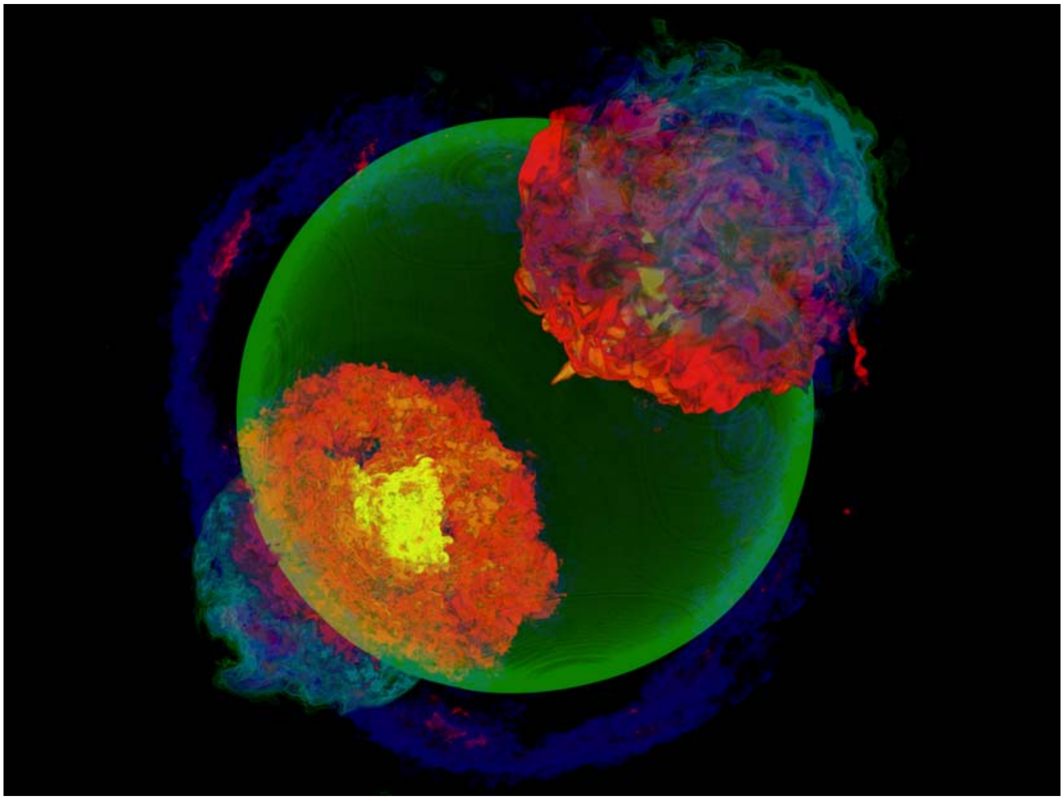
ASC/ALLIANCES CENTER FOR ASTROPHYSICAL THERMONUCLEAR FLASHES AT THE UNIVERSITY OF CHICAGO

YEAR 9 ACTIVITIES REPORT



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Abstract

We summarize the Year 9 activities at the University of Chicago Center for Astrophysical Thermonuclear Flashes. A detailed strategic plan for the next one years was developed and adopted early in the year.

Major milestones achieved by the code group include: (1) release of pre-alpha and alpha versions of *Flash* 3.0; (2) substantial progress in developing other parts of *Flash* 3.0, (3) extensive online documentation for the users, (4) provision of crucial support for the large-scale simulations carried out by the astrophysics group.

Major milestones achieved by the comp phys group include: (1) progress in developing a low Mach number solver suitable for following the pre-explosion smoldering phase of Type Ia supernovae; (2) development of a 3-D radiation transfer module; (3) validation simulations of the Michigan shock-tube experiments which use a powerful laser to drive the R-M and R-T instabilities; (4) simulations of R-T–driven turbulent nuclear burning; (5) 2-D hydro simulations of the deflagration and detonation phases of Type Ia supernovae within the gravitationally confined detonation (GCD) model; and (6) 2-D radiation transfer simulations of the light curves and spectra predicted by the GCD model.

Major milestones achieved by the astro group include: (1) development and extensive verification of a new advection-diffusion-reaction (ADR) flame model that is quieter, more stable, and exhibits less curvature effects than the top-hat model previously used by workers in the Type Ia supernova field, including the Flash Center; (2) development of an improved treatment of the energy release in a nuclear flame; (3) development of a new 3-stage nuclear flame that is quieter, and that tracks the nuclear statistical equilibrium and treats neutronization in the nuclear flame and afterward; (4) a parameter space survey of the effect of initial conditions on the outcome of the deflagration phase of Type Ia supernovae in the gravitationally confined detonation model; (5) exploration of the early phase of nova outbursts; and (6) study of the effect of gravitational settling of heavy elements on X-ray bursts.

Major milestones achieved by the computer science group include (1) development of a collective operation verification library; (2) enhancement of our scalable performance visualization software; and (3) preparation of libraries and tools for next-generation architectures.

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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 is composed of six groups: Code, Computational Physics, Astrophysics, Computer Science, Visualization, and Basic Physics.

2 Code

Participants: K. Antypas, A. Dubey (Group Leader), M. Ganapathy, L. Reid, D. Sheeler, N. Taylor K. Weide

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 design, develop and maintain FLASH, a public domain multiphysics code used in astrophysical simulations, and to support the research of the Astrophysics Group. 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 to 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.

This year, the code group work included two preliminary releases of the newest version of the code, FLASH 3. Many new algorithms and capabilities were added to the code, and extensive online documentation was created in preparation for the releases. This year also saw the first Science run being done with FLASH3. In December 2005, FLASH3 was used to do a large isotropic turbulence simulation on LLNL BGL machine using 32K nodes. In addition the code group was involved in external collaborations, and conducted a tutorial in the summer AAS meeting in Calgary, Canada.

2.2 FLASH 3

Major achievements of the year included

- Release of the pre-alpha and alpha versions of FLASH3, with extensive online documentation for user support. The release also included a developer's section in the documentation to provide guidance to the more advanced users.
- Use of FLASH3 for the large 3D turbulence calculation run on the LLNL BG/L machine. This was the first major scientific simulation done using FLASH 3.
- FLASH tutorial in the summer meeting of the American Astronomical Society
- Making the framework of FLASH available as one click download
- Public release of Flashtest, a tool for regression testing of the FLASH code and other similar codes.
- Getting FLASH3 ready for the 3 dimensional GCD runs.

The pre-alpha release of FLASH3 had all the infrastructural units, and many of the most important physics units. The Grid unit to manage the mesh supports an in-house Uniform Grid and versions 2 and 3 of Paramesh. Most applications can choose between various meshes at the time of setup. The enhancements to the Grid unit include an ability to initialize AMR mesh in parallel. The more usual mode with Paramesh creates the initial blocks on the master PE, and then lets them be distributed to other processors through the refinement process. This approach has obvious limits when the number of processors and the size of the problem grow. The new algorithm allows the initial blocks to be created is a distributed manner. Another significant improvement involves more integrated handling of curvilinear coordinates and corresponding interpolation. We also do the conversion between primitive and conservative variables more consistently. The IO unit supports two parallel IO libraries, HDF5 and pNetCDF. There is also the last resort direct IO implementation which allows each processor to checkpoint itself.

The physics units in the releases included the PPM based hydrodynamics solver and the ideal gas gamma law Equation of State, an 8 wave MHD solver, a multipole based Poisson solver for gravity, Helmholtz equation of State, nuclear burning, and Lagrangian tracer particles for the Uniform Grid. Few more additions to the code were made to facilitate the transition of center's core simulations from FLASH 2.5 to FLASH 3. Most of these additions relate to the white dwarf simulations which moved over to FLASH 3 in early fall 2006. To facilitate this transition, we included a unit for handling the flame, and the white dwarf setup which includes customized boundary conditions and refinement procedures. The tracer particles were extended to run with AMR with a completely new suite of algorithms to manage the movement of particles data.

The new algorithms are efficient, provably scalable and robust. We also enabled density based initialization of tracer particles for these simulations, and added ability to discard particles in mid run. The code group worked with the scientists in the Astrophysics group to eliminate errors, and machine and compiler based quirks, to enable the simulations. Several algorithmic optimizations were also made to the code.

2.3 Collaborations

The code group has an ongoing collaboration with the DEISA project in Europe. The DEISA project is a consortium of universities and supercomputer centers across Europe that are interested in studying performance of platforms and the machines that run on them. They have selected FLASH as their primary application code for this work. The first part of this project involved porting the code to all the major supercomputer installations and profiling them. In the last year, the project has graduated to applying some of the profiling insights to optimization of the code. This collaboration is likely to result in significant performance improvement in the self gravity solver using the multigrid method. In addition we have a working relationship with Paul Ricker, whose student Zarija visited the Flash center for a month in late summer/ early fall to import some of his and Paul Ricker's work into the code. Kevin Olson contributed a tree based self gravity solver, which is in FLASH3 and will be released when Kevin approves. We continue to work with Tau group at University of Oregon on code performance issues.

2.4 Tools

The setup tool has been significantly enhanced, to allow the permutations of units to be done more smoothly. For example if an application selects Paramesh as the Grid unit of choice, then setup script can determine the appropriate implementations of the IO and tracer particles data movement units without explicit specifications. The setup script is also more aggressive in determining and warning about potential errors. Several new tools have been developed to flag coding violations, to provide online link to all the Units' API functions, and runtime parameters. These links provide access to automatically generated information directly from the source tree.

Direct IO capability was added to the code as a last resort when all parallel file systems failed to scale for the large simulation run on the BG/L machine. In this method, each processor writes to, and reads from its own separate file. Several tools were developed to be able to read and process this information. We developed a new algorithm for sorting the trajectories of the Lagrangian tracer particles, which is extensible to IO with parallel file systems.

FlashTest, the tool for nightly regression testing of FLASH has been generalized to be usable with any code that uses steps similar to FLASH in building. If a code has configuration followed by compilation steps, and has an ability to produce benchmarks to test against, it can use FlashTest. We also created several tools to assist in maintenance of the code. An important one is a coding-violations check that runs every night and identifies violations of FLASH coding standards. It also checks for consistency in the API documentation that appears online.

The code releases included extensive on-line documentation. In additions to User's guide, all the units have detailed description of their interface routines, with direct link to the source tree. These descriptions include the list of input output arguments, the functionality of the routine and usage examples where applicable. Links also exist for the runtime parameters relevant to the units, and quick reference tips on IO, code architecture, naming conventions etc. The developer's section of the online documentation includes a"HowTo" section that includes a fully worked out example of the unit architecture of FLASH. It includes explanation of FLASH keywords, the inheritance rules and data management through examples. Additionally there are instructions on migrating code from FLASH2 to FLASH3, including the mapping of the variable and routine names.

2.5 Workshop/Tutorial

The Flash center organized a FLASH code tutorial as a part of the summer AAS meeting. The audience was a mix of people new to the code, and some fairly sophisticated users. Katie, Anshu and Dan from code group and Alan Calder from the Astro group represented the FLASH center.

2.6 Outreach

Anshu Dubey continued to be a part of "Museum Presentation of Science" effort with Leo Kadanoff. One of the movies created as a part of this effort was shown at the American Physical Society annual meeting.

3 Computational Physics and Validation

Participants: T. Dupont (Group Leader), T. Plewa, J. Zhang N. Hearn

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

Considerable effort has been devoted to the development of a low Mach number reactive flow solver to allow simulation of the smoldering phase before a WD runs away. We would like to be able to simulate long periods before “ignition”, but even short periods, say a few minutes, are likely to add to our understanding of the conditions in a WD shortly before it starts on the path to becoming a SN Ia. For a considerable period of time the effort was mostly the work of Hua Pan, who has now left the center. At this point Ju Zhang is doing most of the hands-on work with guidance from Tomasz Plewa and Todd Dupont.

The current solver uses a solver known by its acronym PIMM (from Pressure Implicit Method). This is based on a simplified version of of the an algorithm due to Colella and Pao [1] . This new algorithm has significant advantages in some situations. The implementation is based on the Xing code of Pan and Plewa. The current version of PIMM includes multispecies advection, stellar equation of state, nuclear networks, and support for cylindrical geometry. Several verification tests have been performed, including standard test problems and comparison with published results in the context of type Ia supernova progenitor by Almgren et al [2].

3.3 3-D Radiation Transfer Module

The group activities extended into astrophysics applications with development of new algorithms, code validation studies, and ultimately also application of new physics modules. In particular, in [3] we presented a three-dimensional radiative transfer method designed specifically for use with parallel adaptive mesh refinement hydrodynamics codes. This new algorithm, which we call hybrid characteristics, introduces a novel form of ray tracing that can neither be classified as long, nor as short characteristics, but which applies the underlying principles, i.e. efficient execution through interpolation and parallelizability, of both. Primary applications of the hybrid characteristics method are radiation hydrodynamics problems that take into account the effects of photoionization and heating due to point sources of radiation.

In [4], the FLASH code has been extensively compared to several other hydrodynamics codes in application to disk-planet interaction problem. We found overall good consistency between the codes. The density profiles agree within about 5 per cent for the Eulerian simulations (including FLASH). The SPH results predict the correct shape of the gap although have less resolution in the low-density regions and weaker planetary wakes. The disk masses after 200 orbital periods agree within 10 per cent.

Collaboration with Palermo group (S. Orlando and collaborators) yielded more complete astrophysical view of a shock-cloud interaction problem [5].

Based on 3-D FLASH simulations, we synthesized the expected X-ray emission, using available spectral codes. We found that the morphology of the X-ray emitting structures is significantly different from that of the flow structures originating from the shock-cloud interaction. The hydrodynamic instabilities are never clearly visible in the X-ray band. Shocked clouds are preferentially visible during the early phases of their evolution. Thermal conduction and radiative cooling lead to two different phases of the shocked cloud: a cold cooling dominated core emitting at low energies and a hot thermally conducting corona emitting in the X-ray band. The thermal conduction makes the X-ray image of the cloud smaller, more diffuse, and shorter-lived than that observed when thermal conduction is neglected.

The FLASH code has been extended to model close binary systems in collaboration with Chris Mauche and his group at LLNL. Preliminary results of a global model of the radiatively-driven photoionized wind and accretion flow of the high-mass X-ray binary Vela X-1 has been presented in [6]. The full model combines FLASH hydrodynamic calculations, XSTAR photoionization calculations, HULLAC atomic data, and Monte Carlo radiation transport. We presented maps of the density, temperature, velocity, and ionization parameter from a FLASH two-dimensional time-dependent simulation of Vela X-1, as well as maps of the emissivity distributions of the X-ray emission lines. This is work in progress and will ultimately include fully 3D studies.

3.4 Validation of FLASH Code for R-M/R-T Instabilities

We continued our efforts toward validating the FLASH code. In [7], we presented two- and three-dimensional simulations involving Richtmyer-Meshkov and Rayleigh-Taylor instabilities run with the FLASH code. Variations in the rate of mixing layer growth due to dimensionality, perturbation modes, and simulation resolution were explored. These simulations are designed for detailed comparisons with experiments run on the Omega laser to gain understanding of the mixing processes and to prepare for validation of the Flash code. The initial conditions used in the above study are motivated by pre-supernova structure of a massive star and were discussed in detail in [8]. Computational tools have been constructed to facilitate the comparison of experimental results with simulations through the generation of synthetic radiographs. We expect that these tools will be useful in planning future experiments as well.

3.5 Planning for Simulations of Shock/Bubble Experiments

There has been planning and code development for validation studies involving experimental work on the interaction of shocks with bubbles of Argon in Nitrogen. Understanding the initial conditions is complicated because of the effects of diffusion. The code development for this effort ties in with the educational activity mentioned in the Basic Science section.

3.6 Rayleigh-Taylor–Driven Turbulent Flames

Ju Zhang has led the effort on studying evolution of Rayleigh-Taylor driven turbulent flames in the context of thermonuclear supernova explosions [9]. In this study, the flame evolution was followed through an extended initial transient phase well into the steady state regime. The properties of the evolution of flame surface were examined. We confirmed the form of the governing equation of the evolution suggested by Khokhlov in 1995. The mechanism of vorticity production and the interaction between vortices and the flame surface were discussed in detail. Previously observed periodic behavior of the flame evolution was reproduced and was found to be caused by the turnover of the largest eddies. The characteristic timescales were found to be similar to the turnover time of these eddies. Relations between flame surface creation and destruction processes and basic characteristics of the flow were discussed. In particular, it was found that the flame surface creation strength is associated with the Rayleigh-Taylor timescale. Also, in fully developed turbulence, the flame surface destruction strength scales as $1/L^3$, where L is the turbulent driving scale. The results of our investigation provided support for Khokhlov's self-regulating model of turbulent thermonuclear flames. Based on these results, one can revise and extend the original model. The revision uses a local description of the flame surface enhancement and the evolution of the flame surface since the onset of turbulence, rendering it free from the assumption of an instantaneous steady state of turbulence. This new model can be applied to the initial transient phase of the flame evolution, where the self-regulation mechanism yet to be fully established.

3.7 Simulations of Type Ia Supernovae

Collaboration with Daniel Kasen, Johns Hopkins University, resulted in generalization of the Gravitationally Confined Detonation scenario originally introduced by Plewa, Calder, & Lamb [10]. The dynamics of the explosion in this gravitationally confined detonation model has been extensively studied for several different initial flame configurations [11]. The results point to a shock-to-detonation as one possible mechanism behind transition to detonation, but other possibilities (e.g. Zel'dovich's gradient mechanism) cannot be excluded. Detonations were not obtained in all cases considered pointing to a possible lack of robustness of the process (and adding more weight to other possible detonation triggers discussed but not studied in this work). Where they overlap, the results of this work were qualitatively confirmed in the independent study by Garching supernova group [12]. The difference in outcomes persists, however, in 3D where Roepke et al. results contrast with recent work by Jordan et al. [13], which shows that the gravitationally confined detonation model robustly reaches detonation conditions for a range of initial conditions.

The above work also presented for the first time approximate nucleosynthetic yields obtained with help of alpha network. These yields were subsequently used to create model observables to validate the DFD scenario [14] .

Using time-dependent multi-dimensional radiative transfer calculations, the synthetic broadband optical light curves, near-infrared light curves, color evolution curves, full spectral time-series, and spectropolarization of one gravitationally confined detonation model were obtained, as seen from various viewing angles. All model observables were critically evaluated against examples of well-observed, standard Type Ia supernovae. The consequences of the intrinsic model asphericity we explored by studying the dependence of the model emission on viewing angle, and by quantifying the resulting dispersion in (and internal correlations between) various model observables. These statistical properties of the model were also evaluated against those of the available observational sample of SNe Ia. On the whole, the gravitationally confined detonation model shows good agreement with a broad range of SN Ia observations. Certain deficiencies are also apparent, and point to further developments within the basic theoretical framework. Several intriguing orientation effects we identified in the model which suggest ways in which the asphericity of SNe Ia may contribute to their photometric and spectroscopic diversity and, conversely, how the relative homogeneity of SNe Ia constrains the degree of asymmetry allowable in the models. The comprehensive methodology adopted in this work proved an essential component of developing and validating theoretical supernova models, and helps motivate and clearly define future directions in both the modeling and the observation of SNe Ia.

3.8 White Dwarf Merger Model for Type Ia Supernovae

One possible scenario for supernova formation is through the merger of two white dwarfs. Nathan Hearn, in collaboration with others, has continued his study of this process using the Tillamook parallel SPH (Soft Particle Hydrodynamics) and n-body code to investigate the dynamics of merging white dwarf stars, and the ability of mergers to trigger Type Ia supernovae events. The partially-degenerate, Helmholtz free-energy equation of state and aprox13 nuclear network has been adapted from the Flash code for use as Tillamook modules. An approximate model for orbital decay from gravitational radiation has also been incorporated. Current simulations are modeling the break up of the secondary white dwarf prior to its merger with the primary. A significant re-write of the asynchronous parallel communications algorithms in Tillamook (using MPI) is nearing completion, which should provide enhanced performance and better stability on massively parallel computing resources.

4 Astrophysics

Participants: A. Calder (Deputy Group Leader), R. Fisher, T. Jena, J. Johnsen[1], E. Hicks[1], D. Lamb, 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]

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[1] Graduate student

4.1 Mission and goals

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

4.2 Verification of ADR Flame Model

A large team led by Shimon Asida, a visitor to the Flash Center from The Hebrew University in Jerusalem, has developed a greatly improved advection-diffusion-reaction (ADR) flame model for use in simulations of Type Ia supernovae [15]. This model meets the essential requirements of any flame model: The speed of the flame model must be the same as that of fully resoled numerical simulations of thermonuclear flames. The flame model must also be sufficiently smooth (quiet) and stable. Finally, since the width of th actual nuclear flame is infinitesimal compared to the size of the finest grids that can be used in Type Ia supernova simulations, th flame model should show little "curvature effects," i.e., the flame speed should be the same, whether the curvature of the flame surface is positive or negative. Extensive simulations carried out by the team showed that a sharpened KPP (SKKP) model, in which the leading and trailing edges of the reaction progress variable are truncated at very small values of the reaction progress variable, gives a flame model that is much quieter, more stable, and exhibits much smaller curvature effects that the top-hat model used by earlier workers, including the Flash Center.

4.3 Nuclear Flame Model

A large team led by Alan Calder and Dean Townsley have developed and calibrated a realistic model flame for hydrodynamical simulations of deflagrations in white dwarf (Type Ia) supernovae [16]. The flame model builds on the advection-diffusion-reaction (ADR) model of Khokhlov and includes electron screening and Coulomb corrections to the equation of state in a self-consistent way. We calibrate this model flame—its energetics and timescales for energy release and neutronization—with self-heating reaction network calculations that include both these Coulomb effects and up-to-date weak interactions. The burned material evolves post-flame due to both weak interactions and hydrodynamic changes in density and temperature. The team developed a scheme to follow the evolution, including neutronization, of the NSE state subsequent to the passage of the flame front. As a result, the flame model is suitable for deflagration simulations over a wide range of initial central densities and can track the temperature and electron fraction of the burned material through the explosion and into the expansion of the ejecta.

4.4 Improved Nuclear Flame Model

A large team led by Dean Townsley and Alan Calder have developed an improved method for tracking the nuclear flame during the deflagration phase of Type Ia supernovae [17]. A simplified 3-stage burning model and a non-static ash state are integrated with an artificially thickened advection-diffusion-reaction (ADR) flame front in order to provide an accurate and highly efficient representation of of the energy release and electron capture in and after the unresolved flame. They demonstrate that both the ADR and energy release methods used do not generate significant acoustic noise, as has been a problem with previous ADR-based schemes.

4.5 2-D Simulations of the Deflagration Phase of Type Ia Supernovae

A large team led by Dean Townsley and Alan Calder have used the improved method for tracking the nuclear flame to study the variation in outcomes expected in the gravitationally confined detonation (GCD) model [17]. They showed that if a detonation occurs in material swept up by the material ejected by the first rising bubble but gravitationally confined to the white dwarf (WD) surface (i.e., the GCD paradigm), the density structure of the WD at detonation is systematically correlated with th distance of the deflagration ignition point fro the center of the star. Coupled to a suitably stochastic ignition process, this correlation may provide a plausible explanation for the variety of nickel masses seen in Type Ia supernovae. This work also paves the way to doing 3-D simulations of the gravitationally confined detonation model of Type Ia supernovae, and provides pathfinder simulations for assessing the computational requirements for the 3-D simulations.

4.6 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. 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 [18]. 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 [19], and constitutes a major roadblock to our understanding of the nova phenomenon. The three commonly recognized mechanisms for such enrichment involve: (1) diffusion; (2) gravity wave driven mixing; and (3) convective overshoot.

In earlier work, researchers at the Flash Center explored the possibility that the required mixing and dredge-up could result from a resonant interaction between large-scale shear flows in the accreted envelope and interfacial gravity waves [20; 21]. From a suite of 2-dimensional simulations, we obtained a measure of the rate of mixing and the maximum mixed mass as a function of the wind velocity. The levels of envelope enrichment achieved via this mechanism were found to be quite compatible with those levels determined observationally to characterize the ejecta of classical novae.

In ongoing studies, researchers are considering an alternative mechanism for such mixing - driven by convective undershooting which might be expected to accompany the final stages of nova thermonuclear runaways as discussed below.

Ami Glasner and Eli Livne (Hebrew University of Jerusalem) and Jim Truran have explored the sensitivity of multidimensional nova calculations to the outer boundary condition [22]. 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 [23]. For this 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. All previous multidimensional simulations of nova thermonuclear runaways (TNR) were able to simulate only stages for which the relevant time-scales are very short (10 to 200 seconds), such that only the last stages of the ignition phase and the runaway to peak temperature/luminosity (from a temperature 100 K to peak) could be investigated. Building on improvements in the hydro solver and better computational resources, they are now able to resolve scales that are already unstable to the shear Kelvin-Helmholtz (KH) instability, thus improving the credibility of the results concerning undershoot mixing. The time scales considered range from a phase close to the onset of convection, when the temperature at the base of the envelope is about 5 x 10^7 K, to the runaway itself. The characteristics of the final evolution were substantially the same for simulations starting at 5, 7, and 9 x 10^7 K. It is this universal behavior of all of our models that is the most significant finding of our study. The numerical results obtained support the conclusion that the overall level pf mixing resulting from convective undershooting is at a level $\sim$ 30-40 %, again consistent with observations of the abundance patterns in classical nova ejecta. At early stages we can also examine the fate of local perturbations related to the convective flow. A major issue for research is the ability of such early perturbations to ignite a flame that engulfs the whole envelope as an advancing burning front. Our limited experience with artificial parametric perturbations, presented in this paper, denies this possibility. A major part of the research is devoted to close examinations of numerical effects that can compete with physical mechanisms. We try to estimate the uncertainty limits on the results, mainly on mixing, due to numerical issues.

4.7 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 $\sim$ 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 the diffusion equations. This early 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}).

F. Peng, E. Brown (MSU), and J. Truran have now completed their studies of how this sedimentation of heavy ions in an accreting neutron star's envelope affects the outcome of unstable hydrogen and helium ignition. The strong surface gravity can partially stratify the accreted neutron star envelope, leading to a reduction of hydrogen at the depth at which unstable ignition occurs. Intriguingly, Peng *et al.* [24] find a range of accretion rates for which the hydrogen burning is unstable but not sufficient for initiating helium burning. As a result, the neutron star will accumulate a deep layer of helium that will eventually ignite, producing an energetic X-ray burst. The range of accretion rates for which this happens matches that of several observed X-ray burst sources. An additional surprise is that the sedimentation affects the abundances at ignition even at accretion rates above 0.1 Eddington. An interesting question is whether the stratification of the atmosphere can be imprinted on the rp-process ashes, since the nuclei synthesized in the rp-process burning are in part determined by the ratio of hydrogen to helium at ignition. For example, in the absence of convective mixing sedimentation will boost the production of ^{12}C by a factor $\approx$ 5; this might alleviate the discrepancy between the amount of ^{12}C nuclei needed for subsequent ”superbursts” and current rp-process models

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.

4.8 Students

The following 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), I. Seitenzahl (supervisor J. Truran), A. Zhiglo (supervisor A. Khokhlov), and J. Zuhone (supervisor D. Lamb). Graduate student F. Peng (supervisor J. Truran) has moved on to a postdoctoral position over the past year.

5 Computer Science

Participants: A. Chan, I. Foster, W. Gropp, E. Lusk (Group Leader), R. Ross, 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. MPI program verification, particularly for collective operations
2. Scalable performance visualization
3. Preparation of libraries and tools for next-generation architectures.

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

5.2 Runtime Program Verification for Collective Operations

The FLASH code and the libraries it relies on make extensive use of the MPI collective operations. It is easy to make programming errors in the use of these functions, and such errors can be difficult to find. We developed an MPI profiling library (an MPI-Standard conforming library for intercepting MPI calls) that can be linked into any MPI code, using any MPI implementation, to check at runtime the consistency of the arguments passed to collective MPI operations such as MPI_Broadcast and MPI_Allreduce. The FLASH code, at least as run on a representative problem, was verified to contain no errors involving the consistency of arguments passed to MPI collective operations.

5.3 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.

Our work this year focused on adapting Jumpshot for the display of multithreaded programs likely to be the norm on the large-scale ASC platforms of the near future. Analysis of multithreaded MPI programs linked with the SLOG logging library can provide understanding of the relationship between multithreading and MPI parallelism.

We also continued to provide user support for users of the Jumpshot performance tools.

5.4 Preparing for Next-Generation Architectures

Multicore architectures are in the future of all high-performance computing, particularly at ASC sites. Although FLASH itself is not currently multithreaded, we are laying the groundwork for future FLASH and FLASH follow=on development by creating lock_free mechanisms for SLOG logging of multithreaded code and Jumpshot display of performance data for multithreaded applications. The current release of our MPE tools library contains multithreaded version of both SLOG logging and Jumpshot display.

We have begun development of ADLB, a multithreaded, asynchronous load-balancing library, as a general tool for writing multithreaded code on very large-scale machines.

5.5 ASC Lab Interactions

We continue to work with the vendors of ASC machines, particularly IBM, on MPI library implementation. IBM's MPI for BG/L (and the coming BG/P) is based on MPICH2, and we interact on a monthly and sometimes weekly basis over the MPI implementation code.

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

6 Visualization

Participants: J. B. Gallagher, C. Glendedin (returned to student status September 2006), 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. A significant portion of this years effort has been focused on production visualization with only a minor effort directed toward research. This year's work focused on three production support for three specific tools:

1. FlashView
2. ParaView
3. VisIt

In the following, we describe our activities using these various tools in more detail. In addition to the tools described below, the effort of one full-time visualization team member has been focused on the analysis of the turbulence dataset. This effort includes a full reconstruction of the particle data to correct for error in the identification handling, reprocessing of turbulence data into a more usable format for the Center and community, and the development of access routines for the data. This work was augmented with the production of numerous images and movies from the dataset. Addition time has been spent on the production of volume rendering images and movies of the latest Supernovae results.

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. Though over the past year bug fixes have been made and support effort has been allocated to help with current users.

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 two years 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.

6.4 VisIt

VisIt is an open source visualization package developed at Lawrence Livermore National Laboratory (LLNL) and is built using the Visualization Toolkit (VTK) and has a slightly different user model than ParaView. Over the last year, use of this tool has been gaining in interest with the Flash scientists. This year we have worked with the LLNL team to add features that the Flash group has deemed needed. These include enhancing the ability to load Flash datasets in their native format and supporting the display of the Morton Curve ordering. Support effort has been applied in working with the Flash scientist's to enable them to use the tool. These include the following list:

1. how to visualize results spherical coordinates,
2. demonstrating the use of normalized settings in 2D graphs,
3. demonstration of proper times and cycles in time series visualizations,
4. locking 2D and 3D views, and
5. displaying block ID for parts of plots.

Additional work as been done to enable users via shell script to automatically generate images using VisIt for running simulation. This allows them to check for problems and progress automatically.

7 Basic Science

Participants: S. Abarzhi, P. Constantin, S. Dorfman T. Dupont (Group Leader), L. Kadanoff, I. Mogultay, L. Ryzhik, N. Vladimirova.

The work of the basic science group has mostly been focused on the study of fluid flow. The importance of instabilities, mixing, and reactions to the Flash project has had a strong influence on the questions addressed. There are several modes of inquiry that we have used. One is a mathematical approach in which the objective is to prove certain properties of the flows. Another involves the interaction of theory (in the sense of physics rather than mathematics) and computation to increase our understanding of the flows we are considering. Yet another consists of building simplified models which capture some of the basic flow properties in a semi-quantitative way. There has been some numerical analytic work and some Flash-motivated teaching as well.

There was basic scientific work on turbulence done in the Flash center. Some of that work is mentioned below, but the work associated with the very large simulation of driven turbulence was done primarily by the members of the astrophysics group and will not be described in this section.

7.1 Reactive Flows

Peter Constantin, Lenya Ryzhik and their collaborators have established in [25] and [26] the existence and stability of non-planar fronts in Boussinesq reactive flows in a variety of geometries and with different kinds of boundary conditions.

The efficiency of mixing of reactive flows and connection to dynamical and spectral properties of the underlying operators is studied in [27].

In [28] the so-called explosion problem was studied in the context of a prescribed flow. The explosion problem concerns the competition between diffusive cooling and blow-up by a strong nonlinearity. It has been known for a long time that when the strength k of nonlinearity is small cooling effects dominate while for $k > k_c$ explosion occurs and solutions cease to exist. In [28] it is shown that additional mixing by a prescribed flow may increase the explosion threshold dramatically and identified the flows such that k_c tends to infinity as the flow amplitude increases. In [29] this study is extended to the reactive Boussinesq system in a bounded domain with a cold boundary. In this problem the flow is result of the reaction and the strength of the influence of the reaction on the flow can be measured by the Rayleigh number, a nondimensional measure of gravity. It turns out that when the Rayleigh number tends to infinity boundary cooling will dominate arbitrarily strong nonlinearity. In terms of an evolution problem this means that when gravity is sufficiently strong solutions will exist globally in time and explosion does not occur. On the other hand, when reaction is of the ignition type it is shown that the flow generated by gravity force will quench the flame if gravity is sufficiently strong. This means that the flame is self-extinguishing for large gravity. The flows generated in such problems are shown to possess other good mixing properties.

In [30] Ryzhik and Zlatos studied the speed-up of reaction-diffusion fronts by flows and identify a sharp condition when a given flow speeds-up the KPP fronts.

The paper [31] introduces compressible effects. In a simple one-dimensional flow the flow-temperature coupling speeds up the propagation for coupling that is not too large. However, there exists a coupling threshold beyond which reaction is killed by the shock and propagation is arrested. The next step is to understand whether these results apply to more realistic models. In this work Vladimirova provided important computational support.

In [32] Perthane and Ryzhik asked how strong dispersion can be relative to dissipation so that solution of a viscous-dispersive conservation law would be close to the entropy solution of the conservation law. It turns out that, at least for traveling front solutions, convergence to entropy solutions holds in a much larger range of dispersion that previously believed.

Constantin and collaborators studied turbulent dissipation of energy and enstrophy in [33] and [34].

One of the interesting effects of the work in the Flash Center on reactive flows is that it attracted H. Berestycki to collaborate with researchers at the University of Chicago. Berestycki, a very distinguished French mathematician, is not a member of the Flash Center, but is a visitor to the math department for a quarter every year. As can be seen from the references here, he contributes to our science. He also contributes to the education of mathematics students in areas related to our work.

Vladamirova has worked on several questions of interest to the Flash center. Some of her work relates the semianalytic model of rising bubble discussed in another section of this report. Her contributions there were based in significant part on a paper that has just appeared electronically [35].

Recently Vladamirova has been collaborating with Chertkov in studying Rayleigh-Taylor instabilities in Boussinesq flows. This work is described in [36] . They are now working on extensions of this work to the case of reactive flows. In particular they study a Rayleigh-Taylor instability between two miscible fluids in the presence of a reaction which transforms heavier fluid into lighter fluid. A novelty here is that the nonreacting RT problem is used as the base case, and the effects of weak/moderate/strong reaction are being quantified using traditional turbulence diagnostics.

Dupont and Mogultay have produced simplified models of thermally driven flows using dimension reduction methods [37]. They are now in the process of trying to extend this work to reactive flows.

7.2 Turbulence and Turbulent Mixing

Abarzhi has been studying turbulence and turbulent mixing in unsteady flows from a theoretical point of view. Her work in this area is based on trying to exploit the invariance of the rate of momentum loss. This approach leads to predictions that differ from traditional approaches. She has suggested some experimental indicators that can help us understand the value of this approach.

She is also studying the effect of noise on chaotic systems. The influence of noise may well be important in understanding the predictive capability of computational and theoretical models of turbulence.

7.3 Convergence of Advection Schemes

Dupont worked with a student S. Dorfman on error estimates for new schemes for advection. Some superconvergence results for so-called back and forth methods were found in simple situations.

7.4 Education and Training

Each year Dupont teaches either a graduate course on the numerical solution of partial differential equations or on numerical hydrodynamics. One of the projects used to teach numerical hydrodynamics is based on slightly compressible flow of two component gases. The code from this project was used in one of our previous validation studies of the shock cylinder experiments run at LANL. The current course involves extending that code to cases in which bubbles are present. This will be used to compute some initial conditions for the simulation of experiments run by our collaborators.

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