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

YEAR 8 ACTIVITIES REPORT

October 2005

Abstract

We summarize the Year 8 activities at the University of Chicago Center for Astrophysical Thermonuclear Flashes. A detailed strategic plan for the next two years was developed and adopted early in the year.

Major milestones achieved by the code group include: (1) release of *Flash* 2.5; (2) 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; (3) optimization of an adaptive mesh multi-grid solver; and (4) 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, including a full-scale three-dimensional numerical model of the experiment.

Major milestones achieved by the astrophysics group include: (1) achievement of an accurate treatment of both of the flame energetics and of the energy production and neutronization associated with the post-flame-front phase of distributed burning; (2) 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; (3) 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 (4) 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 and in understanding flame physics.

Major milestones achieved by the computer science group include (1) achievement of scalable performance visualization; (2) enhancement of the scalability of FLASH on large numbers of processors; and (3) 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.

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1 Introduction

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

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

2 Code

Participants: K. Antypas, A. Dubey (Group Leader), M. Ganapathy[1], J. Joshi, L. Reid, K. Riley, D. Sheeler, N. Taylor

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 Astrophysics and Computational Physicists. Members from all groups contribute the future direction of the Flash 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, final release of FLASH 2, development and enhancement of many support tools, external collaborations and tutorial/workshops.

2.2 FLASH 3

One of major achievements of this year's FLASH 3 development was proving its extensibility, and hence its potential usefulness in the wider community. There were two collaborations: One was with Dongwook Lee from university of Maryland, and the other was with Andy Wissink of LLNL, that tested the adaptability and extensibility of code. Dongwook was able to interface a staggered mesh

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[1] Graduate student

MHD module with FLASH 3, while Andy, Katie Antypas and Anshu Dubey are making progress in including SAMRAI as an alternative mesh package in the code. FLASH 3 is stable, and supports several applications, including shock cylinder, which is part of the Flash center's ongoing validation research. Lynn Reid, who joined the group earlier this year, is handling the shock cylinder.

Some of the other enhancements in the code include functional and well tested non-fixed blocksize capability, fully supported IO in hdf5 and pnetcdf formats, a unit test framework, a significantly enhanced setup tool and several new units that have been moved from FLASH 2.

FLASH 2.5, the final version of FLASH 2 was released in February 2005. The enhancements in this version include a new relativistic hydrodynamics solver, new IO module using pnetcdf (parallel IO library distributed by ANL), improved time integration for the passive tracer particles support, and a new provable deadlock free block redistribute algorithm. The release was supervised by Dan Sheeler.

2.3 Collaborations

There are two ongoing external collaborations in the center in which the code group is participating. One is with the group at Catania, Italy to interface FLASH with FLY, their tree code. Dan Sheeler did the bulk of the work for this collaboration. The second effort is with the group in Leiden, Netherlands, for a radiation modules. Anshu is the code group representative in this project. The radiation module has its own characteristic interprocessor communication pattern, and involved development of a new parallel algorithm. Since the pattern is considerably different from the typical FLASH communications, Sameer Shende of the Tau group got interested in its analysis using their tool, this is ongoing work.

Katherine Riley had extensive collaboration with IBM during the development of compilers and other systems software development for their Blugene/Light machine. The FLASH code was instrumental in uncovering several issues in IBM software.

2.4 Tools

FLASH 3 moved from CVS to subversion for version control. Subversion is more flexible and user friendly. 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. There is a new set of idl based routines that can be used for diagnostic purposes, developed by Robert Fisher, that Lynn has adapted for use with FLASH.

The setup tool has been significantly enhanced through Murali Ganapathy's efforts. Some of the important improvements include ability to seamlessly handle internal and external libraries and retention of object files between two builds. The second feature is extremely useful while doing parameter comparisons or benchmarking, since only a few files change. In earlier versions, the setup would kill all the object files, whereas now, the bulk of the files stay, thus considerably reducing build time. This could make our nightly testing significantly faster.

FLASH 3 is under nightly regression testing, using a new tool developed by Noel Taylor. It is a very flexible tool with a user friendly interface, that we intend to release with the code. The performance benchmark tool is operational and in use. Noel is further enhancing it to track the day to day performance of the code by storing some of the daily test suite results. This would enable us to pin point the changes in code that lead to specific performance changes.

The on line documentation has been made clean and consistent. There is a new "HowTo" that succinctly explains the module architecture of FLASH. It includes explanation of FLASH keywords, the inheritance rules and data management through examples.

2.5 Workshop/Tutorial

The FLASH center was invited by CITA (university of Toronto) and McMaster University to hold 2-day long tutorial/workshops at each venue. The audience was a mix of people new to the code, and some fairly sophisticated users. Katie and Anshu from code group and Alan Calder and Bronson Messer from the Astro groups represented the FLASH center.

In September 2005, we held an internal FLASH tutorial for the new arrivals in the center.

2.6 Outreach

Anshu Dubey was a part of "Museum Presentation of Science" effort under Leo Kadanoff. As a part of this effort, she gave a presentation to a group of people from Exploratorium in San Fransisco and Scitech in Aurora. Two movies were created based on FLASH results, one of which is scheduled to become a part of an exhibit at Scitech, and the other one is on view at FLASH center. This year, this effort has expanded to include the Museum of Science and Industry.

3 Computational Physics and Validation

Participants: T. Dupont (Group Leader), A. Haque, P. Hua, G. Jordan, T. Plewa, D. Yu, J. Zhang

3.1 Mission and goals

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

3.2 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 Nuclear Network Capabilities

George Jordan is improving the Flash Center's nuclear network capabilities. The addition of Timmes' "pphotcno" network is appropriate for modeling the runaway phase of a novae and the addition of Timmes' temperature coupled version of "aprox13" is a step to eliminating instabilities in the abundance and temperature profiles (among other quantities) brought about by detonations.

3.6 Validation studies

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

3.7 Validation studies

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 even though numerical models are capable of capturing overall morphology of the system, including velocity evolution, in cases of some experimental configurations single diagnostics used so far may not be sufficient for making meaningful comparisons. To facilitate such comparisons, extended three-fluid numerical models will be constructed. The group also obtained the first three-dimensional model of the whole experiment which indicates possible existence of three-dimensional effects (Widnall-like vortex instability). In what follows we present more detailed description of the experimental setups and numerical results.

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

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

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

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

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

Jordan is continuing these 3-d shock cylinder simulations with the addition of tracer particles.

4 Astrophysics

Participants: N. Boittin[2], A. Calder (Deputy Group Leader), R. Fisher, T. Jena, J. Johnsen[1], E. Hicks[1], D. Lamb, B. Messer, A. Mignone[1], J. Morgan[1], F. Peng[1], A. Poludnenko, R. Rosner, I. Seitenzahl[1], D. Townsley, J. Truran (Group Leader), 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 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

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[2] Undergraduate student

[1] Graduate student

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 eighth 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 $^{12}\mathbf{C}$ and $^{16}\mathbf{O}$ 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 $^{12}\mathbf{C}$ and $^{16}\mathbf{O}$, 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**H** and 4**He** are stored faithfully in the table. The mass fraction of a neutron rich nucleus, such as ^{54}**Fe** is then adjusted to give the correct Y_e. Mass fractions of two other self conjugate nuclei, such as ^{56}**Ni** and ^{24}**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.

Additional technology for better extracting results from the simulations was obtained with the development of a code module for FLASH for the evolution of Lagrangian tracer particles. A. Calder and T. Plewa from the Flash Center worked with P. Ricker, now at UIUC, to incorporate a second-order particle advancement scheme in Flash. The goal of this effort is to allow the recording of density and temperature histories during the course of a Flash simulation. These trajectories can be post-processed with a

The post-processing of the particle trajectories will integrate the material through the temperature and density with a detailed nuclear network. Preliminary results of this study were presented by Ed Brown at the Eighth International Symposium on Nuclei in the Cosmos July 19-23, 2004 in Vancouver, BC, Canada. The preliminary results will appear in the proceedings (Brown et al. 2005).

4.3.2 Octant Resolution and AFL Parameter Studies

To better understand the dynamics of the deflagration phase of type Ia supernovae, we initiated a resolution study of three-dimensional simulations of the deflagration phase of type Ia supernovae. This study focuses on three-dimensional simulations that assume octant symmetry, that is the simulations are of one octant of the star.

Subgrid models are an essential component of all supernova simulations run today. These subgrid models provide the flame speed as well as the burned mass inside cells unresolved in simulations, which in turn lead to the total burned mass and energy released over the entire star. We study the characteristics of the subgrid model in the manner described by Khokhlov (1991a,b,1994,1995; see also Gamezo et al. 2003).

The AFL setup of the FLASH code is in effect one cell; it is a rectangular setup in which the initial configuration is in hydrostatic equilibrium. We then perturb the initial conditions by imposing a sine wave of burned ash at the bottom. A flame front starts to propagate upwards and we can explore the dependences of various parameters on the flame propagation. The parameters of particular interest are the box size L, the resolution, the perturbation wavelength Λ and the amplitude of the initial perturbation. We ran simulations with a maximum resolution of approximately 2.3 cm which we have verified is sufficient to ensure convergence of the quantities of interest to us here: the burned mass, the rate of burning and the burning (surface) area. We keep the initial perturbation with $\Lambda = 5.0\text{x}10^5$ cm with an amplitude $A = 1.0\text{x}10^4$ cm. The height of the box was typically between 8 and 16 times the length, enough to allow the flame to reach self regulation.

We have used the above setup to study the effect of the cell size on the subgrid model predictions of the burned mass and the burning rate. We used the AFL setup, keeping all parameters constant for successive runs except the length of the box. Three simulations were performed for the choices of box size: 6Λ, 7Λ and 11Λ. Critical to our consideration of the formulation of a realistic subgrid model was the finding that the normalized burning rate is not independent of box size. This would seem to imply that the burned mass and hence the energy released in full supernova simulations would depend on the cell size of the simulations, even if the cell size is small enough for the hydrodynamics to have converged. Our continuing investigation will explore how we might modify the subgrid model in such a way that the scaled burning rate becomes independent of the cell size.

4.3.3 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.

4.3.4 Metallicity dependence of Type Ia luminosities

A critical question with regard to the use of Type Ia supernovae as standard candles is whether there might exist a metallicity dependence that could influence observations of events at high red shift (lower metallicity populations). Frank Timmes, Ed Brown, and Jim Truran (Timmes et al. 2003) have explored the idea that the observed variations in the peak luminosities of Type Ia supernovae originate in part from a scatter in metallicity of the main-sequence stars that become white dwarfs. Previous numerical studies have not self-consistently explored metallicities greater than solar. One-dimensional Chandrasekhar mass models of SNeIa produce most of their ^{56}Ni in a burn to nuclear statistical equilibrium between the mass shells $0.2\mathrm{M}_\odot$ and $0.8\mathrm{M}_\odot$, for which the electron to nucleon ratio $\mathrm{Y_e}$ is constant during the burn. We were able to demonstrate analytically that, under these conditions, charge and mass conservation constrain the mass of ^{56}Ni produced to depend *linearly* on the original metallicity of the white dwarf progenitor. Detailed post-processing of W7-like models confirmed this linear dependence. The effect that we have identified is most evident at metallicities larger than solar, and is in agreement with previous self-consistent calculations over the metallicity range common to both calculations. The observed scatter in the metallicity (approximately 1/3rd $\mathrm{Z}_\odot$–3 $\mathrm{Z}_\odot$) of the solar neighborhood is enough to induce a 25% variation in the mass of ^{56}Ni ejected by Type Ia supernova. This is sufficient to vary the peak V-band brightness by $|\Delta M_V| \approx 0.2$. This scatter in metallicity is present out to the limiting redshifts of current observations ($z \lesssim 1$). Sedimentation of neon can possibly amplify the variation in ^{56}Ni mass to $\lesssim 50\%$. Further numerical studies can determine if other metallicity-induced effects, such as a change in the mass of the ^{56}Ni-producing region, offset or enhance the variation we identify.

4.3.5 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.

4.3.6 Turbulent Heating of Supernova Ejecta by ^{56}Ni Decay

Justin Johnsen and Alexei Khokhlov are currently involved in research focused on modeling the ejecta from a Type Ia supernovae. They want to address the possibility of turbulent mixing of the ejecta due to heating of the material through Ni-56 radioactive decay. To do this, they are writing a one-dimensional simulation code that uses Alexei Khokhlov's package for the equation of state. Starting with conditions from a supernovae simulation 1.7 seconds after ignition, they will evolve it until several hours or days in simulation time. They anticipate that heating causes turbulence in a certain range of bubble sizes, and continues until the material becomes transparent to the gamma rays that transport the heat.

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. 2004a).

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.

4.4.1 One-dimensional nova models

Having identified critical features of the wave breaking and mixing mechanism, we then incorporated our findings into a "global" nova simulation. In order to explore the global properties and implications of this local mixing mechanism, we computed several one-dimensional models of a novae with a modified version of the KEPLER stellar evolution code (Weaver et al. 1978). For the underlying white dwarf, we used a mass of 1.0 $M_{\odot}$, a radius of 5000 km, and a luminosity of 10^{31} ergs s^{-1}. The white dwarf was composed of a 50%/50% carbon/oxygen mixture. The accreted material was assumed to be of solar composition, and the accretion rate was 10^{-9} $M_{\odot}$. Convection was modeled using the Ledoux criterion for stability and mixing length theory, and possible effects of convective overshooting were not considered.

Two scenarios were investigated for generating the gravity wave induced mixed layer (Alexakis et al. 2004b).

1. In the first case, we considered the possibility that the shear arises when, during the early stages of the runaway and heating of the envelope, the convective cells drive a wind at the interface between the H-rich atmosphere and the C/O substrate. If mixing were to occur at this stages, convection would be able to distribute the material throughout the convective zone. In fact, the convective region encounters the interface only well after the peak of the runaway and thus no significant enrichment occurs.

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

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

4.4.2 Multidimensional Simulations of Nova Thermonuclear Runaways

Ami Glasner, Eli Livne, and Jim Truran (Glasner et al. 2005) have explored the sensitivity of multidimensional nova calculations to the outer boundary condition. In general, multidimensional reactive flow models of accreted hydrogen-rich envelopes on top of degenerate cold white dwarfs are very effective tools for the study of critical, non-spherically symmetric behaviors during the early stages of nova outbursts. Such models can shed light on both the mechanism responsible for the heavy-element enrichments observed to characterize nova envelope matter and the role of perturbations during the early stages of ignition of the runaway. The complexity of convective reactive flow in multi-dimensions makes the computational model itself complex and sensitive to the details of the numerics. In this study, these authors demonstrate that the imposed outer boundary condition can have a dramatic effect on the solution. Several commonly used choices for the outer boundary conditions are examined. It is shown that the solutions obtained from Lagrangian simulations, where the envelope is allowed to expand and mass is being conserved, are consistent with spherically symmetric solutions. In Eulerian schemes, which utilize an outer boundary condition of free outflow, the outburst can be artificially quenched.

Ami Glasner, Eli Livne, and Jim Truran are also exploring the early stages of evolution of nova runaways. Previous multidimensional calculations of nova thermonuclear runaways have been able to simulate only stages for which the relevant time-scales become very short (seconds). Therefore, only the final phases of the ignition stage and the runaway itself were studied. For their current study, a 1D hydrostatic fully convective ideal profile, for which the convective flux was defined according to the Mixing Length Theory, was used as an initial model. This work profoundly extends the previous studies, since it examines the multidimensional effects of early mixing and of local early perturbations. The time-scales considered are from a phase close to the onset of convection when the temperature at the base of the envelope is about $4 \times 10^7 K$ to the runaway itself.

The results obtained to date indicate: (1) the amplitude of the velocities in the convective flow and the amount of mixing from the core strongly correlate with the reaction rates. As long as reaction rates (and implied rates of energy generation) are low, the convective velocities are small and enrichment by mixing is small. Most of the mixing occurs in the runaway itself when the rate of energy input is high. The small level of early mixing does shorten somewhat he time interval for the runaway to take place but doesn't effect the nature of the runaway itself; and (2) local early perturbations of various amplitudes are spread around the envelope on a very short time-scale (seconds), ensuring the sphericity of the runaway and effecting the overall evolution only by a slight increase of the mixing.

4.5 X-ray bursts

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

4.5.1 Sedimentation and X-ray Bursts

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 $\sim$ 10 sources with extremely low persistent luminosities, $L_X < 10^{36}$ $\mathrm{erg\,s^{-1}}$. 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 (Fang et al. 2005) 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 $\sim$ 1000 times more energetic and last $\sim$ 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.

4.6.1 Analytic Studies of Flame Stretching

Currently A. Zhiglo is studying burning in two-dimensional systems with flame stretching. Previous analytic consideration showed that there may exist a solution with flat thin flame (i.e. fuel concentration f=f(x,t)) and with the gas velocity having uniform gradient of the component along the flame $dv_y/dy(x,t)$. Demonstrating this numerically is proving challenging as a limiting procedure is impossible. (One must solve for velocities and concentration, whereas without stretch the velocity was expressed analytically $v = v(f)$). Current thinking holds that the problem stems from using Newton's method for root finding, and the numerical integration is not so precise to provide derivatives accurate enough. As a possible solution, we will use the asymptotic solutions from far before the front. These may depend on unphysical parameters, which are defined so that the $dv_y/dy(y = \infty)$ had prescribed values. The approach is to solve inverse problem: just vary these parameters with some step, for a given (thus) asymptotics find the corresponding flame speed D (a one dimensional problem, without newton's algorithm) and $dv/dy(y = \infty)$, and then to reconstruct (from thus parametrically defined) D as a function of this gradient (=stretch). For this to succeed, among other things, the integration scheme must be invertible, that is the value of grad v from the parameters in asymptotics must be reliable. Verifying this approach is the subject of present research.

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 I have 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 have also done some work on collisions between galaxies using FLASH's particle mesh N-body algorithm.

4.7.3 Early Evolution of Globular Clusters

Although globular clusters have been observed for decades, their formation still remains a mystery. Two alternative theories have generally been put forward. One assumes that the stars in the clusters formed from already enriched material. An alternative model (Brown et al 1991,1995) suggests self-enrichment within the pristine proto-globular-cluster cloud (PGCC), caused by supernova explosions of an earlier generation of stars in the cluster. According to Fall and Rees (1985), thermal instabilities in the proto-galactic medium lead to a structure consisting of cold dense clouds at a temperature of around $10^4 K$, surrounded by a hot intercloud medium at $10^6 K$. Within these clouds a first generation of stars forms. The massive stars explode as supernovae, and their ejecta merge in a supershell that sweeps up the cloud gas on its way out. The shock quickly sweeps up enough material to go into the Sedov self-similar stage as in the case of supernova remnants. Later in the evolution it will evolve to a radiative phase where a cold, high density shell will form behind it. The material from the ejecta mixes with the pristine gas on the shell through turbulent processes, most likely caused by instabilities on the shell. Gravitational instabilities will presumably lead to the fragmentation of the shell, making it possible for a second generation of stars to form. In some of these PGCC the stars will form a bound globular cluster system whose properties can be compared to the low metallicity halo globular clusters clouds in the galaxy.

A. Medina, V. Dwarkadas, and J. Truran are using FLASH to address this problem. They are considering a 2 dimensional simulation. It is assumed that the density in the cloud can be approximated as constant at the center followed by a $1/r^2$ profile to the edge of the cloud. Their simulations begin in the Sedov stage of expansion at a small initial radius within the constant density medium and are evolved all the way to the hot intercloud medium. Radiative cooling is included. In this way they will be able to examine such instabilities as may arise, and determine whether or not these will completely disrupt the shell.

4.7.4 The Helium Flash with Flash

Laurent Piau and Alan Calder are making progress in the use of the FLASH code in studies of the helium flash. The helium flash is a thermonuclear runaway induced by the helium ignition in the degenerate core of a low mass star when it reaches the top of the red giant branch. This dynamic event cannot properly be addressed with the classical stellar evolution codes, the main reason being the interplay between convection and the runaway process. The phenomenological theories of convection used in stellar evolution codes do not provide a priori information on the thermal structure of convection zones, on the transitory regimes, or on the precise extent of the convective motions. These features are however crucial to the determination of the violence of the runaway during the flash and the subsequent nucleosynthesis and mixing. Being an explicit multidimensional hydrodynamical code devoted to explosive processes in stars, the FLASH code can likely provide new and realistic insights on the helium flash. They plan to address the helium flash by coupling FLASH with CESAM the stellar evolution code that Laurent Piau has used intensively in the past. They first have followed the evolution of low mass stars from the zero age main sequence to the top of the RGB. Subsequently they have mapped the output of the CESAM code in the FLASH code to obtain models in hydrostatic equilibrium. They are currently exploring the initial conditions that define the early stages of burning and, in particular, the development of convective motion associated to the helium burning runaway.

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

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

5 Computer Science

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

5.1 Mission and goals

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

Our goals are to conduct computer science research in certain areas relevant to the 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

5.4 New Data Distribution Technology

Experimentation with FLASH on large numbers of processors led to the invention of a new algorithm for data distribution. The problems arises in FLASH because it is an AMR code, and periodically redistributes its global data for load balancing purposes. Blue Gene's limited memory per node provides additional constraints. The study of this problem led to a new, provably correct algorithm and general-purpose software that implements it, called PADRE.

The PADRE (Parallel Data Redistribution) Toolkit is a collection of portable MPI-based algorithms for efficient scalable parallel data redistribution in limited memory environments (such as one finds with most HPC codes). That is, given a locally decomposed global array and a source/destination map, PADRE carries out the data movement assuming minimal temporary storage. The framework allows the client application to easily explore different redistribution strategies which might have advantages on certain platforms or for certain classes of redistribution maps, memory limit, number of processors, etc. PADRE is designed with a highly modular object framework that easily allows the integration of new algorithms as they become available, and thus is constantly updated and serves as an point of organization for research in this field in general.

5.5 ASC Lab Interactions

We are currently working with IBM and Livermore to run FLASH on the full-size BG/L at Livermore, providing insight into how to utilize very large numbers of processors. This is the FLASH contribution to pushing the envelope of scientific simulation on petaflops-scale machines.

We have continued to interact with all the ASC labs, particularly Sandia, in the area of parallel file systems.

Our MPI implementation MPICH, continues to form the foundation for the vendor MPI implementations on Red Storm and BG/L.

6 Visualization

Participants: J. B. Gallagher, C. Glendedin (added in October 2005), 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 three specific areas:

1. Production Visualization
    (a) FlashView
    (b) ParaView
2. Research Visualization

(a) System Integration

(b) Volume Rendering

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

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.

6.3 ParaView

ParaView is an open source visualization package developed by Kitware Inc. that is built on top of the Visualization Toolkit (VTK) that has a standard graphical user-interface for access to the system. ParaView provides an excellent building block to develop a production visualization environment for the Flash Center. Over the past year we have extended the user interface of ParaView to make it easier to use for the the Flash scientists. The new GUI for ParaView retains all of the existing ParaView functionality while adding a simple interface to 90% of the functionality the average Flash user is looking for without being overwhelmed by more information than is needed. The new simplified interface walks the user through the visualization process. Asking first what Flash file the user wants to work with, followed by which of the variables they are interested in, finally presenting them with a final image that can be saved to disk. Since nothing was removed from the tool, as the users become more and more comfortable with the tool, they can still make use of the all of ParaView's features. ParaView works in a client server mode, which like FlashView is essential for the large datasets that are produced. In addition to the developments in the user interface, the Center has begun investigate the use of ParaView's support for AMR datasets. This effort required interaction with the Kitware staff to move from the use of unstructured representation of the data to a hierarchical box format. Over time this format will will support the direct volume rendering of the data within the end user tool. This new format also supports the viewing of data at all levels of refinement.

6.4 System Integration

This year with the help of summer student Chad Glendedin (added as staff in October), the Center has begun to explore the development of a visualization pipeline that would take data as output from the simulation and begin processing immediately. The pipeline would automate the transfer of data, preprocessing of information, management of datafile storage, and management of visualization metadata. Many of the pieces for the pipeline have been constructed, this includes the automatic management of data placement given a set of data resources. The preprocessing data is handled with the output stored in a database for retrieval by visualization programs at a later date. The transfer of files has also been automated and can make use of both scp and GridFTP for transfers.

6.5 Volume Rendering

The Center has begun to develop the next generation of custom Flash volume rendering systems. This system is built using the Volume Rendering Library (VL) is a general purpose framework for supporting volume rendering. The library leverages existing efforts within the visualization group. The framework implements a set of classes making extensive use of inheritance models to support generalization and easy extension of functionality. While maintaining flexibility, key design decisions have also been made to increase performance on current-generation commodity hardware.

The development of the VL framework is ongoing; however the foundation is complete, as are some initial implementations of visualization algorithms. The current framework provides the following tools:

1. A mechanism for supporting variable spatial representations of the data volume
2. A tree-based volume segmentation algorithm
3. Enforced back-to-front rendering of segmented volume data
4. A set of OpenGL Shading Language-based algorithms for performing volume rendering using the accelerated graphics hardware available in modern gaming cards
5. A set of primitives for performing math routines involving matrices and vectors
6. A mechanism for supporting real-time manipulation of all volume rendering parameters, including the look-up-table used for segmentation and color mapping

7. A mechanism for supporting accurate cut plane functionality
8. A mechanism for specifying a reduced region of interest, and accelerated rendering when such a region is specified

One of the primary purposes for the development of VL involves taking advantage of accelerated graphics hardware available in commodity systems today. In order to reach this goal, specialized shader algorithms, constructed to operate within the graphics hardware itself, had to be developed. The choice of the OpenGL Shading Language for this development leads to a set of algorithms that are platform-independent, easy to read and maintain, and well placed for support into the foreseeable future. Additionally, because of the fundamental structure of the OpenGL Shading Language, applications built using the VL framework will not need to be re-compiled to take advantage of advances in graphics hardware that may be present on any given machine. Finally, the cut plane and region-of-interest functionality, being built directly into the volume rendering framework, allow for accurate volume rendering in hardware even in the presence of these vital features. By taking advantage of certain characteristics of the fragment and vertex shaders developed for hardware-optimized volume rendering, acceleration is even possible when individual voxels are clipped from the data set.

7 Basic Science

Participants: S. Abarzhi, 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.

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[1] Graduate student

- How does interface mixing work? Can computations reliably compute the "saturated state"? This is relevant for the Nova problem, both in the energetics and composition.
- How much physics is needed to capture "fast reconnection"? This is a key question for understanding dissipation and topological restructuring of fields in magnetospheres. Will this supply a cutoff in non-MHD models?
- Can one formalize the process of validation? A question of importance in many areas where we need to build confidence in our codes and modeling.

7.2 Propagation of flame in porous media

Gordon has investigated a regime of low velocity deflagration in hydraulically-resisted flows as those occurring in porous beds is considered. An asymptotic expression for the deflagration velocity is derived. The obtained dependency elucidates the mechanism controlling the gradual enhancement of the propagation velocity prior to the abrupt transition from slow to fast combustion. This enhancement is caused by the drag-induced diffusion of pressure ahead of the advancing front. The time of transition from the slow to fast propagation is estimated.

7.3 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.

7.4 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.

Quenching in cellular flows. We have previously shown that strong shear flows are capable of extinguishing a large flame. This happens when the flow enhances mixing so much that temperature drops everywhere below the ignition threshold. We have extended this result to the cellular flows.

Reacting systems with a boundary heat-loss. Very few rigorous results are available for reaction-diffusion systems in a prescribed flow, as opposed to a single reaction-diffusion-advection equation that has been extensively studied in the last decade. We consider a KPP-type system of equations for temperature and concentration with a boundary heat-loss in a shear flow. We show that the propagation speed is independent of the Lewis number and prove existence of non-planar traveling fronts when Lewis number is equal to one. Note that this is a genuine system even in the equidiffusive case, as the boundary conditions do not support the reduction to one equation that is possible in the adiabatic case. The former result for the propagation speed has been extended to periodic flows and studied numerically.

The reactive Boussinesq system. We have continued an ongoing study of solutions of the reactive Boussinesq system. We have previously obtained uniform bounds on solutions of the Cauchy problem and studied the linear stability of the planar front solution. We have established existence of non-planar traveling fronts for all Rayleigh numbers and have also obtained lower bounds on the speed of propagation of such fronts. In particular, we show that the front speed grows both in the Rayleigh number and in the domain size.

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Figure 1: The flow field density illustrates the vortex structure induced in a column of sulfur hexafluoride 825 microseconds after the passage of a Mach 1.2 shock wave. The shock induces vertical motions because of the misalignment between pressure and density gradients characteristic of the shock wave and the column material. Small-scale irregularities also develop because of fluid dynamic instabilities. The data is from a three-dimensional numerical simulation that was carried out using the FLASH code running on the ASC Q machine. The initial conditions match experiments carried out at Los Alamos National Laboratory. FLASH is a parallel adaptive-mesh-refinement numerical hydrodynamics code developed at the ASC Alliances Center for Thermonuclear Flashes at the University of Chicago. Visualization was produced using software developed in collaboration with Argonne National Laboratory.

Figure 2: Image from the 2 km octant simulation at t = 1.31 s. The simulation was performed with 500,000 Lagrangian tracer particles. The particle trajectories are being post-processed with a detailed nuclear network that will follow their trajectories density and temperature. The image on the left is a volume rendering of the mass scalar variable that controls carbon burning. The image on the right is of particles in the burned region. The color map goes from red to green to blue as the temperature goes from 3.0×10^9 K to 1.2×10^{10} K. The reddish particles toward the front are the cooler particles just beginning to burn. The unburned particles at temperatures well below the range are not visible. The length scale of both images is about 1000 km.

Figure 3: Plot of burned mass versus time for simulations of the deflagration phase of a type Ia supernova. Shown are results for simulations at effective resolutions of 0.5, 1, 2, 4, 8, and 16 km. The left panel shows the early time detail and the right panel shows the complete evolution. The simulations show a trend toward convergence.