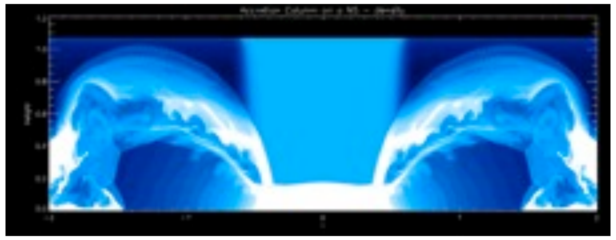
The Center for Astrophysical Thermonuclear Flashes

Capabilities and Applications

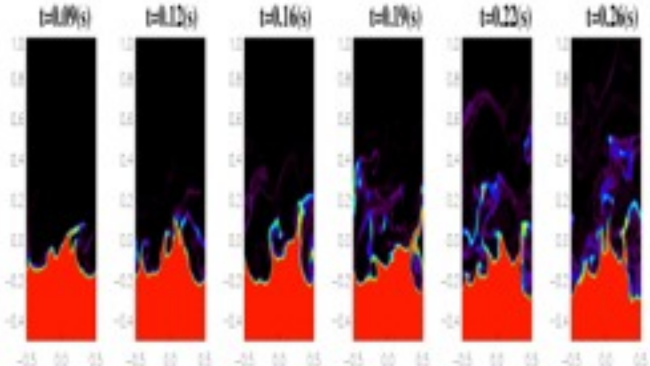
Sean Couch

An Advanced Simulation & Computing (ASC)
Academic Strategic Alliances Program (ASAP) Center
at The University of Chicago

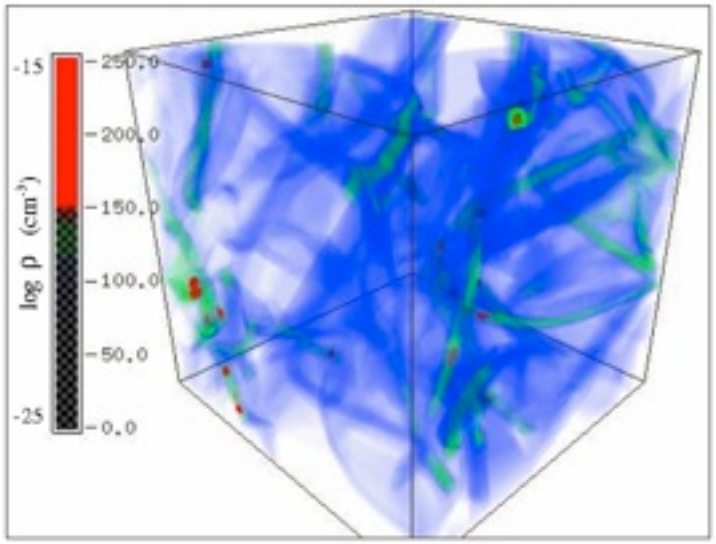
FLASH Capabilities Span a Broad Range…



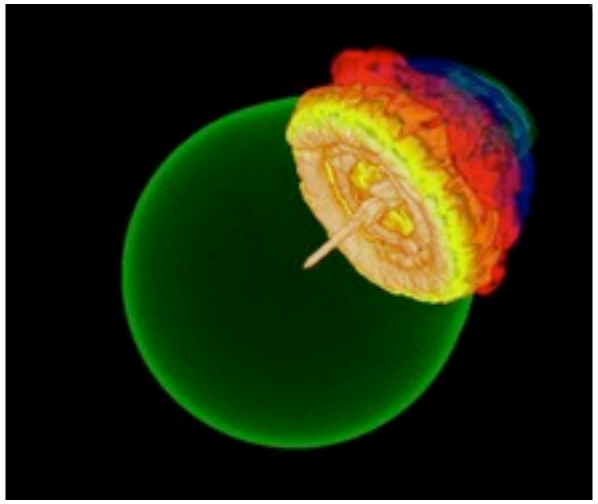
Shortly: Relativistic accretion onto NS



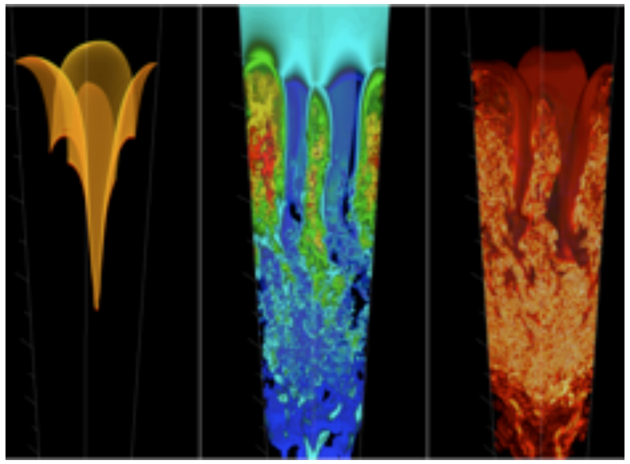
Wave breaking on white dwarfs



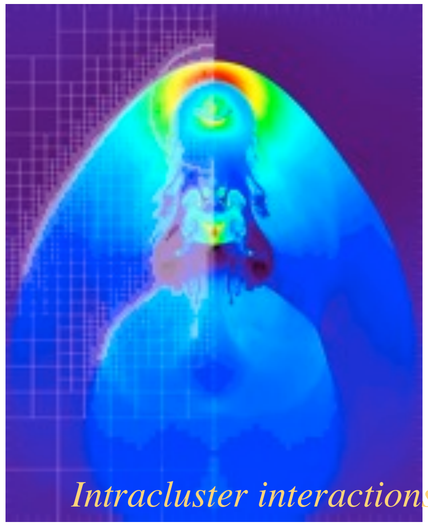
Gravitational collapse/Jeans instability



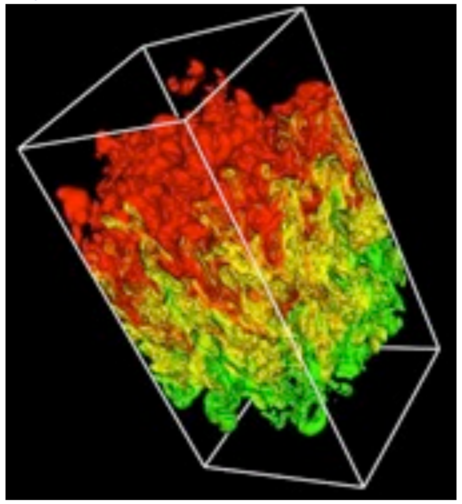
Gravitationally confined detonation



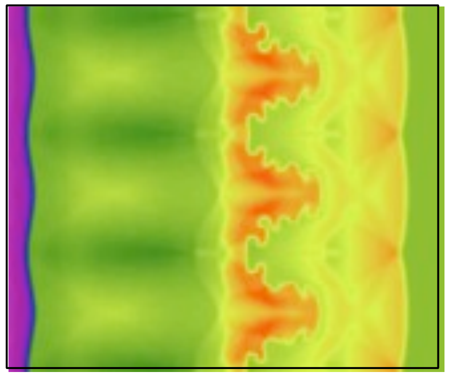
Turbulent Nuclear Burning



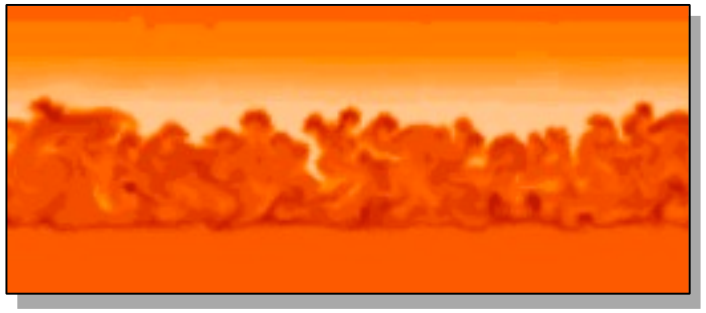
Intracluster interactions



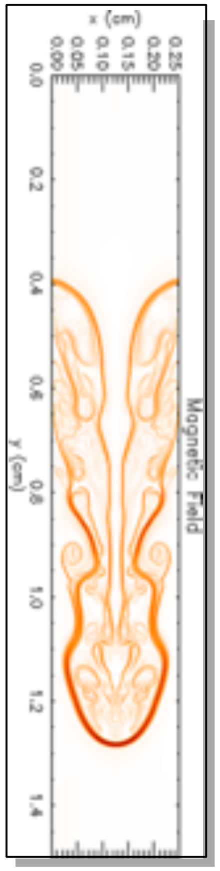
Rayleigh-Taylor instability



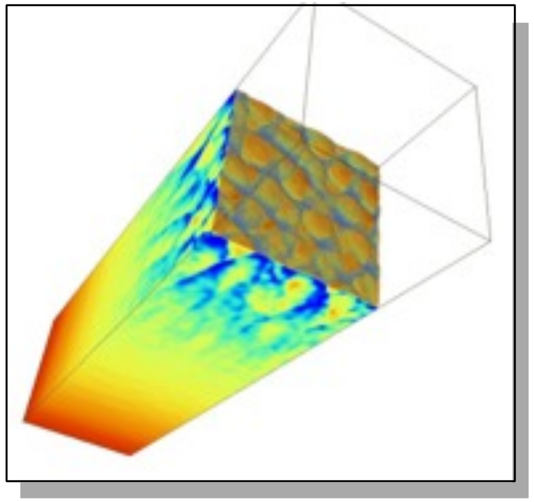
Laser-driven shock instabilities



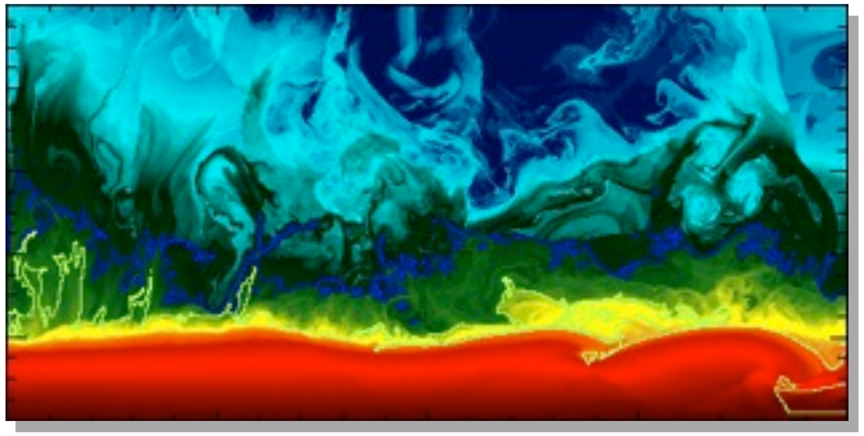
Nova outbursts on white dwarfs



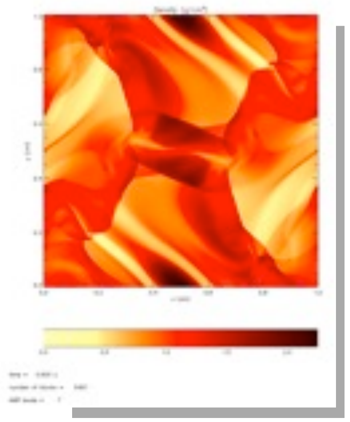
Magnetic Rayleigh-Taylor



Cellular detonation



Helium burning on neutron stars



Orzag/Tang MHD vortex

Richtmyer-Meshkov instability

The ASC/Alliances Center for Astrophysical Thermonuclear Flashes
The University of Chicago

Capabilities

- Infrastructure
  - Configuration (setup)
  - Mesh Management
  - Parallel I/O
  - Monitoring
    - Performance and progress
  - Verification
    - FlashTest
      - Unit and regression testing

- Physics
  - Hydrodynamics, MHD, RHD
  - Equation of State
  - Nuclear Physics and other Source Terms
  - Gravity
  - Particles, active and passive
  - Material Properties
  - Cosmology

Physics Capabilities

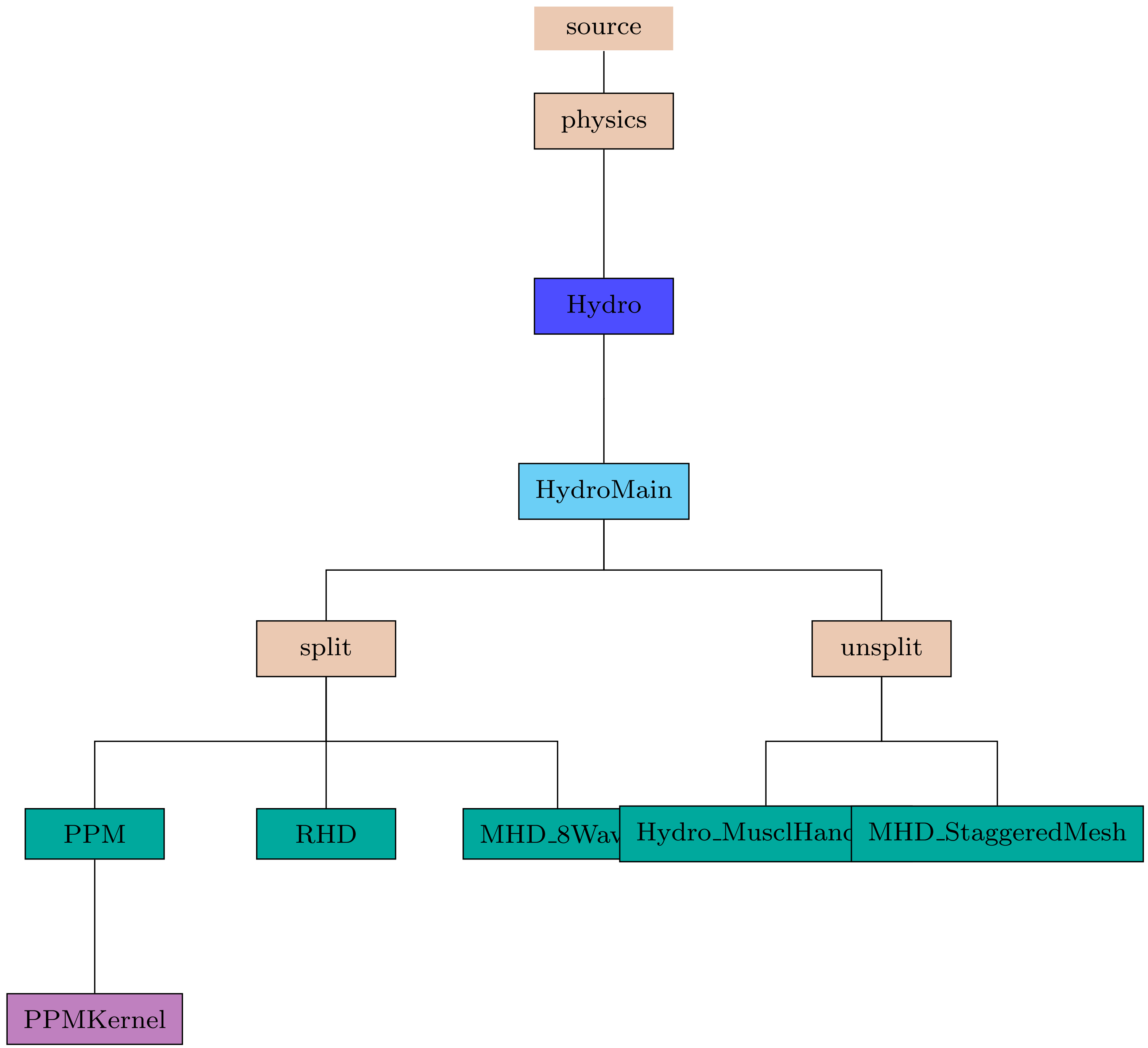


Figure 13.1: The `Hydro` unit directory tree.

Physics Capabilities

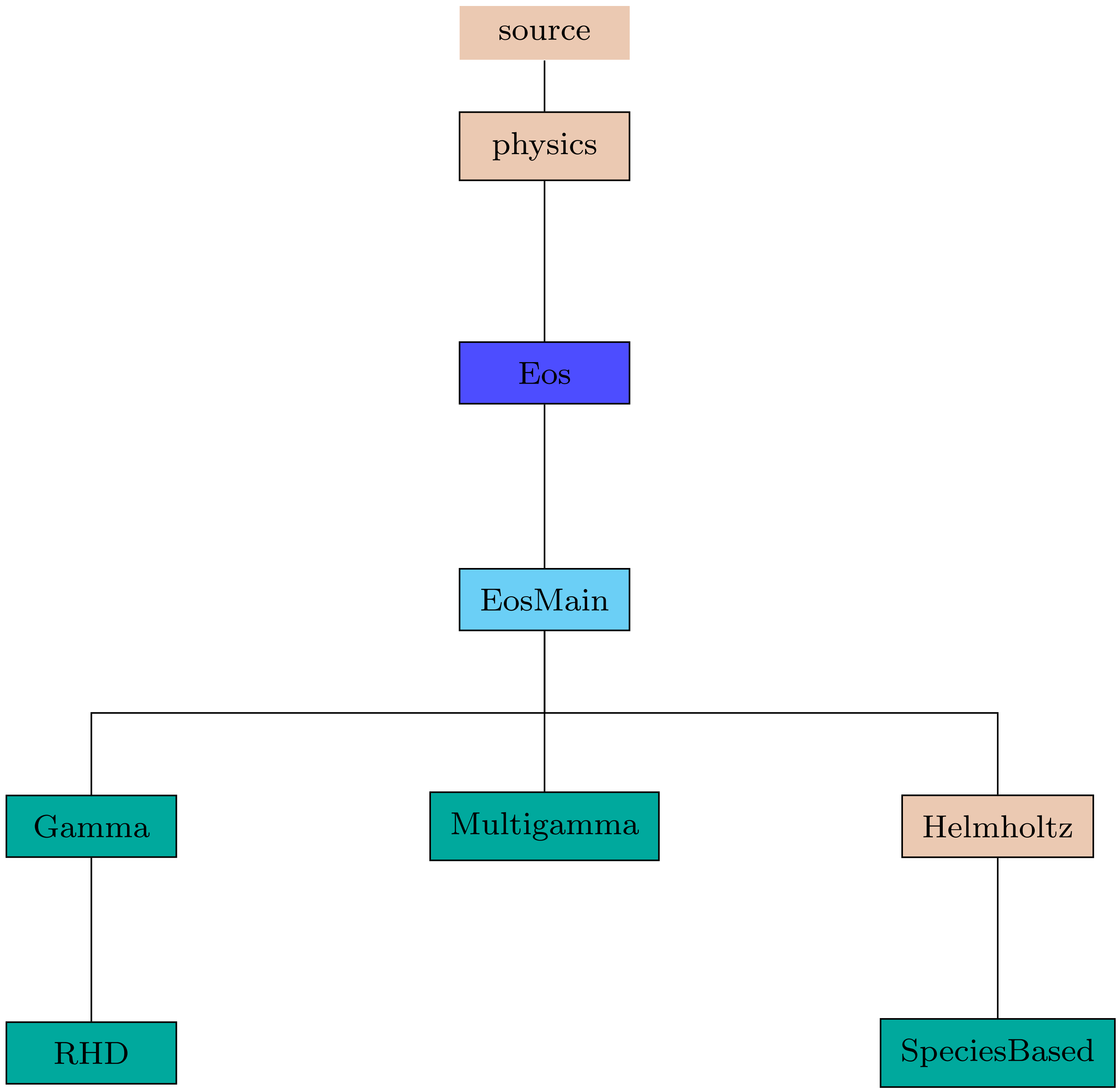


Figure 14.1: The `Eos` directory tree.

Physics Capabilities

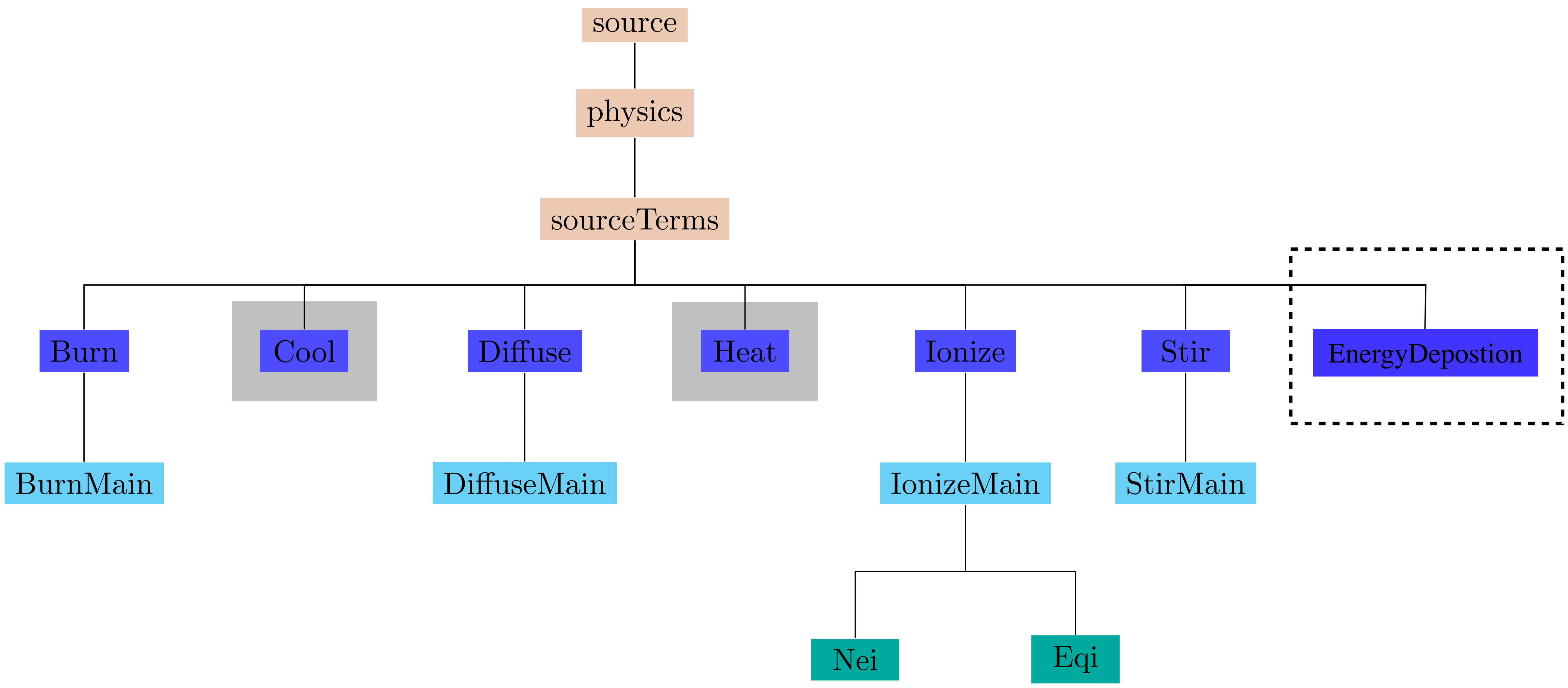


Figure 15.1: The organizational structure of physics source terms, which include units such as `Burn` and `Stir`. Shaded units include only stub implementations.

Physics Capabilities

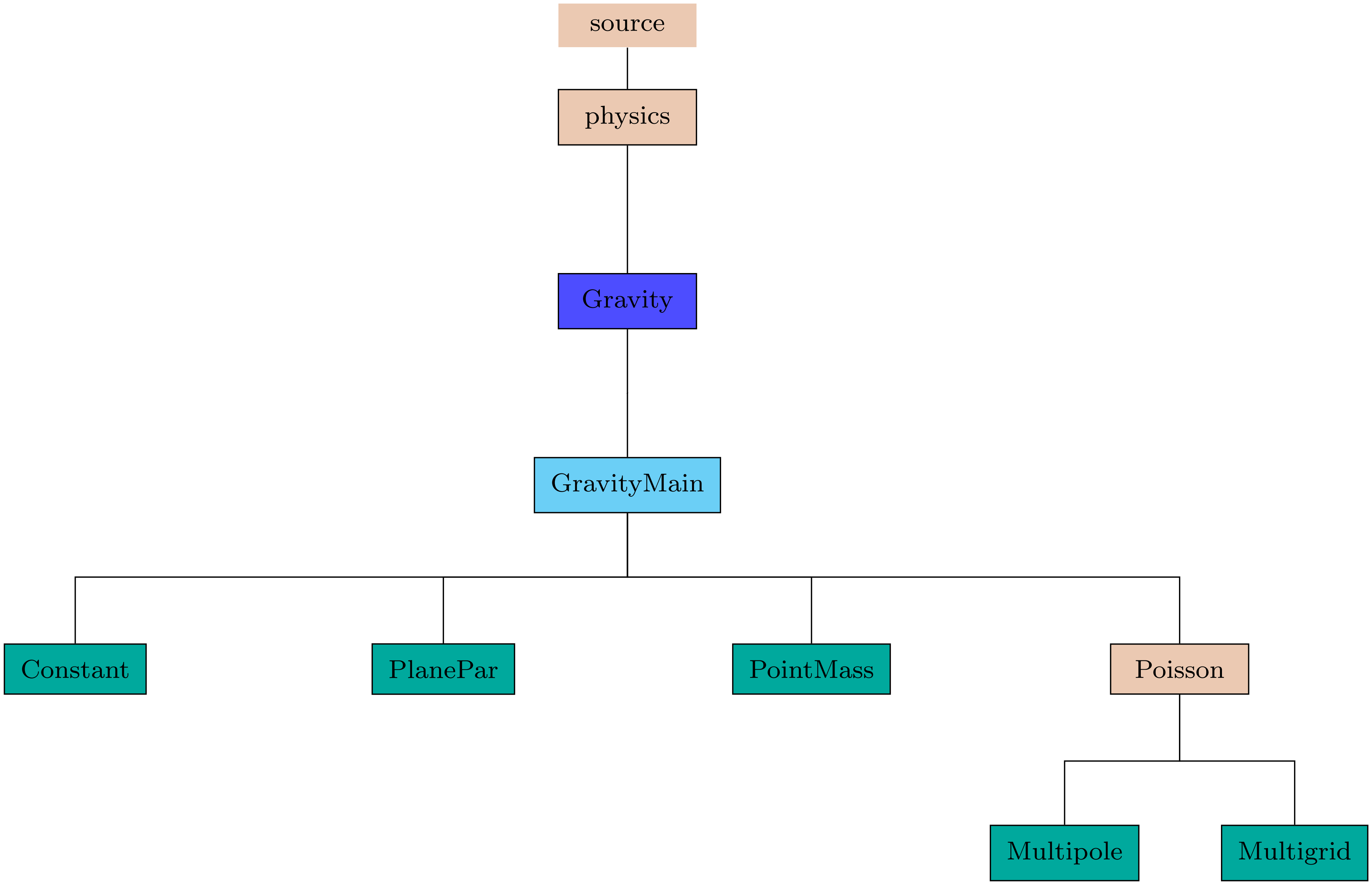


Figure 16.1: The `Gravity` unit directory tree.

Physics Capabilities

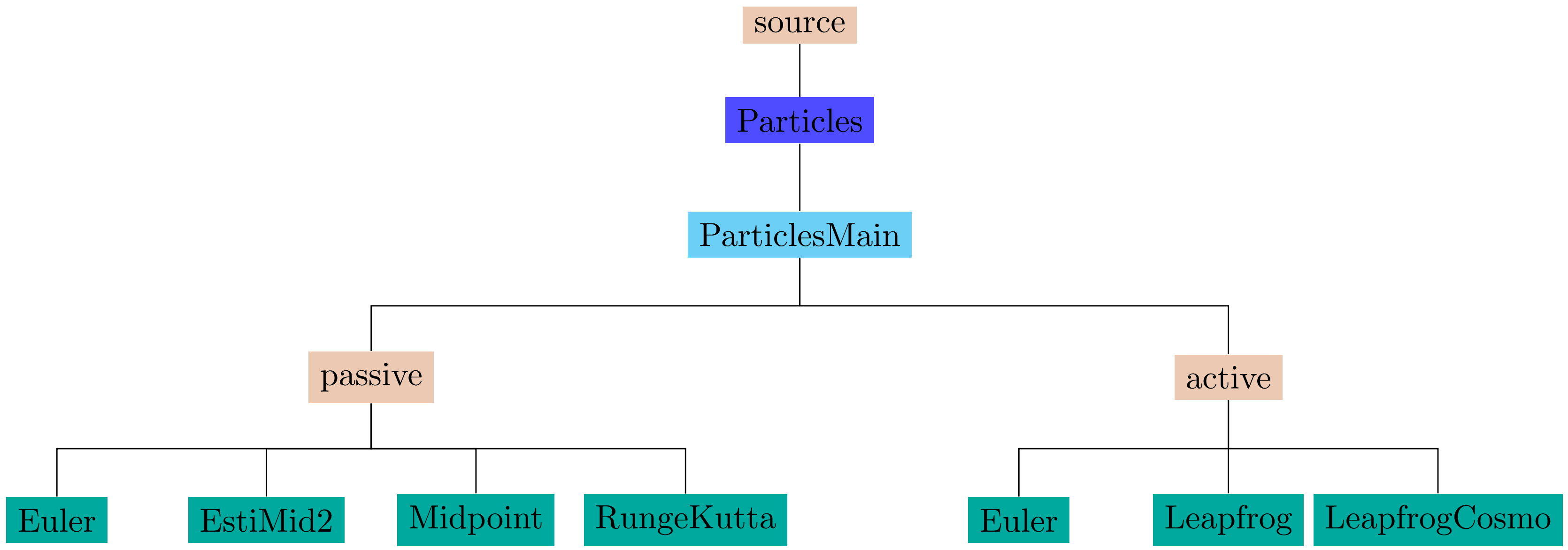


Figure 17.1: The `Particles` unit main subunit.

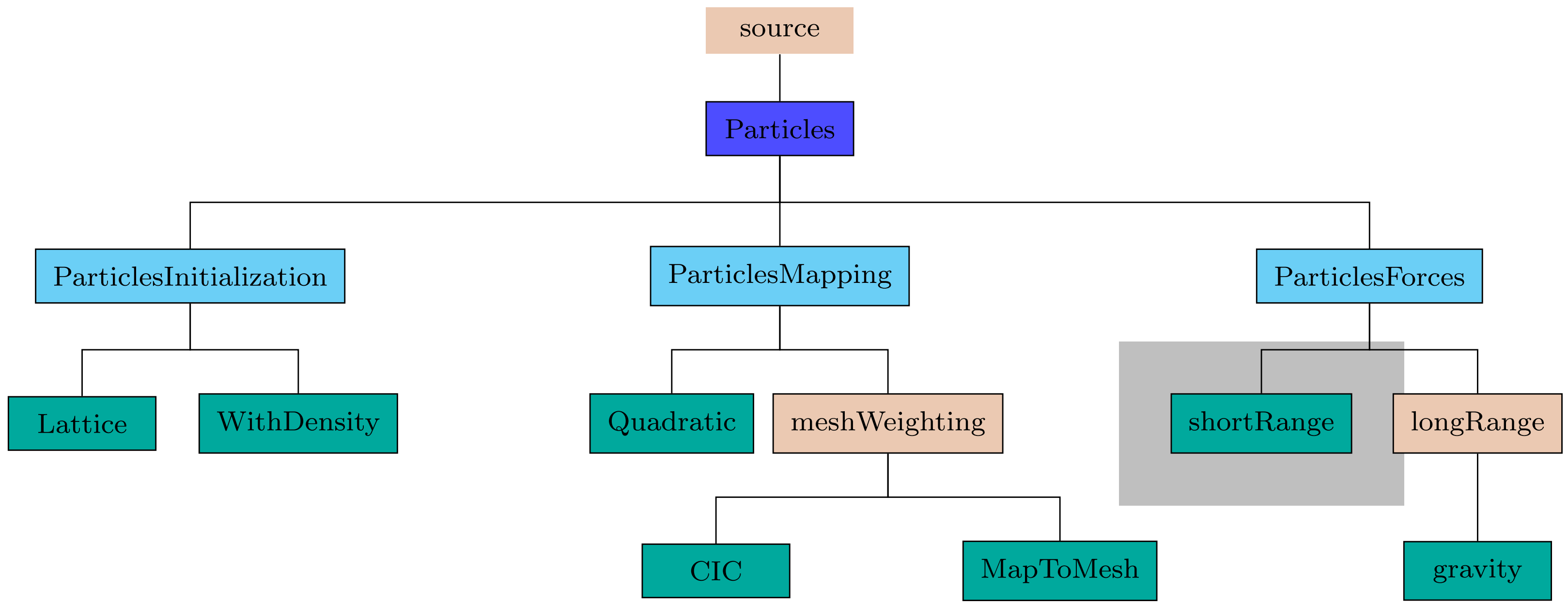


Figure 17.2: The `Particles` unit with ParticlesInitialization and ParticlesMapping subunits.

Physics Capabilities

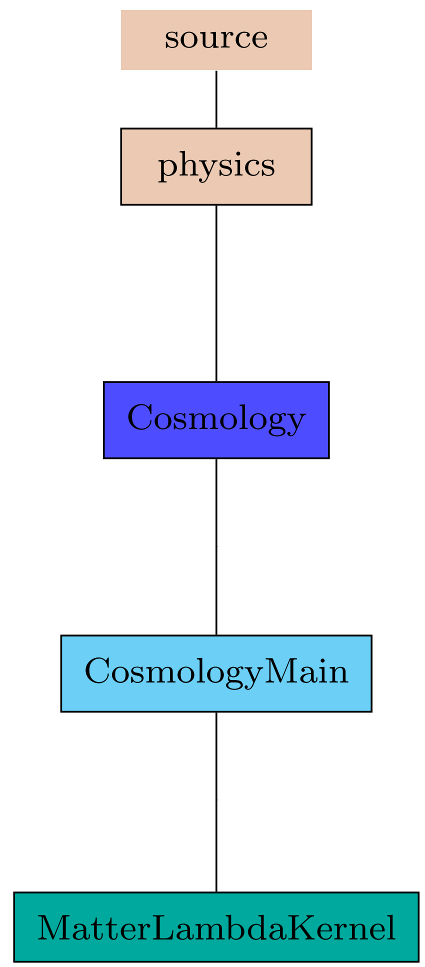


Figure 18.1: The `Cosmology` unit tree.

Physics Capabilities

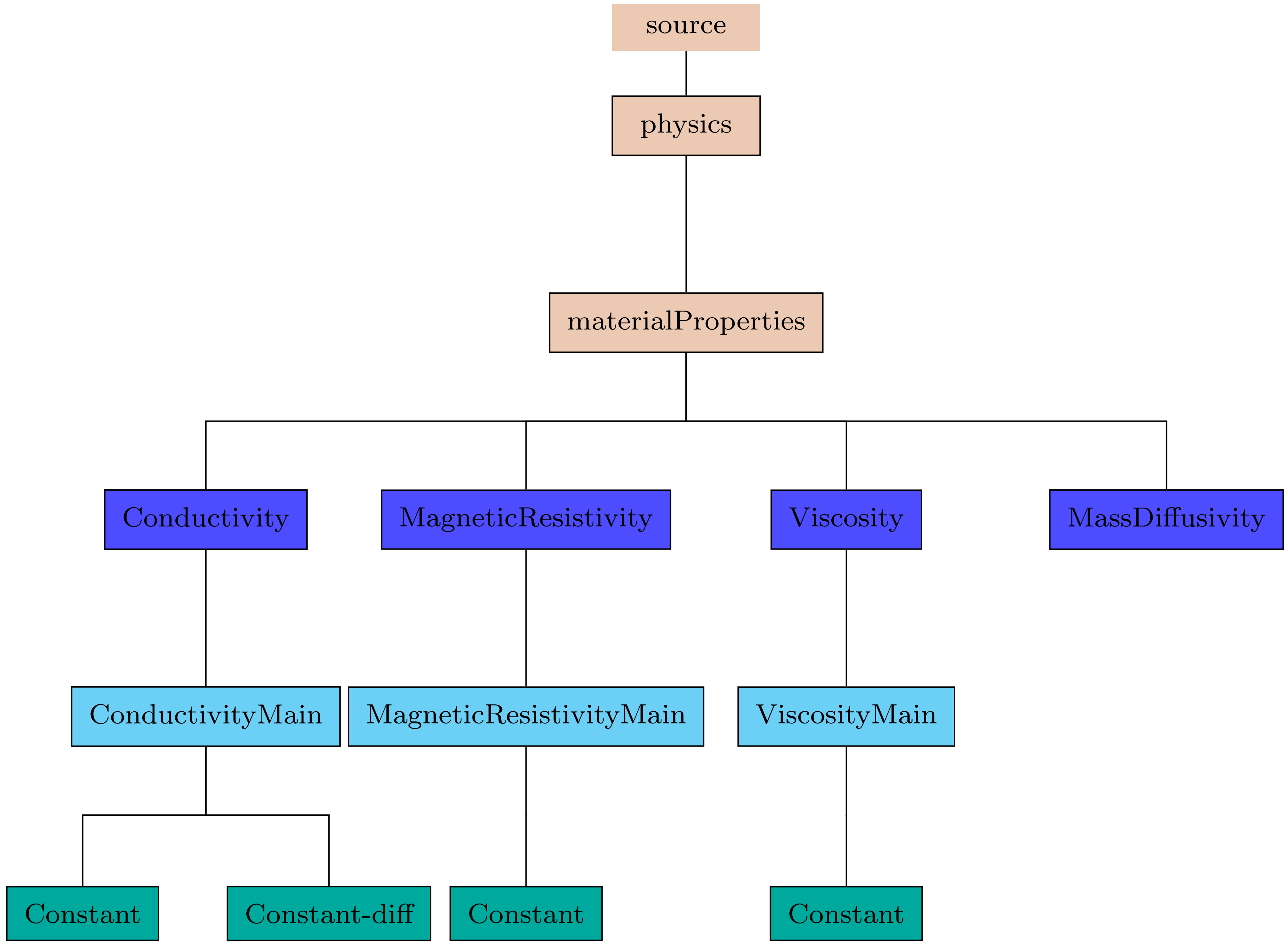
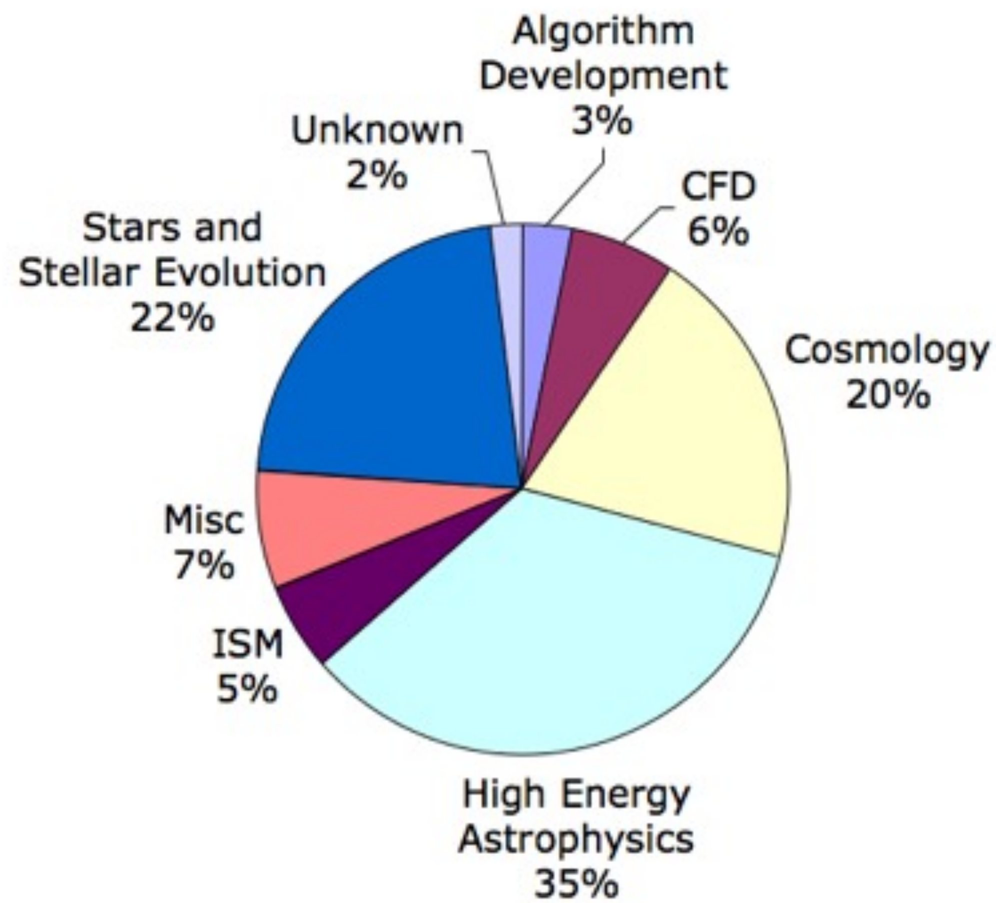


Figure 19.1: The `materialProperties` directory tree.

FLASH Users Community (2007 survey)



Breakdown of FLASH code research areas for primary research tool users

The Simulation Unit

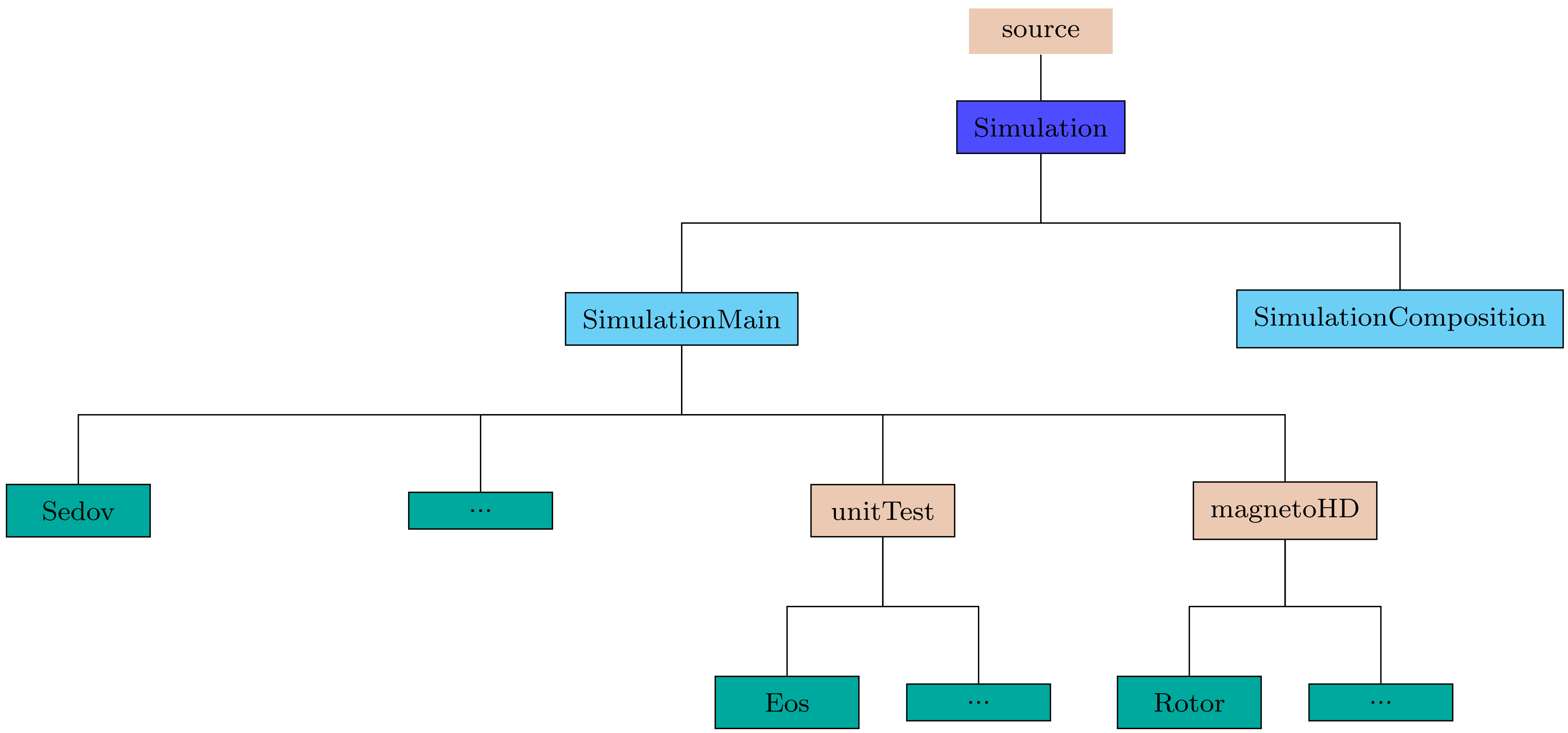


Figure 22.1: The `Simulation` unit directory tree. Only some of the provided simulation implementations are shown. Users are expected to add their own simulations to the tree.

The Simulation Unit

- Typical Unit, obeys architecture, naming conventions, inheritance, etc. rules.
- Special Unit in that it always “wins” inheritance and parameter wars.
- FLASH problems is defined by directories in FLASH3/ source/Simulation/SimulationMain.
- The Simulation directory gives people working on a particular problem a place to put problem specific code that replaces the default functionality in the main body of the code
- It’s also a place to tell the setup script which units this problem will need from the rest of the code

What's in the Simulation Directory?

- Normal UnitMain implementation requirements
  - Simulation_data, Simulation_init, (Simulation_finalize), Simulation_initBlock
  - Makefile (with usually Simulation_data only)
  - Config file
  - Possibly other API functions: e.g. Simulation_initSpecies
- Specific to simulations:
  - Parameter files flash.par, testUG.par, etc.
  - Replacements for routines located elsewhere in directory tree
  - Routines that implement local functions e.g. sim_derivedVariables.F90

Required Code for a New Simulation

- There are certain pieces of code that all simulations must implement:
  - Simulation_data.F90: Fortran module which stores data and parameters specific to the Simulation.
  - Simulation_init.F90: Reads the runtime parameters, and performs other necessary unit initializations.
  - Simulation_initBlock.F90: Sets initial conditions in a single block.
- Optionally, a simulation could implement:
  - Simulation_initSpecies.F90: To give the properties of the species involved in a multispecies simulation

Customized Code for a new Simulation

- In a FLASH simulation directory, you can place code that overrides the functionality you would pick up from other code units
- In the custom code you can modify:
  - Boundary conditions (Grid_applyBCEdge.F90)
  - Refinement criterion (Grid_markRefineDerefine.F90)
  - Diagnostic integrated quanties for output (in the flash.dat file), e.g., total mass (a default) or vorticity (IO_writeIntegralQuantities.F90)
  - Diagnostics to compute new grid scope variables (Grid_computeUserVars.F90)
- In general, this is a place to hack the code in ways specific to your problem, and you can hack basically anything

Creating New Problems

- A new FLASH problem is created by making a directory for it in FLASH3/source/Simulation/SimulationMain. This is where the setup script looks for the problem specific files.
- The source files in a simulation directory that a user will need to modify are:
  - Simulation_data.F90: Fortran module which stores data and parameters specific to the Simulation.
  - Simulation_init.F90: Fortran routine which reads the runtime parameters, and performs other necessary initializations.
  - Simulation_initBlock.F90: Fortran routine for setting initial conditions in a single block.
  - Simulation_initSpecies.F90: Optional Fortran routine for initializing species properties if multiple species are being used.
- Custom implementation of any kernel routine in FLASH can be placed here.

Simulation_data

- A Fortran module containing all data specific to the simulation unit.
- All names should be prefixed with sim_ to make it clear that data belongs to the simulation unit.
- Remember to use the save attribute to prevent data going out of scope.

```
module Simulation_data
  implicit none
  real, save :: sim_pAmbient, sim_xAngle, sim_yAngle, sim_zAngle
end module Simulation_data
```

Simulation_init

- Initializes the simulation unit.
  - Called once at the beginning of the simulation in both new and restarted application runs.
  - Eliminates the need for FLASH2 "*if (firstcall)*" code fragments.

- Example usage:
  - Stores runtime parameter values in Simulation_data private variables.
  - Calculates any runtime parameter derived quantities.
  - Reads a lookup table from a file.

The Config file and Simulation_init

Config file declares the runtime parameters.

```
D sim_pAmbient      Initial ambient pressure
PARAMETER sim_pAmbient    REAL    1.E-5
```

Simulation_init extracts the value of runtime parameters.

The runtime parameter's default value can be overridden in a flash.par

```
subroutine Simulation_init(myPE)
  use Simulation_data
  use RuntimeParameters_interface, ONLY : &
       RuntimeParameters_get

  implicit none
#include "constants.h"
#include "Flash.h"

  integer, intent(in) :: myPE
  call RuntimeParameters_get('sim_pAmbient', &
                             sim_pAmbient)
end subroutine Simulation_init
```

Simulation_initBlock

- Applies initial conditions to the physical domain
  - Initializes Grid data one block at a time.
  - Only called in new application runs (not in restarts).

- Block abstraction allows it to be used with different Grid implementations
  - Called once in UG simulations.
  - Called many times in AMR simulations.

- Generating an initial grid in AMR simulations:
  - Simulation_initBlock is applied to all blocks at the base refinement level.
  - Grid unit refines blocks if refinement criteria met.
    - Simulation_initBlock is re-applied to <u>all</u> blocks.

Repeats {

Simulation_initBlock: Finding cell types

- The Grid API contains a portable way to find the internal cells and guard cells in a particular block.
  - Essential for NFBS Uniform grid mode where block sizes are not always the same size.

Grid_getBlkIndexLimits(blockId, blkLimits, blkLimitsGC, optional: gridDataStruct)

- The arrays *blkLimits* and *blkLimitsGC* contain the lower and upper bounds of a block. For cell-centered PARAMESH data:

blkLimits(LOW,IAXIS)=NGUARD+1; blkLimits(HIGH,IAXIS)=NXB+NGUARD
blkLimitsGC(LOW,IAXIS)=1; blkLimitsGC(HIGH,IAXIS)=NXB+2*NGUARD

- The input argument *gridDataStruct* specifies the underlying grid datastructure, e.g. cell-centered, face-centered, scratch data structure.

Simulation_initBlock: Accessing each cell

- Many Grid API functions available to read / write Grid data:
  - Grid_getPointData, Grid_putPointData
  - Grid_getRowData, Grid_putRowData
  - Most general is Grid_getBlkPtr:

Grid_getBlkPtr(blockID, dataPtr, optional: gridDataStruct)

- Sets the pointer *dataPtr* to the block indicated by *blockID* for the data structure *gridDataStruct*. Free the pointer using Grid_releaseBlkPtr (has same arguments as Grid_getBlkPtr).

- To obtain actual cells coordinates use Grid_getCellCoords:
  Grid_getCellCoords(axis, blockID, edge, guardcell, coordinates, size)

- This stores coordinates for the cells on axis *axis* (IAXIS, JAXIS, KAXIS) at cell location *edge* (LEFT_EDGE, RIGHT_EDGE, CENTER) in the array *coordinates(size)*.

Excerpt from a Simulation_initBlock

```
subroutine Simulation_initBlock(blockID, myPE)
...
call Grid_getBlkIndexLimits(blockID,blkLimits,blkLimitsGC)
sizeX = blkLimitsGC(HIGH,IAXIS) - blkLimitsGC(LOW,IAXIS) + 1 !Num cells inc. guard.
allocate(xCoord(sizeX))
call Grid_getCellCoords(IAXIS, blockID, CENTER, .true., xCoord, sizeX)

call Grid_getBlkPtr(blockId,solnData)
!Loop over each internal cell and initialize data
...
do  i = blkLimits(LOW,IAXIS), blkLimits(HIGH,IAXIS)
   If (xCoord(i) > sim_xpos) solnData(DENS_VAR,i,j,k) = …
end do
call Grid_releaseBlkPtr(blockID,solnData)

end subroutine Simulation_initBlock
```

Simulation_initSpecies

- Implementation only required when working with multiple species.
  - Called from Multispecies_init to initialize fluid properties.
  - Called in new and restarted application runs.
  - Called before Simulation_init.

- General purpose Simulation_initSpecies implementations are available for nuclear networks and ionization (See Simulation/SimulationComposition directory).

- May want to create derived quantities in Simulation_init from the fluids initialized in Simulation_initSpecies.

The Config file and Simulation_initSpecies

Config file declares the species.

```
SPECIES FLD1
SPECIES FLD2
```

Simulation_initSpecies initializes fluid properties.

```
subroutine Simulation_initSpecies()
  use Multispecies_interface, ONLY : Multispecies_setProperty

  implicit none
#include "Flash.h"
#include "Multispecies.h"

  call Multispecies_setProperty(FLD1_SPEC, A, 1.)
  call Multispecies_setProperty(FLD1_SPEC, Z, 1.)
  call Multispecies_setProperty(FLD1_SPEC, GAMMA, &
1.66666666667e0)

  call Multispecies_setProperty(FLD2_SPEC, A, 4.0)
  call Multispecies_setProperty(FLD2_SPEC, Z, 2.0)
  call Multispecies_setProperty(FLD2_SPEC, GAMMA, 2.0)

end subroutine Simulation_initSpecies
```

Working with block lists

- A single processor contains some portion of the total grid data in one or more blocks.
  - Possible to access data in a grid-package specific way.
  - However, we recommend using Grid API functions so that code is independent of a particular grid-package.

Grid_getListOfBlocks(blockType, listofBlocks, count, optional: refinementLevel)

- Returns the actual block IDs in *listOfBlocks* and the number of block IDs in *count.* The returned block IDs must satisfy the criteria set by *blockType* and *refinementLevel* input arguments.

- NOTE: Any code using this function must “use” the function prototype because this function has an optional argument.