FLASH User's Guide

Version 1.0

October 1999

ASCI Flash Center
University of Chicago

Contents

Acknowledgments

The FLASH Code Group is supported by the ASCI Flash Center at the University of Chicago under U. S. Department of Energy contract B341495. Some of the test calculations described here were performed using the Origin 2000 computer at Argonne National Laboratory and the ASCI Blue Mountain computer at Los Alamos National Laboratory.

1 Introduction

The Center for Astrophysical Thermonuclear Flashes, or Flash Center, was founded at the University of Chicago in 1997 under contract to the United States Department of Energy as part of its Accelerated Strategic Computing Initiative (ASCI). The goal of the Center is to solve several problems related to thermonuclear flashes on the surfaces of compact stars (neutron stars and white dwarfs), in particular X-ray bursts, Type Ia supernovae, and novae. To solve these problems requires the participants in the Center to develop new simulation tools capable of handling the extreme resolution and physical requirements imposed by conditions in these explosions, and to do so while making efficient use of the parallel supercomputers developed by the ASCI project, the most powerful constructed to date.

The FLASH code represents an important step along the road to this goal. FLASH is a modular, adaptive, parallel simulation code capable of handling general compressible flow problems in astrophysical environments. FLASH has been designed to allow users to configure initial and boundary conditions, change algorithms, and add new physical effects with minimal effort. It uses the PARAMESH library to manage a block-structured adaptive grid, placing resolution elements only where they are needed most. FLASH uses the Message-Passing Interface (MPI) library to achieve portability and scalability on a variety of different message-passing parallel computers.

This user's guide is designed to enable individuals unfamiliar with the FLASH code to quickly get acquainted with its structure and to move beyond the simple test problems distributed with FLASH, customizing it to suit their own needs. The second section briefly describes the equations and algorithms used by the physics modules distributed with FLASH. It assumes that the reader has some familiarity both with the basic physics involved and with numerical hydrodynamics methods. This familiarity is absolutely essential in using FLASH (or any other simulation code) to arrive at meaningful solutions to physical problems. The novice reader is directed to an introductory text such as Patrick Roache's *Fundamentals of Computational Fluid Dynamics* (Hermosa, 1998) or C. A. J. Fletcher's *Computational Techniques for Fluid Dynamics* (Springer-Verlag, 1991). The advanced reader who wishes to know more specific information about the various algorithms is directed to the literature references in this section.

The third section discusses how to quickly get started with FLASH, describing how to configure, build, and run the code with one of the included test problems, then examine the resulting output. Users familiar with the capabilities of FLASH who wish to quickly 'get their feet wet' with the code can skip directly to this section. The fourth section describes in more detail the use of the configuration and analysis tools distributed with FLASH. The fifth section describes the different test problems distributed with FLASH. The sixth section describes the FLASH code structure at length and gives detailed instructions for extending FLASH's capabilities by adding new problem setups. This section also discusses the code modules included with FLASH 1.0 and describes how new solvers may be integrated into the code. Finally, the seventh section gives guidance on contacting the authors of FLASH.

2 Algorithmic overview

FLASH provides a general simulation framework capable of incorporating several different types of physics module (e.g., hydrodynamics on structured or unstructured meshes, N-body solvers, reactive source terms, etc.) and initial or boundary conditions. However, it has been built to solve a particular class of problems, namely reactive, compressible flows in astrophysical environments. Thus, FLASH 1.0 is distributed with a particular set of algorithms to handle compressible hydrodynamics on a block-structured adaptive mesh, together with an appropriate nuclear equation of state and nuclear reaction network. We treat each of these elements in turn.

2.1 Hydrodynamics

The hydrodynamic module in FLASH 1.0 is based on the PROMETHEUS code (Fryxell, Müller, and Arnett 1989). This code solves Euler's equations for compressible gas dynamics in one, two, or three spatial dimensions. These equations can be written in conservative form as

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{v} = 0 \tag{1}$$

$$\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot \rho \mathbf{v}\mathbf{v} + \nabla P = \rho \mathbf{g} \tag{2}$$

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho E + P)\,\mathbf{v} = \rho \mathbf{v} \cdot \mathbf{g} \tag{3}$$

where ρ is the fluid density, $\mathbf{v}$ is the fluid velocity, P is the pressure, E is the sum of the internal energy ϵ and kinetic energy per unit mass,

$$E = \epsilon + \frac{1}{2}v^2, \tag{4}$$

$\mathbf{g}$ is the acceleration due to gravity, and t is the time coordinate. The pressure is obtained from the energy and density using the equation of state. For the case of an ideal gas equation of state, the pressure is given by

$$P = (\gamma - 1)\rho\epsilon, \tag{5}$$

where γ is the ratio of specific heats. More general equations of state are discussed below.

For reactive flows, a separate advection equation must be solved for each chemical or nuclear species:

$$\frac{\partial \rho X_\ell}{\partial t} + \nabla \cdot \rho X_\ell \mathbf{v} = 0 \ , \tag{6}$$

where X_ℓ is the mass fraction of the ℓth species, with the constraint that $\sum_\ell X_\ell = 1$. The quantity ρX_ℓ represents the partial density of the ℓth fluid. The code does not explicitly track interfaces between the fluids, so a small amount of numerical mixing can be expected during the course of a calculation.

The equations are solved using a modified version of the Piecewise-Parabolic Method (PPM), which is described in detail in Woodward and Colella (1984) and Colella and Woodward (1984). PPM is a higher-order version of the method developed by Godunov (1959).

Godunov's method uses a finite-volume spatial discretization of the Euler equations together with an explicit forward time difference. Time-advanced fluxes at cell boundaries are computed using the analytic solution to Riemann's shock tube problem at each boundary. Initial conditions for each Riemann problem are determined by assuming the nonadvanced solution to be piecewise constant in each cell. Using the Riemann solution has the effect of introducing explicit nonlinearity into the difference equations and permits the calculation of sharp shock fronts and contact discontinuities without introducing significant nonphysical oscillations into the flow. Since the value of each variable in each cell is assumed to be constant, Godunov's method is limited to first-order accuracy in both space and time.

PPM improves on Godunov's method by representing the flow variables with piecewise parabolic functions. It also uses a monotonicity constraint rather than artificial viscosity to control oscillations near discontinuities, a feature shared with the MUSCL scheme of van Leer (1979). Although this could lead to a method which is accurate to third order, PPM is formally accurate only to second order in both space and time, as a fully third-order scheme proved not to be cost-effective. Nevertheless, PPM is considerably more accurate and efficient than most formally second-order algorithms.

PPM is particularly well-suited to flows involving discontinuities, such as shocks and contact discontinuities. The method also performs extremely well for smooth flows, although other schemes which do not perform the extra work necessary for the treatment of discontinuities might be more efficient in these cases. The high resolution and accuracy of PPM are obtained by the explicit nonlinearity of the scheme and through the use of intelligent dissipation algorithms, such as monotonicity enforcement, contact steepening, and interpolant flattening. These algorithms are described in detail by Colella and Woodward (1984).

A complete description of PPM is beyond the scope of this user's guide. However, for comparison with other codes, we note that the implementation of PPM in FLASH 1.0 uses the direct Eulerian formulation of PPM and the technique for allowing nonideal equations of state described by Colella and Glaz (1985). For multidimensional problems, FLASH 1.0 uses second-order operator splitting (Strang 1968). FLASH also implements PPM on a block-structured adaptive mesh, which is described in the following section.

2.2 Adaptive mesh refinement

We have used a package known as PARAMESH (MacNeice et al. 1999) for the parallelization and adaptive mesh refinement (AMR) portion of FLASH. PARAMESH consists of a suite of subroutines which handle refinement/derefinement, distribution of work to processors, guard cell filling, and flux conservation. In this section we briefly describe this package and the ways in which it has been modified for use with FLASH.

PARAMESH uses a block-structured adaptive mesh refinement scheme similar to others in the literature (e.g., Parashar 1999; Berger & Oliger 1984; Berger & Colella 1989; DeZeeuw & Powell 1993) as well as to schemes which refine on an individual cell basis (Khokhlov 1997). In block-structured AMR, the fundamental data structure is a block of uniform cells arranged in a logically Cartesian fashion. Each cell can be specified using a block identifier (processor number and local block number) and a coordinate triple (i, j, k), where $i = 1 \ldots \texttt{nxb}$, $j = 1 \ldots \texttt{nyb}$, and $k = 1 \ldots \texttt{nzb}$. The complete computational grid consists of a collection of blocks with different physical cell sizes, related to each other in a hierarchical fashion using a tree data structure. The blocks at the root of the tree have the largest cells, while their children have smaller cells and are said to be refined. Two rules govern the establishment of refined child blocks in PARAMESH. First, the cells of a refined child block must be one-half as large as those of its parent block. Second, a block's children must be nested; that is, the child blocks must fit within their parent block and cannot overlap one another, and the complete set of children of a block must fill its volume. Thus, in d dimensions a given block can have at most 2^d children.

Each block contains `nxb` $\times$ `nyb` $\times$ `nzb` interior cells and a set of guard cells. The guard cells contain boundary information needed to update the interior cells. These can be obtained from physically neighboring blocks, externally specified boundary conditions, or both. The number of guard cells needed depends upon the interpolation scheme and differencing stencil used for the hydrodynamics algorithm; for the explicit PPM algorithm distributed with FLASH, four guard cells are needed in each direction. PARAMESH handles the filling of guard cells with information from other blocks or a user-specified external boundary routine. If a block's neighbor has the same level of refinement, PARAMESH fills its guard cells using a direct copy from the neighbor's interior cells. If the neighbor has a different level of refinement, the neighbor's interior cells are used to interpolate guard cell values for the block. If the block and its neighbor are stored in the memory of different processors, PARAMESH handles the appropriate parallel communication (blocks are not split between processors). PARAMESH supports only linear interpolation for guard cell filling at jumps at refinement, but it is easily extended to allow other interpolation schemes; for example, for FLASH we have added a quadratic interpolation scheme. Once each block's guard cells are filled, it can be updated independently of the other blocks.

PARAMESH also enforces flux conservation at jumps in refinement, as described by Berger and Colella (1989). At jumps in refinement, the fluxes of mass, momentum, energy, and nuclear abundances across boundary cell faces are averaged across the fine cells at that face and provided to the corresponding coarse face on the neighboring block. These averaged fluxes are then used to update the values of the coarse block's local flow variables.

Each processor decides when to refine or derefine its blocks by computing a user-defined error estimator for each block. Refinement involves creation of between one and 2^d refined child blocks, while derefinement involves deletion of a block. As child blocks are created, they are temporarily placed at the end of the processor's block list. After the refinements and derefinements are complete, the blocks are redistributed among the processors using a work-weighted Morton space-filling curve in a manner similar to that described by Warren and Salmon (1987) for a parallel treecode. During the distribution step each block is assigned a work value (an estimate of the relative amount of time required to update the block). The Morton number of the block is then computed by interleaving the bits of its integer coordinates as described by Warren and Salmon (1987); this determines its location along the space-filling curve. The Morton numbers of all of the blocks in the problem are then sorted using a parallel bitonic sort. Finally, the list of all blocks is partitioned among the processors using the block weights, equalizing the estimated workload of each processor. During the sorting step, only Morton numbers and not block data are communicated between processors; blocks are only moved (if necessary) after the sort. Changes in refinement are typically performed every ten timesteps.

The refinement criterion used by PARAMESH is adapted from Löhner (1987). Löhner's error estimator was originally developed for finite element applications and has the advantage that it uses an entirely local calculation. Furthermore, the estimator is dimensionless and can be applied with complete generality to any of the field variables of the simulation or any combination of them (by default, PARAMESH uses the density and pressure). Löhner's estimator is a modified second derivative, normalized by the average of the gradient over one computational cell. In one dimension on a uniform mesh it is given by

$$E_i = \frac{\mid u_{i+1} - 2u_i + u_{i-1} \mid}{\mid u_{i+1} - u_i \mid + \mid u_i - u_{i-1} \mid + \epsilon[\mid u_{i+1} \mid -2 \mid u_i \mid + \mid u_{i-1} \mid]} , \tag{7}$$

where u_i is the refinement test variable's value in the ith cell. The last term in the denominator of this expression acts as a filter, preventing refinement of small ripples. The constant ϵ is given a value of 10^{-4}. Although PPM is formally second-order and its leading error terms scale as the third derivative, we have found the second derivative criterion to be very good at detecting discontinuities in the flow variable u. When extending this criterion to multidimensions, all cross derivatives are computed, and the following generalization of the above expresion is used:

$$E_i = \left[\sum_{k,l} \frac{\left(\frac{\partial^2 u}{\partial x_k \partial x_l} \right)}{\left[(\mid \frac{\partial u}{\partial x_k} \mid_{i+1} + \mid \frac{\partial u}{\partial x_k} \mid_i) / \Delta x_l + \epsilon \mid \frac{\partial^2 u}{\partial x_k \partial x_l} \mid \right]^2} \right]^{1/2} , \tag{8}$$

where the sums are carried out over the coordinate directions. If the maximum value of E_i in a block is larger than an adjustable constant, CTORE, the block is marked for refinement. If the maximum value of E_i is less than a second constant (CTODE), the block is marked for derefinement. PARAMESH uses the default values CTORE $= 0.8$ and CTODE $= 0.2$. For each block, the error estimator is calculated for all interior cells plus two layers of guard cells, helping to ensure that blocks refine in advance of discontinuities.

2.3 Equation of state

It is common to call an equation of state routine more than 10^9 times when calculating two- and three-dimensional hydrodynamic models of stellar phenomena. Thus, it is very desirable to have an equation of state that is as efficient as possible, yet accurately represents the relevant physics. While FLASH is easily capable of including any equation of state, here we discuss three equation of state (henceforth EOS) routines which are supplied with FLASH 1.0: the ideal-gas or gamma-law EOS, the Nadyozhin EOS, and the Helmholtz EOS.

Each EOS routine takes as input the temperature T, density ρ, mean number of nucleons per isotope $\bar{A}$, and mean charge per isotope $\bar{Z}$. Each routine then returns as output the scalar pressure (P_{tot}, specific thermal energy ϵ_{tot}, and entropy S_{tot}. In addition to these quantities, the EOS routines return partial derivatives of the pressure, specific thermal energy, and entropy with respect to the density and temperature:

$$\left.\frac{\partial P_{tot}}{\partial T}\right|_\rho , \quad \left.\frac{\partial P_{tot}}{\partial \rho}\right|_T , \quad \left.\frac{\partial \epsilon_{tot}}{\partial T}\right|_\rho , \quad \left.\frac{\partial \epsilon_{tot}}{\partial \rho}\right|_T , \quad \left.\frac{\partial S_{tot}}{\partial T}\right|_\rho , \quad \left.\frac{\partial S_{tot}}{\partial \rho}\right|_T . \tag{9}$$

Quantities such as the specific heats and the adiabatic indices can be determined once these partial derivatives are known. When solving the energy equation, the temperature usually is obtained by iteration, and the thermodynamic derivatives must be available in order to implement efficient iteration schemes. Confirming that an EOS routine numerically satisfies thermodynamic consistency also demands that the derivatives be available.

An EOS is thermodynamically consistent if its outputs satisfy the Maxwell relations:

$$P = \rho^2 \frac{\partial \epsilon}{\partial \rho}\bigg|_T + T \frac{\partial P}{\partial T}\bigg|_\rho \tag{10}$$

$$\frac{\partial \epsilon}{\partial T}\bigg|_\rho = T \frac{\partial S}{\partial T}\bigg|_\rho \tag{11}$$

$$-\frac{\partial S}{\partial \rho}\bigg|_T = \frac{1}{\rho^2} \frac{\partial P}{\partial T}\bigg|_\rho \ . \tag{12}$$

Thermodynamic inconsistency can manifest itself in the unphysical buildup (or decay) of the entropy (or temperature) during numerical simulations of what should be an adiabatic flow. Entropy-sensitive models (e.g., core-collapse supernovae) may suffer inaccuracies if thermodynamic consistency is significantly violated over sufficiently long time scales. The equations of state supplied with FLASH satisfy the Maxwell relations to a good degree of precision (in some cases to the limits of 64-bit arithmetic).

The gamma-law EOS provided with FLASH represents a simple ideal gas with constant adiabatic index γ:

$$P = \frac{N_a\, k}{\bar{A}} \rho T \qquad \epsilon = \frac{1}{\gamma - 1}\, \frac{P}{\rho} \qquad S = \frac{P/\rho + \epsilon}{T} \ , \tag{13}$$

where N_a is the Avogadro number, and k is the Boltzmann constant. Because it requires no iteration in order to obtain the temperature, this EOS is quite inexpensive to evaluate.

More complex equations of state are necessary for realistic models of X-ray bursts, Type Ia supernovae, classical novae, and other stellar phenomena, where the electrons and positrons may be relativistic and/or degenerate and where radiation contributes significantly to the thermodynamic state. The Nadyozhin and Helmholtz EOS routines address this need. The Nadyozhin EOS, summarized by Nadyozhin (1974) and explained in detail by Blinnikov et al. (1996), was found by Timmes and Arnett (1999) in a comparison of five different analytic EOS schemes to give the best tradeoff among accuracy, thermodynamic consistency, and speed. The Helmholtz EOS (Timmes & Swesty 1999) uses interpolation from a two-dimensional table of the Helmholtz free energy $F(\rho, T)$, obtaining comparable accuracy, better thermodynamic consistency, and about twice the speed of the Nadyozhin EOS.

For stellar phenomena, the pressure, specific thermal energy, and entropy contain contributions from several components:

$$P_{\rm tot} = P_{\rm rad} + P_{\rm ion} + P_{\rm ele} + P_{\rm pos} \tag{14}$$

$$\epsilon_{\rm tot} = \epsilon_{\rm rad} + \epsilon_{\rm ion} + \epsilon_{\rm ele} + \epsilon_{\rm pos} \tag{15}$$

$$S_{\rm tot} = S_{\rm rad} + S_{\rm ion} + S_{\rm ele} + S_{\rm pos} \ . \tag{16}$$

Here the subscripts "rad," "ion," "ele," and "pos" represent radiation, nuclei, electrons, and positrons, respectively. The radiation portion is that of a blackbody in local thermodynamic equilibrium:

$$P_{\rm rad} = \frac{aT^4}{3} \qquad \epsilon_{\rm rad} = \frac{3P_{\rm rad}}{\rho} \qquad S_{\rm rad} = \frac{(P/\rho + \epsilon)}{T} \tag{17}$$

where a is the Stefan-Boltzmann energy constant, and c is the speed of light. The ion contribution is that of an ideal gas with $\gamma = 5/3$. The electrons and positrons are treated as a non-interacting Fermi gas; the number densities of free electrons $N_{\rm ele}$ and positrons $N_{\rm pos}$ are given by

$$N_{\rm ele} = \frac{8\pi\sqrt{2}}{h^3}\, m_e^3\, c^3\, \beta^{3/2} \left[F_{1/2}(\eta,\beta) + F_{3/2}(\eta,\beta)\right] \tag{18}$$

$$N_{\rm pos} = \frac{8\pi\sqrt{2}}{h^3}\, {\rm m_e}^3\, c^3\, \beta^{3/2} \left[F_{1/2}\left(-\eta - 2/\beta, \beta\right) + \beta\, F_{3/2}\left(-\eta - 2/\beta, \beta\right)\right] , \tag{19}$$

where h is the Planck constant, m_e is the electron rest mass, $\beta = kT/(m_e c^2)$ is the relativity parameter, $\eta = \mu/kT$ is the normalized chemical potential energy μ for electrons, and $F_k(\eta,\beta)$ is the Fermi-Dirac integral

$$F_k(\eta,\beta) = \int_0^\infty \frac{x^k\,(1 + 0.5\,\beta\,x)^{1/2}\,dx}{\exp(x-\eta)+1} \ . \tag{20}$$

Because the electron rest mass is not included in the chemical potential, the positron chemical potential must have the form $\eta_{\rm pos} = -\eta - 2/\beta$. For complete ionization, the number density of free electrons in the matter is

$$N_{\rm ele,matter} = \frac{\bar{Z}}{\bar{A}}\, N_a\, \rho = \bar{Z}\, N_{\rm ion} \ , \tag{21}$$

and charge neutrality requires

$$N_{\rm ele,matter} = N_{\rm ele} - N_{\rm pos} \ . \tag{22}$$

Solving this equation with a standard one-dimensional root-finding algorithm determines η. Once η is known, the Fermi-Dirac integrals can be evaluated, giving the pressure, specific thermal energy, and entropy due to the free electrons and positrons.

The Nadyozhin EOS routine uses polynomial or rational functions to evaluate the thermodynamic quantities. The temperature-density plane is decomposed into 5 regions (see Figure 12 of Blinnikov et al. 1996), with different expansions or fitting functions applied to each region. The methods used in the 5 regions are (1) a perfect gas approximation with the first-order corrections for degeneracy, (2) expansions of the half-integer Fermi-Dirac functions, (3) Chandrasekhar's (1939) expansion for a degenerate gas, (4) relativistic asymptotics, and (5) Gaussian quadrature for the thermodynamic quantities. The perturbation expansions, asymptotic relations, and fitting functions for the 5 regions are combined, with extraordinary care given to making sure that transitions between the regions are continuous, smooth, and thermodynamically consistent. All of the partial derivatives are obtained analytically.

The electron-positron Helmholtz free energy table used by the Helmholtz EOS was generated by using the Timmes EOS routine (Timmes & Arnett 1999). The Fermi-Dirac integrals, along with their derivatives with respect to η and β, were calculated to at least 18 significant figures using the quadrature schemes of Aparicio (1998). Newton-Raphson iteration was used to solve for η to at least 15 significant figures. The thermodynamic derivatives were computed analytically. Searches through the free energy table are avoided by computing hash indices from the values of any given $(T, \rho\bar{Z}/\bar{A})$ pair. No computationally expensive divisions are required in interpolating from the table; all of them can be computed and stored the first time the EOS routine is called.

2.4 Thermonuclear reactions

Modelling thermonuclear flashes typically requires the energy generation rate due to nuclear burning over a large range of temperatures, densities and compositions. The average energy generated or lost over a period of time is found by integrating a system of ordinary differential equations (the nuclear reaction network) for the abundances of important nuclei and the total energy release. In some contexts, such as Type II supernova models, the abundances themselves are also of interest. In either case, the coefficients that appear in the equations typically are extremely sensitive to temperature. The resulting stiffness of the system of equations requires the use of an implicit time integration scheme.

Timmes (1999) has reviewed several methods for solving stiff nuclear reaction networks, providing the basis for the reaction network solver included with FLASH. The scaling properties and behavior of three semi-implicit time integration algorithms (a traditional first-order accurate Euler method, a fourth-order accurate Kaps-Rentrop method, and a variable order Bader-Deuflhard method) and eight linear algebra packages (LAPACK, LUDCMP, LEQS, GIFT, MA28, UMFPACK, and Y12M) were investigated by running each of these 24 combinations on seven different nuclear reaction networks (hard-wired 13- and 19-isotope networks and table-lookup networks using 47, 76, 127, 200, and 489 isotopes). Timmes' analysis suggested that the best balance of accuracy, overall efficiency, memory footprint, and ease-of-use was provided by the choice of a 13- or 19-isotope reaction network, the variable order Bader-Deuflhard time integration method, and the MA28 sparse matrix package. The default FLASH distribution uses this combination of methods, which we describe in this section.

We begin by describing the equations solved by the nuclear burning module. We consider material which may be described by a density ρ and a single temperature T and contains a number of isotopes i, each of which has Z_i protons and A_i nucleons (protons + neutrons). Let n_i and ρ_i denote the number and mass density, respectively, of the ith isotope, and let X_i denote its mass fraction, so that

$$X_i = \rho_i/\rho = n_i A_i/(\rho N_A) \ , \tag{23}$$

where N_A is the Avogadro number. Let the molar abundance of the ith isotope be

$$Y_i = X_i/A_i = n_i/(\rho N_A) \ . \tag{24}$$

Mass conservation is then expressed by

$$\sum_{i=1}^{N} X_i = 1 \tag{25}$$

At the end of each timestep, FLASH checks that the stored abundances satisfy equation (25) to machine precision in order to avoid the unphysical buildup (or decay) of the abundances or energy generation rate. Roundoff errors in this equation can lead to significant problems in some contexts (e.g., classical nova envelopes) where trace abundances are important.

The general continuity equation for the ith isotope is given in Lagrangian formulation by

$$\frac{dY_i}{dt} + \nabla \cdot (Y_i \mathbf{V}_i) = \dot{R}_i \ . \tag{26}$$

In this equation $\dot{R}_i$ is the total reaction rate due to all binary reactions of the form *i(j,k)l*,

$$\dot{R}_i = \sum_{j,k} Y_l Y_k \lambda_{kj}(l) - Y_i Y_j \lambda_{jk}(i) \ , \tag{27}$$

where λ_{kj} and λ_{jk} are the reverse (creation) and forward (destruction) nuclear reaction rates, respectively. Contributions from three-body reactions, such as the triple-α reaction, are easy to append to equation (27). The mass diffusion velocities $\mathbf{V}_i$ in equation (26) are obtained from the solution of a multicomponent diffusion equation (Chapman & Cowling 1970; Burgers 1969; Williams 1988) and reflect the fact that mass diffusion processes arise from pressure, temperature, and/or abundance gradients as well as external gravitational or electrical forces.

The case $\mathbf{V}_i \equiv 0$ is important for two reasons. First, mass diffusion is often unimportant when compared to other transport process such as thermal or viscous diffusion (i.e., large Lewis numbers and/or small Prandtl numbers). Such a situation obtains, for example, in the study of laminar flame fronts propagating through the quiescent interior of a white dwarf. Second, this case permits the decoupling of the reaction network solver from the hydrodynamical solver through the use of operator splitting, greatly simplifying the algorithm. This is the method used by the default FLASH distribution. Setting $\mathbf{V}_i \equiv 0$ transforms equation (26) into

$$\frac{dY_i}{dt} = \dot{R}_i \ , \tag{28}$$

which may be written in the more compact and standard form

$$\dot{\mathbf{y}} = \mathbf{f}\ (\mathbf{y}) \ . \tag{29}$$

Stated another way, in the absence of mass diffusion or advection, any changes to the fluid composition are due to local processes.

Because of the highly nonlinear temperature dependence of the nuclear reaction rates, and because the abundances themselves often range over several orders of magnitude in value, the values of the coefficients which appear in equations (28) and (29) can vary quite significantly. As a result, the nuclear reaction network equations are "stiff." A system of equations is stiff when the ratio of the maximum to the minimum eigenvalue of the Jacobian matrix $\tilde{\mathbf{J}} \equiv \partial \mathbf{f} / \partial \mathbf{y}$ is large and imaginary. This means that at least one of the isotopic abundances changes on a much shorter timescale than another. Implicit or semi-implicit time integration methods are generally necessary to avoid following this short-timescale behavior, requiring the calculation of the Jacobian matrix.

It is instructive at this point to look at an example of how equation (28) and the associated Jacobian matrix are formed. Consider the ^{12}C(α,γ)^{16}O reaction, which competes with the triple-α reaction during helium burning in stars. The rate R at which this reaction proceeds is critical for evolutionary models of massive stars since it determines how much of the core is carbon and how much of the core is oxygen after the initial helium fuel is exhausted. This reaction sequence contributes to the right-hand side equation (29) through the terms

$$\begin{aligned} \dot{Y}(^4He) &= -Y(^4He)\; Y(^{12}C)\; R + \ldots \\ \dot{Y}(^{12}C) &= -Y(^4He)\; Y(^{12}C)\; R\; + \ldots \quad , \\ \dot{Y}(^{16}O) &= +Y(^4He)\; Y(^{12}C)\; R\; + \ldots \end{aligned} \tag{30}$$

where the ellipsis indicate additional terms coming from other reaction sequences. The minus signs indicate that helium and carbon are being destroyed, while the plus sign indicates that oxygen is being created. Each of these three expressions contributes two terms to the Jacobian matrix $\tilde{\mathbf{J}}$=$\partial \mathbf{f}/\partial \mathbf{y}$:

$$\begin{aligned} J(^4He,^4He) &= -Y(^{12}C)\; R\; + \ldots & \qquad J(^4He,^{12}C) &= -Y(^4He)\; R\; + \ldots \\ J(^{12}C,^4He) &= -Y(^{12}C)\; R\; + \ldots & \qquad J(^{12}C,^{12}C) &= -Y(^4He)\; R\; + \ldots \quad . \\ J(^{16}O,^4He) &= +Y(^{12}C)\; R\; + \ldots & \qquad J(^{16}O,^{12}C) &= +Y(^4He)\; R\; + \ldots \end{aligned} \tag{31}$$

Entries in the Jacobian matrix represent the flow, in number of nuclei s^{-1}, into (positive) or out of (negative) an isotope. All of the temperature and density dependence is included in the reaction rate R. The Jacobian matrices that arise from nuclear reaction networks are neither positive-definite nor symmetric since the forward and reverse reaction rates are generally not equal. However, the magnitudes of the matrix entries change as the abundances, temperature, or density change with time.

The default FLASH distribution includes two reaction networks. The 13-isotope α-chain plus heavy-ion reaction network is suitable for most multi-dimensional simulations of stellar phenomena where having a reasonably accurate energy generation rate is of primary concern. The 19-isotope reaction network has the same α-chain and heavy-ion reactions as the 13-isotope network, but it includes additional isotopes to accommodate some types of hydrogen burning (PP and CNO chains), along with some aspects of photodisintegration into ^{54}Fe. This reaction network is described in Weaver, Zimmerman, & Woosley (1978). Both the networks supplied with FLASH are examples of "hard-wired" reaction networks, where each of the reaction sequences are carefully entered by hand. This approach is suitable for small networks when minimizing the CPU time required to run the reaction network is a primary concern, although it suffers the disadvantage of inflexibility.

The Jacobian matrices of nuclear reaction networks tend to be sparse, and they become more sparse as the number of isotopes increases. Implicit time integration schemes require the inverse of the Jacobian matrix, so we need to use a sparse linear algebra package to compute this inverse. To control the iteration count for a prespecified accuracy, FLASH uses a direct sparse matrix solver. Direct methods typically divide the solution of $\tilde{\mathbf{A}} \cdot \mathbf{x} = \mathbf{b}$ into a symbolic LU decomposition, numerical LU decomposition, and a backsubstitution phase. In the symbolic LU decomposition phase the pivot order of a matrix is determined, and a sequence of decomposition operations which minimize the amount of fill-in is recorded.

Fill-in refers to zero matrix elements which become nonzero (e.g., a sparse matrix times a sparse matrix is generally a denser matrix). The matrix is not (usually) decomposed; only the steps to do so are stored. Since the nonzero pattern of a chosen nuclear reaction network does not change, the symbolic LU decomposition is a one-time initialization cost for reaction networks. In the numerical LU decomposition phase, a matrix with the same pivot order and nonzero pattern as a previously factorized matrix is numerically decomposed into its lower-upper form. This phase must be done only once for each staged set of linear equations. In the backsubstitution phase, a set of linear equations is solved with the factors calculated from a previous numerical decomposition. The backsubstitution phase may be performed with as many right-hand sides as needed, and not all of the right-hand sides need to be known in advance.

The MA28 linear algebra package used by FLASH is described by Duff, Erisman, & Reid (1986). It uses a combination of nested dissection and frontal envelope decomposition to minimize fill-in during the factorization stage. An approximate degree update algorithm that is much faster (asymptotically and in practice) than computing the exact degrees is employed. One continuous real parameter sets the amount of searching done to locate the pivot element. When this parameter is set to zero, no searching is done and the diagonal element is the pivot, while when set to unity, complete partial pivoting is done. Since the matrices generated by reaction networks are usually diagonally dominant, the routine is set in FLASH to use the diagonal as the pivot element. Several test cases showed that using partial pivoting did not make a significant accuracy difference, but were less efficient since a search for an appropriate pivot element had to be performed. MA28 accepts the nonzero entries of the matrix in the $(i, j, a_{i,j})$ coordinate system, and typically uses uses 70−90% less storage than storing the full dense matrix.

The time integration method used by FLASH for evolving the reaction networks is the variable order Bader-Deuflhard method (e.g., Bader & Deuflhard 1983; Press et al. 1992). The reaction network is advanced over a large time step H from $\mathbf{y}_n$ to $\mathbf{y}_{n+1}$ by the following sequence of matrix equations. First,

$$\begin{aligned} h &= H/m \\ (\tilde{\mathbf{1}} - \tilde{\mathbf{J}}) \cdot \Delta_0 &= h\mathbf{f}(\mathbf{y}_n) \\ \mathbf{y}_1 &= \mathbf{y}_n + \Delta_0 \ . \end{aligned} \tag{32}$$

Then from $k = 1, 2, \ldots, m-1$

$$\begin{aligned} (\tilde{\mathbf{1}} - \tilde{\mathbf{J}}) \cdot \mathbf{x} &= h\mathbf{f}(\mathbf{y}_k) - \Delta_{k-1} \\ \Delta_k &= \Delta_{k-1} + 2\mathbf{x} \\ \mathbf{y}_{k+1} &= \mathbf{y}_k + \Delta_k \ , \end{aligned} \tag{33}$$

and closure is obtained by the last stage

$$\begin{aligned} (\tilde{\mathbf{1}} - \tilde{\mathbf{J}}) \cdot \Delta_m &= h[\mathbf{f}(\mathbf{y}_m) - \Delta_{m-1}] \\ \mathbf{y}_{n+1} &= \mathbf{y}_m + \Delta_m \ . \end{aligned} \tag{34}$$

This staged sequence of matrix equations is executed at least twice with m=2 and m=6, yielding a fifth-order method. The sequence may be executed a maximum of seven times, which yields a fifteenth-order method. The exact number of times the staged sequence is executed depends on the accuracy requirements (set to one part in 10^6 in FLASH) and the smoothness of the solution. Estimates of the accuracy of an integration step are made by comparing the solutions derived from different orders. The minimum cost of this method — which applies for a single time step that met or exceeded the specified integration accuracy — is one Jacobian evaluation, eight evaluations of the right-hand side, two matrix decompositions, and ten backsubstitutions. This minimum cost can be increased at a rate of one decomposition (the expensive part) and m backsubstitutions (the inexpensive part) for every increase in the order $2k + 1$. The cost of increasing the order is compensated for, hopefully, by taking a correspondingly larger (but accurate) time step. The controls for order versus step size are a built-in part of the Bader-Deuflhard method. The cost per step of this integration method is at least twice as large as the cost per step of either a traditional first-order accurate Euler method or a fourth-order accurate Kaps-Rentrop (essentially an implicit Runge-Kutta) method, However, if the Bader-Deuflhard method can take accurate time steps that are at least twice as large, then this method will be more efficient globally. Timmes (1999) shows that this is typically the case. Note that in equations (32) — (34) not all of the right-hand sides are known in advance since the sequence of linear equations is staged. This staging feature of the integration method will make some matrix packages, such as MA28, a more efficient choice.

The energy generation rate is given by the sum

$$\dot{\epsilon}_{\rm nuc} = N_A \sum_i \frac{dY_i}{dt} \ . \tag{35}$$

Note that a nuclear reaction network does not need to be evolved in order to obtain the instantaneous energy generation rate, since only the right hand sides of the ordinary differential equations need to be evaluated. It is more appropriate in the FLASH program to use the average nuclear energy generated over a time step

$$\dot{\epsilon}_{\rm nuc} = N_A \sum_i \frac{\Delta Y_i}{\Delta t} \ . \tag{36}$$

In this case, the nuclear reaction network does need to be evolved. The energy generation rate, after subtraction of any neutrino losses, is returned to the FLASH program for use with the operator splitting technique.

Finally, the tabulation of Caughlan & Fowler (1988) is used in FLASH for most of the key nuclear reaction rates. Modern values for some of the reaction rates were taken from the reaction rate library of Hoffman (1999, priv. comm.). Nuclear reaction rate screening effects as implemented by Wallace, Woosley, & Weaver (1982), and decreases in the energy generation rate $\dot{\epsilon}_{\rm nuc}$ due to neutrino losses as given by Itoh et al. (1985) are included in calculations done with FLASH.

3 Quick start

This section describes how to quickly get up and running with FLASH, showing how to configure and build it to solve the Sedov explosion problem, how to run it, and how to examine the output using IDL. To begin, verify that you have the following:

- A copy of the FLASH source code distribution. This is most likely available either as a Unix tar file or as a local Concurrent Versions System (CVS) source tree. When FLASH is made publicly available, you will be able to download the tar file from the Flash Center web site at `http://www.flash.uchicago.edu/flashcode/`.
- A Fortran 90 compiler and a C compiler. Most of FLASH is written in Fortran 90.
- An installed copy of the Message-Passing Interface (MPI) library. A freely available implementation of MPI has been created at Argonne National Laboratory and can be accessed on the World Wide Web at `http://www-unix.mcs.anl.gov/mpi/mpich/`.
- If you plan to use the Hierarchical Data Format (HDF) for output files (the default), you will need an installed copy of the freely available HDF library. Currently FLASH supports HDF version 4. As of this writing, later versions of HDF are not yet compatible with HDF 4. HDF is available from the HDF Project of the National Computational Science Alliance at `http://hdf.ncsa.uiuc.edu/`. The contents of HDF output files produced by the FLASH `io/hdf` module are described in detail in section 6.1.6.
- To use the output analysis tools described in this section, a copy of the IDL language from Research Systems, Inc. (`http://www.rsinc.com/`). IDL is a commercial product. However, it is not required for the analysis of FLASH output. The FLASH code group is currently working with members of the Mathematics and Computer Science Division at Argonne National Laboratory to develop more sophisticated visualization tools to distribute either as part of or alongside FLASH.

FLASH has been tested on the following Unix-based platforms. In addition, it may work with others not listed (see section 6.4).

- SGI systems running IRIX (`irix` machine type)
- Intel-based systems running Linux (`linux` machine type)
- Cray/SGI T3E running UNICOS (`t3e` machine type)
- The ASCI Blue Mountain machine, built by SGI (`asci_bluemtn` machine type)
- The ASCI Blue Pacific machine, built by IBM (`asci_blue` machine type)
- The ASCI Red machine, built by Intel (`asci_red` machine type)

In this section we will use `irix` as an example of the machine type. Substitute your machine type for `irix` wherever it appears.

To begin, unpack the FLASH source code distribution. If you have a Unix tar file, type '`tar xvf FLASHX.tar`' (without the quotes), where `X` is the FLASH major version number (for example, use `FLASH1.tar` and `FLASH1/` for FLASH version 1.0). If you are working with a CVS source tree, use '`cvs checkout FLASHX`' to obtain a personal copy of the tree. You may need to obtain permission from the local CVS administrator to do this. In either case you will create a directory called `FLASHX/`. Type '`cd FLASHX`' to enter this directory.

Next, configure the FLASH source tree for the Sedov explosion problem. Type

```
# runtime parameters

lrefine_max = 4
basenm = "sedov_4_"
restart = .false.
trstrt = 0.005
nend = 1000
tmax = 0.02
gamma = 1.4
xlboundary = -21 # code -21 is outflow
xrboundary = -21
ylboundary = -21
yrboundary = -21
```

Figure 1: FLASH parameter file contents for the quick start example.

```
./setup sedov irix -defaults
```

This configures FLASH for the `sedov` problem, using the default hydrodynamic solver, equation of state, and I/O format defined for this problem. The source tree is configured to create a two-dimensional code by default.

The next step is to edit the file `object/Makefile.h`. This file contains all of the site-dependent and architecture-dependent parts of the Makefile. Verify that the compiler settings (`FCOMP`, `CCOMP`, and `CPPCOMP`) and the library paths (`LIB`) are correct for your system. No other changes should be necessary at this stage (later on you may wish to fiddle with the compiler optimization settings). Future versions of FLASH may make use of the GNU `configure` program to handle this step.

From the FLASH root directory (ie. the directory from which you ran `setup`), execute `make`. This will compile the FLASH code. If you should have problems and need to recompile, '`make clean`' will remove all object files from the `object/` directory, leaving the source configuration intact; '`make realclean`' will remove all files and links from `object/`. After '`make realclean`,' a new invocation of `setup` is required before the code can be built.

Assuming compilation and linking were successful, you should now find an executable named `flashX_sedov_irix` in the `object/` directory. (Remember to replace `irix` with your machine type.) You may wish to check that this is the case.

FLASH expects to find a flat text file named `flash.par` in the directory from which it is run. This file sets the values of various runtime parameters which determine the behavior of FLASH. If it is not present, FLASH will use default values for the runtime parameters, which may or may not produce desirable results. Here we will create a simple `flash.par` which sets a few parameters and allows the rest to take on default values. With your text editor, create `flash.par` in the main FLASH directory with the contents of Figure 1. This instructs FLASH to use up to four levels of adaptive mesh refinement (AMR) and to name the output files appropriately. We will not be starting from a checkpoint file (this is the default, but here it is explicitly set for purposes of illustration). Output files are to be written every

0.005 time units, and we will integrate until $t = 0.02$ or 1000 timesteps have been taken, whichever comes first. The ratio of specific heats for the gas (γ) is taken to be 1.4, and all four boundaries of the two-dimensional grid have outflow (zero-gradient or Neumann) boundary conditions. Note the format of the file: each line is a comment (denoted by a hash mark, `#`), blank, or of the form *variable* = *value*. String values are enclosed in double quotes ("). Boolean values are indicated in the Fortran style, `.true.` or `.false.`

We are now ready to run FLASH. To run FLASH on `N` processors, type

```
mpirun -np N object/flashX_sedov_irix
```

remembering to replace `N`, `X`, and `irix` with the appropriate values. Some systems may require you to start MPI programs with a different command; use whichever command is appropriate to your system. The FLASH executable can take one command-line argument, the name of the runtime parameter file. The default parameter file name is `flash.par`.

You should see a number of lines of output indicating that FLASH is initializing the Sedov problem, listing the initial parameters, and giving the timestep chosen at each step. At the end FLASH prints a summary of the CPU time spent in various parts of the code and terminates. In the current directory you should now find several files:

- `flash.log` echoes the runtime parameter settings and indicates the run time, the build time, and the build machine.
- `flash.dat` contains a number of quantities as functions of time: total mass, total energy, total momentum, etc. This file can be used directly by plotting programs such as `gnuplot`; note that the first line begins with a hash (`#`) and thus is ignored by `gnuplot`.
- `sedov_4_000*` are the different checkpoint files. These are complete dumps of the entire simulation at intervals of `trstrt`, suitable for use in restarting the simulation. They are also the primary output products of FLASH.

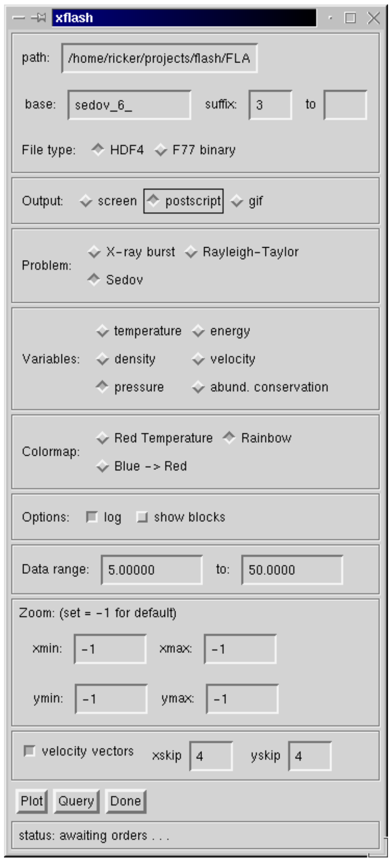
We will use the `xflash` routine under IDL to examine the output. Before doing so, we need to set the values of two environment variables, `IDL_PATH` and `XFLASH_DIR`. Under `csh` this can be done using the commands

```
setenv XFLASH_DIR "$PWD/tools/idl"
setenv IDL_PATH "${XFLASH_DIR}:$IDL_PATH"
```

If you get a message indicating that `IDL_PATH` is not defined, just enter

```
setenv IDL_PATH "$XFLASH_DIR"
```

Now run IDL (`idl`) and enter `xflash` at the `IDL>` prompt. You should see a control panel widget as shown in Figure 2. The path entry should be filled in for you with the current directory. Enter `sedov_4_` as the base filename and enter `4` as the suffix. (`xflash` can generate output for a number of consecutive files, but if you fill in only the beginning suffix, only one file is read.) Our output files are in HDF format, so make sure the HDF button is selected. Choose the image format (screen, Postscript, GIF) and the problem type (in our



path: /home/ricker/projects/flash/FLA

base: sedov_6_ suffix: 3 to

File type: [✓ HDF4] F77 binary

Output: screen [✓ postscript] gif

Problem: X-ray burst Rayleigh-Taylor [✓ Sedov]

Variables: temperature energy density velocity [✓ pressure] abund. conservation

Colormap: Red Temperature [✓ Rainbow] Blue -> Red

Options: [✓ log] show blocks

Data range: 5.00000 to: 50.0000

Zoom: (set = −1 for default)

xmin: −1 xmax: −1

ymin: −1 ymax: −1

[✓ velocity vectors] xskip 4 yskip 4

status: awaiting orders . . .

Figure 2: Control panel for the xflash visualization tool under IDL.

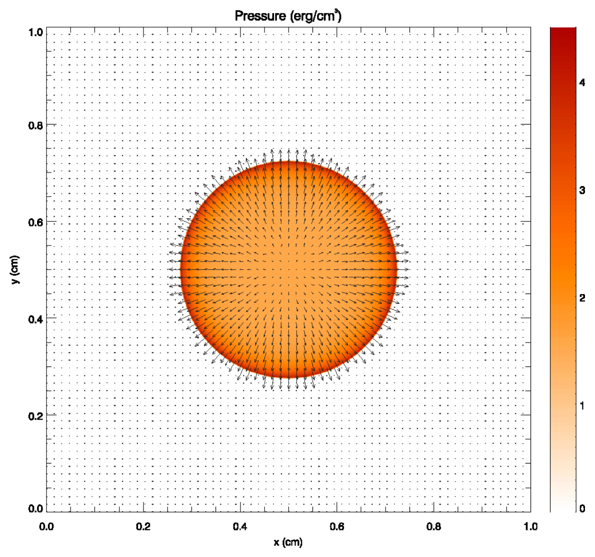


Figure 3: Example of `xflash` output for the Sedov problem with eight levels of refinement.

case, Sedov). Selecting the problem type is only important for choosing default ranges for our plot; plots for other problems can be generated by ignoring this setting and overriding the default values for the data range and the coordinate ranges. Select the desired plotting variable and colormap. The 'abundance conservation' variable produces a plot of the sum of the nuclear abundances, useful for comparison with the expected value (unity). Under 'Options,' select whether to plot the logarithm of the desired quantity, and select whether to plot the outlines of the AMR blocks. For very highly refined grids the block outlines can obscure the data, but they are useful for verifying that FLASH is putting resolution elements where they are needed. Finally, check 'velocity vectors' to overlay the velocity field. The 'xskip' and 'yskip' parameters enable you plot only a fraction of the vectors so that they do not obscure the background plot.

When the control panel settings are to your satisfaction, click the 'Plot' button to generate the plot. For Postscript and GIF output, a file is created in the current directory. The result should look something like Figure 3, although this figure was generated from a run with eight levels of refinement rather than the four used in the quick start example run. With fewer levels of refinement the Cartesian grid causes the explosion to appear somewhat diamond-shaped.

FLASH is intended to be customized by the user to work with interesting initial and boundary conditions. In the following sections we will cover in more detail the structure of FLASH and the sample problems and tools distributed with it.

4 FLASH tools

In this section we describe several of the tools distributed with FLASH. The source code for these programs (except for `setup`) can be found in the main FLASH source tree under the `tools/` directory.

4.1 The FLASH configuration script (setup)

The `setup` script, found in the FLASH root directory, provides the primary command-line interface to the FLASH source code. It configures the source tree for a given problem and target machine and creates files needed to parse the runtime parameter file and make the FLASH executable. More description of what `setup` does may be found in Section 6.1. Here we describe its basic usage.

Running `setup` without any options prints a message describing the available options:

```
[sphere 5:09pm] % ./setup
usage:  setup problem-name machine-type [options]

          problems:  2blast advect mach rt sedov sod xrayburst
          machines:  asci_blue asci_bluemtn asci_red irix linux t3e
          options:  -verbose -portable -defaults -[123]d -maxblocks=#
```

Available values for the two mandatory options, the name of the problem to configure and the type of machine to configure for, are determined by scanning the `setups/` and `source/systems/` directories, respectively.

A "problem" consists of a set of initial and boundary conditions, possibly additional physics (e.g., a subgrid model for star formation), and a set of adjustable parameters. The directory associated with a problem contains source code files which implement the initial and boundary conditions and extra physics, together with a configuration file, read by `setup`, which contains information on required physics modules and adjustable parameters.

A "machine type" consists of an architecture and an associated operating system. Normally it does not refer to a specific machine, but in the case of the ASCI machines (Blue Pacific, Blue Mountain, and Red), the particular machine is unique and is treated as a separate architecture. The directory for each machine type contains a makefile fragment (`Makefile.h`) which sets command names, compiler flags, and library paths, and any replacement or additional source files needed to compile FLASH for that machine type.

`setup` uses the problem and machine type, together with a user-supplied file called `Modules` which lists the code modules to include, to generate a directory called `object/` which contains links to the appropriate source files and makefile fragments. It also creates the master makefile (`object/Makefile`) and several Fortran include files (`object/rt_*`) which are needed by the code in order to parse the runtime parameter file. After running `setup`, the user can make the FLASH executable by running `make` in the `object/` directory (or from the FLASH root directory, if the `-portable` option is not used with `setup`). The optional command-line modifiers have the following interpretations:

`-verbose`	Normally `setup` echoes to the standard output summary messages indicating what it is doing. Including the `-verbose` option causes it to also list the links it creates.
`-portable`	This option creates a portable build directory. Instead of `object/`, `setup` creates `object_`*problem*_*machine*`/`, and instead of creating links to the source files in `source/` and `setups/`, it copies files from those directories into the build directory. The resulting build directory can be placed into a `tar` archive and sent to another machine for building. Because the makefile in the FLASH root directory is generic and does not know what problem or machine has been selected, it cannot be used to make code which has been configured with `-portable`.
`-defaults`	Normally `setup` requires that the user supply a plain text file called `Modules` (in the FLASH root directory) which specifies which code modules to include. A sample `Modules` file appears in Figure 4. Each line is either a comment (preceded by a hash mark (`#`)) or a module include statement of the form `INCLUDE` *module*. Sub-modules are indicated by specifying the path to the sub-module in question; in the example, the sub-module `gamma` of the `eos` module is included. If a module has a default sub-module, but no sub-module is specified, `setup` automatically selects the default using information provided by the module's configuration file. The purpose of the `-defaults` option is to enable `setup` to generate a "rough draft" of a `Modules` file for the user. The configuration file for each problem setup specifies a number of code module requirements; for example, a problem may require the perfect-gas equation of state (`eos/gamma`) and an unspecified hydro solver (`hydro`). With `-defaults`, `setup` creates a `Modules` file by converting these requirements into module include statements. In addition, it checks the configuration files for the required modules and includes any of *their* required modules, eliminating duplicates. This is only done for one level of requirement, but usually this is enough. Most users configuring a problem for the first time will want to run `setup` with `-defaults` to generate a `Modules` file, then edit `Modules` directly to specify different sub-modules (e.g., hydro solvers or I/O formats). After editing `Modules` in this way, re-run `setup` without `-defaults` to incorporate the changes into the code configuration.

```
# Modules file constructed for rt problem by setup -defaults

INCLUDE driver
INCLUDE eos/gamma
INCLUDE grav
INCLUDE paramesh
INCLUDE mmpi
INCLUDE mpi_amr
INCLUDE hydro
INCLUDE io
```

Figure 4: Example of the `Modules` file used by `setup` to determine which code modules to include.

`-[123]d`	By default `setup` creates a makefile which produces a FLASH executable capable of solving one- or two-dimensional problems (equivalent to `-2d`). To generate a makefile with options appropriate to three-dimensional problems, use `-3d`. The resulting code will be able to solve 1D, 2D, or 3D problems. To generate a one-dimensional code, use `-1d`. While `-3d` provides maximum flexibility, it also allocates the most memory at runtime. It is generally very wasteful of memory to solve a 1D or 2D problem using an executable compiled with `-3d`. These options are mutually exclusive and cause `setup` to add the appropriate compilation option to the makefile it generates.
`-maxblocks=#`	This option is also used by `setup` in constructing the makefile compiler options. It determines the amount of memory allocated at runtime to the adaptive mesh refinement (AMR) block data structure. For example, to allocate enough memory on each processor for 500 blocks, use `-maxblocks=500`. If the default block buffer size is too large for your system, you may wish to try a smaller number here (the defaults are currently defined in `source/driver/physicaldata.fh`). Alternatively, you may wish to experiment with larger buffer sizes if your system has enough memory.

After configuring the source tree with `setup` and using `make` to create an executable in the build directory, look in the build directory for a file named `rt_parms.txt`. This contains a complete list of all of the runtime parameters available to the executable, together with their variable types, default values, and comments. To set runtime parameters to values other than the defaults, create a runtime parameter file named `flash.par` in the directory from which FLASH is to be run. The format of this file is described in Section 3.

4.2 FLASH output comparison utility (`focu`)

The FLASH output comparison utility, or `focu` (pronounced *faux-coup*), is a command-line utility which compares FLASH output files according to specified criteria (e.g., local or global error criterion on any of the hydrodynamical variables) and reports whether they are the same or not. This is useful in determining whether a change to FLASH (or to the value of a runtime parameter) has changed the results obtained with a given problem.

4.2.1 Building `focu`

The `focu` executable is configured and built in much the same way as is FLASH: obtain source tree, run `setup` to configure the source tree for a given architecture, and run `make` in the build directory. FLASH and `focu` are different in that `focu` is problem-independent, so only a machine type needs to be specified, and in that (at least at the present time) all of the modules included with `focu` are used, so `setup` is always run with the `-defaults` option. (See Section 4.1 for details regarding the usage of `setup`.) To summarize the steps in building `focu`:

1. Move to the `focu` root directory (`tools/focu/` relative to the FLASH root directory).

2. Run `./setup` *machine-type* `-defaults`, where *machine-type* is the name of the architecture for which you are configuring `focu` (run `setup` without options for a list). Do not use the setup script in the FLASH root directory.

3. Edit `object/Makefile.h` to set compiler flags and the locations of libraries. Since `focu` contains routines to read both HDF and Fortran unformatted output, you must have the HDF library installed.

4. Run `make`. If compilation is successful, you should find an executable named `focu_`*machine-type* in the current directory.

Additional setup options are available and are interpreted as described in Section 4.1.

4.2.2 Using `focu`

Running `focu` is very similar to running FLASH itself. First prepare a runtime parameter file, then run `focu` using

`mpirun -np` *N* `focu_`*machine-type parameter-file*

(or use the command used by your system to start MPI programs). Here *N* is the number of processors to use (which need not be the same as the number of processors used by the FLASH job which produced the output files to be read), and *machine-type* is the machine type specified in the setup step. If the *parameter-file* argument is not supplied, `focu` looks for a parameter file named `focu.par` in the current directory. The format of this file is identical to that used by FLASH (see Section 3).

The runtime parameters understood by `focu` are as follows. Default values are listed in brackets following each description.

`file1`	Base file name for the first file to compare. The file name will be constructed by appending the file number, padded with zeros to four places, to the base file name. ["file1"]
`num1`	The file number for the first file to compare. [0]
`format1`	The format of the first file: "HDF" for Hierarchical Data Format, "F77" for Fortran unformatted. ["HDF"]
`file2`	Base file name for the second file to compare. ["file2"]
`num2`	File number for the second file. [0]
`format2`	Format for the second file. ["HDF"]
`variable`	The name of the hydrodynamical variable to examine. Available values are "density," "pressure," "x velocity," "y velocity," "z velocity," "temperature," "energy," "kinetic energy," "internal energy," "x momentum," "y momentum," "z momentum," and "abundance *N*," where *N* is the index of the abundance to use. ["density"]
`criterion`	The error criterion to apply in comparing the files. This must be of the form "*A B*", where *A* is either "local" or "global," and *B* is either "sum," "min," or "max." For the global criteria, `focu` first computes the volume-weighted average, minimum value, or maximum value of `variable` for each file, then computes the L1 deviation between the two global quantities. For the local criteria, the files are compared on a zone-by-zone basis. Consequently the AMR block structures of the two files must be the same in order for the comparison to succeed. If `criterion` is "local sum," the volume-weighted average of the local L1 deviations is compared to `threshold` to determine success or failure. If `criterion` is "local min" or "local max," the minimum or maximum L1 deviation is compared. The L1 deviation for two quantities X_1 and X_2 is defined as $\|X_2 - X_1\|/\max\{\frac{1}{2}\|X_1 + X_2\|, 10^{-99}\}$. ["global sum"]
`threshold`	The error threshold to use in deciding success or failure. [10^{-6}]
`outfile`	The name of the output file to create when generating the comparison report. Setting this to "stdout" causes `focu` to write to standard output. ["stdout"]

The output of `focu` is a short report listing the volume-averaged sum, minimum, and maximum deviations (local or global, depending on the setting of `criterion`) and reporting SUCCESS or FAILURE according to the supplied threshold. For example, if two runs of FLASH are performed using the Sedov problem, one with HDF output and one with Fortran

```
FOCU: Flash Output Comparison Utility

Comparing:  "sedov_4_f77_" # 3
            "sedov_4_hdf_" # 3

Variable:   density
Criterion:  local sum
Threshold:  1.0000000000000E-09

Result:
  Error:    0.0000000000000E+00
  Minimum:  0.0000000000000E+00
  Maximum:  0.0000000000000E+00
  SUCCESS
```

Figure 5: Example of `focu` output format.

unformatted output, the resulting output files should be identical. The report generated by a `focu` comparison of two such files is shown in Figure 5. Note that the last line of the report begins with SUCCESS or FAILURE, making it easy for a script to test the results. For example, with `csh` one might use

```
set result = `mpirun -np 2 focu_irix focu_sedov.par | grep SUCCESS`
if ("result" == "SUCCESS") then
...
endif
```

`focu` is used by the automated FLASH test script (Section 5.1) to compare FLASH outputs to the reference results supplied as part of the test suite.

4.3 IDL routines for the analysis of FLASH output (`fidlr`)

`fidlr` is a set of routines, written in the IDL language, which provide tools for plotting results obtained with FLASH. The routines include programs which can be run from the IDL command line to read 2D or 3D FLASH datasets and interpolate them onto uniform grids. An IDL program called `xflash` provides a graphical interface to these routines, enabling users to read and plot 2D AMR datasets without interpolating onto a uniform mesh.

4.3.1 Configuring your environment to use the IDL routines

The FLASH IDL routines are located in the `tools/fidlr/` subdirectory of the FLASH root directory. To use them you must set two environment variables. First set the value of `XFLASH_DIR` to the location of the FLASH IDL routines; for example, under `csh`, use

`setenv XFLASH_DIR` *flash-root-path*`/tools/fidlr` where *flash-root-path* is the absolute path of the FLASH root directory. Next add this directory to your IDL_PATH variable:

```
setenv IDL_PATH "${XFLASH_DIR}:$IDL_PATH"
```

If you have not previously defined IDL_PATH, omit :$IDL_PATH from the above command. You may wish to include these commands in your .cshrc file (or profile if you use another shell) to avoid having to reissue them every time you log in.

To begin using the routines, start IDL (idl). You may wish to make use of the program start.pro included with fidlr; this forces the use of an eight-bit colormap on 24-bit displays which have the ability to maintain two color depths (such as those found on SGIs). To use this program, start IDL using idl start.pro.

4.3.2 Using the xflash graphical plotting tool

xflash provides a graphical interface to IDL for plotting one or several 2D AMR datasets. It plots variables using a shaded colormap and can overlay the outline of the AMR block structure or arrows showing the velocity field. It also enables users to zoom in to different regions of the dataset and to probe the dataset.

To use the graphical tool, from the IDL command line (idl>) execute xflash. The widget is divided into sections controlling the file location, output type, problem, variable to plot, colormap, plot options, data range, zooming, and velocity vectors. At the bottom is a status display. See Figure 2 for an example of the appearance of the xflash window.

File location

The files to be read are specified by entering a path (by default the current IDL working directory), a base name, and a range of suffixes. If only the first suffix is entered, only that one is used; otherwise all integers between the beginning and ending suffix are used. Select the file type by choosing "HDF" for Hierarchical Data Format or "F77" for Fortran unformatted output. At present the Fortran reader does not convert little-endian files to big-endian or vice versa.

Output device

It is possible to direct output to the screen, to a Postscript file, or to a GIF image. The plotting routine will determine the orientation (portrait or landscape) using the aspect ratio of the domain to be plotted, and it will plot the largest area that maintains this ratio.

Problem

The problem buttons load default data ranges, axis orientation, and velocity information for different problems. New problems can be added quite easily by modifying the file tools/fidlr/xflash_defaults.pro. It is not necessary to add a problem in order to plot a dataset. The problem selection exists only to provide rational default values for data ranges;

these values can be overridden through the widget.

Variables

Presently the following variables can be plotted: temperature, density, pressure, total energy, velocity magnitude, and abundance conservation error. The latter is the difference between the sum of the nuclear abundances in a zone and unity. The choice of problem and variable affects the default data range chosen.

Colormap

The colormaps used by `xflash` differ from the standard IDL colormaps. The first 12 colors are uniform across the colormaps and contain standard colors (red, green, blue, white, black) that are used to set the background color, text color, and so forth.

Plotting options

Two plotting options are currently available. The "log" option plots the common logarithm of the chosen variable, while the "show blocks" option overlays the boundaries of the AMR block structure on the colormap used to represent the variable. For AMR grids with many levels of refinement, the block boundaries can completely obscure the colormap; however, this option can be useful for verifying that resolution elements are being placed where they are needed.

Data range

The default data range may be overridden if desired by entering a new minimum or maximum value here. The values of the defaults are set in `tools/fidlr/xflash_defaults.pro`.

Zoom

A value of -1 here indicates that the default position for the corresponding limit is to be used. Leave each limit at -1 to plot the entire grid, or enter different limits to plot a smaller part of the grid.

Velocity vectors

If this box is checked, velocity arrows will be overlaid on the colormap. The arrow lengths are scaled according to a "typical" velocity magnitude, and magnitudes outside of a specified range are not plotted. The values of the typical velocity and the clipping range are set in `tools/fidlr/xflash_defaults.pro`. If the velocity vector box is checked, the xskip and yskip options become selectable. These options set the number of zones to skip in each direction when plotting arrows. For highly refined meshes this can help one to avoid obscuring the colormap with arrows.

Control buttons

Once all of the options are set, press the “Plot” button to produce the plot. The status of the plot appears in the status window below the buttons. If only a single plot is made (ie. only one suffix was specified), additional plots can be made without reading in the dataset again. This permits one to easily experiment with color tables, data ranges, and so forth. Once the plot is complete, press the “Query” button and click anywhere in the plot to probe the dataset. Mouse clicks will bring up a window showing the position of the click and the values of the hydrodynamical variables at that position.

Press the “Quit” button to terminate the widget.

4.3.3 Other IDL routines

Following is a description of each of the IDL routines included with the FLASH IDL tools in the `tools/fidlr` subdirectory.

Main programs

`xflash.pro`	Widget routine and event handler.
`xflash_defaults.pro`	Contains problem-specific defaults.
`xplot_amr.pro`	Main plotting routine, called by `xflash`.

Reading routines

`read3_amr.pro`	Reads block-structured AMR data from an HDF 4 file. The data are stored in common blocks.
`read_amr_f77.pro`	Reads block-structured AMR data from a Fortran unformatted file. The data are stored in common blocks.
`def_common.pro`	Defines the common blocks which hold the AMR data. Run this from the command line in order to access the AMR data structure directly (e.g., in order to pass a variable name to one of the uniform resampling routines).

Data manipulation routines

`merge_amr.pro`	Resamples a given AMR data structure on a uniform grid of a given coarseness. Currently the only way to manipulate 3D data.
`scale2_amr.pro`	Resamples a given AMR data structure on a uniform grid, producing a byte array for plotting purposes.

Plotting routines

`partvelvec.pro`	Plots velocity vectors.
`draw_blocks.pro`	Plots the outline of the AMR block structure.
`colorbar2.pro`	Produces a horizontal color key.
`vcolorbar.pro`	Produces a vertical color key.

Utility routines

`cmcongrid.pro`	A special version of `congrid` used by `tvimage`.
`color_gif.pro`	Captures a window and saves it to a GIF file.
`nolabel.pro`	A hack to allow unlabelled axes.
`start.pro`	When run at the start of an IDL session, sets up an eight-bit X visual on a 24-bit display (when supported by the X server).
`tvimage.pro`	Similar to the IDL `tv` command, but allows a byte array to be drawn on the screen or directly into a Postscript file.
`undefine.pro`	Frees up memory used by AMR data structures.

5 The supplied problems

5.1 Running the FLASH test suite

To verify that FLASH works as expected, and to debug changes in the code, we have created a suite of standard test problems. Most of these problems have analytical solutions which can be used to test the accuracy of the code. The remaining problems do not have analytical solutions, but they produce well-defined flow features which have been verified by experiments and are stringent tests of the code. The test suite configuration code is included with the FLASH source tree (in the `setups/` directory), so it is easy to configure and run FLASH with any of these problems 'out of the box.' Sample runtime parameter files are also included. Files containing reference results for the test suite tend to be large and so are distributed separately (via the `FLASH_TEST` CVS tree or in archive form as `FLASH_TEST.tar`). The `FLASH_TEST` tree also contains the runtime parameter files needed to reproduce the reference results.

Included with the test suite results is a script named `flash_test` which automates the process of comparing test suite results with the reference results. `flash_test` takes one argument, the machine type (run `flash_test` with no arguments for a list of available types). It automatically configures and builds FLASH for each of the test problems, builds the `focu` output comparison utility (Section 4.2), runs FLASH with each test problem, and uses `focu` to compare the results. It prepares a report for the entire suite of problems, flagging compilation problems, catastrophic runtime errors, and erroneous results. Since `flash_test` can be quite time-consuming to execute for the full test suite, it is generally a good idea to execute it as a batch job on the target system. Note that the tests may be run individually using the runtime parameter files provided with the FLASH test suite. Plots similar to those in this section can be produced using IDL routines provided with the test suite; these make use of the FLASH IDL tools (Section 4.3).

5.2 The Sod shock-tube problem

The Sod problem (Sod 1978) is an essentially one-dimensional flow discontinuity problem which provides a good test of a compressible code's ability to capture shocks and contact discontinuities with a small number of zones and to produce the correct density profile in a rarefaction. It also tests a code's ability to correctly satisfy the Rankine-Hugoniot shock

Table 1: Runtime parameters used with the `sod` test problem.

Variable	Type	Default	Description
`rho_left`	real	1	Initial density to the left of the interface (ρ_L)
`rho_right`	real	0.125	Initial density to the right (ρ_R)
`p_left`	real	1	Initial pressure to the left (p_L)
`p_right`	real	0.1	Initial pressure to the right (p_R)
`u_left`	real	0	Initial velocity (perpendicular to interface) to the left (u_L)
`u_right`	real	0	Initial velocity (perpendicular to interface) to the right (u_R)
`xangle`	real	0	Angle made by interface normal with the x-axis (degrees)
`yangle`	real	90	Angle made by interface normal with the y-axis (degrees)
`posn`	real	0.5	Point of intersection between the interface plane and the x-axis

jump conditions. When implemented at an angle to a multidimensional grid, it can also be used to detect irregularities in planar discontinuities produced by grid geometry or operator splitting effects.

We construct the initial conditions for the Sod problem by establishing a planar interface at some angle to the x and y axes. The fluid is initially at rest on either side of the interface, and the density and pressure jumps are chosen so that all three types of flow discontinuity (shock, contact, and rarefaction) develop. To the "left" and "right" of the interface we have

$$\begin{array}{rclrcl} \rho_\mathrm{L} & = & 1 & \rho_\mathrm{R} & = & 0.125 \\ p_\mathrm{L} & = & 1 & p_\mathrm{R} & = & 0.1 \end{array} \tag{37}$$

The ratio of specific heats γ is chosen to be 1.4 on both sides of the interface.

In FLASH, the Sod problem (`sod`) uses the runtime parameters listed in Table 1 in addition to the regular ones supplied with the code. For this problem we use the `eos/gamma` equation of state module and set the value of the parameter `gamma` supplied by this module to 1.4. The default values listed in Table 1 are appropriate to a shock with normal parallel to the x-axis which initially intersects that axis at $x = 0.5$ (halfway across a box with unit dimensions).

Figure 6 shows the result of running the Sod problem with FLASH on a two-dimensional grid, with the analytical solution shown for comparison. The hydrodynamical algorithm used here is the directionally split piecewise-parabolic method (PPM) included with FLASH. In this run the shock normal is chosen to be parallel to the x-axis. With six levels of refinement, the effective grid size at the finest level is 256^2, so the finest zones have width 0.00390625. At $t = 0.2$ three different nonlinear waves are present: a rarefaction between $x \approx 0.25$ and $x \approx 0.5$, a contact discontinuity at $x \approx 0.68$, and a shock at $x \approx 0.85$. The two

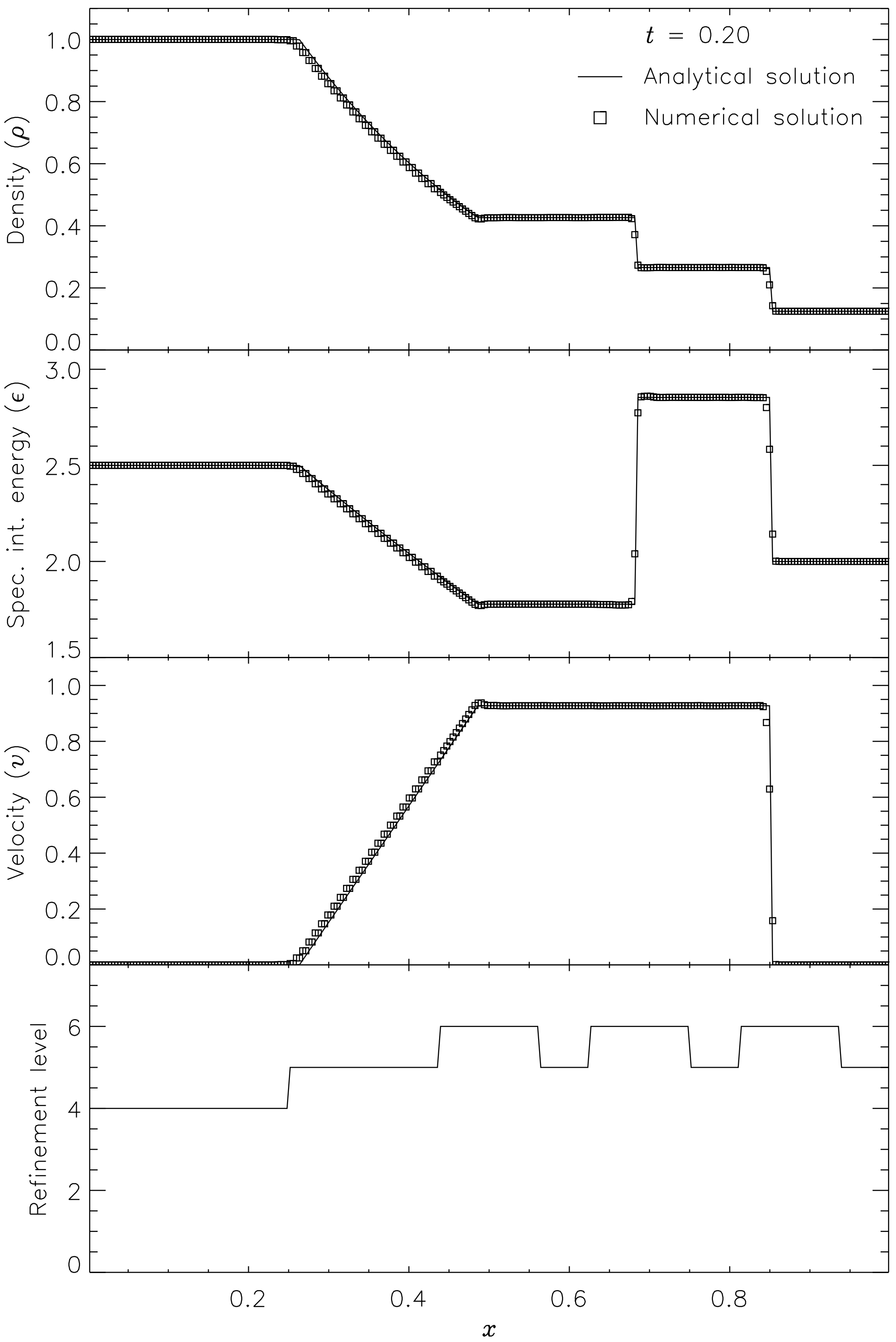


Figure 6: Comparison of numerical and analytical solutions to the Sod problem. A 2D grid with six levels of refinement is used. The shock normal is parallel to the x-axis.

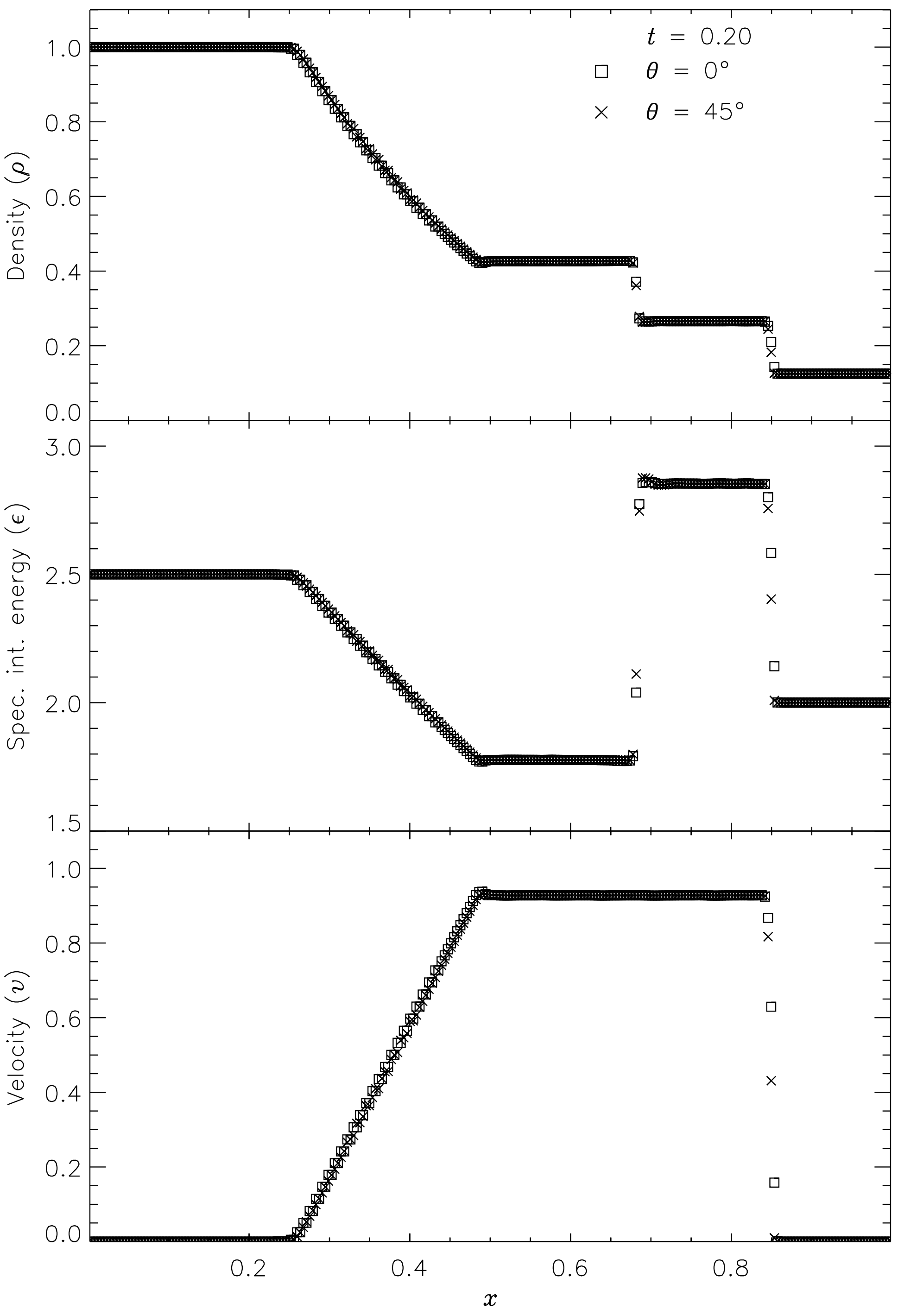


Figure 7: Comparison of numerical solutions to the Sod problem for two different angles (θ) of the shock normal relative to the x-axis. A 2D grid with six levels of refinement is used.

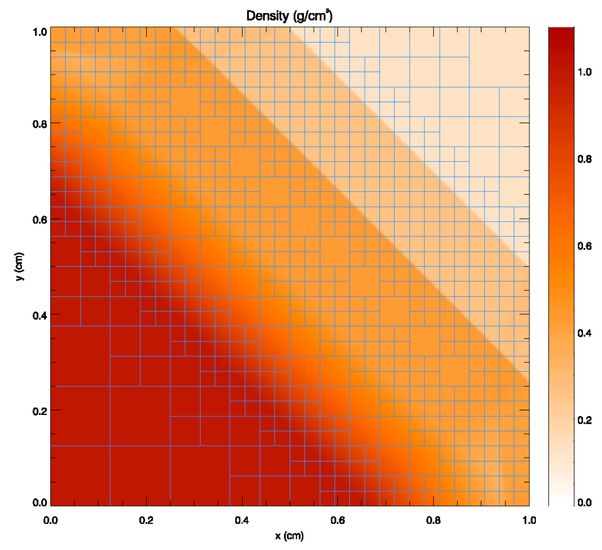


Figure 8: Density in the diagonal 2D Sod problem with six levels of refinement at $t = 0.2$. The outlines of AMR blocks are shown (each block contains 8×8 zones).

sharp discontinuities are each resolved with approximately three zones at the highest level of refinement, demonstrating the ability of PPM to handle sharp flow features well. Near the contact discontinuity and in the rarefaction we find small errors of about $1 - 2\%$ in the density and specific internal energy, with similar errors in the velocity inside the rarefaction. Elsewhere the numerical solution is exact; no oscillation is present.

Figure 7 shows the result of running the Sod problem on the same two-dimensional grid with different shock normals: parallel to the x-axis ($\theta = 0°$) and along the box diagonal ($\theta = 45°$). For the diagonal solution we have interpolated values of density, specific internal energy, and velocity to a set of 256 points spaced exactly as in the x-axis solution. This comparison shows the effects of the second-order directional splitting used with FLASH on the resolution of shocks. At the right side of the rarefaction and at the contact discontinuity the diagonal solution undergoes slightly larger oscillations (on the order of a few percent) than the x-axis solution. Also, the value of each variable inside the discontinuity regions differs between the two solutions by up to 10% in most cases. However, the location and thickness of the discontinuities is the same between the two solutions. In general shocks at an angle to the grid are resolved with approximately the same number of zones as shocks parallel to a coordinate axis.

Figure 8 presents a grayscale map of the density at $t = 0.2$ in the diagonal solution together with the block structure of the AMR grid in this case. Note that regions surrounding the discontinuities are maximally refined, while behind the shock and discontinuity the grid has de-refined as the second derivative of the density has decreased in magnitude. Because zero-gradient outflow boundaries were used for this test, some reflections are present at the upper left and lower right corners, but at $t = 0.2$ these have not yet propagated to the center of the grid.

5.3 The Woodward-Colella interacting blast-wave problem

This problem was originally used by Woodward and Colella (1984) to compare the performance of several different hydrodynamical methods on problems involving strong, thin shock structures. It has no analytical solution, but since it is one-dimensional, it is easy to produce a converged solution by running the code with a very large number of zones, permitting an estimate of the self-convergence rate when narrow, interacting discontinuities are present. For FLASH it also provides a good test of the adaptive mesh refinement scheme.

The initial conditions consist of two parallel, planar flow discontinuities. Reflecting boundary conditions are used. The density in the left, middle, and right portions of the grid ($\rho_{\rm L}$, $\rho_{\rm M}$, and $\rho_{\rm R}$, respectively) is unity; everywhere the velocity is zero. The pressure is large to the left and right and small in the center:

$$p_{\rm L} \;=\; 1000 \qquad p_{\rm M} \;=\; 0.01 \qquad p_{\rm R} \;=\; 100\;. \tag{38}$$

The equation of state is that of a perfect gas with $\gamma = 1.4$.

Figure 9 shows the density and velocity profiles at several different times in the converged solution, demonstrating the complexity inherent in this problem. The initial pressure discontinuities drive shocks into the middle part of the grid; behind them, rarefactions form and propagate toward the outer boundaries, where they are reflected back onto the grid and interact with themselves. By the time the shocks collide at $t = 0.028$, the reflected rarefactions have caught up to them, weakening them and making their post-shock structure more complex. Because the right-hand shock is initially weaker, the rarefaction on that side reflects from the wall later, so the resulting shock structures going into the collision from the left and right are quite different. Behind each shock is a contact discontinuity left over from the initial conditions (at $x \approx 0.50$ and 0.73). The shock collision produces an extremely high and narrow density peak; in the Woodward and Colella calculation the peak density is slightly less than 30. Even with ten levels of refinement, FLASH obtains a value of only 18 for this peak. Reflected shocks travel back into the colliding material, leaving a complex series of contact discontinuities and rarefactions between them. A new contact discontinuity has formed at the point of the collision ($x \approx 0.69$). By $t = 0.032$ the right-hand reflected shock has met the original right-hand contact discontinuity, producing a strong rarefaction which meets the central contact discontinuity at $t = 0.034$. Between $t = 0.034$ and $t = 0.038$ the slope of the density behind the left-hand shock changes as the shock moves into a region of constant entropy near the left-hand contact discontinuity.

Figure 10 shows the self-convergence of density and pressure when FLASH is run on this problem. For several runs with different maximum refinement levels, we compare the density, pressure, and total specific energy at $t = 0.038$ to the solution obtained using FLASH with ten levels of refinement. This figure plots the L1 error norm for each variable u, defined using

$$\mathcal{E}(N_{\rm ref}; u) \equiv \frac{1}{N(N_{\rm ref})} \sum_{i=1}^{N(N_{\rm ref})} \left| \frac{u_i(N_{\rm ref}) - u_i(10)}{u_i(10)} \right| \;, \tag{39}$$

against the effective number of zones ($N(N_{\rm ref})$) at the highest level of refinement $N_{\rm ref}$. In computing this norm, both the 'converged' solution $u(10)$ and the test solution $u(N_{\rm ref})$ are interpolated onto a uniform mesh having $N(N_{\rm ref})$ zones. Values of $N_{\rm ref}$ between 2 (corresponding to cell size $\Delta x = 1/16$) and 9 ($\Delta x = 1/2048$) are shown. Although PPM is

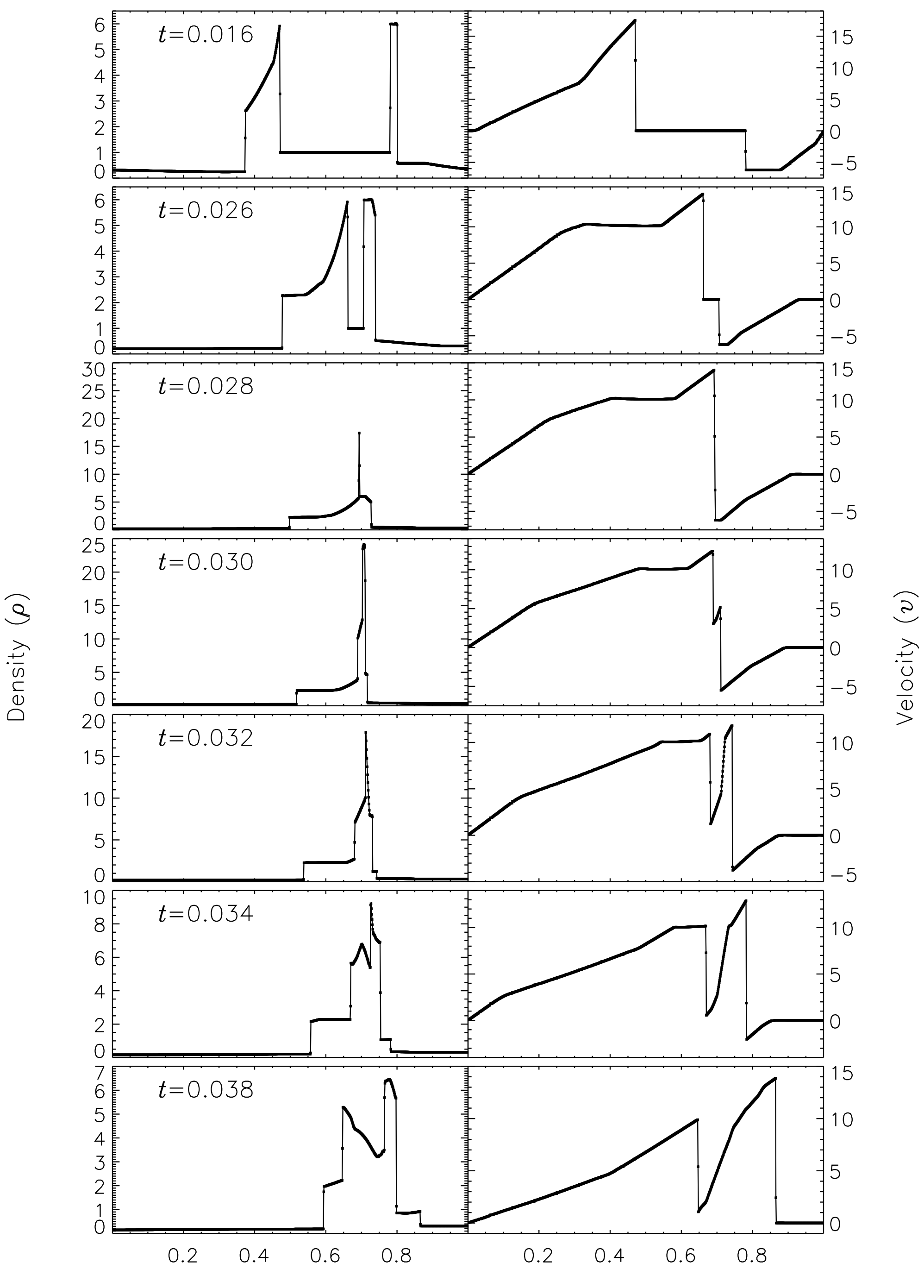


Figure 9: Density and velocity profiles in the Woodward-Colella interacting blast-wave problem, as computed by FLASH using ten levels of refinement.

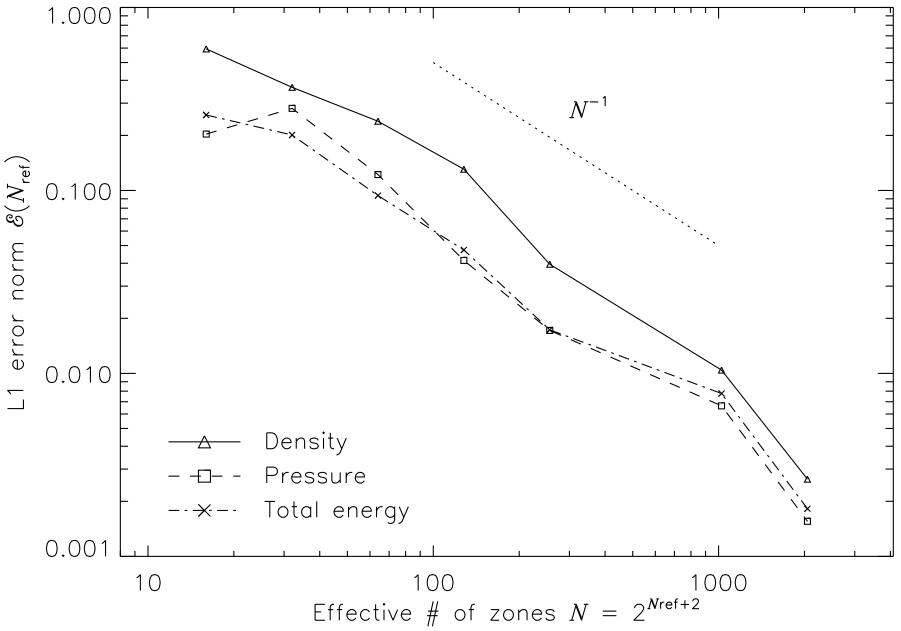


Figure 10: Self-convergence of the density, pressure, and total specific energy in the `2blast` test problem.

Table 2: Runtime parameters used with the `2blast` test problem.

Variable	Type	Default	Description
`rho_left`	real	1	Initial density to the left of the left interface (ρ_L)
`rho_mid`	real	1	Initial density between the interfaces (ρ_M)
`rho_right`	real	1	Initial density to the right of the right interface (ρ_R)
`p_left`	real	1000	Initial pressure to the left (p_L)
`p_mid`	real	0.01	Initial pressure in the middle (p_M)
`p_right`	real	100	Initial pressure to the right (p_R)
`u_left`	real	0	Initial velocity (perpendicular to interface) to the left (u_L)
`u_mid`	real	0	Initial velocity (perpendicular to interface) in the middle (u_L)
`u_right`	real	0	Initial velocity (perpendicular to interface) to the right (u_R)
`xangle`	real	0	Angle made by interface normal with the x-axis (degrees)
`yangle`	real	90	Angle made by interface normal with the y-axis (degrees)
`posnL`	real	0.1	Point of intersection between the left interface plane and the x-axis
`posnR`	real	0.9	Point of intersection between the right interface plane and the x-axis

formally a second-order method, one sees from this plot that, for the interacting blast-wave problem, the convergence rate is only linear. Indeed, in their comparison of the performance of seven nominally second-order hydrodynamic methods on this problem, Woodward and Colella found that only PPM achieved even linear convergence; the other methods were worse. The error norm is very sensitive to the correct position and shape of the strong, narrow shocks generated in this problem.

The additional runtime parameters supplied with the `2blast` problem are listed in Table 2. This problem is configured to use the perfect-gas equation of state (`eos/gamma`), and it is run in a two-dimensional unit box with `gamma` set to 1.4. Boundary conditions in the y direction (transverse to the shock normals) are taken to be periodic.

5.4 The Sedov explosion problem

The Sedov explosion problem (Sedov 1959) is another purely hydrodynamical test in which we check the code's ability to deal with strong shocks and non-planar symmetry. The problem involves the self-similar evolution of a cylindrical or spherical blast wave from a delta-function initial pressure perturbation in an otherwise homogeneous medium. To initialize the code, we deposit a quantity of energy $E = 1$ into a small region of radius δr at the center of the grid. The pressure inside this volume, p_0', is given by

$$p_0' = \frac{3(\gamma - 1)E}{(\nu + 1)\pi\, \delta r^{\nu}} \ , \tag{40}$$

where $\nu = 2$ for cylindrical geometry and $\nu = 3$ for spherical geometry. We set $\gamma = 1.4$. (In running this problem we choose δr to be 3.5 times as large as the finest adaptive mesh resolution in order to minimize effects due to the Cartesian geometry of our grid.) Everywhere the density is set equal to $\rho_0 = 1$, and everywhere but the center of the grid the pressure is set to a small value, $p_0 = 10^{-5}$. The fluid is initially at rest. In the self-similar blast wave which develops for $t > 0$, the density, pressure, and radial velocity are all functions of $\xi \equiv r/R(t)$, where

$$R(t) = C_\nu(\gamma) \left(\frac{Et^2}{\rho_0}\right)^{1/(\nu+2)} \ . \tag{41}$$

Here C_ν is a dimensionless constant depending only on ν and γ; for $\gamma = 1.4$, $C_2 \approx C_3 \approx 1$ to within a few percent. Just behind the shock front at $\xi = 1$ we have

$$\begin{aligned} \rho = \ \rho_1 &\equiv \frac{\gamma+1}{\gamma-1}\rho_0 \\ p = \ p_1 &\equiv \frac{2}{\gamma+1}\rho_0 u^2 \\ v = \ v_1 &\equiv \frac{2}{\gamma+1}u \ , \end{aligned} \tag{42}$$

where $u \equiv dR/dt$ is the speed of the shock wave. Near the center of the grid,

$$\begin{aligned} \rho(\xi)/\rho_1 &\propto \xi^{\nu/(\gamma-1)} \\ p(\xi)/p_1 &= \text{constant} \ . \\ v(\xi)/v_1 &\propto \xi \end{aligned} \tag{43}$$

Figure 11 shows density, pressure, and velocity profiles in the two-dimensional Sedov problem at $t = 0.05$. Solutions obtained with FLASH on grids with 2, 4, 6, and 8 levels of refinement are shown in comparison with the analytical solution. In this figure we have computed average radial profiles in the following way. We interpolated solution values from the adaptively gridded mesh used by FLASH onto a uniform mesh having the same resolution as the finest AMR blocks in each run. Then, using radial bins with the same width as the zones in the uniform mesh, we binned the interpolated solution values, computing the average value in each bin. At low resolutions, errors show up as density and velocity overestimates behind the shock, underestimates of each variable within the shock, and a numerical precursor spanning 1–2 zones in front of the shock. However, the central pressure is accurately determined, even for two levels of refinement; because the density goes to a finite value rather than its correct limit of zero, this corresponds to a finite truncation of the temperature (which should go to infinity as $r \to 0$). As resolution improves, the artificial

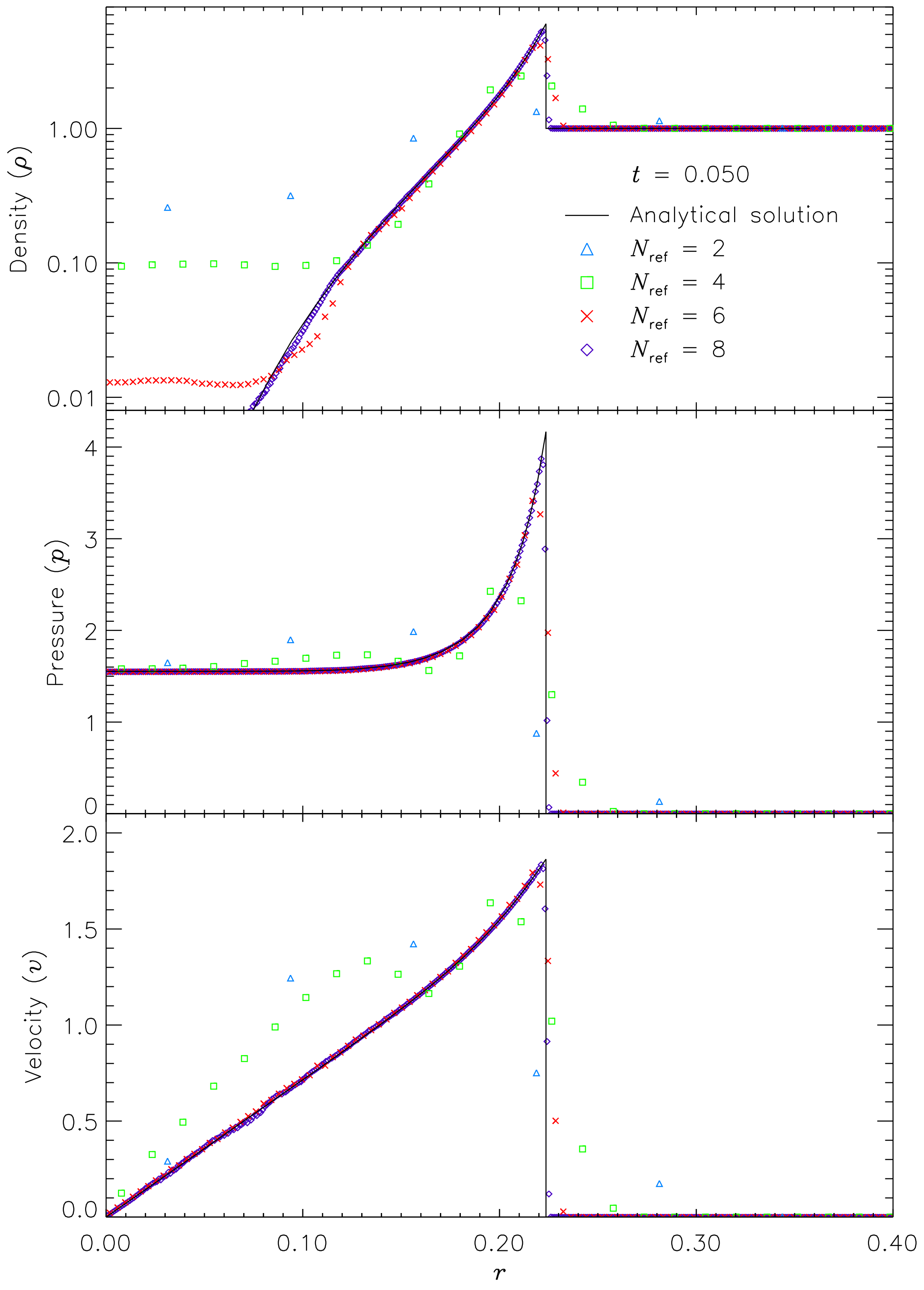


Figure 11: Comparison of numerical and analytical solutions to the Sedov problem in two dimensions. Numerical solution values are averages in radial bins at the finest AMR grid resolution in each run.

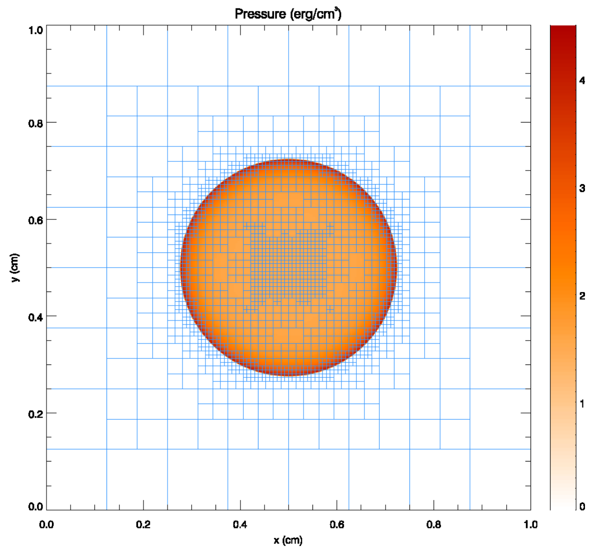


Figure 12: Pressure field in the 2D Sedov explosion problem with 8 levels of refinement at $t = 0.05$. Overlaid on the pressure colormap are the outlines of the AMR blocks.

finite density limit decreases; by $N_{\rm ref} = 6$ it is less than 0.2% of the peak density. Except for the $N_{\rm ref} = 2$ case, which does not show a well-defined peak in any variable, the shock itself is always captured with about two zones. The region behind the shock containing 90% of the swept-up material is represented by four zones in the $N_{\rm ref} = 4$ case, 17 zones in the $N_{\rm ref} = 6$ case, and 69 zones for $N_{\rm ref} = 8$. However, because the solution is self-similar, for any given maximum refinement level the shock will be four zones wide at a sufficiently early time. The behavior when the shock is underresolved is to underestimate the peak value of each variable, particularly the density and pressure.

Figure 12 shows the pressure field in the 8-level calculation at $t = 0.05$ together with the block refinement pattern. Note that a relatively small fraction of the grid is maximally refined in this problem. Although the pressure gradient at the center of the grid is small, this region is refined because of the large temperature gradient there. This illustrates the ability of PARAMESH to refine grids using several different variables at once.

We have also run FLASH on the spherically symmetric Sedov problem in order to verify the code's performance in three dimensions. The results at $t = 0.05$ using five levels of grid refinement are shown in Figure 13. In this figure we have plotted the root-mean-square (RMS) numerical solution values in addition to the average values. As in the two-dimensional runs, the shock is spread over about two zones at the finest AMR resolution in this run. The width of the pressure peak in the analytical solution is about 1 1/2 zones at this time, so the maximum pressure is not captured in the numerical solution. Behind the shock the numerical solution average tracks the analytical solution quite well, although the Cartesian grid geometry produces RMS deviations of up to 40% in the density and velocity in the derefined region well behind the shock. This behavior is similar to that exhibited in the two-dimensional problem at comparable resolution.

The additional runtime parameters supplied with the `sedov` problem are listed in Table

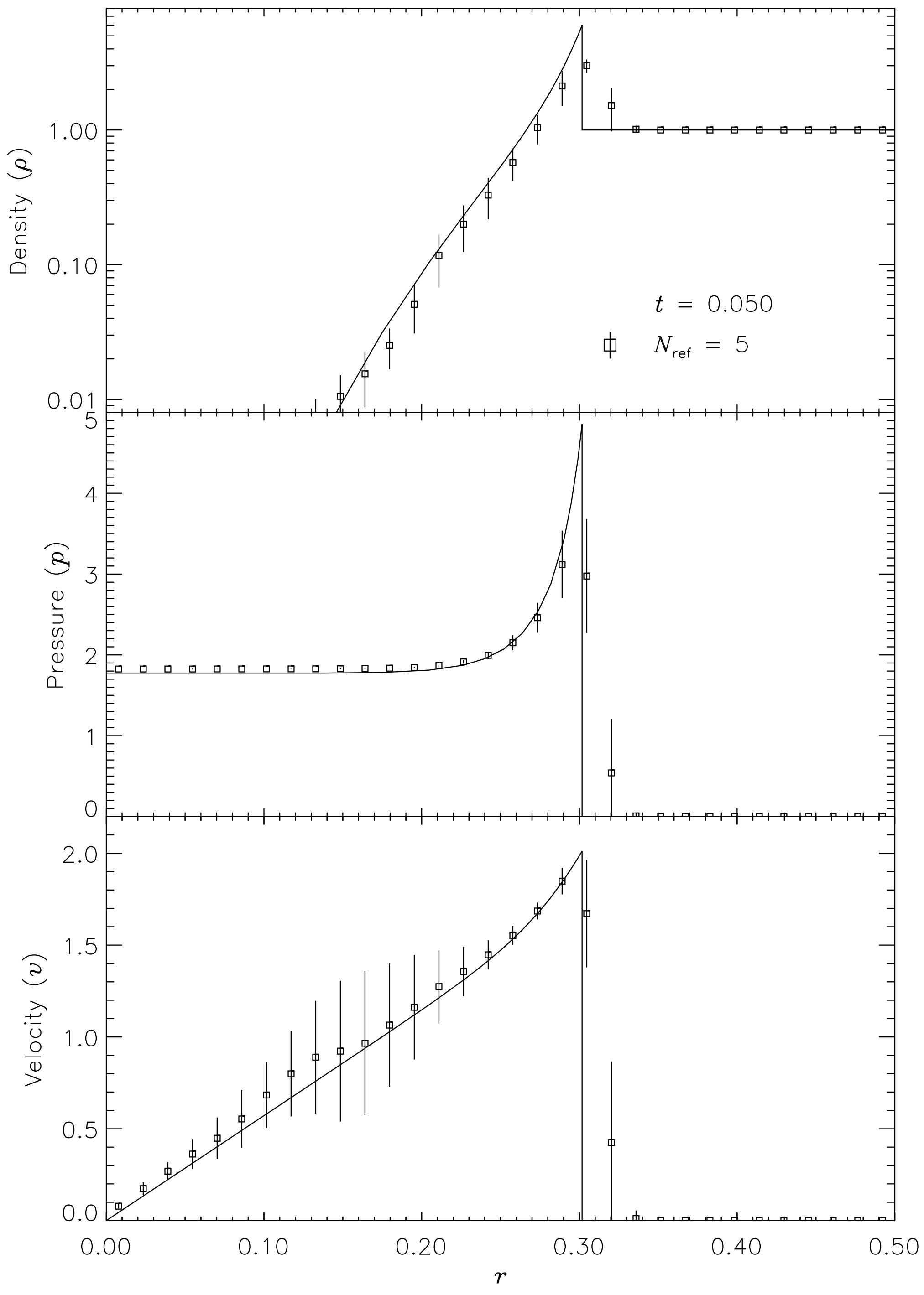


Figure 13: Comparison of numerical and analytical solutions to the spherically symmetric Sedov problem. A 3D grid with five levels of refinement is used.

Table 3: Runtime parameters used with the `sedov` test problem.

Variable	Type	Default	Description
`p_ambient`	real	10^{-5}	Initial ambient pressure (p_0)
`rho_ambient`	real	1	Initial ambient density (ρ_0)
`exp_energy`	real	1	Explosion energy (E)
`r_init`	real	0.05	Radius of initial pressure perturbation (δr)
`xctr`	real	0.5	x-coordinate of explosion center
`yctr`	real	0.5	y-coordinate of explosion center
`zctr`	real	0.5	z-coordinate of explosion center

3. This problem is configured to use the perfect-gas equation of state (`eos/gamma`), and it is run in a unit box with `gamma` set to 1.4.

5.5 The advection problem

In this problem we create a planar density pulse in a region of uniform pressure p_0 and velocity $\mathbf{u}_0$, with the velocity normal to the pulse plane. The density pulse is defined via

$$\rho(s) = \rho_1\phi(s/w) + \rho_0\left[1 - \phi(s/w)\right] \ , \tag{44}$$

where s is the distance of a point from the pulse midplane, w is the characteristic width of the pulse, and the pulse shape function ϕ is, for a square pulse,

$$\phi_{\rm SP}(\xi) = \begin{cases} 1 & |\xi| < 1 \\ 0 & |\xi| > 1 \end{cases} \ , \tag{45}$$

and for a Gaussian pulse,

$$\phi_{\rm GP}(\xi) = e^{-\xi^2} \ . \tag{46}$$

For these initial conditions the Euler equations reduce to a single wave equation with wave speed u_0; hence the density pulse should move across the computational volume at this speed without changing shape. Advection problems similar to this were first proposed by Boris and Book (1973) and Forester (1977).

The advection problem tests the ability of the code to handle planar geometry, as does the Sod problem. It is also like the Sod problem in that it tests the code's treatment of flow discontinuities which move at one of the characteristic speeds of the hydrodynamical equations. (This is difficult because noise generated at a sharp interface, such as the contact discontinuity in the Sod problem, tends to move with the interface, accumulating there as the calculation advances.) However, unlike the Sod problem it compares the code's treatment of leading and trailing contact discontinuities (for the square pulse), and it tests the treatment of narrow flow features (for both the square and Gaussian pulse shapes). Many hydrodynamical methods have a tendency to clip narrow features or to distort pulse shapes by introducing artificial dispersion and dissipation (Zalesak 1987).

Table 4: Runtime parameters used with the `advect` test problem.

Variable	Type	Default	Description
`rhoin`	real	1	Characteristic density inside the advected pulse (ρ_1)
`rhoout`	real	10^{-5}	Ambient density (ρ_0)
`pressure`	real	1	Ambient pressure (p_0)
`velocity`	real	10	Ambient velocity (u_0)
`width`	real	0.1	Characteristic width of advected pulse (w)
`pulse_fctn`	integer	1	Pulse shape function to use: 1=square wave, 2=Gaussian
`xangle`	real	0	Angle made by pulse plane with x-axis (degrees)
`yangle`	real	90	Angle made by pulse plane with y-axis (degrees)
`posn`	real	0.25	Point of intersection between pulse mid-plane and x-axis

The additional runtime parameters supplied with the `advect` problem are listed in Table 4. This problem is configured to use the perfect-gas equation of state (`eos/gamma`), and it is run in a unit box with `gamma` set to 1.4. (The value of γ does not affect the analytical solution, but it does affect the timestep.)

To demonstrate the performance of FLASH on the advection problem, we have performed tests of both the square and Gaussian pulse profiles with the pulse normal parallel to the x-axis ($\theta = 0°$) and at an angle to the x-axis ($\theta = 45°$) in two dimensions. The square pulse used $\rho_1 = 1$, $\rho_0 = 10^{-3}$, $p_0 = 10^{-6}$, $u_0 = 1$, and $w = 0.1$. With six levels of refinement in the domain $[0, 1] \times [0, 1]$, this value of w corresponds to having about 52 zones across the pulse width. The Gaussian pulse tests used the same values of ρ_1, ρ_0, p_0, and u_0, but with $w = 0.015625$. This value of w corresponds to about 8 zones across the pulse width at six levels of refinement. For each test we performed runs at two, four, and six levels of refinement to examine the quality of the numerical solution as the resolution of the advected pulse improves. The runs with $\theta = 0°$ used zero-gradient (outflow) boundary conditions, while the runs performed at an angle to the x-axis used periodic boundaries.

Figure 14 shows, for each test, the advected density profile at $t = 0.4$ in comparison with the analytical solution. The upper two frames of this figure depict the square pulse with $\theta = 0°$ and $\theta = 45°$, while the lower two frames depict the Gaussian pulse results. In each case the analytical density pulse has been advected a distance $u_0 t = 0.4$, and in the figure the axis parallel to the pulse normal has been translated by this amount, permitting comparison of the pulse displacement in the numerical solutions with that of the analytical solution.

The advection results show the expected improvement with increasing AMR refinement level $N_{\rm ref}$. Inaccuracies appear as diffusive spreading, rounding of sharp corners, and clipping. In both the square pulse and Gaussian pulse tests, diffusive spreading is limited to about

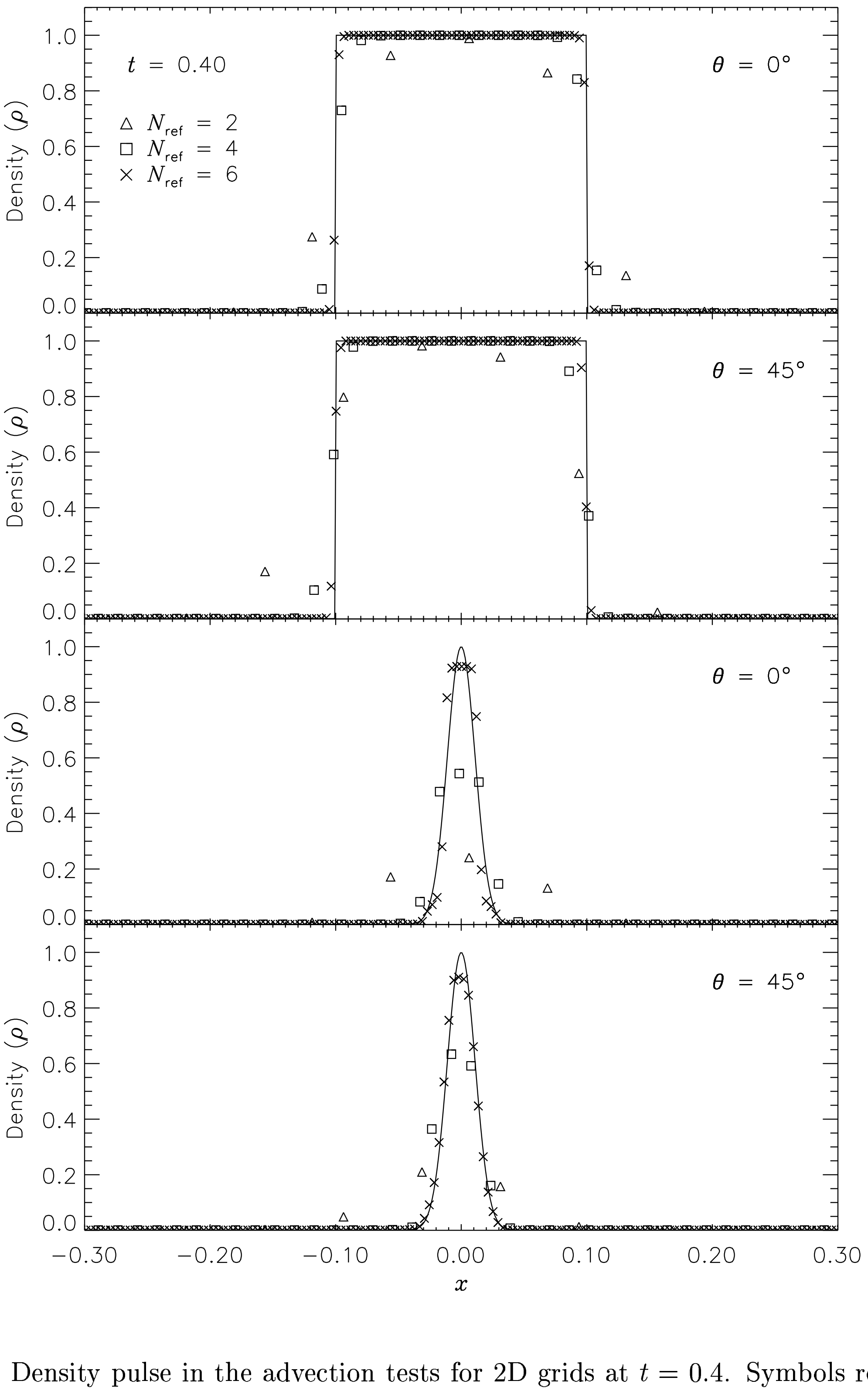


Figure 14: Density pulse in the advection tests for 2D grids at $t = 0.4$. Symbols represent numerical results using grids with different levels of refinement $N_{\rm ref}$ (2, 4, and 6).

one zone on either side of the pulse. For $N_{\rm ref} = 2$ the rounding of the square pulse and the clipping of the Gaussian pulse are quite severe; in the latter case the pulse itself spans about two zones, which is the approximate smoothing length in PPM for a single discontinuity. For $N_{\rm ref} = 4$ the treatment of the square pulse is significantly better, but the amplitude of the Gaussian is still reduced by about 50%. In this case the square pulse discontinuities are still being resolved with 2–3 zones, but the zones are now a factor of 25 smaller than the pulse width. With six levels of refinement the same behavior is observed for the square pulse, while the amplitude of the Gaussian pulse is now 93% of its initial value. The absence of dispersive effects (ie. oscillation) despite the high order of the PPM interpolants is due to the enforcement of monotonicity in the PPM algorithm.

The diagonal runs are consistent with the runs which were parallel to the x-axis, with the possibility of a slight amount of extra spreading behind the pulse. However, note that we have determined density values for the diagonal runs by interpolation along the grid diagonal. The interpolation points are not centered on the pulses, so the density does not always take on its maximum value (particularly in the lowest-resolution case).

These results are consistent with earlier studies of linear advection with PPM (e.g., Zalesak 1987). They suggest that, in order to preserve narrow flow features in FLASH, the maximum AMR refinement level should be chosen so that zones in refined regions are at least a factor 5–10 smaller than the narrowest features of interest. In cases in which the features are generated by shocks (rather than moving with the fluid), the resolution requirement is not as severe, as errors generated in the preshock region are driven into the shock rather than accumulating as it propagates.

5.6 The problem of a wind tunnel with a step

The problem of a wind tunnel containing a step was first described by Emery (1968), who used it to compare several hydrodynamical methods which are only of historical interest now. Woodward and Colella (1984) later used it to compare several more advanced methods, including PPM. Although it has no analytical solution, this problem is useful because it exercises a code's ability to handle unsteady shock interactions in multiple dimensions. It also provides an example of the use of FLASH to solve problems with irregular boundaries.

The problem uses a two-dimensional rectangular domain three units wide and one unit high. Between $x = 0.6$ and $x = 3$ along the x-axis is a step 0.2 units high. The step is treated as a reflecting boundary, as are the lower and upper boundaries in the y direction. For the right-hand x boundary we use an outflow (zero gradient) boundary condition, while on the left-hand side we use an inflow boundary. In the inflow boundary zones we set the density to ρ_0, the pressure to p_0, and the velocity to u_0, with the latter directed parallel to the x-axis. The domain itself is also initialized with these values. For the Emery problem we use

$$\rho_0 = 1.4 \qquad p_0 = 1 \qquad \gamma = 1.4 \qquad u_0 = 3\ , \tag{47}$$

which corresponds to a Mach 3 flow. Because the outflow is supersonic throughout the calculation, we do not expect reflections from the right-hand boundary.

The additional runtime parameters supplied with the `windtunnel` problem are listed in Table 5. This problem is configured to use the perfect-gas equation of state (`eos/gamma`)

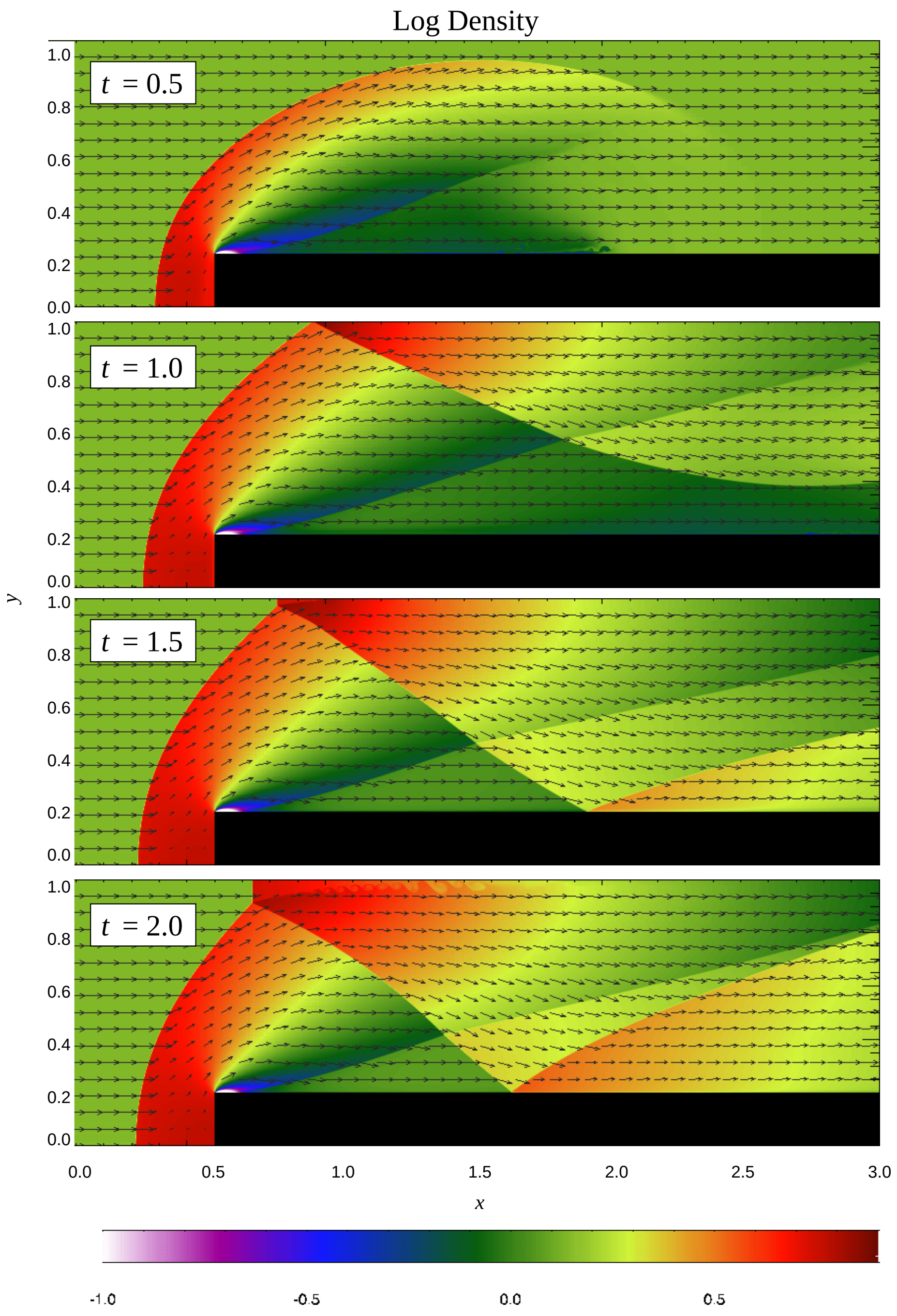


Figure 15: Density and velocity in the Emery wind tunnel test problem, as computed with FLASH. A 2D grid with five levels of refinement is used.

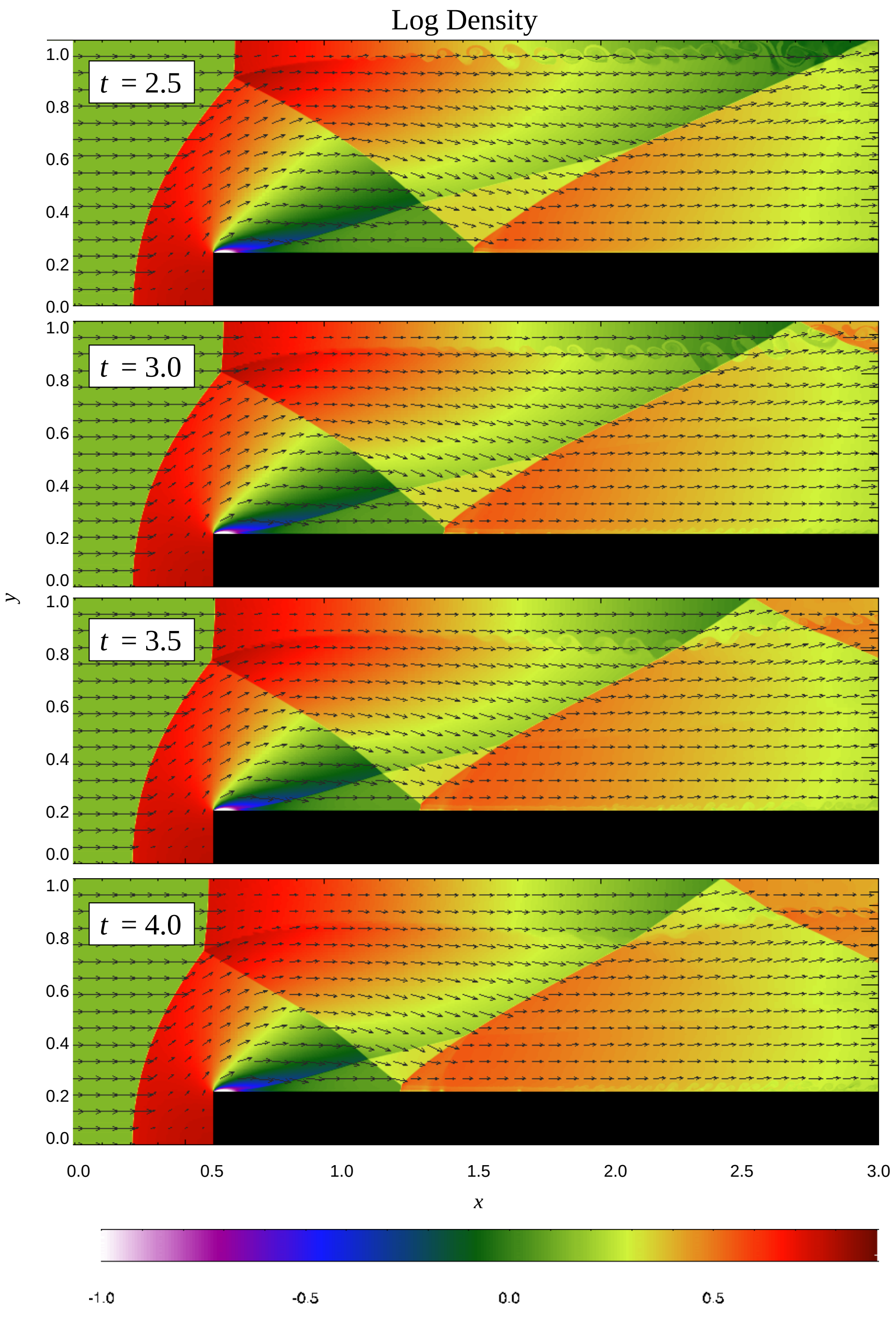


Figure 15: Density and velocity in the Emery wind tunnel test problem (continued).

with `gamma` set to 1.4. We also set `xmax` = 3, `ymax` = 1, `Nblockx` = 15, and `Nblocky` = 4 in order to create a grid with the correct dimensions. The version of `divide_domain` supplied with this problem adds three top-level blocks along the lower left-hand corner of the grid to cover the region in front of the step. Finally, we use `xlboundary` = −23 (user boundary condition) and `xrboundary` = −21 (outflow boundary) to instruct FLASH to use the correct boundary conditions in the x direction. Boundaries in the y direction are reflecting (−20).

Until $t = 12$ the flow is unsteady, exhibiting multiple shock reflections and interactions between different types of discontinuity. Figure 15 shows the evolution of density and velocity between $t = 0$ and $t = 4$ (the period considered by Woodward and Colella). Immediately a shock forms directly in front of the step and begins to move slowly away from it. Simultaneously the shock curves around the corner of the step, extending farther downstream and growing in size until it strikes the upper boundary just after $t = 0.5$. The corner of the step becomes a singular point, with a rarefaction fan connecting the still gas just above the step to the shocked gas in front of it. Entropy errors generated in the vicinity of this singular point produce a numerical boundary layer about one zone thick along the surface of the step. Woodward and Colella reduce this effect by resetting the zones immediately behind the corner to conserve entropy and the sum of enthalpy and specific kinetic energy through the rarefaction. However, we are less interested here in reproducing the exact solution than in verifying the code and examining the behavior of such numerical effects as resolution is increased, so we do not apply this additional boundary condition. The errors near the corner result in a slight overexpansion of the gas there and a weak oblique shock where this gas flows back toward the step. At all resolutions we also see interactions between the numerical boundary layer and the reflected shocks which appear later in the calculation.

By $t = 1$ the shock reflected from the upper wall has moved downward and has almost struck the top of the step. The intersection between the primary and reflected shocks begins at $x \approx 1.45$ when the reflection first forms at $t \approx 0.65$, then moves to the left, reaching $x \approx 0.95$ at $t = 1$. As it moves, the angle between the incident shock and the wall increases until $t = 1.5$, at which point it exceeds the maximum angle for regular reflection (40° for $\gamma = 1.4$) and begins to form a Mach stem. Meanwhile the reflected shock has itself reflected from the top of the step, and here too the point of intersection moves leftward, reaching $x \approx 1.65$ by $t = 2$. The second reflection propagates back toward the top of the grid, reaching it at $t = 2.5$ and forming a third reflection. By this time in low-resolution runs we see a second Mach stem forming at the shock reflection from the top of the step; this results from the interaction of the shock with the numerical boundary layer, which causes the angle of incidence to increase faster than in the converged solution. Figure 16 compares the density field at $t = 4$ as computed by FLASH using several different maximum levels of refinement. Note that the size of the artificial Mach reflection diminishes as resolution improves.

The shear zone behind the first ("real") Mach stem produces another interesting numerical effect, visible at $t = 3$ and $t = 4$: Kelvin-Helmholtz amplification of numerical errors generated at the shock intersection. The wave thus generated propagates downstream and is refracted by the second and third reflected shocks. This effect is also seen in the calculations of Woodward and Colella, although their resolution was too low to capture the detailed eddy structure we see. Figure 17 shows the detail of this structure at $t = 3$ on grids with several different levels of refinement. The effect does not disappear with increasing resolution, for

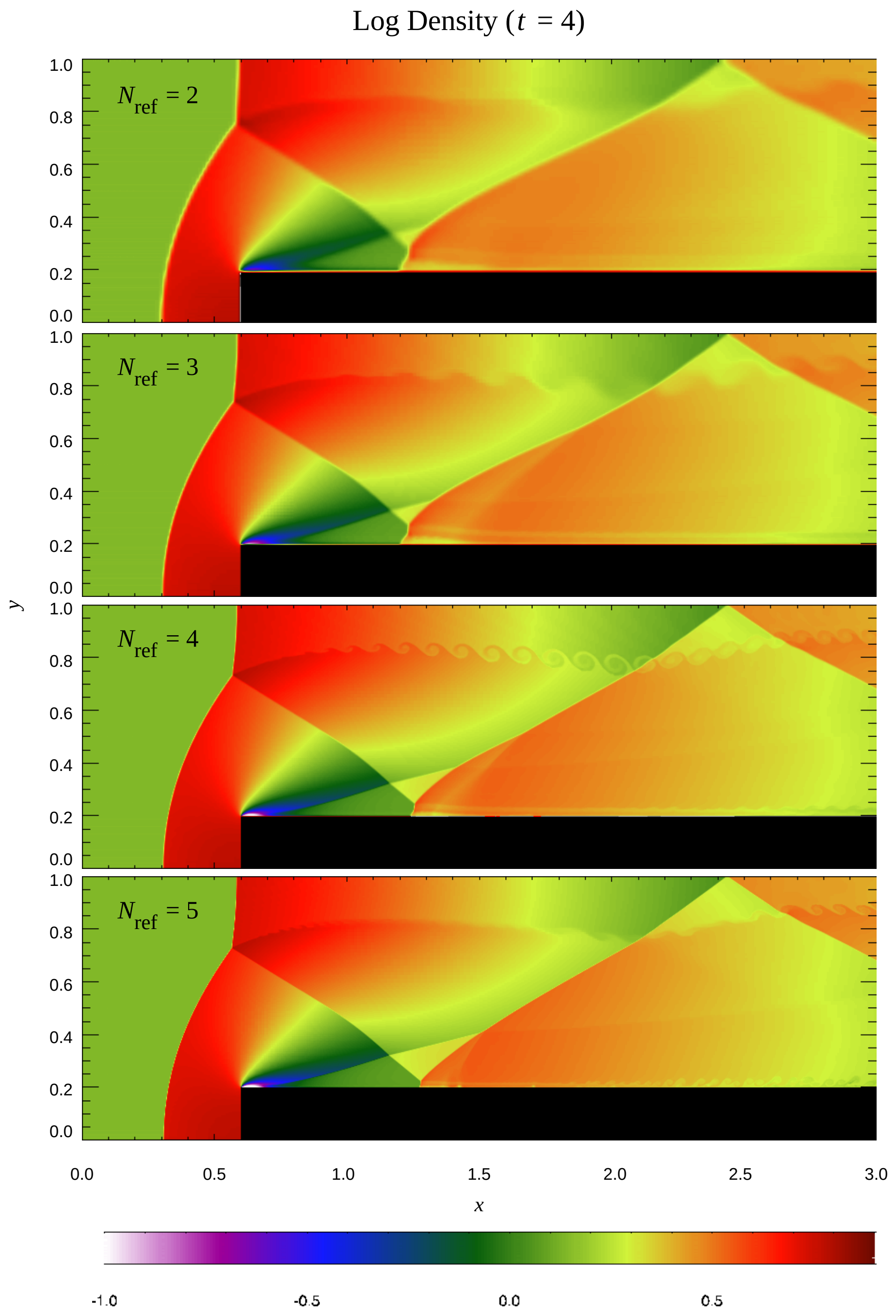


Figure 16: Density at $t = 4$ in the Emery wind tunnel test problem, as computed with FLASH using several different levels of refinement.

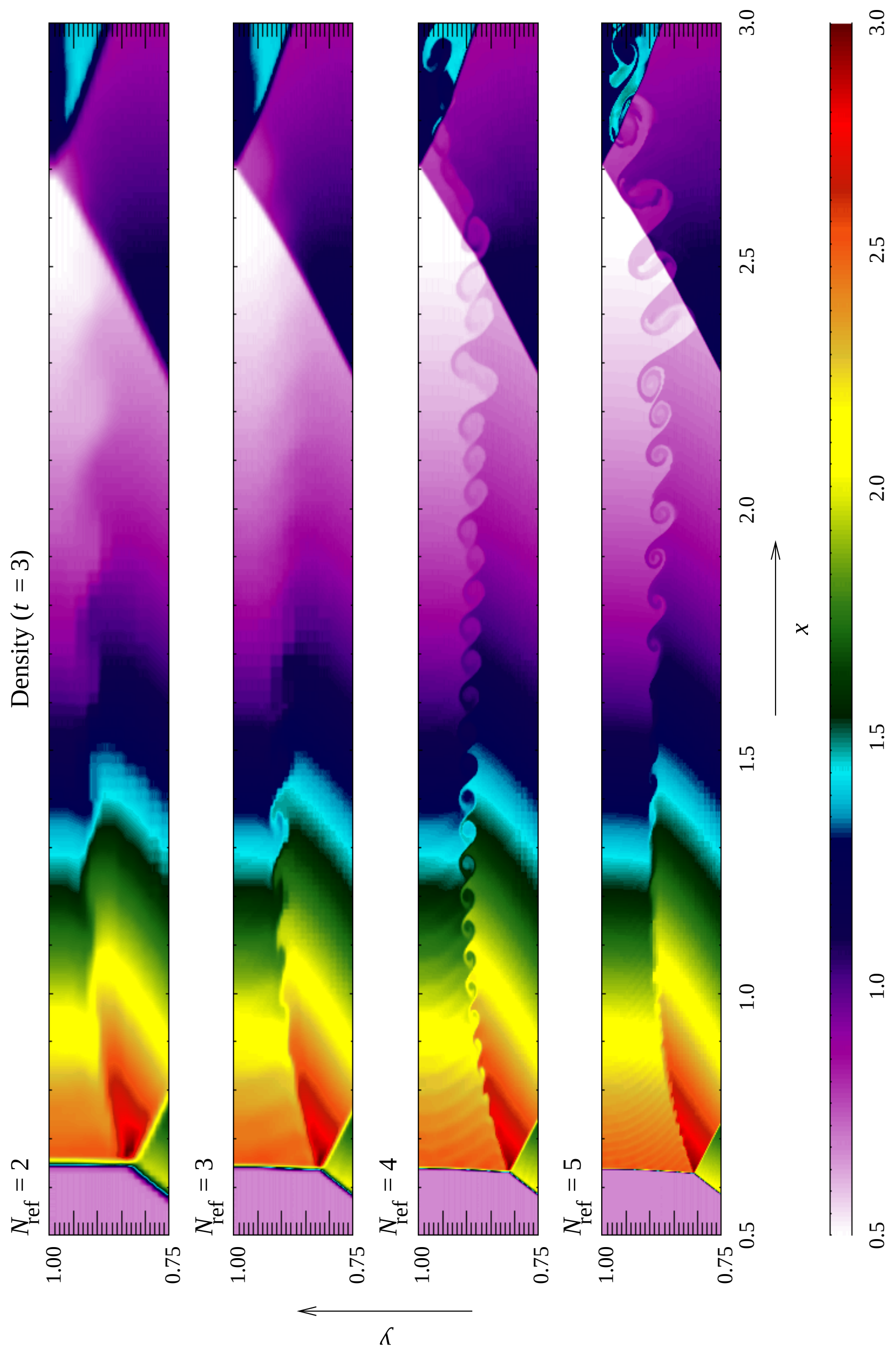


Figure 17: Detail of the Kelvin-Helmholtz instability seen at $t = 3$ in the Emery wind tunnel test problem for several different levels of refinement.

Table 5: Runtime parameters used with the `windtunnel` test problem.

Variable	Type	Default	Description
`p_ambient`	real	1	Ambient pressure (p_0)
`rho_ambient`	real	1.4	Ambient density (ρ_0)
`wind_vel`	real	3	Inflow velocity (u_0)

two reasons. First, the instability amplifies numerical errors generated at the shock intersection, no matter how small. Second, PPM captures the slowly moving, nearly vertical Mach stem with only 1–2 zones on any grid, so as it moves from one column of zones to the next, artificial kinks form near the intersection, providing the seed perturbation for the instability. This effect can be reduced by using a small amount of extra dissipation to smear out the shock, as discussed by Colella and Woodward (1984). This tendency of physical instabilities to amplify numerical noise vividly demonstrates the need to exercise caution when interpreting features in supposedly converged calculations.

Finally, we note that in high-resolution runs with FLASH we also see some Kelvin-Helmholtz rollup at the numerical boundary layer along the top of the step. This is not present in Woodward and Colella's calculation, presumably because their grid resolution is lower (corresponding to two levels of refinement for us) and because of their special treatment of the singular point.

6 Going further with FLASH

FLASH is designed to be easy to configure, use, and extend. Configuration and use involve selecting particular sets of initial and boundary conditions, physics modules, and solution algorithms, as well as setting the values of parameters which control the simulation. Extension involves the addition of new problems, physics, and algorithms to suit the user's requirements. In this section we describe in some detail the structure of the FLASH source code, the format of the configuration files, and the runtime parameters and output formats available. We also discuss the steps a user needs to take in order to customize the code.

6.1 The FLASH code architecture

FLASH 1.0 consists of several modules which perform various high-level tasks, such as driving the code, solving the Euler equations, and solving the nuclear network equations. Figure 18 schematically represents the relationships between these modules. In this figure, a line connecting a higher block to a lower block indicates that the routines in the higher block call routines in the lower block. While most of the modules are represented by a single block, the three major functions of the driver module (initialization, evolution, and input/output) are broken out into separate blocks. This reflects the fact that the driver module included with FLASH 1.0 is oriented toward hyperbolic systems of equations. The PARAMESH library functions as the adaptive mesh refinement (AMR) module in FLASH 1.0 (see Section 2.2 for

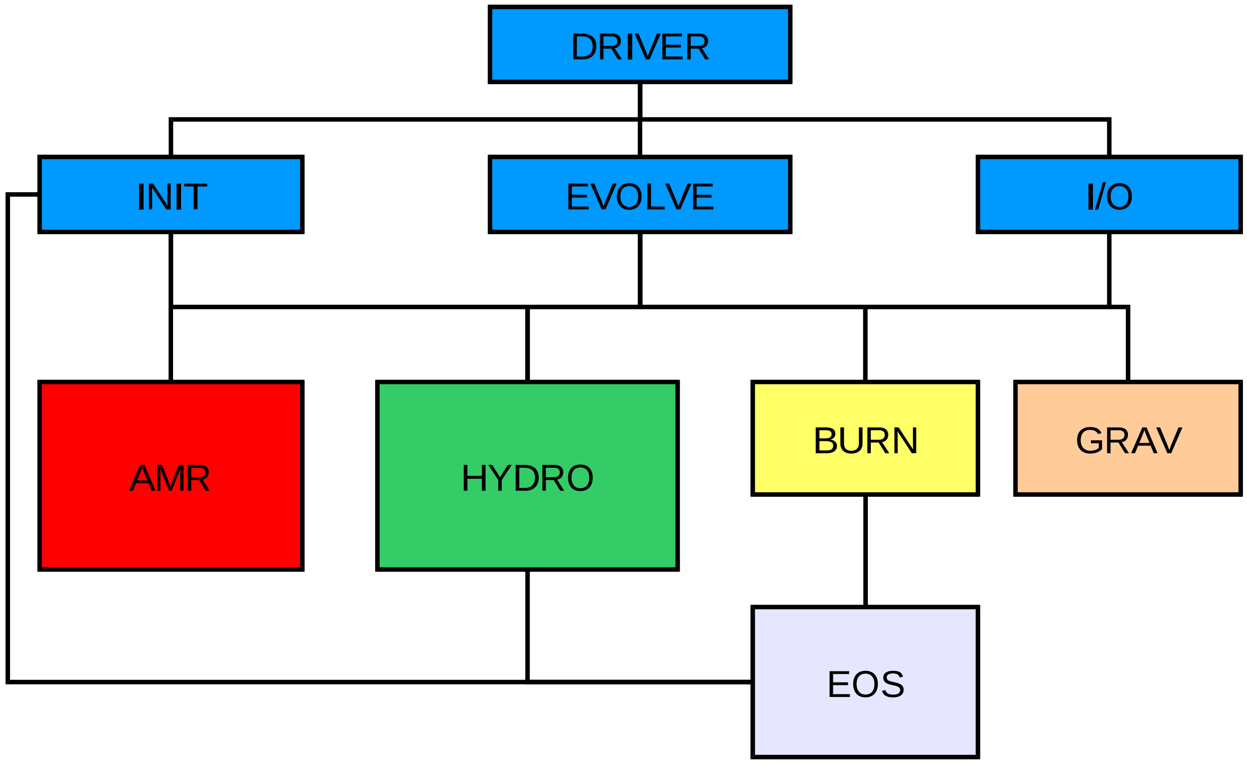


Figure 18: Module interrelationships in the FLASH code.

details).

While modules in FLASH carry out generic high-level functions, often it is desirable to carry out these functions with different types of solver or choices of physics. FLASH uses sub-modules to implement this capability. A sub-module is an optional or alternative collection of routines which implements a specific instance of the general functionality represented by its parent module. Modules can have multiple sub-modules, which may or may not be mutually exclusive. Sub-modules may themselves have sub-modules. Figure 19 shows two examples of module/sub-module relationships in FLASH; one (the EOS) uses sub-modules to implement different physics, while the other (HYDRO) uses sub-modules to implement different types of solver. Code associated with a module is inherited by its sub-modules, so modules can serve as an interface layer between their sub-modules and the rest of the code. This allows different types of solver to be readily plugged in to FLASH, and when no solver for a given piece of physics is needed, the interface layer can provide empty stub routines to other parts of the code which reference the module. The following section provides more detailed information on the organization of FLASH into modules and sub-modules.

Currently data are shared among the different modules in FLASH by means of included common blocks which are part of each module. The driver module supplies the AMR mesh data structure and all runtime parameters globally to all other modules. However, variables used only within a module are declared in that module's include files, which are not included by other modules. While this mechanism does enable module data to be kept "private" if

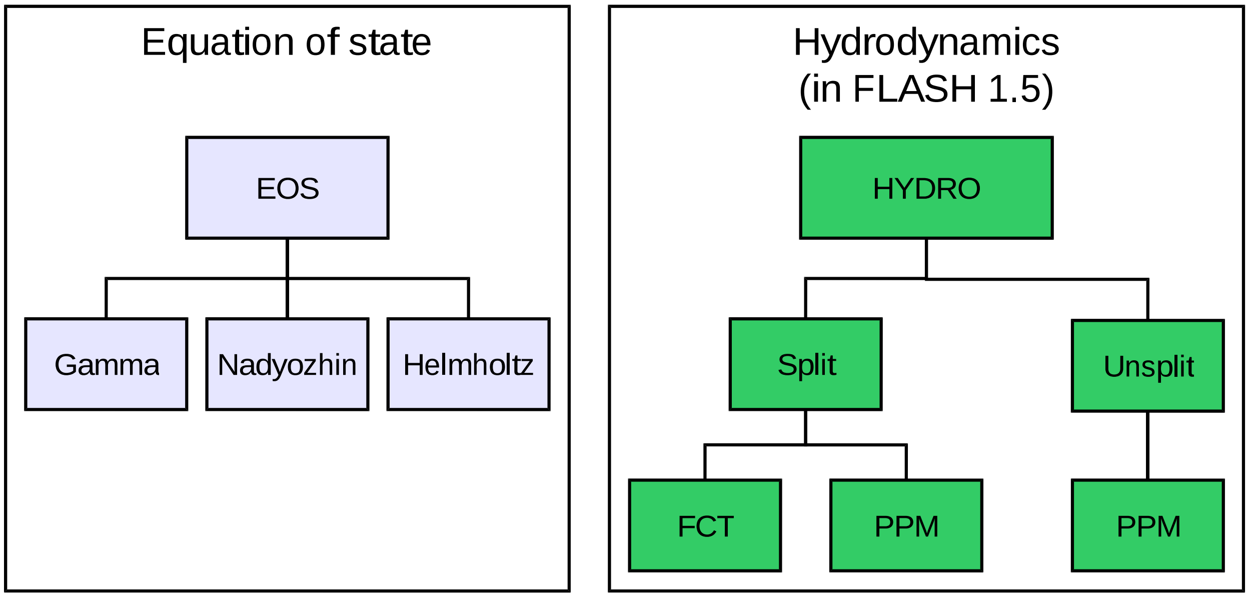


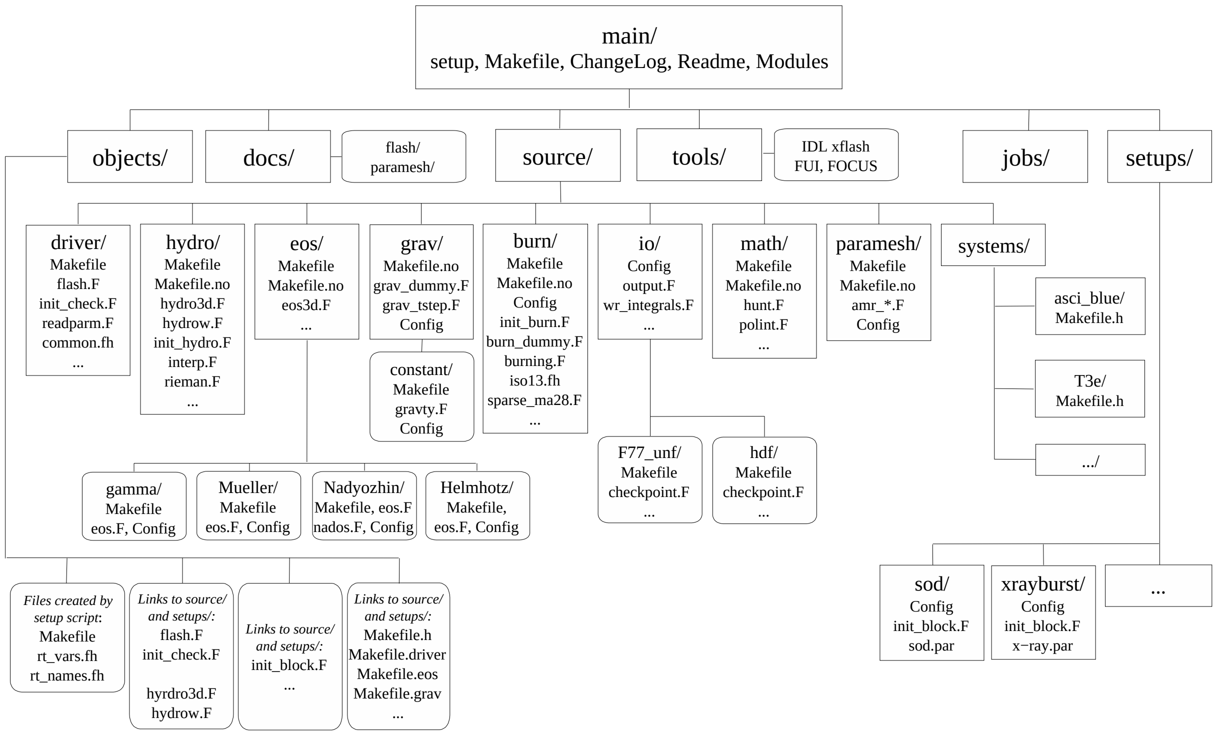
Figure 19: Examples of two uses of sub-modules in FLASH. FLASH 1.5 is the current development version of the code.

module programmers are disciplined, the use of global variables leaves open the possibility that new modules will attempt to redefine variables provided by the driver. In the current development version of FLASH (1.5) we are experimenting with ways to overcome this difficulty without hurting the code's performance. We expect the next version of FLASH to incorporate the use of Fortran 90 derived data types passed as arguments to modules by the driver, with no common blocks shared between modules.

6.1.1 Code infrastructure

The structure of the FLASH source tree is used to organize the source code into (more or less) independent code modules, as shown in Figure 20. The general plan is that source code is organized into one set of directories, while the code is built in a separate directory using links to the appropriate source files. The links are created by a source configuration script called `setup`, which makes the links using options selected by the user and then creates an appropriate makefile in the build directory. The user then builds the executable with a single invocation of `make`.

Source code for each of the different code modules is stored in subdirectories under `source/`. The code modules implement different physics, such as hydrodynamics, nuclear burning, and gravity, or different major program components, such as the main driver code and the input/output code. Each module directory contains source code files, makefile fragments indicating how to build the module, and a configuration file (see Section 6.1.2). For each module, the makefile fragment `Makefile` is used when the module is included in the code, while `Makefile.no` is used when the module is not included (generally it builds a dummy source file containing subroutine stubs).



main/
setup, Makefile, ChangeLog, Readme, Modules
objects/
docs/
flash/ paramesh/
source/
tools/
IDL xflash FUI, FOCUS
jobs/
setups/
driver/ Makefile flash.F init_check.F readparm.F common.fh ...
hydro/ Makefile Makefile.no hydro3d.F hydrow.F init_hydro.F interp.F rieman.F ...
eos/ Makefile Makefile.no eos3d.F ...
grav/ Makefile.no grav_dummy.F grav_tstep.F Config
constant/ Makefile gravty.F Config
burn/ Makefile Makefile.no Config init_burn.F burn_dummy.F burning.F iso13.fh sparse_ma28.F ...
io/ Config output.F wr_integrals.F ...
math/ Makefile Makefile.no hunt.F polint.F ...
paramesh/ Makefile Makefile.no amr_*.F Config
systems/
asci_blue/ Makefile.h
T3e/ Makefile.h
.../
gamma/ Makefile eos.F, Config
Mueller/ Makefile eos.F, Config
Nadyozhin/ Makefile, eos.F nados.F, Config
Helmhotz/ Makefile, eos.F, Config
F77_unf/ Makefile checkpoint.F ...
hdf/ Makefile checkpoint.F ...
Files created by setup script: Makefile rt_vars.fh rt_names.fh
Links to source/ and setups/: flash.F init_check.F hyrdro3d.F hydrow.F
Links to source/ and setups/: init_block.F ...
Links to source/ and setups/: Makefile.h Makefile.driver Makefile.eos Makefile.grav ...
sod/ Config init_block.F sod.par
xrayburst/ Config init_block.F x−ray.par
...

Figure 20: Structure of the FLASH source tree.

Each module subdirectory may also have additional sub-module directories underneath it. These contain code, makefiles, and configuration files specific to different variants of the module. For example, the `hydro/` module directory can contain files which are generic to hydrodynamical solvers, while its `ppm/` subdirectory contains files specific to the piecewise-parabolic method and its `fct/` subdirectory contains files specific to the flux-corrected transport method. Configuration files for other modules which need hydrodynamics can specify `hydro` as a requirement without mentioning a specific solver; the user can then choose one solver or the other when building the code (via the `Modules` file; Section 6.1.3). When `setup` configures the source tree it treats each sub-module as inheriting all of the source code and the configuration file in its parent module's directory, so generic code does not have to be duplicated. However, makefiles in the parent directory are not inherited. Sub-modules can themselves have sub-modules, so for example one might have `hydro/split/ppm` and `hydro/unsplit/ppm`.

New solvers and new physics can be added. At the current stage of development of FLASH it is probably best to consult the authors of FLASH (see Section 7) for assistance in this. Some general guidelines for adding solvers to FLASH 1.0 may be found in Section 6.1.5 and Section 6.3.

An additional subdirectory of `source/` called `systems/` contains code specific to different architectures (eg., `irix` and `t3e`), each of which has its own directory under `systems/`. Each of these directories contains a makefile fragment called `Makefile.h` which is used to set machine-dependent compilation flags and so forth. In addition, special versions of any routines which are needed for each architecture are included in these directories. For example, the T3E needs a special version of `getarg.f`, so `systems/t3e/` contains this file.

The `setups/` directory has a structure similar to that of `source/`. In this case, however, each of the "modules" represents a different initial model or problem, and the problems are mutually exclusive; only one is included in the code at a time. Also, the problem directories have no equivalent of sub-modules. A makefile fragment specific to a problem need not be present, but if it is, it is called `Makefile`. Section 6.2 describes how to add new problem directories.

The setup script creates a directory called `object/` in which the executable is built. In this directory `setup` creates links to all of the source code files found in the specified module and sub-module directories as well as the specified problem directory. (A source code file has the extension `.c`, `.C`, `.f`, `.F`, `.fh`, or `.h`.) Because the problem setup directory and the machine-dependent directory are scanned last, links to files in these directories override the "defaults" taken from the `source/` tree. Hence special variants of routines needed for a particular problem can be used in place of the standard versions by simply giving the files containing them the same names.

Using information from the configuration files in the specified module and problem directories, `setup` creates three files needed to parse the runtime parameter file. The first two, `rt_vars.fh` and `rt_names.fh`, are Fortran include files which declare and set the default values of the parameters and associate them with character strings used for parsing the runtime parameter file. The third, `rt_parms.txt`, concatenates all of the PARAMETER statements found in the appropriate configuration files and so can be used as a "master list" of all of the runtime parameters available to the executable.

`setup` also creates links in `object/` to all of the appropriate makefile fragments (ie.

```
# Configuration file for hydro module

DEFAULT ppm

REQUIRES driver
REQUIRES eos
REQUIRES paramesh

PARAMETER cfl REAL 0.8 # Courant factor
```

Figure 21: Example of a `Config` file used by `setup` to configure a hydro solver module.

`Makefile` for included modules, `Makefile.no` for non-included modules, `Makefile.h` in the system-dependent directory, and `Makefile` in the problem directory). The link names in `object/`, `Makefile.`*module*, are associated with the appropriate fragments in the source directories. The setup script creates a master makefile (`Makefile`) in `object/` which includes all of these fragments.

The master makefile created by `setup` creates a temporary subroutine, `buildstamp.f`, which echoes the date, time, and location of the build to the FLASH log file when FLASH is run. To ensure that this subroutine is regenerated each time the executable is linked, the makefile deletes `buildstamp.f` immediately after compiling it.

The setup script can be run with the `-portable` option to create a directory with real files which can be collected together with `tar` and moved elsewhere for building. In this case the build directory is assigned the name `object_`*problem_machine*`/`. Further information on the options available with `setup` may be found in Section 4.1.

Additional directories included with FLASH are `tools/`, which contains tools for working with FLASH and its output (Section 4); `docs/`, which contains documentation for FLASH (including this user's guide) and the PARAMESH library; and `jobs/`, which contains example job submission scripts for various machines.

6.1.2 Configuration files

Information about module dependencies, default sub-modules, runtime parameter definitions, and so on is stored in plain text files named `Config` in the different module directories. These are parsed by `setup` when configuring the source tree and are used to create the Fortran code needed to implement the runtime parameters, choose sub-modules when only a generic module has been specified, and to flag problems when dependencies are not resolved by some included module. In the future they may contain additional information about module interrelationships. An example `Config` file appears in Figure 21.

The syntax of the configuration files is as follows. Arbitrarily many spaces and/or tabs may be used, but all keywords must be in uppercase. Lines not matching an admissible pattern are ignored. (Someday soon they will generate a syntax error.)

comment A comment. Can appear at the end of a line.

`DEFAULT` *sub-module*

Specify which sub-module of the current module is to be used as a default if a specific sub-module has not been indicated in the `Modules` file (Section 6.1.3). For example, the `Config` file for the `eos` module specifies `gamma` as the default sub-module. If no sub-module is explicitly included (ie. `INCLUDE eos` is placed in `Modules`), then this command instructs `setup` to assume that the `gamma` sub-module was meant (as though `INCLUDE eos/gamma` had been placed in `Modules`).

`REQUIRES` *module[/sub-module[/sub-module...]]*

Specify a module requirement. Module requirements can be general, not specifying sub-modules, so that module dependencies can be independent of particular algorithms. For example, the statement `REQUIRES eos` in a module's `Config` file indicates to `setup` that the `eos` module is needed by this module. No particular equation of state is specified, but some EOS is needed, and as long as one is included by `Modules`, the dependency will be satisfied. More specific dependencies can be indicated by specifying sub-modules. For example, `eos` is a module with several possible sub-modules, each corresponding to a different equation of state. To specify a requirement for, eg., the Nadozhin EOS, use `REQUIRES eos/nadozhin`. Giving a complete set of module requirements is helpful to the end user, because `setup` uses them to generate the `Modules` file when invoked with the `-defaults` option.

`PARAMETER` *name type default*

Specify a runtime parameter. Parameter names are unique up to 20 characters and may not contain spaces. Admissible types are REAL (or DOUBLE), INTEGER, STRING, and BOOLEAN (or LOGICAL). Default values for REAL and INTEGER parameters must be valid numbers, or compilation will fail. Default STRING values can be unquoted (in which case only the first word is recognized) or enclosed in double quotes ("). Default BOOLEAN values must be TRUE or FALSE to avoid compilation errors. Once defined, runtime parameters are available to the entire code; currently there is no mechanism for making them available only to some modules and not to others.

6.1.3 Module files

The `Modules` file, which is created in the FLASH root directory either by the user or by `setup -defaults`, is used by `setup` to specify the particular code modules (and sub-modules) to include. It allows the user to combine desired variants of the different code modules or to use different solution algorithms while still satisfying the dependencies of the different modules. The setup script terminates with an error if all of the dependencies of the different included modules are not satisfied by some other included module. The format of this file is similar to that of the configuration files (Section 6.1.2), but only two types of instruction are recognized:

`#` *comment*	A comment. Can appear at the end of a line.
`INCLUDE` *module[/sub-module[/sub-module...]]*	Specify a module (and optionally a sub-module) to include in the source configuration. If no sub-module is specified, and the configuration file for the specified module has a default sub-module, then that default will be used. For example, if the `eos` module is specified, then its default sub-module `gamma` will be used; if `eos/nadozhin` is specified, then the `nadozhin` sub-module will be used.

An example `Modules` file appears in Figure 4.

6.1.4 Runtime parameters

Runtime parameters are used to control the initial model, the various physics modules, and the behavior of the simulation. They are made available to FLASH via the setup configuration files described in Section 6.1.2. Their values can be set at runtime through the runtime parameter file and can be changed without requiring the user to rebuild the executable.

The runtime parameter file is a plain text file with the following format. Each line is either a comment (denoted by a hash mark, `#`), blank, or of the form *variable* = *value*. String values are enclosed in double quotes (`"`). Boolean values are indicated in the Fortran style, `.true.` or `.false.` Comments may appear at the end of a variable assignment line. An example parameter file may be found in Figure 1.

By default FLASH looks for a parameter file named `flash.par` in the directory from which it is run. An alternative file name can be specified as a command-line argument when FLASH is run.

In Section 6.1.5, Tables 6–11 list the runtime parameters made available by the different code modules included with FLASH. Please see Section 5 for more information on runtime parameters specific to each of the test problems supplied with FLASH.

6.1.5 Code modules

In this section we describe in turn each of the code modules included with FLASH, together with its available sub-modules and runtime parameters. We also discuss the ways in which new solvers or new physics modules must interact with each module in order to work with FLASH 1.0. Tables 6–11 list the runtime parameters for each module. More detailed descriptions of the algorithms included with FLASH may be found in Section 2.

Driver module (`driver`*)*

This module contains the main program and administrative subroutines which are not tied to any specific physics module. The driver module in FLASH 1.0 is oriented toward hyperbolic problems. Hence its major functions include setting initial conditions, calling output routines (which are handled by the `io` module) periodically, and managing the forward time advance of the simulation (including the calculation of the timestep).

The driver module also provides the global data context for FLASH. Most physics modules access this context by including the file `common.fh`, which itself includes the other include files needed by the driver (hence these other files need not be explicitly included). Since `common.fh` and its brethren use preprocessor statements, subroutines which include it have

```
#include "common.fh"
```

as their first statement. The include files included by `common.fh` are:

> `readparm.fh`, which contains declarations needed by the runtime parameter parser, including the runtime parameter buffers;
>
> `rt_vars.fh`, which is generated by `setup` and includes all runtime parameter declarations, their default settings, and their equivalences to the runtime parameter buffers;
>
> `constants.fh`, which contains declarations and settings for physical constants;
>
> `definitions.fh`, which contains code constant declarations;
>
> `physicaldata.fh`, `tree.fh`, `workspace.fh`, and `block_boundary_data.fh`, which contain constant and array declarations for the block-structured mesh data structure used by the code; and
>
> `mpif.h`, which contains Fortran constant declarations for use with the Message-Passing Interface library. This file is provided as part of the MPI distribution, not with FLASH.

Users wishing to use or extend FLASH need not edit any of these files. However, the file `physicaldata.fh` sets two constants, `maxblocks` and `nuc2`, which are important. `maxblocks` sets the maximum number of AMR blocks which may be allocated to a given processor. Normally this may be set at compile time using `setup -maxblocks`. The second constant, `nuc2`, determines the number of nuclear abundances to track. The default value is 13. For problems not requiring nuclear burning, it may be desirable to set this to a smaller value in order to reduce memory usage; however, this is not required. At present `nuc2` can only be changed by editing `physicaldata.fh`. (Note that if you wish to *increase* `nuc2` and turn nuclear burning on, you should also increase the `ionmax` parameter, which is set in `iso13.fh`.)

The main program is contained in the file `flash.F`. It first reads the runtime parameter file and initializes the AMR library and physics modules. Then, depending upon the setting of the `restart` parameter, it calls init_from_scratch() to initialize the grid using the specified initial conditions or init_from_checkpoint() to read the initial conditions from a checkpoint file. The most important functions carried out by init_from_scratch() are the call to divide_domain(), which allocates top-level AMR blocks, and the call to init_block(), which initializes a single block (and is part of the `hydro` module). All problem setups must provide

Table 6: Runtime parameters used with the `driver` module.

Variable	Type	Default	Description
`basenm`	string	chkpnt_	File name prefix for checkpoint files (including the file to start from, if `restart = .true.`)
`nend`	integer	100	Maximum number of timesteps to take before halting the simulation
`nrstrt`	integer	10000	Maximum number of steps to take before creating a checkpoint file
`restart`	boolean	.false.	Set to .true. to restart the simulation from a checkpoint file
`tmax`	real	1	Maximum simulation time to advance before halting the simulation
`trstrt`	real	1	Maximum simulation time to advance before creating a checkpoint file
`dtini`	real	10^{-10}	Initial timestep
`small`	real	10^{-10}	Generic small cutoff value for positive definite quantities
`smlrho`	real	10^{-10}	Cutoff value for density
`smallp/e/t/u/x`	real	10^{-10}	Cutoff values for pressure, energy, temperature, velocity, and nuclear abundances
`nsdim`	integer	2	Grid dimensionality
`x/y/zmin`	real	0	Minimum x, y, and z coordinates for grid
`x/y/zmax`	real	1	Maximum x, y, and z coordinates for grid
`igeomx/y/z`	integer	0	Grid geometry in x, y, and z directions: 0=Cartesian
`nuc`	integer	0	Number of nuclear species to track
`igrav`	integer	0	If set to 1, use gravity
`iburn`	integer	0	If set to 1, use nuclear burning
`CPNumber`	integer	0	Initial checkpoint file number. If restarting from a checkpoint, set this to the number of the file to restart from
`x/y/zlboundary`	integer	-20	Type of external boundary in the $-x$, $-y$, and $-z$ directions: -20=reflecting, -21=outflow, -22=periodic, -23=user-defined
`x/y/zrboundary`	integer	-20	Type of external boundary in the $+x$, $+y$, and $+z$ directions

Table 6: Runtime parameters used with the `driver` module (continued).

Variable	Type	Default	Description
`iref1`	integer	5	Variable to use for the first AMR refinement pass. The second spatial derivative is used to select blocks for refinement. 0=none, 1=density, 2=x-velocity, 5=pressure, 6=energy, 7=temperature, 11=He abundance, 13=Ni abundance
`iref2`	integer	1	Variable for the second AMR pass
`iref3/4`	integer	0	Variables for the third and fourth AMR passes
`Nblockx/y/z`	integer	1	Number of top-level blocks in the x, y, and z directions

a version of init_block(). On the other hand, the divide_domain() subroutine provided with FLASH is fairly general and can set up a top-level mesh with `Nblockx`×`Nblocky`×`Nblockz` blocks. For irregular domains (such as in the `windtunnel` test problem), a special version of divide_domain() should be provided as part of the problem setup. (See Section 6.2 for a discussion of creating new problem setups. The files containing the replacement routines should be given the same names as the originals.)

After initialization the main program calls output_initial() (part of the `io` module) to write a checkpoint file containing the initial conditions and to create the scalar/global file, to which FLASH writes the total energy and other quantities at the end of each timestep.

Following the initial output in `flash.F` is the main evolution loop, consisting of a call to hydro_3d() (which advances the system one timestep), a call to timestep() (which determines the size of the next timestep according to constraints provided by each of the solver modules), and a call to output() (which writes to the scalar/global file and produces checkpoint files at specified intervals). In FLASH 1.0 the evolution routine hydro_3d() is part of the `hydro` module, which is essentially the evolution part of the PROMETHEUS code (Section 2.1). The loop terminates either when `nend` timesteps have been taken or when the simulation time exceeds `tmax`. The last things the main program does are to checkpoint the final timestep and print CPU timing information.

Currently the hydrodynamics, equation of state, gravity, and nuclear burning routines are all called from within hydro_3d(). In FLASH 1.5 the evolution function is taken over from hydro_3d() by a routine called evolve() which is part of the `driver` module. However, since evolution in FLASH 1.0 is handled by a routine which is properly part of the `hydro` module, FLASH 1.0 should always be built with hydrodynamics included. (Alternatively, a new non-hydro physics module might supply a replacement for hydro_3d().) Users wishing to implement new physics modules within FLASH 1.0 should insert calls to their solver routines in hydro_3d(). In order to access the block-structured mesh data, global variables (such as the simulation time and the number of processors), and runtime parameters, new module routines should include `common.fh` as discussed above. With the data structure and modularity enhancements coming in FLASH 1.5 we expect the process of adding a new solver to become much simpler. See Section 6.3 for further general guidelines on adding solvers to FLASH.

Hydrodynamics module (`hydro`*)*

The `hydro` module solves the Euler equations of hydrodynamics (see Section 2.1). The solver included with FLASH 1.0 is directionally split and is based on the piecewise-parabolic method (PPM; Colella & Woodward 1984). Future versions will include sub-modules to handle unsplit PPM and perhaps other hydro algorithms.

As discussed in the previous section, in its current form the `hydro` module handles the evolution function of the `driver` module through the routine hydro_3d(). This routine performs one-dimensional sweeps in the x, y, and z directions, calls the nuclear burning routine (burn()), and then applies these operators in reverse order. Hydrodynamical boundary conditions are set before each 1D sweep by a call to the PARAMESH routine amr_guardcell(). For each sweep, the code cycles through the leaf-node blocks, applying the 1D hydro operator to each in turn. For a single block, hydro_3d() loops over the coordinates transverse to the sweep direction, copying rows of data from the block array to a 1D sweep array (via getrwx(), getrwy(), and getrwz()). For each row, hydrodynamical fluxes are computed with a call to hydrow(); these fluxes are then used to update zones in the interior of the block with update_soln() and in the guard cells with update_soln_boun(). Following the application of each 1D hydrodynamical operator, the hydrodynamical fluxes are corrected to ensure conservation at jumps in refinement with a call to the PARAMESH routine amr_flux_conserve(). At the end hydro_3d() tests the grid refinement with several calls to the PARAMESH amr_test_refinement() routine, then initiates changes in refinement with a call to the PARAMESH amr_refine_derefine() routine.

Three other externally visible routines in the `hydro` module are init_hydro(), which initializes the module by setting the hydrodynamical variables to zero; init_block(), which sets the initial conditions in a single block; and tot_bnd(), which is called by the PARAMESH guard cell filling routines when an external boundary is encountered. The latter two routines are the most important from the standpoint of users wishing to construct a new problem setup (Section 6.2).

In addition to the global common file `common.fh`, the hydrodynamical routines include three other common files: `common_hydro.fh`, which contains declarations for variables specific to 1D hydrodynamical schemes (appropriate to the operator-split implementation in FLASH 1.0); `common_ppm.fh`, which contains declarations specific to the piecewise-parabolic method; and `iso13.fh`, the common file exported by the nuclear burning module and containing information on the nuclear isotopes to track (only used by hydro_3d()).

Equation of state module (`eos`*)*

The `eos` module implements the equation of state needed by the hydrodynamical and nuclear burning solvers. Three sub-modules are available in FLASH 1.0: `gamma`, which implements a perfect-gas equation of state; `nadozhin`, which implements an equation of state appropriate to partially degenerate material at nuclear densities in thermal equilibrium with

Table 7: Runtime parameters used with the `hydro` module.

Variable	Type	Default	Description
`cfl`	real	0.8	Courant-Friedrichs-Lewy (CFL) factor; must be $<$ 1 for stability in explicit schemes
PPM-specific parameters			
`epsiln`	real	0.33	PPM shock detection parameter ϵ
`omg1`	real	0.75	PPM dissipation parameter ω_1
`omg2`	real	10	PPM dissipation parameter ω_2
`igodu`	integer	0	If set to 1, use the Godunov method (completely flatten all interpolants)
`vgrid`	real	0	Scale factor for dissipative grid velocity
`nriem`	integer	10	Number of iterations to use in Riemann solver
`cvisc`	real	0.1	Artificial viscosity constant

Table 8: Runtime parameters used with the `eos` module.

Variable	Type	Default	Description
`gamma`	real	1.6667	Ratio of specific heats for the gas (γ)

radiation (Nadyozhin 1974); and `helmholtz`, which uses a fast Helmholtz free-energy table interpolation to handle the same physics as `nadozhin` (Timmes & Swesty 1999).

The primary interface routine for the `eos` module in FLASH 1.0 is eos3d(), which sets the pressure in an entire block of zones by calling the eos() routine supplied by each equation of state sub-module. The input data for this routine are the density, temperature, and thermal energy for the block (the block's local identification number is passed as an argument, and the block data are referenced through the global common blocks). Usually eos3d() is called when these values have been changed (e.g., by the hydro routines) and the pressure must be made consistent with them again. The eos() routine performs this computation for a row of zones. (Routines in the `eos` module include common files exported by the `hydro` and `burn` modules. For this [and physics] reasons, sensible use of `eos` requires the `hydro` module [and, for `nadozhin` and `helmholtz`, the `burn` module] to be included.) Each sub-module also supplies a routine called eos_fcn() which enables the pressure to be returned for specified values of the density, temperature, energy, and composition, without reference to the grid.

Nuclear burning module (`burn`*)*

The nuclear burning module uses a sparse-matrix semi-implicit ordinary differential equation (ODE) solver to calculate the nuclear burning rate and update the fluid variables accordingly (Timmes 1999). The primary interface routines for this module are init_burn(),

Table 9: Runtime parameters used with the `burn` module.

Variable	Type	Default	Description
`tnucmin`	real	1.1×10^{8}	Minimum temperature in K for burning to be allowed
`tnucmax`	real	1.0×10^{12}	Maximum temperature in K for burning to be allowed
`dnucmin`	real	1.0×10^{-10}	Minimum density (g/cm^3) for burning to be allowed
`dnucmax`	real	1.0×10^{14}	Maximum density (g/cm^3) for burning to be allowed
`ni56max`	real	0.4	Maximum Ni^{56} mass fraction for burning to be allowed

Table 10: Runtime parameters used with the `grav/constant` module.

Variable	Type	Default	Description
`gconst`	real	-981	Gravitational acceleration constant (cm/s^2)

which calls routines to set up the nuclear isotope tables needed by the module; and burn(), which calls the ODE solver and updates the hydrodynamical variables in a single row of a single AMR block. In addition to the global common file `common.fh` and the 1D hydrodynamical common file `common_hydro.fh`, the burning routines include a common file named `iso13.fh` which declares variables shared within the burning module.

Gravity module (`grav`)

The `grav` module sets up the gravitational field; the effects of gravity are handled by the `hydro` module. In FLASH 1.0 the only gravitational field sub-module is `constant`, which creates a uniform acceleration in the x-direction. The next version of FLASH will include a Poisson solver to compute the gravitational field due to the matter on the computational grid. This module supplies two routines: gravty(), which sets the gravitational acceleration in a row of zones, and tstep_grav(), which sets the timestep constraint due to gravitation (currently a no-op).

Input/output module (`io`)

The `io` module handles the output produced by FLASH, in particular the periodic checkpoints and the regular output of total energy, mass, and momentum information. It has two sub-modules, `hdf`, which selects the Hierarchical Data Format (HDF) for checkpoint files, and `f77_unf`, which selects Fortran 77 unformatted output. The HDF output produced by

Table 11: Runtime parameters used with the `paramesh` module.

Variable	Type	Default	Description
`lrefine_max`	integer	1	Maximum number of levels of adaptive mesh refinement (AMR)
`lrefine_min`	integer	1	Minimum AMR refinement level
`nrefs`	integer	2	Number of timesteps to advance before adjusting the grid refinement

`io/hdf` is described in Section 6.1.6.

The primary interface routines for the `io` module are output_initial(), which handles output just after initialization and before the main FLASH timestep loop is entered; output(), which handles periodic output inside the timestep loop; output_final(), which handles output following the completion of the timestep loop; and wr_integrals(), which computes the totals of several quantities, including energy, mass, momentum, and so on, then writes them to an ASCII file named `flash.dat` at the end of each timestep. The checkpoint routines provided by the two sub-modules of `io` are checkpoint_wr(), which writes checkpoint files, and checkpoint_re(), which reads them in.

PARAMESH and related modules (`paramesh`*,* `mmpi`*,* `mpi_amr`*)*

The `paramesh` module supplies the adaptive mesh-refinement (AMR) library used by the rest of FLASH (MacNeice et al. 1999). It supplies a block-structured grid with factor-of-two refinement between levels, as described in Section 2.2. The `mmpi` and `mpi_amr` modules supply routines for translating the shared-memory subroutine calls used by PARAMESH into Message-Passing Interface (MPI) calls. The next version of PARAMESH, which will be included with a future version of FLASH, relies only upon MPI calls, and these modules will cease to be included. See the PARAMESH home page at

`http://esdcd.gsfc.nasa.gov/ESS/macneice/paramesh/paramesh.html`

for further details.

The next version of FLASH will also include a general mesh interface layer, permitting other adaptive mesh packages to be exchanged with PARAMESH if desired.

Math library module (`math`*)*

The `math` module contains miscellaneous mathematical routines which are useful in the other modules, such as a polynomial interpolation routine and a list-searching routine, both drawn from Press et al. (1992).

6.1.6 HDF output produced by FLASH

Currently two output formats for checkpoint files are supported by FLASH: Hierarchical Data Format (HDF) version 4 and Fortran 77 unformatted. HDF is preferred because HDF files are more portable and the format is more extensible. In this section we describe the structure of HDF checkpoint files produced by FLASH so that users can read FLASH output files into programmable visualization packages of their choosing.

With HDF, several different types of data can be combined within the same file. Data objects are specified within a file by means of character labels, and they can be read in any order using the routines provided as part of the HDF interface. See the HDF documentation for further details. Table 12 lists the data objects which FLASH writes to HDF output files. Along with the label of each object is listed its size and type (4-byte integer or 8-byte real). For reference, note that:

`tot_blocks`	=	total number of blocks
`nxb, nyb, nzb`	=	zones/block in each direction
`dimen`	=	number of dimensions
`nvar`	=	number of variables
`nfaces`	=	number of faces/block (= 2×`dimen`)
`nchild`	=	maximum number of child blocks per block ($= 2^{\texttt{dimen}}$)

6.2 Creating new problems

In general, creating new sets of initial conditions is quite straightforward. Most users need only duplicate one of the existing setups and then edit it to suit their needs. Here we list the steps needed in order to create a new problem from scratch; at any step you may wish to copy a file from a similar existing setup and use it as a starting point. For example, to create a problem with plane-parallel symmetry, but in which the plane normal is adjustable, it may be helpful to start with files from the `sod` test problem. Similarly, for cylindrically or spherically symmetric initial conditions the `sedov` problem is a useful starting point.

1. Create a directory in `setups/` with the name of the problem. Move to this directory.

2. Create a setup configuration file named `Config`. The format of this file is described in Section 6.1.2. This tells the setup script which optional code modules are required and which runtime parameters to create.

3. Create code files to set up the problem and do anything else needed. If hydrodynamics is included, at a minimum you must have a file named `init_block.F`, containing a subroutine named init_block() which sets up the density, pressure, velocity, etc. for the gas. If your problem requires special boundary conditions, you should also have a version of the file `tot_bnd.F`, which contains a routine to set the values of fluid variables in the guard cells. If your problem has an irregular boundary, you need a version of the file `divide_domain.F`, which creates the top-level AMR block structure. See one of the supplied problem setups for examples.

   For any files you create in the problem's setup directory with extensions `.C`, `.c`, `.F`, `.f`, `.h`, or `.fh`, the setup script will automatically create links in the `object/` directory. However, they will only be compiled and linked into the executable if you create a makefile for the problem. Files such as `init_block.F`, which have the same name as a

Table 12: Contents of HDF 4 files produced by FLASH.

HDF label	Variable size and type	Description
'total blocks'	1 (int)	Total number of blocks in the calculation
'time'	1 (real)	Simulation time
'timestep'	1 (real)	Timestep taken
'timers'	7 (real)	CPU timing information: 1 – guard cell filling 2 – hydro computations 3 – tree computations 4 – flux computations 5 – eos 6 – burning 7 – io
'number of steps'	1 (int)	Number of steps taken
'refine level'	`tot_blocks` (int)	Refinement level of each block
'node type'	`tot_blocks` (int)	Type of node in the tree structure; node type = 1 is 'good data'
'gid'	`nfaces` + 1 + `nchild`×`tot_blocks` (int)	`gid(:,iblock)` contains the global block IDs of neighbors of block `iblock`. The first argument gives the direction: 1 – minimum x direction 2 – maximum x direction 3 – minimum y direction 4 – maximum y direction 5 – minimum z direction 6 – maximum z direction
'coordinates'	`dimen`×`tot_blocks` (real)	Center coordinates of each block: `coord(1,iblock)` : x coordinate `coord(2,iblock)` : y coordinate `coord(3,iblock)` : z coordinate
'block size'	`dimen`×`tot_blocks` (real)	Dimensions of each block: `size(1,iblock)` : x dimension `size(2,iblock)` : y dimension `size(3,iblock)` : z dimension
'bounding box minimum'	`dimen`×`tot_blocks` (real)	Minimum coordinate values in each block: `bnd_min(1,iblock)` : x minimum `bnd_min(2,iblock)` : y minimum `bnd_min(3,iblock)` : z minimum

Table 12: Contents of HDF 4 files produced by FLASH (continued).

HDF label	Variable size and type	Description
'bounding box maximum'	`dimen`×`tot_blocks` (real)	Maximum coordinate values in each block: `bnd_max(1,iblock)` : x maximum `bnd_max(2,iblock)` : y maximum `bnd_max(3,iblock)` : z maximum
'unknowns'	`nvar`×`nxb`×`nyb`× `nzb`×`tot_blocks`	Simulation data: `unk(n,i,j,k,b)` contains the `b`th block, `n`th variable, zone `(i,j,k)`. Currently `n` has the following interpretation: 1 – density 2 – x velocity 3 – y velocity 4 – z velocity 5 – pressure 6 – energy 7 – temperature 8 – $\gamma_{\rm e}$ 9 – $\gamma_{\rm c}$ 10 – old temperature 11+ – nuclear abundances

file in the included source directories, will simply replace the default files and do not require special treatment. For other files, create a short Makefile (call it that) in the problem setup directory with the contents

```
#-------special files for problem-------
problem = list of object files
#-------end special files---------------
```

where *problem* is the name of your problem.

6.3 Adding new solvers

Adding new solvers (either for new or existing physics) to FLASH is similar in some ways to adding a problem configuration. In general one creates a subdirectory for the solver, placing it under the source subdirectory for the parent module if the solver implements currently supported physics, or creating a new module subdirectory if it does not. Put the source files required by the solver into this directory, then create the following files:

`Makefile`: The make include file for the module should set a macro with the name of the module equal to a list of the object files in the module. Optionally (recommended), add a list of dependencies for each of the source files in the module. For example, the `burn` module's make include file is

```
burn = burning.o odeint_net.o sparse_ma28.o init_burn.o tstep_burn.o

burning.o :  burning.F iso13.fh
odeint_net.o :  odeint_net.F
sparse_ma28.o :  sparse_ma28.F
init_burn.o :  init_burn.F common.fh iso13.fh
tstep_burn.o :  tstep_burn.F common.fh
```

Note that if you are adding a sub-module to a module which previously had no sub-modules, you should move the `Makefile` from the module directory into the sub-module directory and add the new filenames to any that are already there. If the module instead already has sub-modules, copy the `Makefile` from one of them and do the same thing. This ensures that the source files in the module directory are built along with the sub-module. Only the `Makefile` in the last sub-module in a directory path is used by `setup`, so sub-modules should each have a separate `Makefile`.

`Makefile.no`: This make include file is used by `setup` when it is instructed not to include the module. Sub-modules need not have a `Makefile.no`; their parent modules should provide one for them. The contents of `Makefile.no` should be

```
module = module_dummy.o module_dummy.o :  module_dummy.F
```

where *module* is the name of the module.

module`_dummy.F`: This file should contain stub routines to use when the module is not included in the code. Stubs only need to be written for routines which are visible outside the module. If you are writing a sub-module for an existing module, make sure the stub routine file for the parent module contains stubs for any sub-module routines which might be visible outside the module.

`Config`: Create a configuration file for the module or sub-module you are creating. All configuration files in a sub-module path are used by `setup`, so in a sense a sub-module inherits its parent module's configuration. `Config` should declare any runtime parameters you wish to make available to the code when this module is included. It should indicate which (if any) other modules your module requires in order to function, and it should indicate which (if any) of its sub-modules should be used as a default if none is specified when `setup` is run. The configuration file format is described in Section 6.1.2.

Finally, if you are creating a new module (not a sub-module of an existing module), you should add the name of the module to the line beginning

```
    set ALLMODULES = "driver io hydro ...
```

in the setup script. This is a messy requirement at the moment; in the next version of FLASH we expect `setup` to determine for itself what modules are available.

This is all that is necessary to add a module or sub-module to the code. However, it is not sufficient to have the module routines called by the code! If you are creating a new solver for an existing physics module, the module itself should provide the interface layer to the rest of the code. As long as your sub-module provides the routines expected by the interface layer, the sub-module should be ready to work. However, if you are adding a new module (or if your sub-module has externally visible routines – a no-no for the future), you will need to add calls to your externally visible routines. It is difficult to give completely general guidance; here we simply note a few things to keep in mind.

If you wish to be able to turn your module on or off without recompiling the code, create a new runtime parameter (e.g., `use_`*module*) in the `driver` module. You can then test the value of this parameter before calling your externally visible routines from the main code. For example, the `burn` module routines are only called if (`iburn .eq. 1`). (Of course, if the `burn` module is not included in the code, setting `iburn` to 1 will result in empty subroutine calls.)

You will need to add `#include "common.fh"` if you wish to have access to the global AMR data structure. Since this is the only mechanism for operating on the grid data (which is presumably what you want to do) in FLASH 1.0, you will probably want to do this. An alternative, if your module uses a pre-existing data structure, is to create an interface layer which converts the PARAMESH-inspired tree data structure used by FLASH into your data structure, then calls your routines. This will probably have some performance impact, but it will enable you to quickly get things working.

You may wish to create an initialization routine for your module which is called before anything (e.g., setting initial conditions) is done. In this case you should call the routine init_*module*() and place a call to it (without any arguments) in the main driver routine, `flash.F`, which is part of the `driver` module. Be sure this routine has a stub available.

If your solver introduces a constraint on the timestep, you should create a routine named `tstep_`*module*() which computes this constraint. Add a call to this routine in `timestep.F` (part of the `driver` module), using your global switch parameter if you have created one. See this file for examples. Your routine should operate on a single block and take three parameters: the timestep variable (a real variable which you should set to the smaller of itself and your constraint before returning), the minimum timestep location (an integer array with five elements), and the block identifier (an integer). Returning anything for the minimum location is optional, but the other timestep routines interpret it in the following way. The first three elements are set to the coordinates within the block of the zone contributing the minimum timestep. The fourth element is set to the block identifier, and the fifth is set to the current processor identifier (`MyPE`). This information tags along with the timestep constraint when blocks and solvers are compared across processors, and it is printed on stdout by the master processor along with the timestep information as FLASH advances.

Since hydro_3d() handles evolution in FLASH 1.0, you will probably need to add a call to your solver in this routine. This will require you to include the `hydro` module when building FLASH. Alternatively, you can provide a different hydro_3d() which handles the evolution your way, but you will need to put it in a file named something other than `hydro3d.F`, since all source files in all top-level module directories are linked to by `setup` (whether they are required by the linked-to makefiles or not).

Try to limit the number of entry points to your module. This will make it easier to update it when the next version of FLASH is released. It will also help to keep you sane.

6.4 Porting FLASH to other machines

Porting FLASH to new architectures should be fairly straightforward for most Unix or Unix-like systems. For systems which look nothing like Unix, or which have no ability to interpret the setup script or makefiles, extensive reworking of the meta-code which configures and builds FLASH would be necessary. We do not treat such systems here; rather than do so, it would be simpler for us to do the port ourselves. The good news in such cases is that, assuming that you can get the source tree configured on your system and that you have a Fortran 90 compiler and the other requirements discussed in Section 3, you should be able to compile the code without making too many changes to the source. We have generally tried to stick to standard Fortran 90, avoiding machine-specific features.

For Unix-like systems, you should make sure that your system has `csh`, a `make` which permits included makefiles, `awk`, and `sed`. You will need to create a directory in `source/systems/` with the name of your machine/OS type. At a minimum this directory should contain a makefile fragment named `Makefile.h`. The best way to start is to copy one of the existing makefile fragments (eg. for `irix`) to your new directory and modify that. `Makefile.h` sets macros which define the names of your compilers, the compiler and linker flags, the names of additional object files needed for your machine but not included in the standard source distribution, and additional shell commands (such as file renaming and deletion commands) needed for processing the master makefile.

For most Unix systems this will be all you need to do. However, in addition to `Makefile.h` you may need to create machine-specific subroutines which override the defaults included with the main source code. As long as the files containing these routines duplicate the existing routines' filenames, they do not need to be added to the machine-dependent object list in `Makefile.h`; `setup` will automatically find the special routine in the system-specific directory and link to it rather than to the general routine in the main source directories.

An example of such a routine is getarg(), which returns command-line arguments and is used by FLASH to read the name of the runtime parameter file from the command line. This routine is not part of the Fortran 90 standard, but it is available on many Unix systems without the need to link to a special library. However, it is not available on the Cray T3E; instead, a routine named pxfgetarg() provides the same functionality. Therefore we have encapsulated the getarg() functionality in a routine named get_arguments(), which is part of the `driver` module in a file named `getarg.f`. The default version simply calls getarg(). For the T3E a replacement `getarg.f` calling pxfgetarg() is supplied. Since this file overrides a default file with the same name, `getarg.o` does not need to be added to the machine-dependent object list in `source/systems/t3e/Makefile.h`.

7 Contacting the authors of FLASH

FLASH is still under active development, so many desirable features have not yet been included (eg., self-gravity, thermal conduction, radiation transport, etc.). Also, you will most likely encounter bugs in the distributed code. A mailing list has been established for reporting problems with the distributed FLASH code. To report a bug, send email to

`flash_bugs@mcs.anl.gov`

giving your name and contact information and a description of the procedure you were following when you encountered the error. Information about the machine, operating system (`uname -a`), and compiler you are using is also extremely helpful. *Please do not send checkpoint files, as these can be very large.* If the problem can be reproduced with one of the standard test problems, send a copy of your runtime parameter file and your setup options. This situation is very desirable, as it limits the amount of back-and-forth communication needed for us to reproduce the problem. We cannot be responsible for problems which arise with a physics module or initial model you have developed yourself, but we will generally try to help with these if you can narrow down the problem to an easily reproducible effect which occurs in a short program run *and* if you are willing to supply your added source code.

At present no address has been set up for general development questions and comments, but we expect this to change in the near future. Documentation (including this user's guide) and support information for FLASH can be obtained on the World Wide Web at

`http://www.flash.uchicago.edu/flashcode/`

8 References

Aparicio, J. M. 1998, ApJS, 117, 627

Bader, G. & Deuflhard, P. 1983, NuMat, 41, 373

Berger, M. J. & Collela, P. 1989, JCP, 82, 64

Berger, M. J. & Oliger, J. 1984, JCP, 53, 484

Blinnikov, S. I., Dunina-Barkovskaya, N. V., & Nadyozhin, D. K. 1996, ApJS, 106, 171

Boris, J. P. & Book, D. L. 1973, JCP, 11, 38

Burgers, J. M. 1969, Flow Equations for Composite Gases (New York: Academic)

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

Chapman, S. & Cowling, T. G. 1970, The Mathematical Theory of Non-uniform Gases (Cambridge: CUP)

Colella, P. & Glaz, H. M. 1985, JCP, 59, 264

Colella, P. & Woodward, P. 1984, JCP, 54, 174

DeZeeuw, D. & Powell, K. G. 1993, JCP, 104, 56

Duff, I. S., Erisman, A. M., & Reid, J. K. 1986, Direct Methods for Sparse Matrices (Oxford: Clarendon Press)

Emery, A. F. 1968, JCP, 2, 306

Fletcher, C. A. J. 1991, Computational Techniques for Fluid Dynamics, 2d ed. (Berlin: Springer-Verlag)

Forester, C. K. 1977, JCP, 23, 1

Fryxell, B. A., Müller, E., & Arnett, D. 1989, in Numerical Methods in Astrophysics, ed. P. R. Woodward (New York: Academic)

Godunov, S. K. 1959, Mat. Sbornik, 47, 271

Itoh, N., Hayashi, H., Nishikawa, A., & Kohyama, Y. 1996, ApJS, 102, 411

Khokhlov, A. M. 1997, Naval Research Lab memo 6406-97-7950

Löhner, R. 1987, Comp. Meth. App. Mech. Eng., 61, 323

MacNeice, P., Olson, K. M., Mobarry, C., de Fainchtein, R., & Packer, C. 1999, CPC, accepted

Nadyozhin, D. K. 1974, Nauchnye informatsii Astron, Sov. USSR, 32, 33

Parashar M., 1999, private communication (http://www/caip.rutgers.edu/~parashar/DAGH)

Press, W. H., Teukolsky, S. A., Vetterling, W. T., & Flannery, B. P. 1992, Numerical Recipes in Fortran, 2d ed. (Cambridge: CUP)

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

Sod, G. 1978, JCP, 27, 1

Strang, G. 1968, SIAM J. Numer. Anal., 5, 506

Timmes, F. X. 1999, ApJS, in press

Timmes, F. X. & Arnett, D. 1999, ApJS, in press

Timmes, F. X. & Swesty, F. D. 1999, ApJS, in press

van Leer, B. 1979, JCP, 32, 101

Wallace, R. K., Woosley, S. E., & Weaver, T. A. 1982, ApJ, 258, 696

Warren, M. S. & Salmon, J. K. 1993, in Proc. Supercomputing 1993 (Washington, DC: IEEE Computer Soc.)

Weaver, T. A., Zimmerman, G. B., & Woosley, S. E. 1978, ApJ, 225, 1021

Williams, F. A. 1988, Combustion Theory (Menlo Park: Benjamin-Cummings)

Woodward, P. & Colella, P. 1984, JCP, 54, 115

Zalesak, S. T. 1987, in Advances in Computer Methods for Partial Differential Equations VI, eds. Vichnevetsky, R. and Stepleman, R. S. (IMACS), 15