The Center for Astrophysical Thermonuclear Flashes

Infrastructure 2: Particles

Chris Daley

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

Particle flavors

- Passive particles trace hydrodynamic flow in the simulation:
  - Velocities obtained from values on the grid.
- Active particles influence the simulation:
  - e.g. forces between particles (N-Body problem).
- 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*

- The *initmethod* and *mapmethod* strings must correspond to a 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 and Particles_mapFromMesh).

- 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.

Example 1

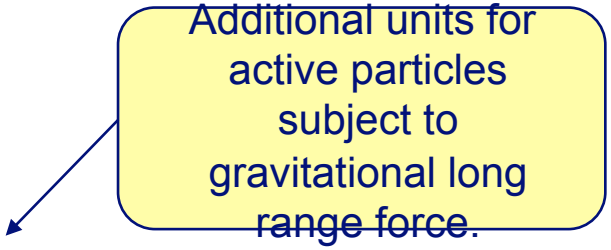
Add Passive particles:

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

Example 2

Add Active particles with your own custom initialization:

REQUIRES Particles/ParticlesMain/active/LeapfrogCosmo
PARTICLETYPE darkmatter INITMETHOD custom MAPMETHOD weighted
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

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 *TYPE variable-name*

(Here, *TYPE* 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 val1

PARTICLEMAP TO val1 FROM MASS_SCALAR val1

PARAMETER particle_attribute_1 STRING “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.