as well as the neutronization rate $\dot{Y}_e$ of the bulk as a function of ρ, T and Y_e. These results, together with the nuclear energy released dQ, are tabulated in a 3-D table for the appropriate range of ρ, T and Y_e. Since 200 nuclei are too numerous to be advected by the hydro, we have chosen a representative set of nuclei to capture all the features of the NSE composition. The mass fractions of the light nuclei $^{1}\mathbf{H}$ and $^{4}\mathbf{He}$ are stored faithfully in the table. The mass fraction of a neutron rich nucleus, such as $^{54}\mathbf{Fe}$ is then adjusted to give the correct Y_e. Mass fractions of two other self conjugate nuclei, such as $^{56}\mathbf{Ni}$ and $^{24}\mathbf{Mg}$ are then adjusted to give the correct average nucleon number $\bar{A}$. These representative nuclei are then stored in the same lookup table.

Neutronization is then implemented explicitly into the code. From the table we get $\dot{Y}_e$ at the old time. The new Y_e is then calculated with a simple Euler step.

Once the flame has passed, the ashes are in NSE, and we enter into the phase of distributed burning. The hydrodynamic evolution of the ashes, however, causes changes in ρ and T. Since the NSE abundances, and hence $\bar{A}$ as well as the nuclear energy released dQ, are functions of ρ and T, it is important to continuously adjust the NSE state of the ashes. This instantaneous adjustment of the ashes is what we call distributed burning. This reactive development of the NSE state has a very different character than either typical nuclear burning or neutronization. In both these latter cases, $\dot{E}$, the rate of internal energy loss or gain for a fluid element, depends only on its state, ρ, T and Y_e. In the case of the NSE ashes, however, $\dot{E}$ also depends on $\dot{\rho}$ and $\dot{T}$, coupling it directly to the hydrodynamic development.

4.3.2 Merging White Dwarf Binary Model of Type Ia Supernovae

In a separate study, N. Hearn has incorporated the Helmholtz equation of state and the APROX13 nuclear networks from Flash into his parallel Smoothed Particle Hydrodynamics code. The Flash modules are being used to perform n-body simulations of merging binary white dwarfs, a long-discussed possible Type Ia supernova mechanism.

4.3.3 Simulations of Rotating/Deformed Supernova Events

Alexei Poludnenko and Alexei Khokhlov are interested in following the evolution of Type Ia supernovae through the stage of free expansion, for the general case of models which include the effects of rotation. Many three-dimensional fluid dynamical problems are characterized by a very large degree of contraction, expansion, and/or rotation of a fluid. Examples include (but not limited to) stellar core collapse, supernova explosions, star and galaxy formation, and inertial confinement. Compression or expansion of matter in these problems may reach many orders of magnitude.

Problems with large degree of deformation are computationally difficult. Local features of a flow in these problems may be significantly compressed, expanded, and advected over large distances. This puts extreme demands on numerical resolution and on the quality of numerical advection algorithms. For a rotating fluid, large compression or expansion may also lead to large numerical errors in conservation of angular momentum.

Three different approaches can be used to overcome some of these computational difficulties: (1) Adaptive mesh refinement (AMR), (2) computations on a moving mesh (MM), and (3) computations in a deforming (non-inertial) reference frame (DRF). In an AMR approach, a computational mesh can be refined or de-refined to counteract contraction or expansion, respectively, thus maintaining numerical resolution of features of interest. In a MM approach, mesh lines can be moved continuously to minimize the relative motion of fluid with respect to the mesh. A limiting case of a MM approach is a Lagrangian approach in which mesh follows the fluid exactly. An arbitrary Eulerian Lagrangian method (ALE) can be classified as MM.

The AMR and MM approaches are fundamentally the same in that they both work with fluid quantities defined in a stationary inertial reference frame. The only difference is that in an AMR approach the fluid moves through a stationary mesh and an additional interpolation is required only when the mesh is refined. In a MM approach fluid quantities must be re-interpolated onto a new mesh every time step either explicitly as an Eulerian step plus re-map, or implicitly by modifying fluxes through boundaries of computational cells. Mesh velocities can be specified arbitrarily. Because fluid variables are defined in a stationary inertial frame, they are not affected by mesh movements.

In the third, DRF approach, fluid velocity is defined with respect to a moving reference frame. Mesh in this approach has two distinct functions. It defines the boundaries of computational cells and at the same time represents a reference frame. The equations of fluid dynamics must be modified in this approach to include the effects of centrifugal and Coriolis forces. If a reference frame is non-inertial, an additional force associated with accelerations of a reference frame must be included, as well.

A best known astrophysical example of a DRF approach is numerical simulations of galaxy formation which are usually carried out in a non-stationary reference frame. In these simulations, the terms accounting for a non-stationary expansion of the universe are known a priori and are explicitly added as source terms to Euler equations of fluid dynamics.

It is impossible to pick up a single "best" numerical approach to solving all fluid dynamics problems. The right choice must depend on a problem in question and often it is a compromise between the accuracy, flexibility, ease of applicability, and code availability. The approaches discussed above can be and are often used in combination. For example, simulations of galaxy formation routinely combine a DRF approach which takes care of a global expansion of the Universe with an AMR or a MM approaches which are used for a more accurate treatment of a structure formation on smaller scales.

In their work, these researchers plan to investigate the applicability of a DRF approach and a combination of a DRF and AMR approaches to such astrophysical problems as contracting expanding and rotating objects, e.g., collapsing stellar cores and supernovae.

They consider non-inertial reference frames which expand or contract spherically-symmetrically with respect to an inertial laboratory frame. A solid (non-differential) rotation of a frame is also allowed. In many practical cases this may be enough to compensate for a bulk motion associated with an implosion or an explosion of a star or an inertial confinement target. They work under a premise that peculiar motions, local deformations, and sharp features – shocks, contact and material discontinuities, and reaction fronts, – present in the flow can be better treated using an AMR applied in a moving non-inertial frame.

4.4 Studies of Nova Outbursts

Classical novae are a manifestation of thermonuclear runaways in accreted hydrogen/helium shells on the surfaces of white dwarfs in close binary systems (see, e.g., the review by Gehrz et al. 1998). Compelling observational data indicate that the material ejected by some classical novae can be significantly enriched in C, N,O, and Ne, by $\gtrsim$30% by mass (Livio & Truran 1994). It was recognized early that such levels of envelope enrichment could best be explained by dredge-up of some of the underlying white dwarf matter, prior to the final stages of the thermonuclear runaway. The question of how this enrichment is realized has, however, challenged theory now for several decades (see, e.g., the review by Livio & Truran 1990), and constitutes a major roadblock to our understanding of the nova phenomenon. One of the more promising of the proposed mechanisms involves shear mixing.

Flash researchers have completed a systematic investigation of one promising mechanism for shear-induced mixing and envelope enrichment in nova white dwarf environments: a resonant interaction between large-scale shear flows in the accreted envelope and interfacial gravity waves (Rosner et al. 2001). The greater compositional buoyancy in the C/O white dwarf means that the interface sustains gravity waves. Miles (1957) showed that in the presence of a shear flow (i.e., a "wind"), gravity waves with a group velocity matching a velocity in the shear flow are resonantly amplified. These waves eventually form a cusp and break. When the waves break, they inject, analogously to ocean waves, a spray of C/O into the H/He atmosphere. The source of the shear could arise from a number of mechanisms, including convection and the accretion process itself. We have explored the effects of such mixing with two dimensional models, in an attempt to demonstrate how the mixed mass depends upon the velocity of the flow, whatever its origin (Alexakis et al. 2004).

From a suite of 2-dimensional simulations, we have obtained a measure of the rate of mixing and the maximum mixed mass as a function of the wind velocity. Representative three dimensional simulations further reveal the characteristics of this mixing process. In the context of one dimensional models of nova outbursts, we then explored two scenarios for the mixing process and their implications for realistic models of nova explosions.

4.5 Sedimentation and X-ray Bursts

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

Type I X-ray bursts are understood as explosive H/He burning of the accreted material from companion stars on the surface of neutron stars. There are X-ray bursts detected from ~ 10 sources with extremely low persistent luminosities, $L_X < 10^{36}$ erg s^{-1}. At such implied low mass accretion rates ($\dot{M} < 10^{-10}\ M_\odot\,\mathrm{yr}^{-1}$), the sedimentation velocity of heavier elements is comparable to the downward flow velocity in the accumulating atmosphere. Motivated by this observation, Fang Peng, Edward Brown (Michigan State University) and Jim Truran worked on the effect of sedimentation on the distribution of isotopes in the atmosphere of an accreting neutron star and on the ignition of H and He. Fang Peng developed a method for solving diffusion equations. This work revealed that sedimentation can have effect even on high mass accretion rates, where X-ray superbursts (similar to X-ray burst but ~ 1000 times more energetic and last ~ 1000 times longer) are observed. In general, sedimentation changes the proton-to-seed ratio at the ignition and then the following rp-process during the bursts. Taking this into account, we proposed that we might explain the short bursts ($\sim 10 - 50$ sec) observed at these low mass accretion sources. This project is motivated by recent discoveries of such Type I X-ray bursts observed from sources at low persistent luminosities ($\lesssim 10^{36}$ erg s^{-1}).

In order to assess the effect of sedimentation on Type I X-ray bursts and on the subsequent evolution of the ashes, it is necessary to include the effect of compositional inertia and multi-burst calculation. For achieving this, Fang Peng is working with Alexander Heger (Los Alamos National Laboratory) and Ed Brown on the sedimentation effect by incorporating the diffusion code into a 1-D Lagrangian hydrodynamical scheme (the KEPLER code). Fang Peng generalized the diffusion code for non-uniform zoning and is now developing a method to diffuse thousands of isotopes in a reasonably short computational time. With the hydrodynamic code coupled with the diffusion code, we could study the long-term effect of sedimentation on burst behavior and the ash products.

4.6 Astrophysical Flame Microphysics

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

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

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

On the other hand, the terrestrial combustion literature has a large body of work on ignition, flames in turbulence, and transitions. An excellent review on turbulent flame velocity, for instance, is provided by Lipatnikov and Chomiak (2002), where it is made clear that the problem is greatly more complicated than the simple scalings used in the current generation of large-scale simulations. The state of terrestrial flame-turbulence research is greatly more sophisticated than the current astrophysical corpus, and we would like to begin placing astrophysical combustion research on the same rigorous footing as terrestrial combustion research.

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

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

4.7 Other Flash Astrophysics Studies

4.7.1 Galaxy Mergers and Cluster Formation

John Morgan is using three dimensional simulations to study ram-stripping of a group of galaxies as it falls into a larger galaxy cluster. To do this, he is using a modified gravity module, which combines multi-grid gravity and an external field. Only a portion of the galaxy cluster is simulated, which is represented as a "tube" of gas in plane-parallel geometry. The cluster dark matter and the unsimulated portion of the cluster are encapsulated by an externally applied gravitational field. The galaxy group is represented by a spherical distribution of gas and particles. This high-resolution study will help us understand important hydrodynamic interactions in hierarchical structure formation.

4.7.2 Collisions Between Galaxies

John Zuhone is concerned with the use of the FLASH code to simulate galaxy formation and evolution, and cosmology. This primarily utilizes the gravity, particle, and hydro modules of the FLASH code. The key ingredient to getting N-body simulations to work on FLASH has been finding the best way to solve Poisson's equation. To this end, this past year, John has been attempting to build a tree code N-body solver for FLASH which uses the basic PARAMESH structure in FLASH to calculate the approximate gravitational force on each particle. He has also done some work on collisions between galaxies using FLASH's particle mesh N-body algorithm.

4.8 ASCI Lab and Other Interactions

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

1. D. Arnett (supernovae, validation; University of Arizona/Tucson)
2. A. Bayliss (novae and X-ray bursts; Northwestern University)
3. A. Burrows (supernovae; University of Arizona/Tucson)
4. A. Glasner (novae; Hebrew University of Jerusalem)
5. W. Hillebrandt (novae and supernovae; MPI Garching bei München)
6. R. Hoffman (reaction networks; LLNL)
7. E. Muller (relativistic astro; MPI Garching bei München)
8. T. Strohmayer (X-ray bursts; NASA Goddard)
9. D. Swesty (radiative transfer; SUNY at Stony Brook)
10. R. Taam (novae and X-ray bursts; Northwestern University)
11. S. Woosley (supernovae and X-ray bursts; University of California at Santa Cruz)

4.9 Students

Five graduate students are currently working on the Astrophysics portion of the Center's research: J. Johnsen (supervisor A. Khokhlov), J. Morgan (supervisor D. Lamb), F. Peng (supervisor J. Truran), A. Zhiglo (supervisor A. Khokhlov), and J. Zuhone (supervisor D. Lamb). Graduate students who have moved on to postdoctoral positions this year include: A. Alexakis (supervisor R. Rosner), J. Dursi (supervisor R. Rosner), and A. Mignone (supervisor R. Rosner).

5 Computer Science

Participants: A. Chan, E. Lusk (Group Leader), K. Riley, A. Siegel

5.1 Mission and Goals

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

Our goals are to conduct computer science research in certain areas relevant to the ASC program in general, and the Flash Center in particular. This year work focused on three specific areas:

1. Scalable performance visualization
2. Scalability enhancements for FLASH on large numbers of processors.
3. New algorithms for data distribution

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

5.2 Scalable Performance Visualization

Our work in this areas consists of various aspects of the Jumpshot project. Jumpshot is a graphical viewer for a scalable logfile format (SLOG) that permits viewing of very large logfiles with excellent interactive performance. Sophisticated data structures within the file itself allow viewing of large or small parts of the file without ever having to read the entire file.

This year both the logging and viewing parts of Jumpshot/SLOG underwent changes to allow for the display of MPI-2 programs. MPI-2 programs are likely to involve multiple communicators and intercommunicators, as well as one-sided, remote memory access operations. Until this year, SLOG logging and Jumpshot display referred only to a single communicator. FLASH itself provided the stimulus for the multiple-communicator display, since FLASH3 uses multiple communicators for its uniform gird variation. We also worked with the University of Oregon to incorporate the Jumpshot/SLOG software into TAU, a general and widely used performance analysis toolkit.

We enhanced SLOG for more portability and scalability, demonstrating its use with both IBM's MPI for BG/L and the LAM cluster-based MPI, as well as its "native" MPI implementation, MPICH2.

5.3 Improved Scalability of the FLASH Code

A major activity this year was experimentation with the FLASH code on IBM's Blue Gene computer. We conducted experiments with the FLASH code on Argonne's 2048-cpu machine and on the 32,000-cpu machine at IBM Watson Research Laboratory. Scalability problems that had not occurred on the smaller ASC machines were uncovered and addressed. The code is now being readied to make use of the 128,000-cpu machine at Livermore. (FLASH runs with one process per 2-processor node, so the largest FLASH runs we hope to make will utilize 64000 processors

6 Visualization

Participants: J. B. Gallagher, R. Hudson, M. E. Papka (Group Leader)

6.1 Mission and Goals

The Visualization component of the Flash Center carries out two major roles, research in visualization and the development of a production visualization environment both stimulated by and supportive of the Flash Center as a whole and relevant to the ASC program in general . This year's work focused on two specific areas:

1. Production Visualization
   (a) FlashView
   (b) ParaView
2. Research Visualization
   (a) System Integration
   (b) Volume Rendering

6.2 FlashView

FlashView is a tool for visualizing Flash datasets on standard Linux workstations. Flash datasets are stored in HDF5 files in a block structured format. The goal of the production visualization environment is to operate on the Flash datasets without requiring a resampling of the data. FlashView is a domain specific application that addresses the needs of the Flash user community to prepare basic images and movies of Flash datasets. The tool is capable of generating isosurface and cutting planes of scalar variables from Flash datasets. The user is also able to view the computational grid that was used to calculate the dataset. The user is capable of manipulating color maps and clipping planes in order to tailor the visualization to their needs. The user is also able to extract basic information about the visualization output, such surface area of the isosurface. The user is also capable of producing animations of the dataset(s), examples include a given isosurface (isovalue) over the entire time series or an animation of isovalues over a given dataset. A perl interface is provided to aid the user in the generation of movies. FlashView has been included with the 2.5 release of the Flash application and is distributed on the Flash Center website. Official development has ceased as the Center moves to the use of ParaView.

7 Basic Science

Participants: A. Caceres[1], A. Calder, F. Cattaneo, P. Constantin, T. Dupont (Group Leader), P. Gordon, L. Kadanoff, M. Lewicka, R. Rosner, L. Ryzhik, N. Vladimirova, B. Winn[1]

7.1 Mission and Goals

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

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

[1] Graduate student

- Can one formalize the process of validation? A question of importance in many areas where we need to build confidence in our codes and modeling.

7.2 Propagation of Combustion Fronts in the Presence of the Flow

Gordon has considered a reaction-diffusion-advection system of the KPP type in a periodic flow with heat-loss through the boundary. We show, that, as in the case of a shear flow, the propagation speed is determined by the linearization ahead of the front and is thus independent of the Lewis number. Moreover, we show that a flame may be blown-off or be extinguished by the presence of a periodic flow. We present an explicit procedure of constructing a flow which leads to the blow-off or extinction of the flame. The period cell size has to be sufficiently small in order for the flow to extinguish a flame if the channel is wider than critical.

7.3 The Reaction-Diffusion Phenomena in Fluids

The overall goal of this research is an understanding of the mixing effects of flows on reaction: the possibility of front speed-up and quenching. The previous work was centered on fronts in prescribed flows while the main thrust of the current work is in flows coupled to the reaction.

Boundary layers in cellular flow at a high Péclet numbers. As a step toward a better understanding of the effects of the cellular flows (flows with closed streamlines) we have considered a particular advection-diffusion boundary value problem with a prescribed boundary data. The normal component of the flow is assumed to vanish along the boundary. It has been known in the physics literature since the work of Childress and others that boundary layers form along the cell separatrices. Integral bounds that are consistent with the above behavior have been obtained in some special periodic cases in the works of Fannjiang and Papanicolaou, and Heinze. We have obtained explicit bounds on the oscillation of the solution along streamlines and have shown that flow becomes approximately uniform at a certain distance from the separatrices. We also construct an asymptotic description of the solution inside the boundary layers and obtain the error bounds. We expect our methods to be useful in other problems involving the high Péclet number flows.

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