

FLASH Code Tutorial

part II

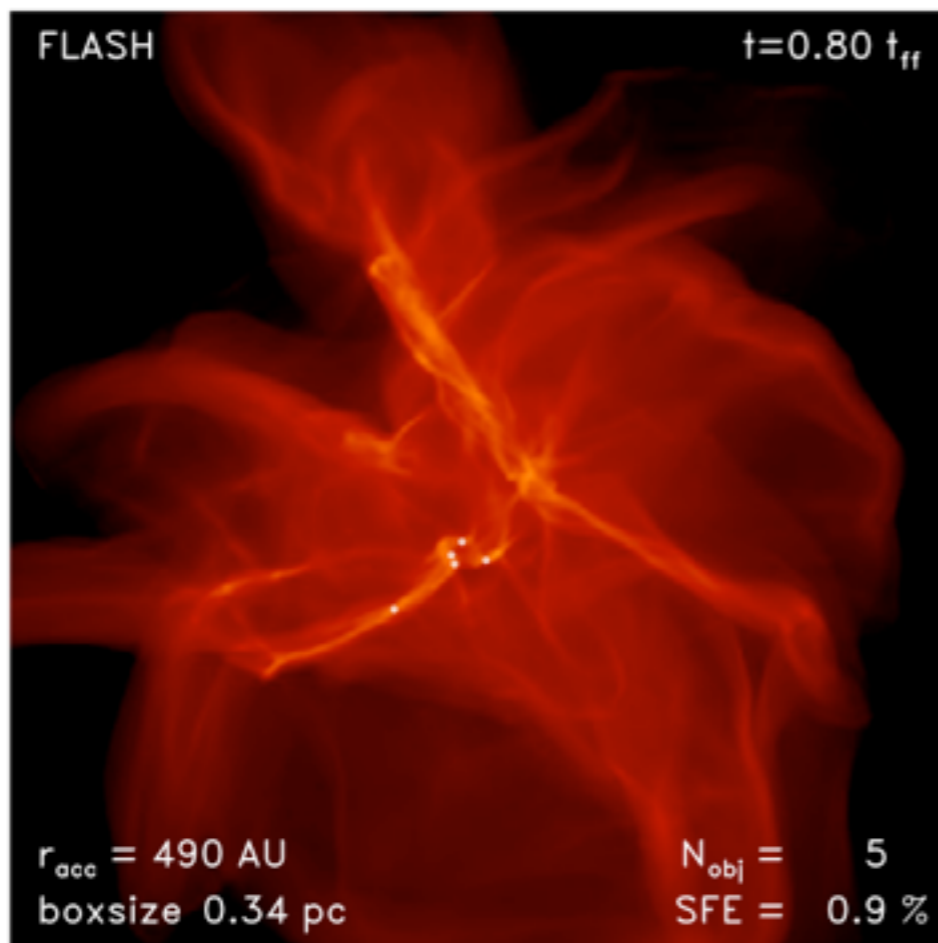
Gravity modules

Robi Banerjee
Hamburger Sternwarte
banerjee@hs.uni-hamburg.de

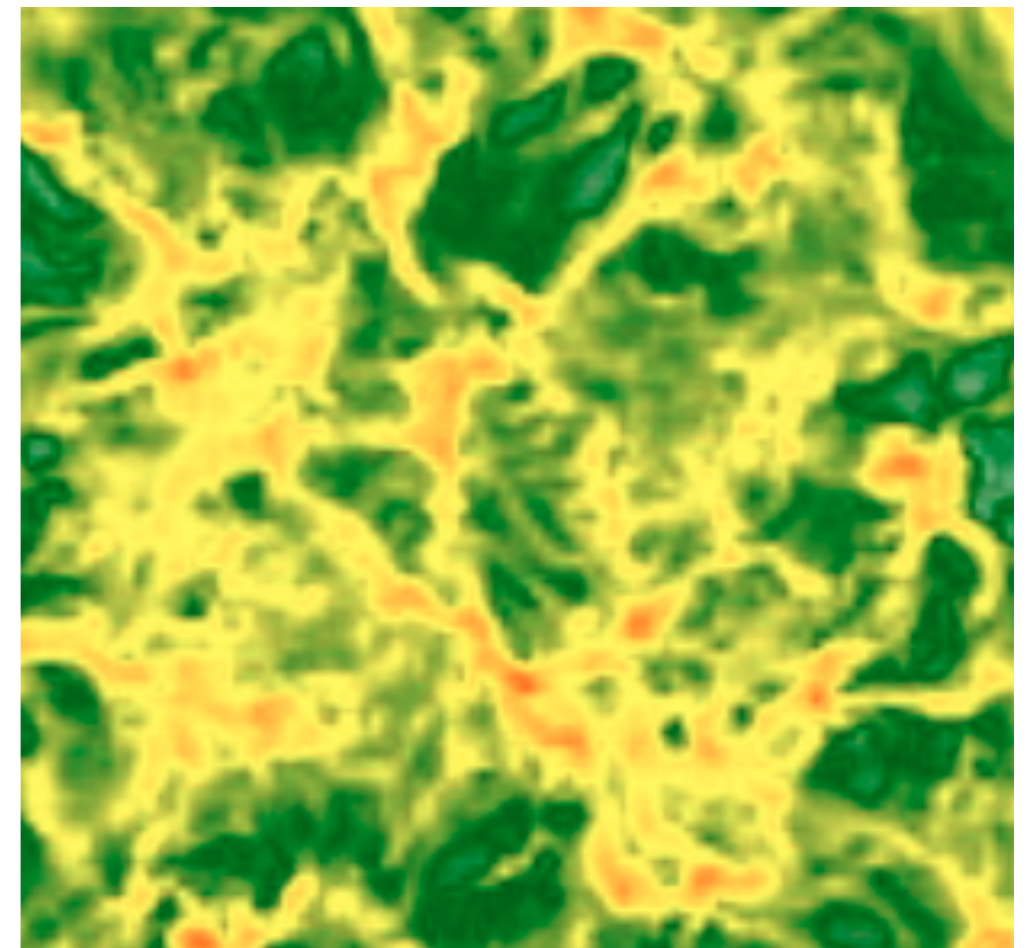
FLASH code: Gravity

Motivation

- dynamics of stratified atmospheres
- N-body dynamics in gaseous media (e.g. stellar cluster, planets)
- collapse of gas cores (e.g. star formation)
- formation of molecular clouds
- ...



collapse of a cloud core



molecular cloud formation

FLASH code: Gravity

- **coupling** to hydro-dynamics / MHD

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$

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

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot [(\rho E + P) \mathbf{v}] = \rho \mathbf{v} \cdot \mathbf{g}$$

g : gravitational acceleration

⇒ via **source** term

⇒ **no explicit** total energy conservation using gravitational potential

FLASH code: Gravity

- Gravity modules
 - `source/physics/Gravity`
 - ⇒ **default**: constant gravitational acceleration
 - `source/Grid/GridSolvers`
 - ⇒ for **self-gravity**
 - Multipole
 - Multigrid
 - BHTree

FLASH code: Gravity

- time-independent **external** fields:
 - `source/physics/Gravity/GravityMain`
 - `Constant`
 $\Rightarrow \mathbf{g} = \text{const}$ in `gdir` = `x,y` or `z` direction
 - `PlanPar`
 $\Rightarrow \mathbf{g} = G_N M / h^2$ `h` = `x,y` or `z`-direction
 - `PointMass`
 $\Rightarrow \mathbf{g} = G_N M / r^2 \mathbf{r}/r$

 \Rightarrow similarly for *sink particles*

FLASH code: Gravity

- Self-gravity:

⇒ source/Grid/GridSolvers

provides gravitational potential $\Phi(\mathbf{x})$ via

- multi-pole solver
- multi-grid solver (Paul Ricker 2008)
- tree-based solver (Richard Wunsch)

$$\Rightarrow \nabla^2 \Phi(\mathbf{x}) = 4\pi G_N \rho(\mathbf{x}) \quad \Rightarrow \mathbf{g}(\mathbf{x}) = -\nabla \Phi(\mathbf{x})$$

$$\begin{aligned} \Rightarrow g_{x;ijk} &= \frac{1}{2\Delta x} (\phi_{i-1,j,k} - \phi_{i+1,j,k}) \\ g_{y;ijk} &= \frac{1}{2\Delta y} (\phi_{i,j-1,k} - \phi_{i,j+1,k}) \\ g_{z;ijk} &= \frac{1}{2\Delta z} (\phi_{i,j,k-1} - \phi_{i,j,k+1}) \end{aligned} \quad \begin{array}{l} \text{implementation via} \\ \text{finite difference} \\ \text{scheme} \end{array}$$

FLASH code: Gravity

- setup with self-gravity:

in `Config` file

⇒ `REQUIRES physics/Gravity/GravityMain/Poisson/Multipole`

or

⇒ `REQUIRES physics/Gravity/GravityMain/Poisson/Multigrid`

or

⇒ `REQUIRES physics/Gravity/GravityMain/Poisson/BHTree`

FLASH code: Gravity

- setup with self-gravity:

boundary conditions

<i>bcTypes</i>	Type of boundary condition
0	Isolated boundaries
1	Periodic boundaries
2	Dirichlet boundaries
3	Neumann boundaries
4	Given-value boundaries

FLASH code: Gravity

- Multipole solver

formal solution of $\nabla^2\Phi(\mathbf{x}) = \alpha \rho(\mathbf{x})$; $\alpha = 4\pi G_N$

$$\Rightarrow \phi(\mathbf{x}) = -\frac{\alpha}{4\pi} \int d^3\mathbf{x}' \frac{\rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|}$$

with Green's function

$$\Rightarrow \frac{1}{|\mathbf{x} - \mathbf{x}'|} = 4\pi \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \frac{1}{2\ell + 1} \frac{r_{<}^{\ell}}{r_{>}^{\ell+1}} Y_{\ell m}^*(\theta', \varphi') Y_{\ell m}(\theta, \varphi)$$

where $Y_{\ell m}(\theta, \varphi)$ are the spherical harmonic functions

$$\Rightarrow \text{origin at center of mass (CM): } \mathbf{x}_{\text{cm}} = \frac{\int \mathbf{x} \rho(\mathbf{x}) d\mathbf{x}}{\int \rho(\mathbf{x}) d\mathbf{x}}$$

FLASH code: Gravity

- Multipole solver

$$\Rightarrow \Phi(\mathbf{x}) \rightarrow \Phi(r, \mu(r))$$

with **source moments** $\mu(r)$

$$\text{e.g. } \mu_{\ell m}^{\text{ei}}(r) \equiv \frac{(\ell - m)!}{(\ell + m)!} \int_{r > r'} d^3 \mathbf{x}' r'^{\ell} \rho(\mathbf{x}') P_{\ell m}(\cos \theta') \cos m \varphi'$$

and $\mu^{\text{oi}}, \mu^{\text{eo}}, \mu^{\text{oo}}$, (even/odd, inner/outer)

\Rightarrow compute μ 's up to l_{max}

\Rightarrow **note:** scales at least as $2 \times N_{\text{grid}} \times l_{\text{max}}^2$

\Rightarrow only useful for low l_{max} , i.e. nearly spherical problems

FLASH code: Gravity

- Multipole solver

- main runtime parameters

Variable	Type	Default	Description
<code>mpole_lmax</code>	integer	10	Maximum multipole moment
<code>quadrant</code>	logical	<code>.false.</code>	Use symmetry to solve a single quadrant in 2D axisymmetric cylindrical (r, z) coordinates, instead of a half domain.

- supported grid geometries:

- ⇒ 1D, spherical

- ⇒ 2D, cylindrical, spherical

- ⇒ 3D, Cartesian, axi-symmetric

FLASH code: Gravity

- Multipole solver

- possible test suit:

`unitTest/Multipole`

⇒ only multipole solver **without** gravity
based on MacLaurin spheroid analytic solution

FLASH code: Gravity

- Multipole solver
 - improved Multipole solver
 - ⇒ `source/Grid/GridSolvers/Multipole_new`
- improvements:
 - efficient memory layout
 - elimination of over- and underflow errors when using astrophysical (dimensions $\approx 10^9$) domains
 - elimination of subroutine call overhead (1 call per cell)
 - ...

FLASH code: Gravity

- **Multigrid solver**

- based on improved *Huang-Greengard* (2000) method by *P. Ricker* (ApJS, 2008)

- **iterative** method

- uses fine-coarse structure of AMR grid

⇒ restrict & interpolate solution
to different refinement levels ⇒ **V-cycle**

- main functions in

`source/Grid/GridSolvers/Multigrid/`
⇒ `gr_hg*.F90`

FLASH code: Gravity

- Multigrid solver: V-cycle

```
!! DESCRIPTION
!! This is the main Poisson solve routine for the Huang & Greengard
!! (2000, SIAM J. Sci. Comput., 21, 1551) algorithm. This routine
!! defines the multigrid cycle as expressed in the article.
!!
!! coarse ^
!!
!!      o----->o          o----->o
!!      ^      s \          ^      s \ c
!!      r|      o o          lr      o o o
!!      e|      l \          le      l \ r
!!      s|      v o          ls      v o r
!!      t|      e \          lt      e \ e
!!      r|              o          lr              o c
!!      i|              \          li              \ t
!!      c|              o          lc              o
!!      t|              \          lt              \
!!
!! src |          o----->o gr_iSlS          o----->...until |r| < rtol
!! fine |_____take residual_____take new residual__>
!!
```

FLASH code: Gravity

- Multigrid solver: more details

- residual
$$R(\mathbf{x}) \equiv 4\pi G\rho(\mathbf{x}) - \nabla^2 \tilde{\phi}(\mathbf{x})$$

- finite difference operator:

$$\mathcal{D}_\ell \tilde{\phi}_{ijk}^{bl} \equiv \frac{1}{\Delta x_\ell^2} \left(\tilde{\phi}_{i+1,jk}^{bl} - 2\tilde{\phi}_{ijk}^{bl} + \tilde{\phi}_{i-1,jk}^{bl} \right) + \dots$$

- restrict operator: fine \rightarrow coarse

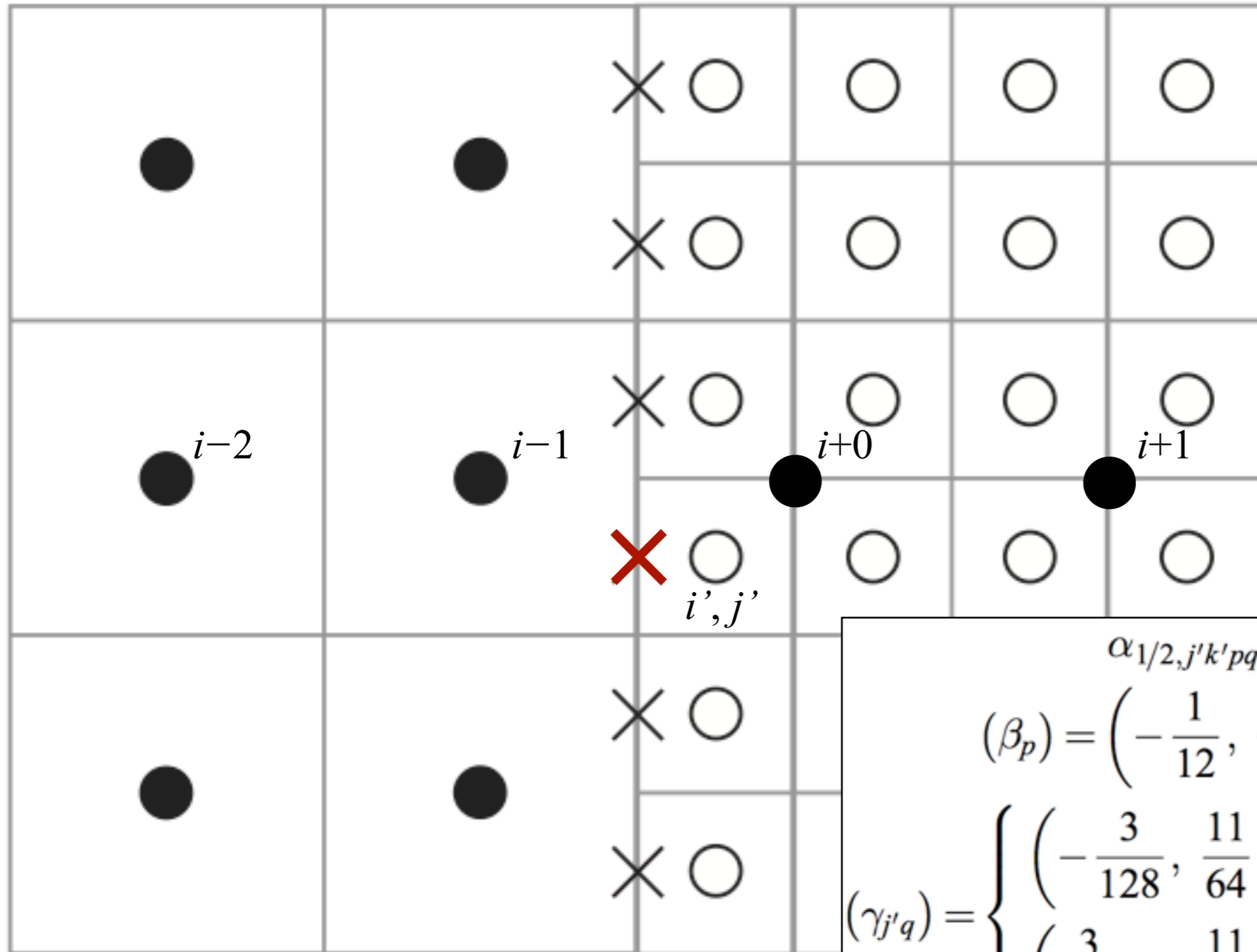
$$(\mathcal{R}_\ell \tilde{\phi})_{ijk}^{\mathcal{P}(c),\ell} \equiv \frac{1}{2^d} \sum_{i'j'k'} \tilde{\phi}_{i'j'k'}^{c,\ell+1}$$

- interpolation operator at block edges: coarse \rightarrow fine

$$(\mathcal{I}_\ell \tilde{\phi})_{i'j'k'}^{c,\ell+1} \equiv \sum_{p,q,r=-2}^2 \alpha_{i'j'k'pqr} \tilde{\phi}_{i+p,j+q,k+r}^{\mathcal{P}(c),\ell}$$

FLASH code: Gravity

- Multigrid solver: Interpolation operator



Example:
 $-x$ boundary

$$\alpha_{1/2, j'k'pqr} = \beta_p \gamma_{j'q} \gamma_{k'r},$$

$$(\beta_p) = \left(-\frac{1}{12}, \frac{7}{12}, \frac{7}{12}, -\frac{1}{12}, 0 \right),$$

$$(\gamma_{j'q}) = \begin{cases} \left(-\frac{3}{128}, \frac{11}{64}, 1, -\frac{11}{64}, \frac{3}{128} \right), & j' \text{ odd,} \\ \left(\frac{3}{128}, -\frac{11}{64}, 1, \frac{11}{64}, -\frac{3}{128} \right), & j' \text{ even} \end{cases}$$

FLASH code: Gravity

- Multigrid solver: more details

1. Restrict the source function $4\pi G\rho$ to all levels. Subtract the global average for the periodic case.
2. *Interpolation step*: For ℓ from 1 to ℓ_{\max} ,
 - (a) Reset the grid so that ℓ is the maximum refinement level
 - (b) Solve $\mathcal{D}_\ell \tilde{\phi}_{ijk}^{b\ell} = 4\pi G\rho_{ijk}^{b\ell}$ for all blocks b on level ℓ . → sin-type Green's function or FFT
 - (c) Compute the residual $R_{ijk}^{b\ell} = 4\pi G\rho_{ijk}^{b\ell} - \mathcal{D}_\ell \tilde{\phi}_{ijk}^{b\ell}$
 - (d) For each block b on level ℓ that has children, prolong face values for $\tilde{\phi}_{ijk}^{b\ell}$ onto each child block.
3. *Residual propagation step*: Restrict the residual $R_{ijk}^{b\ell}$ to all levels.
4. *Correction step*: Compute the discrete L_2 norm of the residual over all leaf-node blocks and divide it by the discrete L_2 norm of the source over the same blocks. If the result is greater than a preset threshold value, proceed with a correction step: for each level ℓ from 1 to ℓ_{\max} ,
 - (a) Reset the grid so that ℓ is the maximum refinement level
 - (b) Solve $\mathcal{D}_\ell C_{ijk}^{b\ell} = R_{ijk}^{b\ell}$ for all blocks b on level ℓ . → sin-type Green's function or FFT
 - (c) Overwrite $R_{ijk}^{b\ell}$ with the new residual $R_{ijk}^{b\ell} - \mathcal{D}_\ell C_{ijk}^{b\ell}$ for all blocks b on level ℓ .
 - (d) Correct the solution on all leaf-node blocks b on level ℓ : $\tilde{\phi}_{ijk}^{b\ell} \rightarrow \tilde{\phi}_{ijk}^{b\ell} + C_{ijk}^{b\ell}$.
 - (e) For each block b on level ℓ that has children, interpolate face boundary values of $C_{ijk}^{b\ell}$ for each child.
5. If a correction step was performed, return to the residual propagation step.

FLASH code: Gravity

- Multigrid solver: more details

1. Restrict the source function $4\pi G\rho$ to all levels. Subtract the global average for the periodic case.
2. *Interpolation step*: For ℓ from 1 to ℓ_{\max} ,
 - (a) Reset the grid so that ℓ is the maximum refinement level
 - (b) Solve $\mathcal{D}_\ell \tilde{\phi}_{ijk}^{bl} = 4\pi G\rho_{ijk}^{bl}$ for all blocks b on level ℓ . → sin-type Green's function or FFT
 - (c) Compute the residual $R_{ijk}^{bl} = 4\pi G\rho_{ijk}^{bl} - \mathcal{D}_\ell \tilde{\phi}_{ijk}^{bl}$
 - (d) For each block b on level ℓ that has children, prolong face values for $\tilde{\phi}_{ijk}^{bl}$ onto each child block.
3. *Residual propagation step*: Restrict the residual R_{ijk}^{bl} to all levels. ←
4. *Correction step*: Compute the discrete L_2 norm of the residual over all leaf-node blocks and divide it by the discrete L_2 norm of the source over the same blocks. If the result is greater than a preset threshold value, proceed with a correction step: for each level ℓ from 1 to ℓ_{\max} ,
 - (a) Reset the grid so that ℓ is the maximum refinement level
 - (b) Solve $\mathcal{D}_\ell C_{ijk}^{bl} = R_{ijk}^{bl}$ for all blocks b on level ℓ . → sin-type Green's function or FFT
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 - (e) For each block b on level ℓ that has children, interpolate face boundary values of C_{ijk}^{bl} for each child.
5. If a correction step was performed, return to the residual propagation step.

FLASH code: Gravity

```
do m = 1, gr_hgMeshRefineMax
  call gr_hgSetMaxLevel(m) ! This is a new FLASH3 routine
  ! call gr_hgNorm(0, 1, gr_iSource, norm_tmp, MG_NODES_LEAF_ONLY)
  call gr_hgSetZeroBoundary(m, gr_iSoln) !oK
  call gr_hgSolveLevel(m, gr_iSource, gr_iSoln, SolveBlock, MG_NODES_ALL_NODES) ! Working here.....
  call gr_hgResidual(m, gr_iSource, gr_iSoln, gr_iSls) !oK
  call gr_hgProlongBndries(m, gr_iSoln, gr_iSoln, 0) ! LBR doesn't wanna know. But we looked at it...
enddo
! Correction step. Restrict residuals from finer levels to coarser levels.
! Solve for correction on these levels and interpolate boundary conditions to
! finer levels. Solve for corrections there and apply. Repeat. Repeat these
! correction steps until the desired residual norm is achieved.
do n = 0, gr_hgMaxCorrections
  call gr_hgNorm(0, 2, gr_iSls, norm_lhs, MG_NODES_LEAF_ONLY)

  if (norm_lhs/norm_rhs <= gr_hgMaxResidualNorm) exit

  do m = gr_hgMeshRefineMax-1, 1, -1
    call gr_hgRestrict(m+1, gr_iSls, gr_iSls)
  enddo

  call gr_hgSetMaxLevel(1)
  call gr_hgSetZeroBoundary(1, gr_iCorr)
  call gr_hgSolveLevel(1, gr_iSls, gr_iCorr, SolveBlock, MG_NODES_ALL_NODES, dt, chi)
  call gr_hgLevelAdd(1, gr_iSoln, gr_iCorr, MG_NODES_LEAF_ONLY) !oK
  call gr_hgProlongBndries(1, gr_iCorr, gr_iCorr, 0) !infamous

  do m = 2, gr_hgMeshRefineMax
    call gr_hgSetMaxLevel(m)
    call gr_hgSetZeroBoundary(m, gr_iCorr)
    call gr_hgSolveLevel(m, gr_iSls, gr_iCorr, SolveBlock, MG_NODES_ALL_NODES)
    call gr_hgResidual(m, gr_iSls, gr_iCorr, gr_iSls) ! not called on top level
    call gr_hgLevelAdd(m, gr_iSoln, gr_iCorr, MG_NODES_LEAF_ONLY)
    call gr_hgProlongBndries(m, gr_iCorr, gr_iCorr, 0)
  enddo
enddo
```

FLASH code: Gravity

- Multigrid solver: Additional fields needed:
 - 'gpot' key GPOT_VAR: actual gravitational potential
 - 'gpot1' key GPOT_VAR: gravitational potential from previous time step \Rightarrow needed to start solution iteration
 - 'isls' key ISLS_VAR: residual potential variable
 - 'icor' key ICOR_VAR: correction potential variable
 - 'imgm' key IMGGM_VAR: image mass for periodic BCs
 - 'imgp' key IMGPP_VAR: image potential for periodic BCs

FLASH code: Gravity

- Multigrid solver:
 - supported geometries
 - ⇒ only Cartesian geometry in 1, 2 and 3 D
 - supported boundary conditions
 - ⇒ isolated
 - ⇒ periodic
 - ⇒ Dirichlet (Φ given at the boundaries)
 - ⇒ Neumann, not yet implemented

FLASH code: Gravity

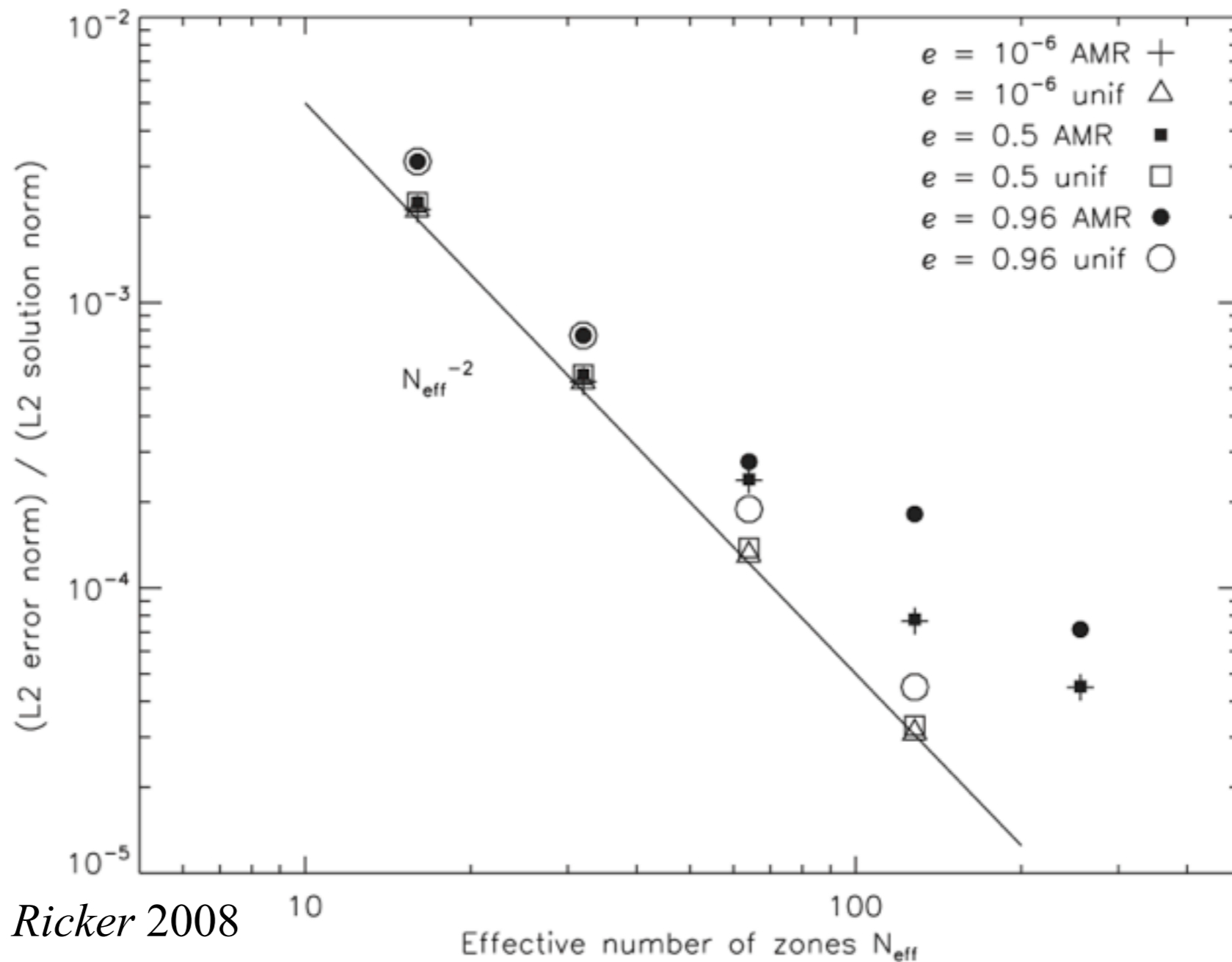
- Multigrid solver: main files

source/Grid/GridSolvers/Multigrid

```
gr_hgBndry.F90
gr_hgData.F90
gr_hgFinalize.F90
gr_hgGuardCell.F90
gr_hgInit.F90
gr_hgInitSource.F90
gr_hgLevelAdd.F90
gr_hgLevelAddScalar.F90
gr_hgLevelMultiplyScalar.F90
gr_hgLevelZero.F90
gr_hgMapBcType.F90
gr_hgNorm.F90
gr_hgPoissonSolve1D.F90
gr_hgPoissonSolve2D.F90
gr_hgPoissonSolve3D.F90
gr_hgPoissonSolveBlock.F90
gr_hgProlongBndries.F90
gr_hgRecordNodeTypeState.F90
gr_hgResidual.F90
gr_hgRestoreNodeTypes.F90
gr_hgRestrict.F90
gr_hgSetExtBoundary.F90
gr_hgSetMaxLevel.F90
gr_hgSetZeroBoundary.F90
gr_hgSolve.F90
gr_hgSolveLevel.F90
gr_hg_amr_1blk_bcset_work.F90
```

FLASH code: Gravity

- Multigrid solver: **Solution convergence**
 - ⇒ UG: truncation error: $O(\Delta x^2)$
 - ⇒ weaker for AMR (here: 5% of vol. on highest refinement level)



FLASH code: Gravity

- **Barns & Hut Tree Solver**
(*Barns & Hut*, Nature 1986)
 - implemented by Richard Wünsch (Prague)
 - based on an oct-tree with monopole moments
⇒ matches oct-tree AMR structure of PARAMESH
- basic properties
 - scaling: $N \log(N)$: N number of grid/mass cells
instead N^2 of for direct summation
 - works only for $NBX = NBY = NBZ$
 - $NBX = 2^n$ (not yet tested for $NBX \neq 8$)

FLASH code: Gravity

- Tree Solver: steps to calculate the gravitational potential:

- **build the tree:**

1. build oct-tree in block (**block-tree**)

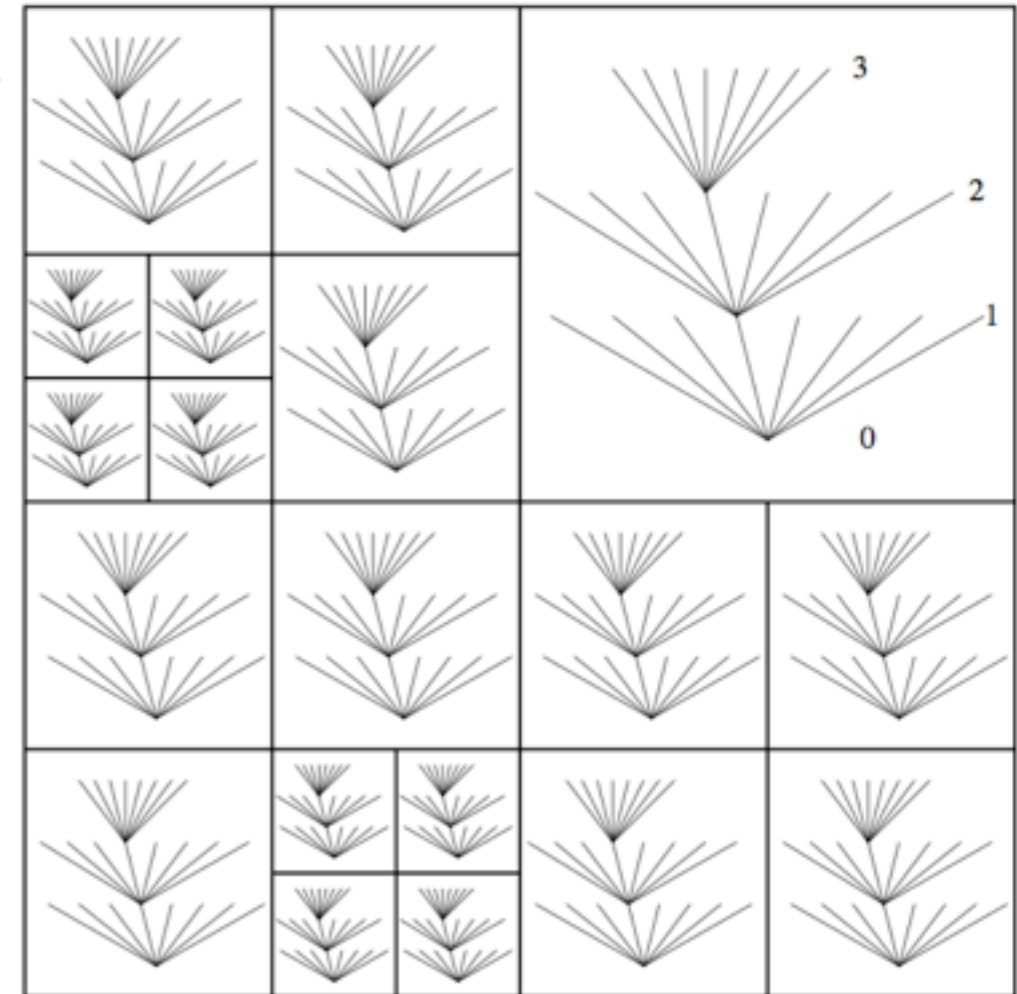
⇒ $\log_2(\text{nbx})$ levels

⇒ stored in `gr_bhTreeArray`

2. **masses** and **CMs** of top nodes are distributed to all processors via `gr_bhTreeParentTree`
(4 , MAXBLOCKS , NPROCS)

3. calculation of **masses** and **CMs** of parent blocks on all CPUs

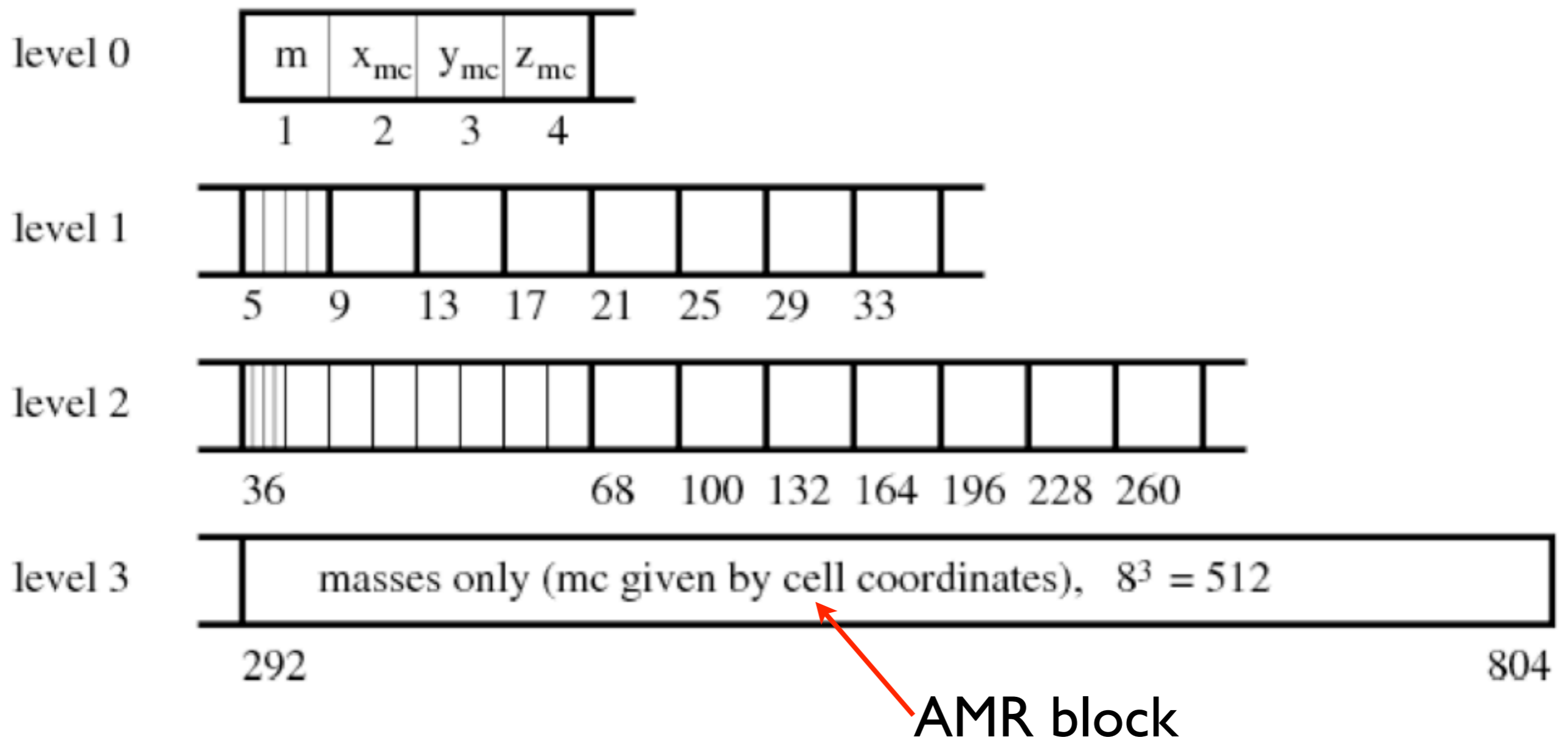
⇒ stored also in `gr_bhTreeParentTree`



⇒ tree down to leaf block information on all CPUs

FLASH code: Gravity

- **block-tree** structure in memory for blocks with $8 \times 8 \times 8$ grid cells
⇒ linear array in memory: size = $8^3 + 4 \times (8^2 + 8^1 + 8^0) = 804$



⇒ access via multi-index

FLASH code: Gravity

- Tree Solver: steps to calculate the gravitational potential:
 - **communication of the tree:**

I. determine which **block-trees** to be communicated:

$$\frac{S_{\text{node}}(l)}{D_{\text{min}}} < \text{gr_bhTreeLimAngle}$$

⇒ $S(l)$: size of the local **block-tree** at level $l = 0..3$

⇒ D_{min} : minimum distance to all remote blocks

all eight corners of both, the local and the remote blocks, are checked

⇒ typical values for **gr_bhTreeLimAngle**: 0.5 ... 1.0

FLASH code: Gravity

- Tree Solver: steps to calculate the gravitational potential:

- **communication of the tree:**

1. determine which **block-tree** levels to be communicated:

$$\frac{S_{\text{node}}(l)}{D_{\text{min}}} < \text{gr_bhTreeLimAngle}$$

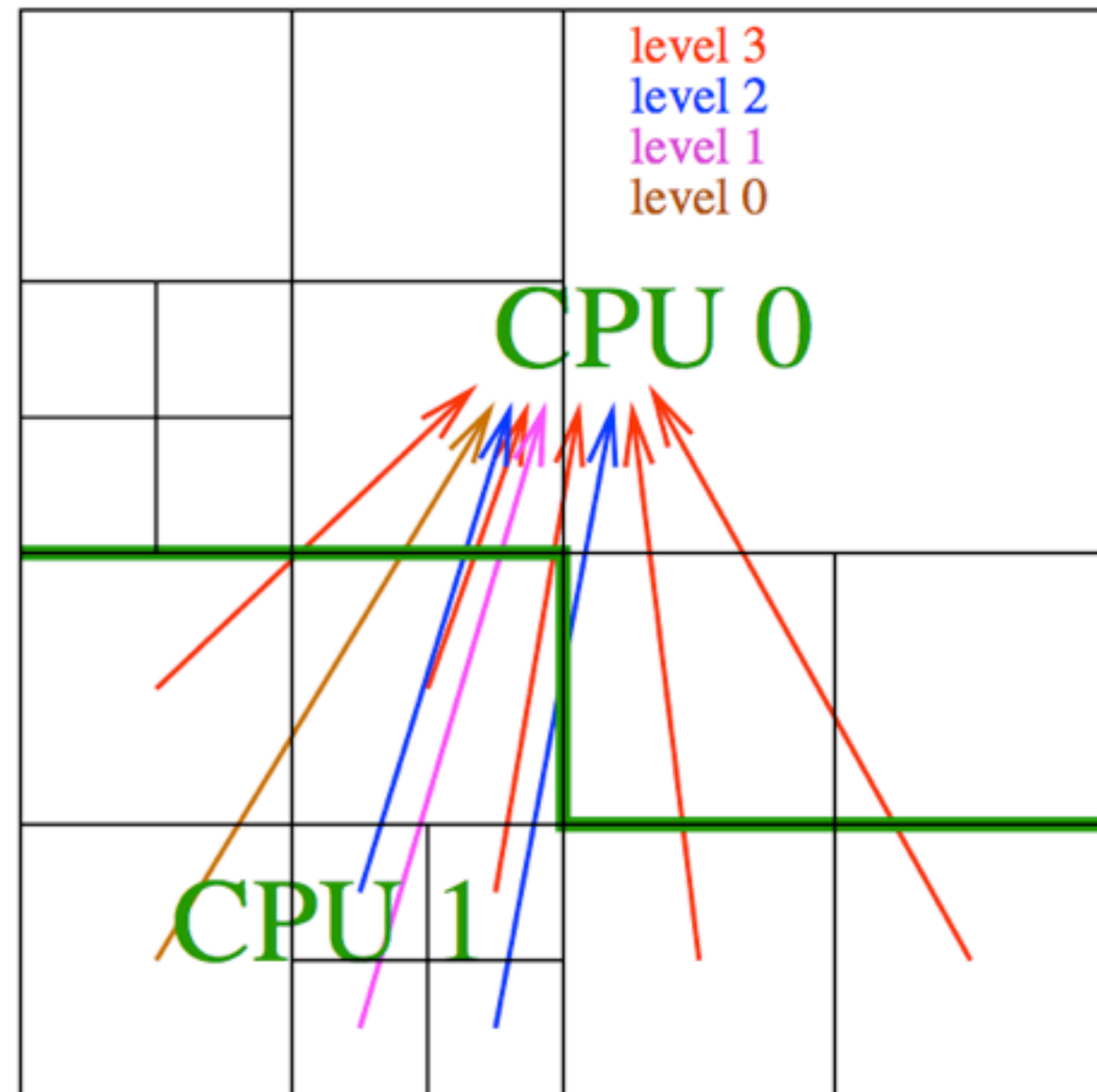
2. communication of **block-tree** levels

⇒ to allocate memory on remote CPUs

⇒ all values for a given CPU in a single message

3. selected **block-tree** nodes are send to remote CPUs

⇒ all **block-tree** nodes are packed into a single message



FLASH code: Gravity

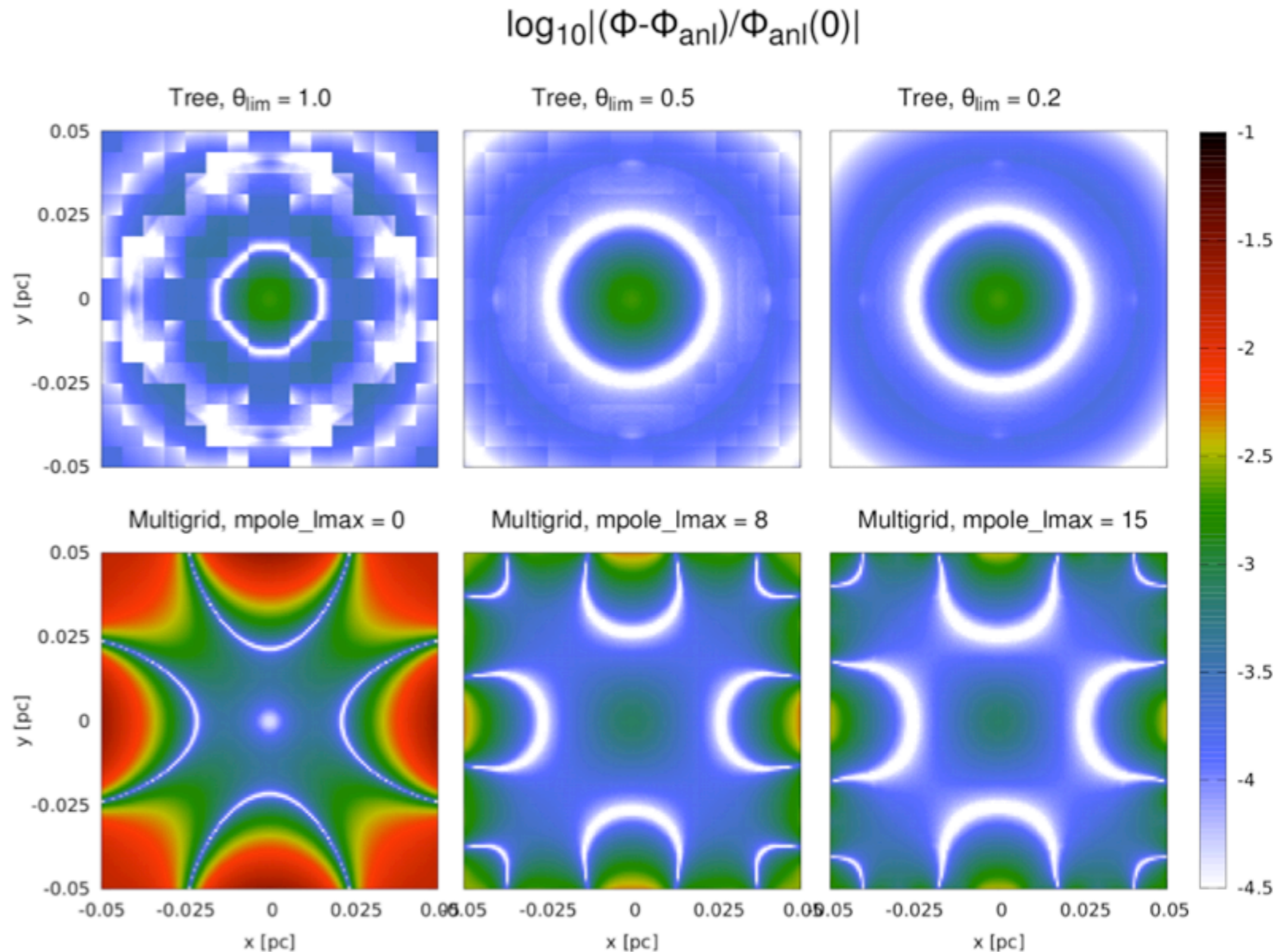
- Tree Solver: steps to calculate the gravitational potential:
 - **calculation of the potential** \Rightarrow the “tree walk”
 - \Rightarrow most time consuming part ($\sim 90\%$ of tree solver)
 - \Rightarrow fully parallel, no more communication needed
 - walk the tree for local block A
 - \Rightarrow start with refinement level one
- B is the currently processed tree node
 - if B is a **parent** block
 - $\Rightarrow S_B/D_{AB} < \theta_{\text{lim}}$ (S_B : size of B , D_{AB} : min distance to CM_B)
 - $\Rightarrow \Delta\Phi_{A,\text{cell}} = -G M_B/D_{\text{cell},B}$
 - else continue with child-blocks of B

FLASH code: Gravity

- Tree Solver: steps to calculate the gravitational potential:
 - if B is a leaf block:
 - \Rightarrow **block tree** of B is walked separately for each level
 - \Rightarrow **block tree** consists of nodes N
 - $\Rightarrow S_N/D_{\text{cell},N} < \theta_{\text{lim}}$ (S_N : size of node N)
 - $\Rightarrow \Delta\Phi_{A,\text{cell}} = -G M_N/D_{\text{cell},N}$
 - else continue with children of N

FLASH code: Gravity

- Tree Solver: Test with Bonnor-Ebert sphere



FLASH code: Gravity

- Tree Solver:

- supported geometry

⇒ so far, only 3D cartesian geometry

- boundary conditions

⇒ isolated

⇒ periodic → generation of 'Ewald' field values necessary

- Parameters

```
PARAMETER gr_bhTreeLimAngle REAL 0.5 [ 0 ... ]
PARAMETER gr_bhIlist INTEGER 0 [ 0, 1 ]
PARAMETER gr_bhEwaldFieldNx INTEGER 64 [ 1 ... ]
PARAMETER gr_bhEwaldFieldNy INTEGER 64 [ 1 ... ]
PARAMETER gr_bhEwaldFieldNz INTEGER 64 [ 1 ... ]
PARAMETER gr_bhEwaldSeriesN INTEGER 10
PARAMETER gr_bhEwaldAlwaysGenerate BOOLEAN TRUE
PARAMETER gr_bhEwaldFName STRING "ewald_field"
PARAMETER gr_bhUseEwaldDecomp BOOLEAN TRUE
PARAMETER gr_bhEwaldIsoFac INTEGER 1000
```

FLASH code: Gravity

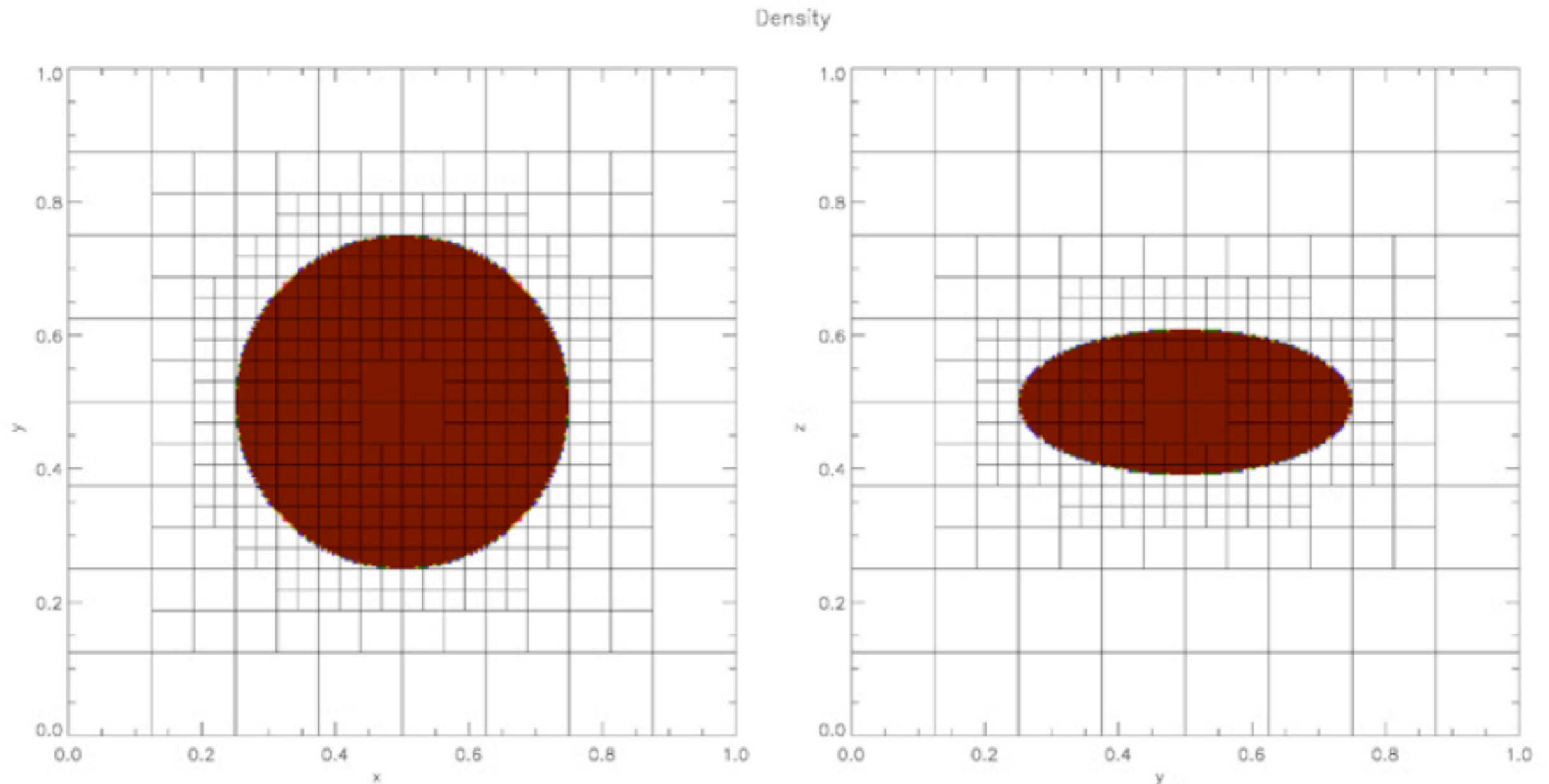
- Tree Solver: the source files
in `source/Grid/GridSolvers/BHTree/Wunsch`

```
Grid_solvePoisson.F90
gr_bhBlockRelationship.F90
gr_bhBuildTree.F90
gr_bhBuildTreeBlock.F90
gr_bhComBlkProperties.F90
gr_bhComParentTree.F90
gr_bhData.F90
gr_bhDestroyTree.F90
gr_bhErfc.F90
gr_bhEwald.F90
gr_bhEwaldField.F90
gr_bhExchangeTrees.F90
gr_bhFinalize.F90
gr_bhFindNeighbours.F90
gr_bhGetTreePos.F90
gr_bhGetTreeSize.F90
gr_bhILContrib.F90
gr_bhInit.F90
gr_bhInitTemplates.F90
gr_bhLeafContrib.F90
gr_bhLocalInterface.F90
gr_bhParentContrib.F90
gr_bhPotential.F90
gr_bhPotentialBlock.F90
```

FLASH code: Gravity

- MacLaurin test problem: collapse of a spheroid

`source/Simulation/SimulationMain/MacLaurin`



spheroid with ellipticity $e = 0.9$

FLASH code: Sinks

tasks

- try **MacLauren** setup with
 - multipole
 - multigrid and
 - BHTree

Poisson solvers

- set up and run a collapse **Bonnor-Ebert** problem:
`source/Simulation/SimulationMain/BonnorEbert`

replace Config with `/pfs/banerjee/Config_BE`