Flash Center for Computational Science

Lagrangian Infrastructure & IO

FLASH Tutorial/Workshop
May 30 – June 1, 2012
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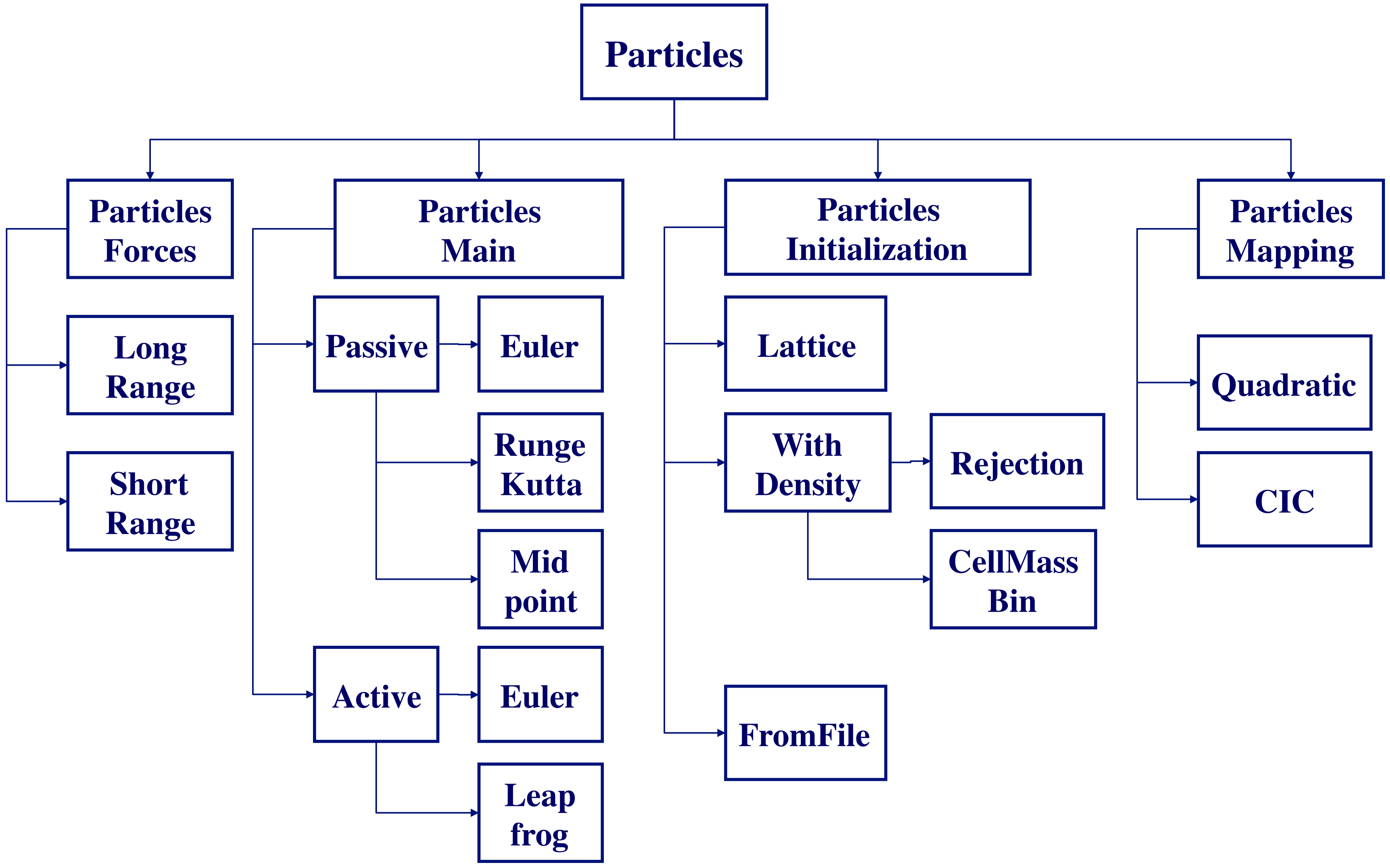
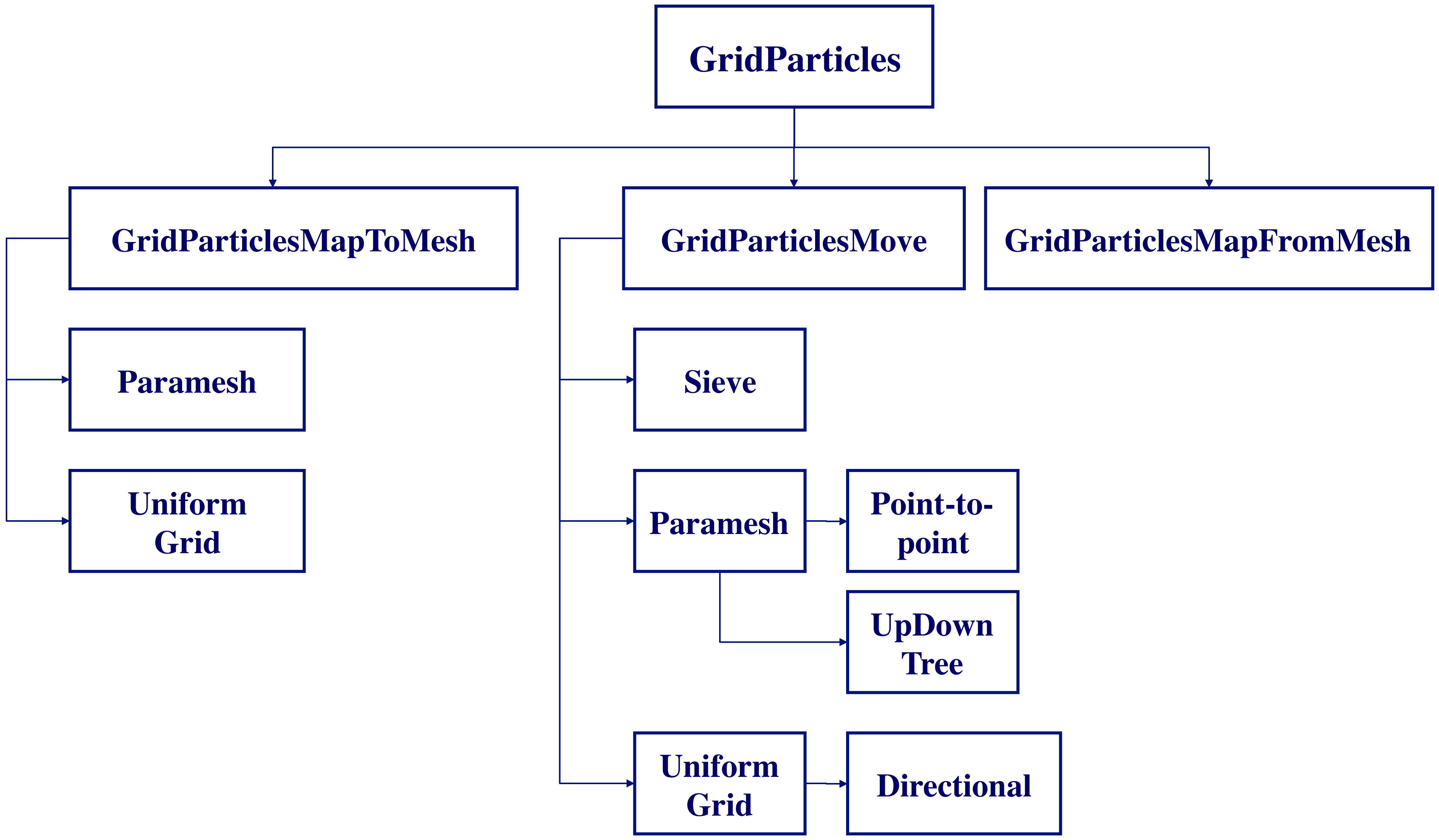
Components of the Framework

- Four sub-units within Particles unit
  - ParticlesMain – unit scope data, time advancement
  - ParticlesInitialization – initializing the unit and particle positions
  - ParticlesMapping – to & from the grid
  - ParticlesForces – from & to other particles and from & to grid
- One sub-unit in the Grid unit
  - GridParticles
  - Three sub-sub-units under it
    - GridParticlesMove – move the particles data structures when their positions change
    - GridParticlesMapFromMesh – interpolate grid variables from the cell or face center to the particle positions
    - GridParticlesMapToMesh – map the particle attribute to relevant cells in the grid variable

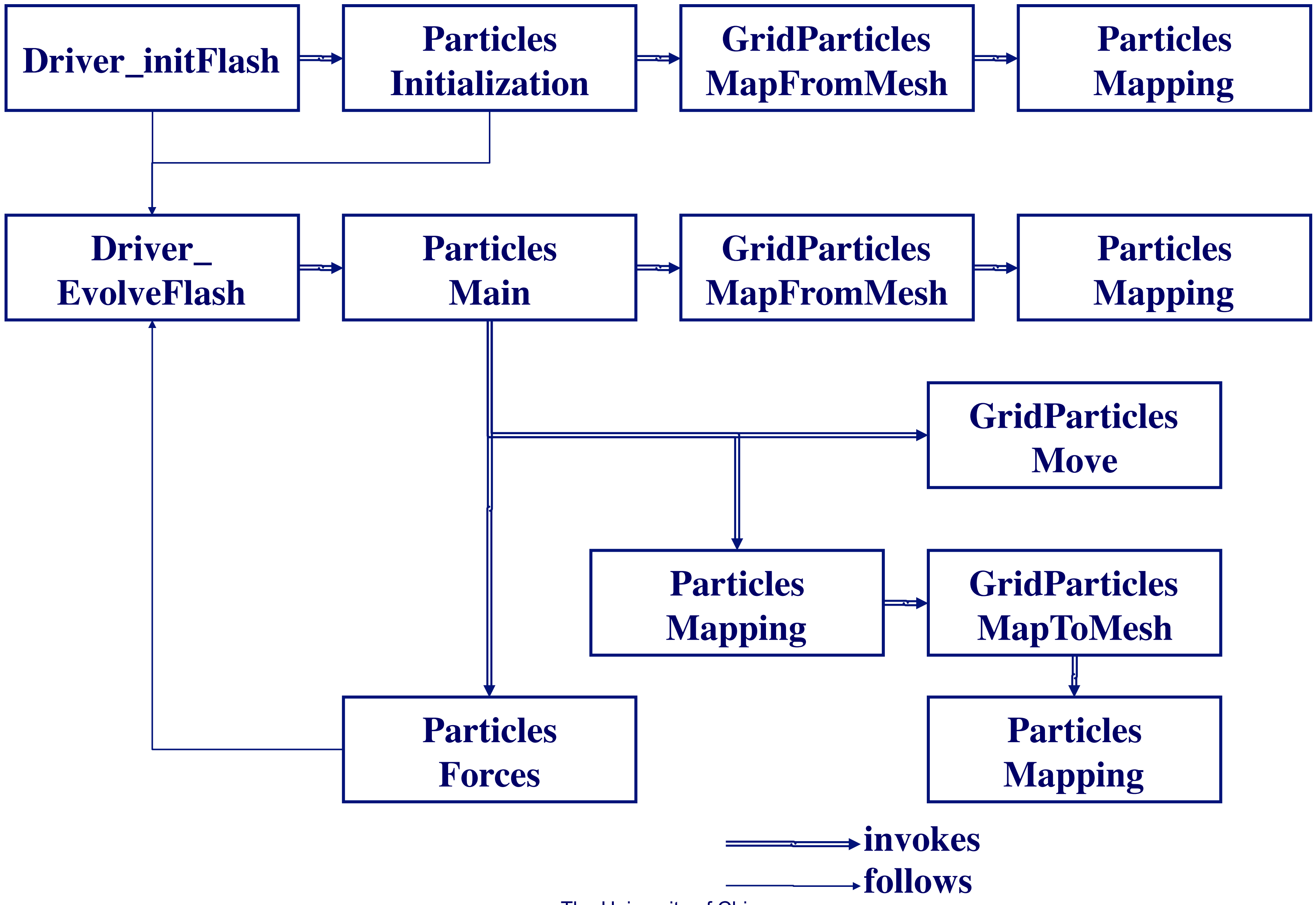
The Particles Unit



The GridParticles Sub-unit



The Control Flow Between Them



Particle flavors

- Passive particles trace and record the history of the flow
- Active particles influence the simulation
  - Massive (dark matter) or Charged (PIC)
- All particles are stored in the same 2-D array:
  - 1st dim: Total number of particle properties (*NPART_PROPS*) . A single property named *TYPE_PART_PROP* indicates particle type.
  - 2nd dim: Maximum number of particles that are allowed on a single processor (*pt_maxPerProc*).

Particle behaviors

- Particle behavior controlled by implementations of:
  - Time advancement
  - Initialization
  - Mapping (Bidirectional for active particles)
- Include the FLASH sub-units providing the desired behavior in your Simulation Config file.
- Register particle behavior with a particular particle type using PARTICLETYPE keyword in your Simulation Config file.

PARTICLETYPE keyword

- PARTICLETYPE *name* INITMETHOD *initmethod* MAPMETHOD *mapmethod* ADVMETHOD *advmethod*

- The *initmethod*, *mapmethod and advmethod* strings must correspond to pre-processor definitions from the file Particles.h.
  - We use these definitions to select the functions that are called for each particle type (see logic in the wrapper functions Particles_initPositions, Particles_mapFromMesh and Particles_advance).

- PARTICLETYPE keyword is not fool-proof!
  - Your responsibility to ensure PARTICLETYPE arguments are consistent with the units being included.
  - Glance over the setup generated files: Particles_specifyMethods.F90 and setup_units.

Initialization

- The wrapper function Particles_initPositions calls the specified initialization function for each particle type.

- We have initialization functions named pt_initPositionsLattice and pt_initPositionsWithDensity.
  - These correspond to *initmethod* strings of:
    - “lattice”: Regularly spaced particle distribution.
    - “with_density”: Density of particles is proportional to the density on the grid.

- You can use your own initialization function:
  - Name it pt_initPositions and place in simulation directory.
  - Use an *initmethod* string of “custom” for each particle type that should use this distribution.

Mapping

- Converts grid based quantities into similar attributes defined on particles (and vice versa for active particles).
  - Particles_mapFromMesh (Mesh → Particles)
  - Particles_mapToMeshOneBlk (Particles → Mesh)

- FLASH supplies the following mapping schemes:
  - Quadratic: Second-order interpolation.
    - Only available for passive particles.
  - Weighted: A linear weighting from nearby points.
    - Default weighting is Cloud-In-Cell (CIC).

- Use *mapmethod* strings of “quadratic” or “weighted”.

Time advancement

- Different time integration schemes for passive and active particles.
  - Only one type of passive and one type of active scheme may be selected in a simulation.

- Advancement of particles' position may require particles move to another block (may be on another processor).
  - Movement is handled by Grid/GridParticles subunit.
    - Also handles particle movement that occurs as a result of refinement / derefinement.

Particle attributes

- Aditional properties can be defined for each particle:

PARTICLEPROP *property-name*

- The new particle property may be used to sample the state of mesh variables:

PARTICLEMAP TO *property-name* FROM *VARTYPE variable-name*

(Here, *VARTYPE* can be GRIDVAR, FACEX, FACEY, FACEZ, VARIABLE, MASS_SCALAR, SPECIES)

- We map from *variable-name* to *property-name* before we write a checkpoint file or a particle file.
- Example: To sample the value of a mass scalar named val1:

MASS_SCALAR val1

PARTICLEPROP pval1

PARTICLEMAP TO pval1 FROM MASS_SCALAR val1

Particle based refinement

- Possible to refine the AMR grid according to the number of particles in each block.
  - May be necessary to avoid exceeding *pt_maxPerProc* in simulations that have significant particle clustering.

- This can be used as the sole refinement criterion or it can be used in conjunction with the standard mesh refinement criterion.

- Use the following runtime parameters:
  - *refine_on_particle_count = .true. / .false.*
  - *max_particles_per_blk = Value*

Useful runtime parameters

Particle options that can be set in flash.par:

useParticles: Logical value that specifies whether to use particles.

pt_maxPerProc: Maximum number of particles that may exist on a single processor. Used to size particles array.

refine_on_particle_count: Logical value that specifies whether particle count should be used as a refinement criterion.

max_particles_per_blk: Refinement criterion for *refine_on_particle_count*. It is the maximum number of particles that may exist on any block.

Example 1

Add Passive particles:

```
REQUESTS Particles/ParticlesMain/passive/RungeKutta
PARTICLETYPE passive INITMETHOD lattice MAPMETHOD quadratic
ADVMETHOD rungekutta
REQUESTS Particles/ParticlesInitialization/Lattice
REQUESTS Particles/ParticlesMapping/Quadratic
REQUESTS Particles/ParticlesMain/passive/RungeKutta
REQUIRES Grid/GridParticles
```

FLASH Simulation : Weakly compressible turbulence

Example 2

Add Active particles with your own custom initialization:

```
REQUIRES Particles/ParticlesMain/active/LeapfrogCosmo
PARTICLETYPE darkmatter INITMETHOD custom MAP
    ADVMETHOD leapfrog
REQUESTES Particles/ParticlesMain/active/massive/Le
```

Additional units for active particles subject to gravitational long range force.

```
REQUESTS Particles/ParticlesMapping/meshWeighting/CIC
REQUIRES Grid/GridParticles/MapToMesh
REQUIRES Particles/ParticlesMapping/meshWeighting/MapToMesh
REQUIRES Particles/ParticlesForces/longRange/gravity/ParticleMesh
REQUESTS physics/Gravity/GravityMain/Poisson/Multigrid
```

Massive Particles Simulations

Galaxy Cluster Simulation

PIC

- External Contribution by Mats Holmström
- Models ions as particles and electrons as massless fluid
- Works only with uniform grid
- Two basic operations
  - Deposit charges and currents into the grid
    - Grid_mapParticlesToMesh
  - Interpolate fields to particle positions
    - Grid_mapMeshToParticles
- Time advancement using predictor-corrector leapfrog

Lagrangian Framework

File Types - Diagnostic Files

- Log File: *flash*.log
  - Generated by the Logfile module
  - Collects events during a run, and often provides more data than stdout/stderr
  - Can also put out individual process logfiles -- good for debugging
- Dat File: *flash*.dat
  - Collection of quantities generated per time step
  - Usually integrated over the physical domain
- amr.log -- Paramesh only!
  - Generated by Paramesh in the event of an error
- Timer summaries: *timer_summary_xxxxx*
  - Allows for the collection of individual processor timing data from FLASH's timers, each processor writes out a file
  - Can be turned off by setting *eachProcWritesSummary* to false

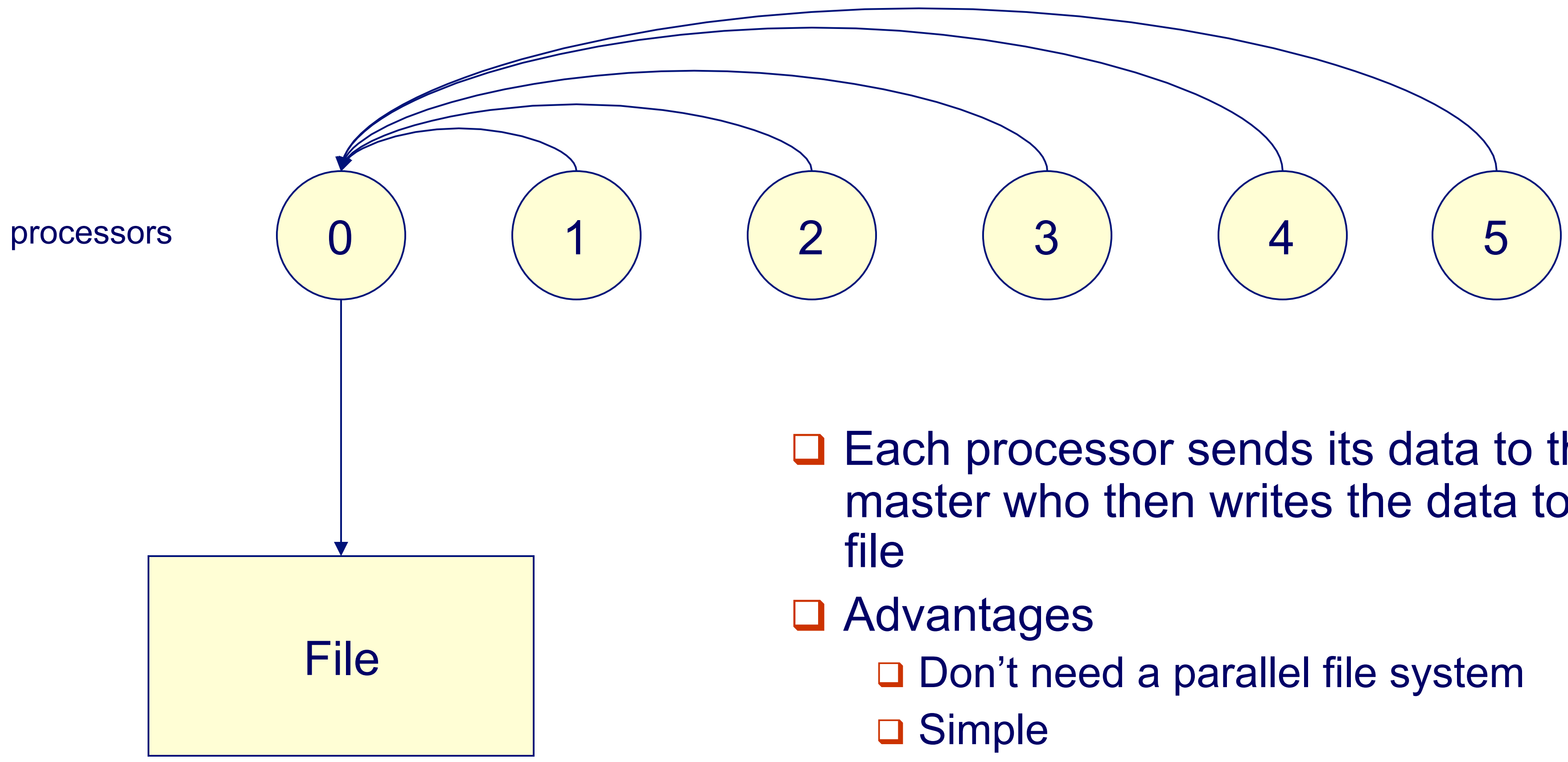
File Types -- Large Files

- Checkpoint files: *basename_filetype*_chk_*xxxx*
  - Contain everything you need to restart outside of a parfile
  - Large, but can save a lot of time and CPU hours
  - Can be set to “roll” via the rollingCheckpoint parameter
- Plot Files: *basename_filetype*_plt_cnt_*xxxx*
  - Contains specific Eulerian quantities specified in your parfile
  - Much smaller and faster to output than a checkpoint
  - By default double-sized floating point data is output in single precision
- Particle files: *basename_filetype*_part_*xxxx*
  - Contains header information, particle metadata and particle data
  - Typically very small and fast to output

Key Flash I/O Feature Overview

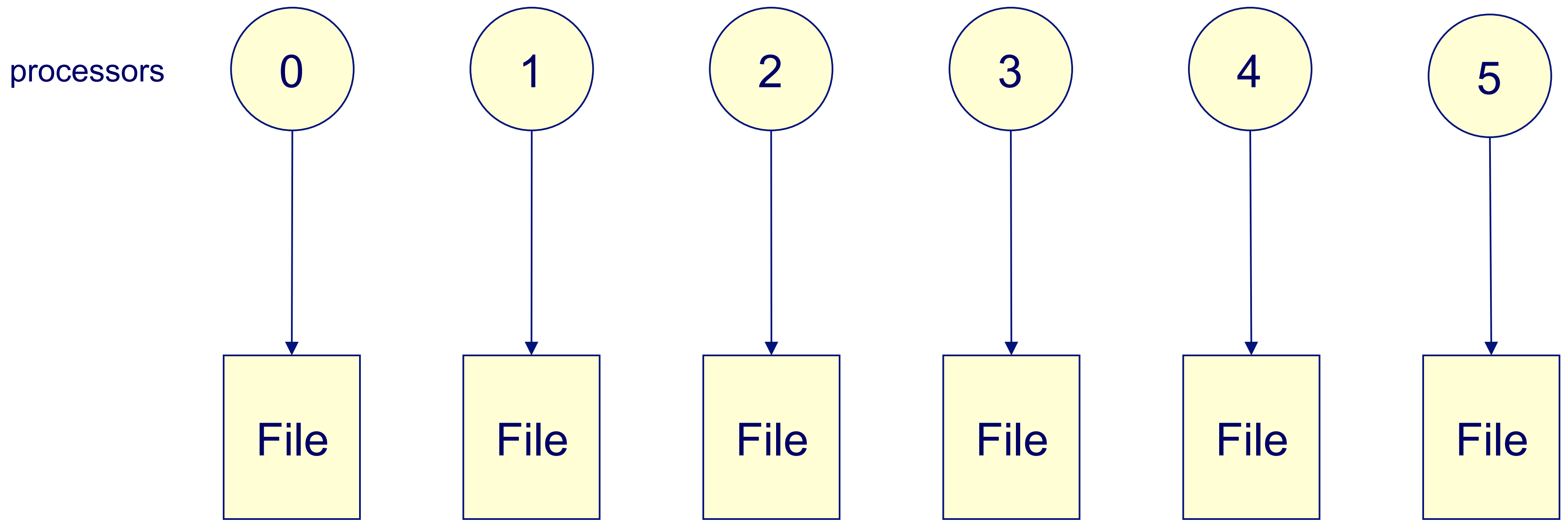
- Multiple I/O Modes
  - Serial, Parallel, Direct
- Multiple I/O Libraries supported
  - HDF5 in serial and parallel mode
  - PnetCDF
  - More can be brought in under FLASH’s architecture
- Transparent Restarting
- Arbitrary I/O File Splitting
- Integral Quantities

Serial I/O



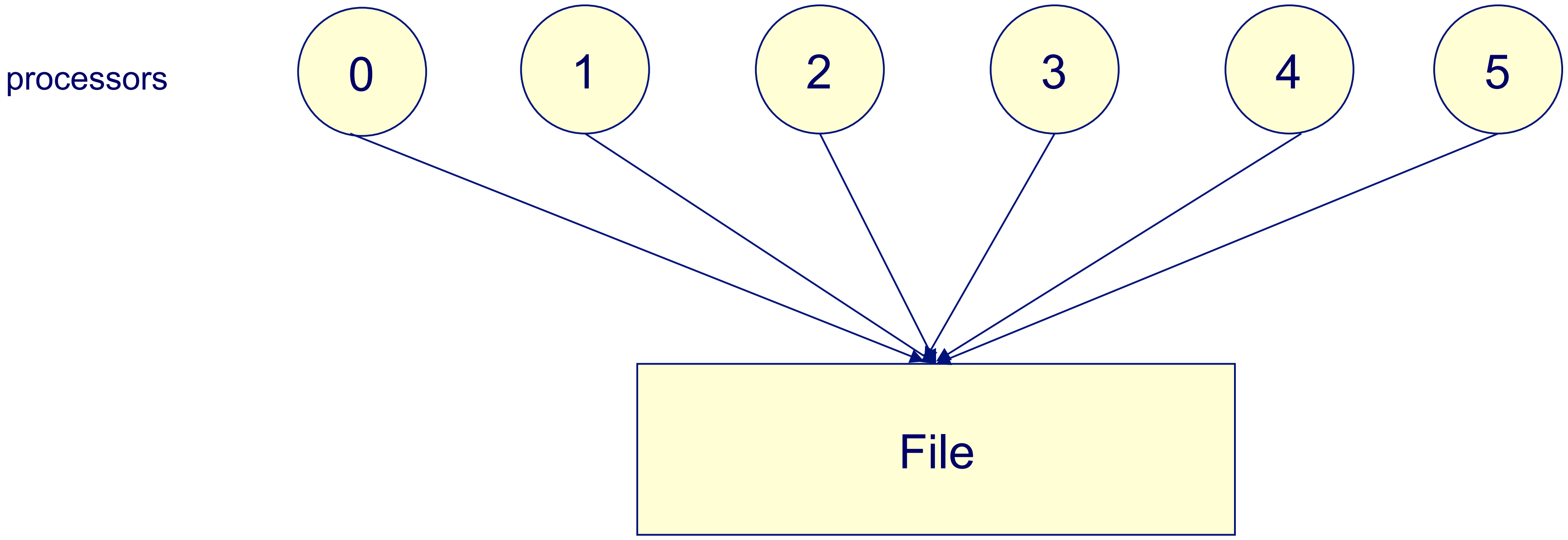
- Each processor sends its data to the master who then writes the data to a file
- Advantages
  - Don’t need a parallel file system
  - Simple
- Disadvantages
  - Not scalable
  - Not Efficient

Parallel I/O: Separate Files



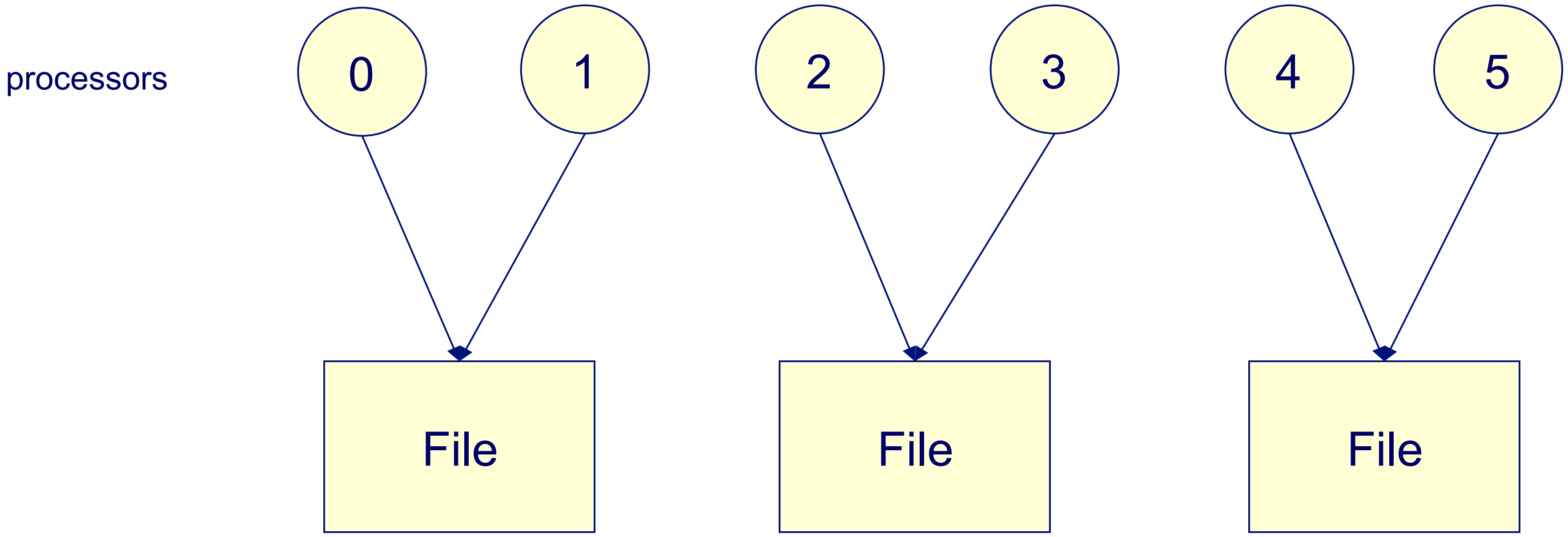
- Each processor writes its own data to a separate file
- Advantages
  - Fast!
- Disadvantages
  - can quickly accumulate many files
  - hard to manage
  - requires post processing

Parallel I/O: Single-file



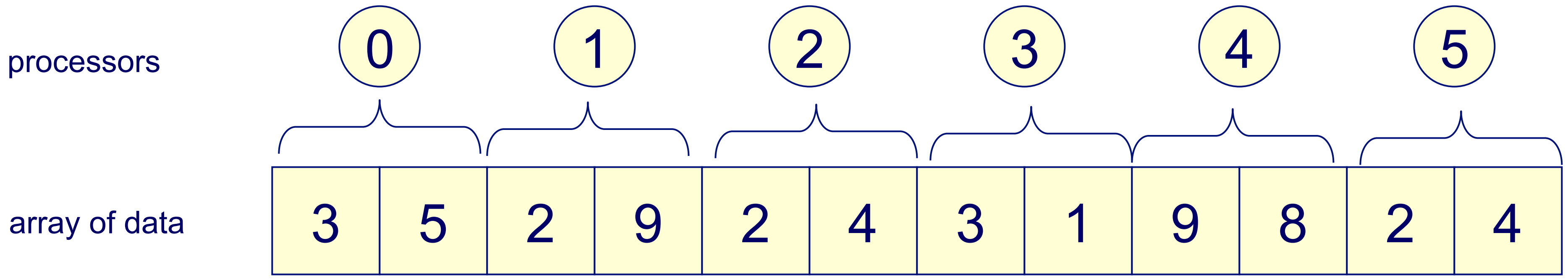
- Each processor writes its own data to the same file using MPI-IO mapping
- Advantages
  - single file
  - scalable
- Disadvantages
  - requires MPI-IO mapping or other higher level libraries

Parallel I/O Split File



- Hybridized model: parallel output to multiple files
- Advantages
  - Potentially more scalable than single file
  - Can take advantage of architecture
- Disadvantages
  - Requires MPI-IO mapping or other higher level libraries
  - Still have multiple files to deal with

Parallel IO single file



Each processor writes to a section of a data array. Each must know its offset from the beginning of the array and the number of elements to write

HDF5

- Library maintained by the HDF group
- Allows for serial and parallel operations
- Primary IO format for FLASH
- Pros:
  - Data is stored with metadata that increases portability
  - Very flexible data format
  - Handles large volumes of data well
  - Most tools for working with FLASH files are written for this format
- Cons:
  - Can be slower than other IO libraries
  - Lots of settings, can be confusing

HDF5: Notes on Parallel Mode

- Parallel HDF5 can be run using an independent access pattern or a collective access pattern
- Collective operations can aggregate reads and writes from multiple processes so that the data can be written in one disk operation
- This can lead to dramatic increases in speed.
- Collective mode may not play nice with other HDF5 features

PnetCDF

- Library maintained by Argonne National Laboratory
- Allows for parallel operations, a CDF library can be used for serial tools.
- Every operation is run in collective mode
- Pros:
  - Very fast if collective operations are enabled, can be faster than HDF5
  - Interface to files is simpler than HDF5
- Cons:
  - Not as flexible
  - Most tools for FLASH do not support PnetCDF files

Direct IO

- Each processor performs a binary write to disk.
- Data split up into *n* files where *n* is the number of processors.
- Pros:
  - Always available.
  - One of the fastest methods available.
- Cons:
  - No automated reader
  - Files will be non-portable
  - Can generate too many files
- Warning:
  - Method of Last Resort!
  - Implementation within FLASH is only an example should this mode be necessary.

Flash Center IO Nightmare…

- Large 32,000 processor run on LLNL BG/L
- Parallel IO libraries not yet available
- Intensive I/O application
    - checkpoint files .7 TB, dumped every 4 hours, 200 dumps
        - used for restarting the run
        - full resolution snapshots of entire grid
    - plotfiles - 20GB each, 700 dumps
        - coarsened by a factor of two averaging
        - single precision
        - subset of grid variables
    - particle files 1400 particle files 470MB each
- 154 TB of disk capacity
- 74 million files!
- Unix tool problems
- 2 Years Later we were still trying to sift though data, sew files together

Integral Quantities

- Individual file output by the master PE
- Collects quantities integrated by volume over the grid
  - Cartesian geometries are supportes along with 2D cylindrical
- Frequently overrode in individual simulations for additional functionality
- If modified, the user is responsible for all MPI needed to marshal data
  - Recommended that you use Flash_mpi.h and FLASH_REAL for MPI calls.
- Also a good place for step-by-step statistics for debugging

Questions?

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