Various Hydro Solvers in FLASH3

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FLASH3 Tutorial
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Hydro Solvers in FLASH3

- In FLASH3, “Hydro” unit houses more than one usual gas dynamics solver:
  - Pure hydrodynamics (i.e., gas dynamics) solvers (PPM & MUSCL-Hancock)
  - Magnetohydrodynamics (MHD) solvers (Unsplit Staggered Mesh & 8-wave)
  - Relativistic hydrodynamics (RHD) solver

- The Hydro unit is organized into two different subunits depending on how you treat multidimensional flux updates:
  - Operator (dimensional) Splitting (Strang, 1968) vs. Unsplit (Colella, 1990; Lee & Deane, 2009)
    - source/Hydro/HydroMain/split (PPM, 8-wave MHD, RHD)
    - source/Hydro/HydroMain/unsplit (Staggered Mesh MHD, MUSCL-Hancock pure-Hydro)

- All these five major different solvers are based on high-order Godunov (1959) method which involves:
  - Finite volume method
  - Predictor-corrector
  - Riemann problem
  - Explicit time advancement
Physics of Hydro Solvers

- Pure hydrodynamics solvers (PPM & MUSCL-Hancock)
  - Compressible reactive gas dynamics
  - Can solve a broad range of (astro)physical problems

- MHD solvers (Unsplit Staggered Mesh & 8-wave)
  - Flows of conducting fluids (ionized gases, liquid metals) in presence of magnetic fields
  - Plasma is a completely ionized gas, consisting of freely moving positively charged ions (or nuclei) and negatively charged electrons
  - Lorentz forces act on charged particles and change their momentum and energy. In return, particles alter strength and topology of magnetic fields.
  - A valid macroscopic model of magnetized plasma $\rightarrow$ MHD

- Relativistic hydrodynamics solver (RHD)
  - A wide variety of astrophysical flows exhibit relativistic behavior
  - Accretion around compact objects, jets in extragalactic radio sources, pulsar winds, gamma ray bursts
Operator Splitting vs. Unsplit Formulations

\[ \frac{\partial U}{\partial t} + \nabla \cdot \text{Flux} = 0 \]

\[ \frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = 0 \]
Operator Splitting vs. Unsplit Formulations

\[ \frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = 0 \]

**Splitting**

\( X^{\Delta t} : \)

PDE: \( U_t + F(U)_x = 0 \)

IC: \( U^n \)

\[ \begin{array}{c}
\Delta t \\
U^{n+1/2}
\end{array} \]

\( Y^{\Delta t} : \)

PDE: \( U_t + G(U)_y = 0 \)

IC: \( U^{n+1/2} \)

\[ \begin{array}{c}
\Delta t \\
U^{n+1}
\end{array} \]

1\textsuperscript{st} order Strang Splitting

\[ U^{n+1} = X^{\Delta t} Y^{\Delta t} U^n \]

2\textsuperscript{nd} order Strang Splitting

\[ U^{n+1} = (X^{\Delta t/2} Y^{\Delta t/2}) (Y^{\Delta t/2} X^{\Delta t/2}) U^n \]

**Unsplit**

PDE: \( U_t + F(U)_x + G(U)_y = 0 \)

IC: \( U(x, y, t^n) = U^n \)
Splitting vs. Unsplit

source/Hydro/HydroMain

/split

• PPM
• MHD_8Wave
• RHD

• Easy to implement
• Robust, stable, efficient
• Less memory and computation
• Good enough for gas dynamics
• Bad for MHD

/unsplit

• Hydro_MusclHancock
• MHD_StaggeredMesh

• Not easy to implement a robust & stable solver
• More memory and computation
• Good for preserving symmetries
• Very important for MHD!
Hydro Solvers Primer – Split solvers

- **Piecewise-parabolic method solver (PPM) (Fryxell et al., 2000)**
  - Parabolic interpolation of data over each cell (Colella and Woodward, 1984)
    - (Ideally) $3^{rd}$ order, (formally) $2^{nd}$ order, (practically) $1^{st}$ order in shocks and discontinuities in spatial discretization
    - High resolution with accuracy (smooth flows)
    - Monotonicity enforcement, interpolant flattening, steepening of contact discontinuities
  - $2^{nd}$ order in explicit time evolution using operator splitting formulation

- Cellular detonation
- Rayleigh-Taylor instability
- Gravitationally confined detonation
- Turbulent Nuclear Burning
Hydro Solvers Primer – Split solvers

- **MHD 8-wave solver (Timur Linde, 1999)**
  - Monotone Upstream-centered Scheme for Conservation Laws (MUSCL) approach (Van Leer, 1977)
    - 2nd order in space, 2nd order in time
    - Magnetic monopoles (8th wave) are convected away, rather than accumulated (Powell et al., 1998) (i.e., $\nabla \cdot B \neq 0$)
  - Non-conservative formulation of the MHD governing equations
  - Incorrect jump conditions and incorrect propagation speeds across discontinuities
  - Robust and accurate (as compared to the basic conservative scheme)

Orszag-Tang  
Shock-Cloud Interaction  
Magnetic reconnection  
Magnetic RT
Hydro Solvers Primer – Split solvers

- **Special Relativistic solver (RHD) (A. Mignone, 2004)**
  - PPM (3rd order in space) and PLM (2nd order) interpolations
  - 2nd order in explicit time evolution using operator splitting formulation
  - (special) relativistic effects are twofold:
    - kinematical, \( v \sim c \) (\( \gamma = 1/(1 - v^2)^{1/2} >> 1 \))
    - thermodynamical, \( c_s \sim c \)
  - Relativistic flows with \( \gamma > (3/2)^{1/2} \) are always supersonic, and therefore shock-capturing methods are essential (Martí and Müller, 2003)

\[ \gamma = 10 \text{ Jet} \]

Relativistic Shock tube

2-D Riemann Problem

Jet through collapsars (GRB), \( \gamma \sim 50 \)

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Hydro Solvers Primer – Unsplit solvers

- **Unsplit pure-Hydro solver (Lee, 2009)**
  - Reduced version of USM-MHD solver without magnetic and electric fields
  - 2nd order MUSCL-Hancock in space and time
  - Preserves better flow symmetries (Roe solver + Carbuncle instability fix)

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Unsplit MUSCL-Hancock

Split PPM
Hydro Solvers Primer – Unsplit solvers

- **Unsplit Staggered Mesh (USM) MHD solver (Lee, 2006; Lee and Deane 2009)**
  - A very efficient new data reconstruction algorithm
    - MUSCL-Hancock (2nd order in space) type characteristic tracing method
    - No extra Riemann problems for transverse fluxes!
  - A new way of treating multidimensional MHD source terms in unsplit formulation
  - Constrained Transport (CT) algorithm (Evans and Hawley, 1988; Balsara and Spicer, 1999) for induction equations to maintain $\nabla \cdot \mathbf{B} = 0$ on a staggered grid
    - cell-centered, face-centered, corner (edge-centered) variables
  - Enhanced solution accuracy in calculating electric fields for the induction equations (modified electric field construction)
    - Added proper amount of numerical dissipation – important!
Hydro Solvers Primer – Unsplit solvers

- **Unsplit Staggered Mesh (USM) MHD solver (Lee. 2006: Lee and Deane 2009)**

![3D Staggered Mesh Diagram]
Why unsplit formulation is necessary for MHD?

- Operator splitting MHD schemes cannot avoid erroneous growth in $B_z$:

$$\frac{\partial B_z}{\partial t} + B_z \frac{\partial u}{\partial x} - B_x \frac{\partial w}{\partial x} - w \frac{\partial B_x}{\partial x} + u \frac{\partial B_z}{\partial x} + B_z \frac{\partial v}{\partial y} - B_x \frac{\partial w}{\partial y} + w \frac{\partial B_y}{\partial y} + v \frac{\partial B_z}{\partial y} = 0$$

$$w \nabla \cdot \mathbf{B} = w(\Delta B_{x,i}/\Delta x + \Delta B_{y,j}/\Delta y)$$

Unsplit Staggered Mesh solver

Split 8-wave solver

2D Field Loop advection test
More on the USM-MHD solver

- **Physics**
  - Ideal and non-ideal flows
    - Magnetic resistivity, thermal conductivity, and viscosity
  - EOS
    - Ideal gamma, multiple gamma, Helmholtz (degenerate EOS)
  - Gravity
  - Multiple species, particles
  - Well tested for wide ranges of plasma flows: \(10^{-6} < \beta \left( \equiv \frac{p}{B_p} \right) < 10^6\)

- **Implementations and algorithms**
  - Riemann solvers
    - Roe (default), HLLE, HLLC, HLLD (robust and accurate, suggested for most plasma flows)
    - Carbuncle, even-odd instability fix for Roe solver
  - Strong shock-rarefaction detect algorithm (Balsara)
  - Various slope limiters (Minmod, MC, Van Leer, hybrid)
  - Two prolongation methods of divergence-free B fields on AMR
  - Use of face-centered variables, and edge-centered variable
  - Wide ranges of CFL limit: CFL < 1 for 1D, 2D and 3D
Applications

High Mach Number MHD Turbulence

Brio-Wu MHD shock-tube

3D Field Loop advection

Rotor

Magnetic Reconnection

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How to Setup a New Problem

- MHD Simulation (especially with the USM solver) should be located in
  - source/Simulation/SimulationMain/magnetoHD/
  - Special prolongation for face-centered variables

- Create Simulation_initBlock.F90 exactly as you would do for hydro. Just do not forget to set magnetic field variables (both cell-centered and cell face-centered) in the initialization routine.
  - Magnetic fields need to satisfy $\nabla \cdot \mathbf{B} = 0$

- Do not add magnetic pressure to total specific energy, because FLASH EOS routines assume a specific expression for it.

- Create Config and flash.par files for your own Simulation directory.

- Special care in writing custom boundary conditions in Grid_bcApplyToRegionSpecialized.F90.

- Write custom functions and do not forget to add them to Makefile. Such custom functions in your Simulation directory will override other standard implementations.
Example – Config

# Configuration file for Orszag Tang MHD vortex problem
# (Orszag and Tang, J. Fluid Mech., 90:129--143, 1979)

REQUIRES physics/Hydro/HydroMain
REQUIRES physics/Eos/EosMain/Gamma

USESETUPVARS withParticles

IF withParticles
    PARTICLETYPE passive INITMETHOD lattice MAPMETHOD quadratic
    
    REQUIRES Particles/ParticlesMain
    REQUESTS IO/IOMain
    REQUESTS IO/IOParticles
    REQUESTS Particles/ParticlesMapping/Quadratic
    REQUESTS Particles/ParticlesInitialization/Lattice
ENDIF

D tiny Threshold value used for numerical zero
PARAMETER tiny REAL 1.e-16

# ------------------ For Resistive MHD setup ------------------#
#REQUIRES physics/materialProperties/Conductivity/ConductivityMain/Constant-diff
#REQUIRES physics/materialProperties/Viscosity/ViscosityMain
#REQUIRES physics/materialProperties/MagneticResistivity/MagneticResistivityMain
#REQUIRES physics/sourceTerms/Diffuse/DiffuseMain

#VARIABLE vecz # vector potential Az
#------------------ End of Resistive MHD setup ------------------#
# DivB control switch
killdivb = .true.

# Flux Conservation for AMR
flux_correct = .true.

# Switches specific to the unsplit staggered mesh MHD solver

## I. Interpolation scheme:
order = 2 # Interpolation order (First/Second order)
slopeLimiter = "mc" # Slope limiters (mimod, mc, vanLeer, hybrid, limited)
LimitedSlopeBeta = 1. # Slope parameter for the "limited" slope by Toro
charLimiting = .true. # Characteristic limiting vs. Primitive limiting

## II. Magnetic (B) and Electric (E) fields:
E_modification = .true. # High order algorithm for E-field construction
energyFix = .true. # Update magnetic energy using staggered B-fields
ForceHydroLimit = .false. # Pure Hydro Limit (B=0)
prolMethod = "injection_prol" # Prolongation method (injection_prol, balsara_prol)

## III. Riemann solvers:
RiemannSolver = "Roe" # Roe, HLL, HLLC, HLLD, LF
shockInstabilityFix = .false. # Carbuncle instability fix for the Roe solver
entropy = .false. # Entropy fix for the Roe solver

## IV. Strong shock handling scheme:
shockDetect = .false. # Shock detect for numerical stability

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Example – setup lines

- ./setup magnetoHD/OrszagTang -auto -2d +usm (+8wave) -opt (-debug)
  -objdir=OT2D -with-unit=Particles +pm3 (+pm4dev) -nxb=8 -nyb=8
  - Irefine_min = 1, Irefine_max = 6

- ./setup magnetoHD/Rotor -auto -2d +usm -opt +ug –nxb=200 –nyb=300
  - iProcs = 2, jProcs = 2

- ./setup magnetoHD/Rotor -auto -2d +usm -opt +nofbs
  - iGridSize = 400, jGridSize = 600, iProcs = 2, jProcs = 2

More shortcuts can be found in
- /bin/setup_shortcuts.txt
- Users can add their own customized shortcut(s) by editing the file
/bin/setup_shortcuts.txt

# Choice of Grid
grid:unit=Grid:
ug:+grid:Grid=UG:
pm2:+grid:Grid=PM2:
pm40:+grid:Grid=PM40:
pm3:+pm40
pm4dev:+grid:Grid=PM4DEV:ParameshLibraryMode=True

# Choice of MHD solver
# NOTE: The 8wave mhd solver only works with the native interpolation.
8wave:--with-unit=physics/Hydro/HydroMain/split/MHD_8Wave:+grid:--grid-interpolation=native

# NOTE: If pure hydro mode used with the USM solver, add +pureHydro in setup
usm:--with-unit=physics/Hydro/HydroMain/unsplit/MHD_StaggeredMesh:--without-unit=physics/Hydro/HydroMain/split/MHD_8Wave
pureHydro:physicsMode=hydro
unsplithydro:--with-unit=physics/Hydro/HydroMain/unsplit/Hydro_MusclHancock
Tips on setting up your problems

- Simulation’s Config file contains all default runtime parameter values specific to your problem
- default.par is also generated in your object directory
- Flash.h, setup_units, setup_vars, setup_params, etc
- Always helpful to read FLASH user’s guide
- Further read/refer references to understand the various roles/effects on using different choices of runtime parameters
  - e.g., Roe vs. HLL-type Riemann solvers
- Use “-debug” for testing
- Many (simple) issues come from wrong initializations and wrong boundary conditions
  - Simplify your issues as much as possible
  - Detailed description on your issues/bugs is always welcome
    - Your simulation files, flash.par, log files, boundary conditions, compilers, setup lines, etc.
Tips in general

- Make sure you know your problem
  - Literature research
  - IC, BC, units
  - Any working example?
  - Working on FLASH3

- Comments, comments, and comments – keep your journal

- Useful books and references:
  - LeVeque, Finite volume methods for hyperbolic problems
  - Toro, Riemann solvers and numerical methods for fluid dynamics
  - Laney, Computational gas dynamics
  - Goedbloed and Poedts, Principles of Magnetohydrodynamics
  - NRL plasma formulary
  - FLASH user’s guide

- Ask around good people!
Ideal MHD Equations

\[
\frac{\partial}{\partial t}\begin{pmatrix}
\rho \\
V \\
\rho E \\
B
\end{pmatrix} + \nabla \cdot \begin{pmatrix}
\rho V \\
\rho VV + (p + \frac{B^2}{2})\mathbf{I} - \mathbf{B}\mathbf{B} \\
V(\rho E + p + \frac{B^2}{2}) - \mathbf{B}(\mathbf{V} \cdot \mathbf{B}) \\
\mathbf{V}\mathbf{B} - \mathbf{B}\mathbf{V}
\end{pmatrix} = 0
\]

**Major Properties:**

- MHD equations form a hyperbolic system \(\rightarrow\) Seven families of waves (entropy, Alfvén and fast and slow magnetoacoustic waves).
- Convex space of physically admissible variables if convex EOS.
- Non-convex flux function \(\rightarrow\) Multiple degeneracies in the eigensystem, possibility of compound waves, shock evolutionarity concerns.

**Important to remember:** Fluid (Euler) equations are not the limiting case of MHD equations in the \(B \to 0\) case in strict mathematical sense.
MHD Equations in FLASH3

\[
\begin{align*}
\frac{\partial \rho}{\partial t} &+ \nabla \cdot (\rho \mathbf{v}) = 0 \\
\frac{\partial \rho \mathbf{v}}{\partial t} &+ \nabla \cdot (\rho \mathbf{v} \mathbf{v} - \mathbf{B} \mathbf{B}) + \nabla p_s = \rho \mathbf{g} + \nabla \cdot \mathbf{\tau} \\
\frac{\partial \rho \mathbf{E}}{\partial t} &+ \nabla \cdot (\mathbf{v} (\rho \mathbf{E} + p_s) - \mathbf{B} (\mathbf{v} \cdot \mathbf{B})) = \rho \mathbf{g} \cdot \mathbf{v} + \nabla \cdot (\mathbf{v} \cdot \mathbf{\tau} + \sigma \nabla T) + \nabla \cdot (\mathbf{B} \times (\eta \nabla \times \mathbf{B})) \\
\frac{\partial \mathbf{B}}{\partial t} &+ \nabla \cdot (\mathbf{v} \mathbf{B} - \mathbf{B} \mathbf{v}) = -\nabla \times (\eta \nabla \times \mathbf{B})
\end{align*}
\]

where

\[
\begin{align*}
p_s &= p + \frac{B^2}{2}, \\
\mathbf{E} &= \frac{1}{2} \mathbf{v}^2 + \epsilon + \frac{1}{2} \frac{B^2}{\rho}, \\
\mathbf{\tau} &= \mu \left( (\nabla \mathbf{v}) + (\nabla \mathbf{v})^T - \frac{2}{3} (\nabla \cdot \mathbf{v}) \right)
\end{align*}
\]

- Advective terms are discretized using slope-limited TVD scheme.
- Diffusive terms are discretized using central finite differences.
- Time integration is done using one-stage Hancock scheme.
- Directions are either split or unsplit.
Overview on Numerical MHD codes

- Numerical MHD
  - Finite difference method (e.g., ZEUS code by Stone & Norman, 1992)
  - High order Godunov method – high resolution shock capturing approach

- Two major algorithmic progresses in high order Godunov based MHD codes
  - Multidimensional integration algorithm
    - split vs. unsplit
    - Donor cell method
    - Corner transport upwind (CTU), Colella 1990

- Divergence-free constraint on B
  - Hodge projection
    - Zachary et al, 1994; Crockett et al, 2005
  - Constrained transport (CT)

- Non-conservative formulation
  - Powell (et al), 1994; 1999; Falle et al, 1998; Dedner et al, 2002
Overview on Numerical MHD codes

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USM scheme
Applications

Orszag-Tang

Shock-Cloud Interaction

Self-Gravitating Plasma

Magnetic RT

Jet Launching

Surface Gravity Wave

Rising bubble

Magnetic reconnection

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Beyond Plain MHD

Plasma effects

- Reduced 2D Hall (Grasso et al, 1999)
- Electron inertia and compressibility
- 3D Hall MHD and two-fluid MHD

\[ E + V \times B = \frac{1}{S} J + \frac{d_e^2 dJ}{n dt} + \frac{d_i}{n} (J \times B - \nabla \cdot \tilde{P}_e) \]

Relativistic MHD

\[ \frac{\partial W}{\partial t} + (\nabla \cdot F)^T = 0 \]

\[ W = \begin{pmatrix} \Gamma \rho \\ \Gamma^2 \frac{e+p}{c^2} u + \frac{1}{c^2} S_A \\ B \\ \left( \Gamma^2 (e+p) - p - \Gamma \rho c^2 + e_A \right) \end{pmatrix}, \quad F = \begin{pmatrix} \Gamma \rho \mathbf{u} \\ \frac{\Gamma^2}{c^2} (e+p) \mathbf{uu} + p \mathbf{1} + \mathbf{P}_A \\ \mathbf{uB} - \mathbf{Bu} \\ \left[ (\Gamma^2 (e+p) - \Gamma \rho c^2) \mathbf{u} + S_A \right] \end{pmatrix}^T \]

\[ \Gamma = \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}}, \quad e_A = \frac{1}{2 \mu_0} \left( B^2 + \frac{1}{c^2} E^2 \right), \]

\[ S_A = \frac{1}{\mu_0} (E \times B), \quad \mathbf{P}_A = e_A \mathbf{I} - \frac{1}{\mu_0} \mathbf{BB} - \frac{1}{\mu_0 c^2} EE. \]
Field Loop advection in 3D
Gardiner & Stone (2008)
Current Sheet Problem with different plasma beta values (magnetic field lines are shown)

$t = 0$
Numerical Results on Benchmarked problems (2)

Current Sheet Problem with different plasma beta values (magnetic field lines are shown)

\[
\begin{align*}
\beta &= 10^{-3} & \beta &= 10^{-4} & \beta &= 10^{-5} & \beta &= 10^{-6} \\
\end{align*}
\]

\[
\begin{align*}
t &= 2 \\
\end{align*}
\]

\[
\begin{align*}
t &= 6 \\
\end{align*}
\]

\[
\begin{align*}
t &= 10 \\
\end{align*}
\]
Other Applications