FLASH Center for Computational Science

FLASH Infrastructure Code Units: Driver, Grid, IO

Flash Tutorial at RAL
May 30, 2012
Klaus Weide

The University of Chicago

Infrastructure Code Topics

- Driver Unit
  - Overview and Function
  - Unsplit vs Split
- Grid Unit
  - Overview: Implementations
  - Overview: blocks, cells,
  - PARAMESH: oct-tree
  - Data structures and Meta-Data
  - Configuring Variables for Grid Data Structures
  - Dimensions and Geometries
  - What the Grid Code Unit Does
  - Filling Guard Cells and Boundary Conditions
- IO Unit preview

Driver Unit

- Overview and Function
- Unsplit vs Split

Driver - Overview and Function

All other code units and their subroutines are called, directly or indirectly, from *Driver*. There are three phases encompassing everything FLASH does:

Initialize – **Simulate** (producing some output,…) – **Finish**

The main F90 program, Flash.F90, invokes the rest of the code like this:

- call Driver_initFlash
  - Initialize parameters, data, Grid incl. variable values, ...
- call Driver_evolveFlash
  - Advance in time (the only kind of "evolution" that FLASH does)
- call Driver_finalizeFlash
  - Clean up nicely

Time Evolution - Unsplit and Split

- FLASH4 provides two variants of time evolution (two *Driver* "implementations"): *Split* and *Unsplit*.
  - Pick the right one for the *Hydro* implementation used

    (normally this is automatically done by the `./setup` command)
  - Driver_evolveFlash implements the main loop of FLASH.
  - The loop ends normally when one of several conditions is satisfied:
    - Loop counter dr_nstep = nstart ... nend
    - Simulation time reaches tmax
    - Wall clock reaches wall_clock_time_limit
  - Time step dt can vary between dtmin and dtmax, Driver_computeDt computes new dt after each loop iteration.
  - Driver_computeDt calls Hydro_computeDt, Particles_computeDt, etc. to honor time step requirements of different code units.

Time Evolution - Unsplit vs Split

- DriverMain/Split/

  Driver_evolveFlash loop for split *Hydro* (PPM, default)

```
Do ...
      call Hydro(...,SWEEP_XYZ)
      call other physics
      .....
      call Hydro(...,SWEEP_ZYX)
      call other physics
      .....
End Do
```

- DriverMain/Unsplit/

  Driver_evolveFlash loop for unsplit *Hydro* (staggered mesh MHD, etc.)

```
Do ...
      call Hydro(...)
      call other physics
      .....

End Do
```

- Each loop iteration advances the solution by 2 dt

- Each loop iteration advances the solution by dt

Grid Unit

- Overview: Purpose
- Overview: Implementations
- Overview: blocks, cells, ...
- PARAMESH: oct-tree
- Data structures and Meta-Data
- Configuring Variables for Grid Data Structures
- Dimensions and Geometries
- What the Grid Code Unit Actually Does
- Filling Guard Cells
- Boundary Conditions

First Look at Paramesh (and UG) Grids

- Purpose of the Grid: represent data
  - Much more on *UNK* variables etc. below
  - More precisely, will be talking about the *GridMain* subunit of Grid
- Each block of data resides on exactly one processor* (at a given point in time)
- At a given point in time, the number of local blocks on a processor lies between 1 and MAXBLOCKS. (or can be 0, at least during initialization)
  - MAXBLOCKS is defined at setup time. This represents a hardwired limit on how many blocks can exist in total.
  - Grid_getLocalNumBlks() returns the current local value.
  - Paramesh attempts to balance blocks across processors so that processor will have approximately equal amounts of work to do.
  - With the FLASH4 Uniform Grid (UG), the number of blocks is always one per processor.

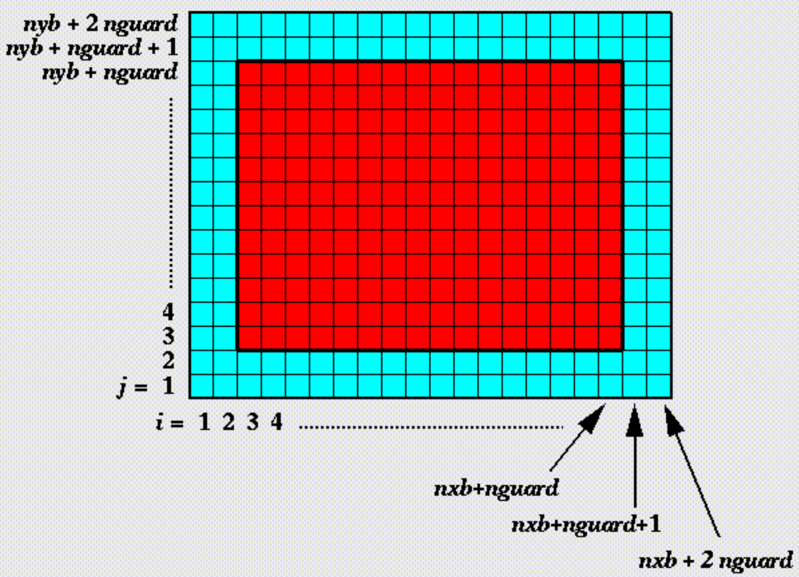
*On notation: processor here means, more correctly: MPI task .

Overview: Implementations

- UG – Uniform Grid
  - Fast, very little overhead
  - Use when your problem does not profit from varying resolution
- Paramesh2 – old AMR for FLASH2 compatibility
- Paramesh4.0 – currently the default Grid Implementation
- Paramesh4dev
  - May become the default soon; recommended for large runs.
  - Same functions as PM4.0, users should see no differences in results. (known exception: very small differences are possible with face variables.)
  - Performance can differ from PM4.0:
    - Faster in handling grid refinement changes
    - Other Grid operations may be slightly slower
- Chombo – patch-based library, experimental

Select implementation: `setup` shortcuts +ug, +pm40, +pm4dev

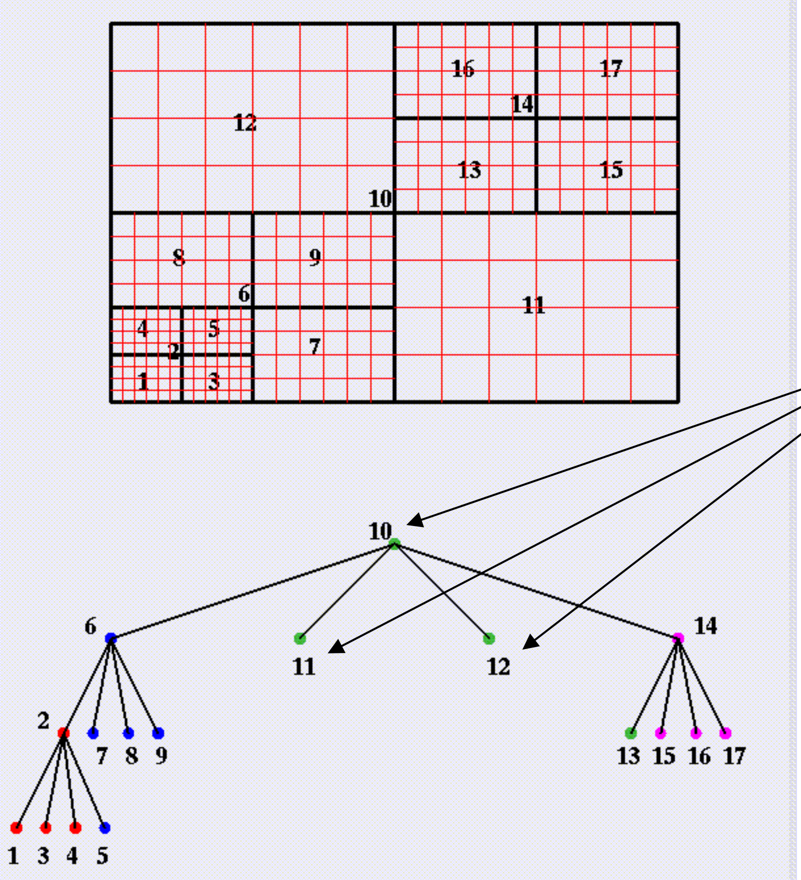
Reminder: blocks and cells



Indexing scheme for a 2D grid block with 2 guard cells (nguard=2) at each block boundary. Interior cells are colored red, guard cells are colored blue.

- The grid is composed of blocks
- FLASH4: In current practice, all blocks are of same size.
- May cover different fractions of the physical domain, depending on a block's resolution.
- Data storage area for each block reserves space for some layers of guard cells.

PARAMESH: An Oct-tree of Blocks



- Paramesh specific design:
  - Block Structured
  - All blocks have same dimensions
  - Blocks at different refinement levels have different grid spacings and thus cover different fractions of the physical domain
  - Fixed sized blocks specified at compile time
- Global block numbers are based on Morton order, approximates "space-filling" behavior. (example numbers for PM2; PM4 is very similar.)
- Storage order within each processor follows this ordering. Re-distribution of blocks after refinement changes, for load balancing.
- Oct-tree in 3D: A node has either 8 children or none. (Quad-tree in 2D, binary in 1D)
- Blocks are of type LEAF, PARENT, or ANCESTOR.
- Data for PARENT and ANCESTOR blocks occupies storage space! (not much in 3D)

In choosing Paramesh, the original FLASH code architects chose simplicity of the Paramesh structure over a patch based mesh.

Limits of Paramesh

- PARAMESH is based on blocks, not general patches.

  - Limitations imposed by Paramesh:
    - Same number of cells in all blocks
    - Same number of guard cell layers in all blocks, all directions
    - Resolution ("Delta") of a block changes by multiples of 2.
    - Resolution of neighbors differs at most by factor of 2.

    (In other words: the local refinement level may change by at most ±1)

How Blocks are Addressed

- At a given time, a block is **globally** uniquely identified by a pair (*proc, BlockID*), where
  - 0 < *proc* < *numprocs*
  - 1 < *BlockID* <= MAXBLOCKS
- **Locally**, *BlockID* is sufficient to specify a block
  - User code can't directly access remote blocks anyway
- Morton Numbers provide another way to identify blocks **globally.**

  (private data of the Grid unit, not exposed to other code at runtime)
- The global block number of a block determines the index of the block's data in output files (checkpoint, plot files). It is not available to user code during run time.

How Blocks are Stored

- Solution data,
- per-block meta data,
- tree information (for local blocks!)

are stored in F90 arrays declared like this:

```
real, dimension(:,:,:,:,MAXBLOCKS) :: UNK
real, dimension(:,MAXBLOCKS)       :: bnd_box
integer, dimension(:,MAXBLOCKS)    :: parent
```

etc. etc.

- MAXBLOCKS is a hardwired constant (from setup time)
- "Inactive" (non-leaf) blocks also use storage
- These structures are internal to the Grid unit and should not be accessed directly by other code.
- Use the appropriate *Grid_something()* subroutine calls instead! (in particular: *Grid_getBlkPtr*, *Grid_getBlkData*)

Grid Data Structures

- **CENTER** (keywords VARIABLE, SPECIES, MASS_SCALAR)
  - The “normal” way to keep fluid variables: logically cell-centered
  - Kept internally in an array UNK of dimensions UNK(NUNK_VARS,NXB+*gcs*,NYB+*gcs*,NZB+*gcs*,sMAXBLOCKS)
- FACEX, FACEY, FACEZ
  - Face-centered variables, currently used by unsplit MHD solver
  - Supported in UG, PM 4.0, PM 4dev
- SCRATCH *(data that is never updated automatically by Grid)*
  - Additional block-oriented storage provided by FLASH (not PM Kernel)
  - Guard cell filling or other communications not supported
- WORK *(only 1 “variable”, not recommended for portability)*
  - Additional block-oriented storage provided by PARAMESH (not in UG)
  - Used internally by some units (currently: geometric multigrid solvers)
- (FLUX – not a permanent data store, for flux corrections by *Hydro*)

Configuring Variables for Grid Data Structures

- Use VARIABLE vvvv in Config for unk(VVV_VAR,:,:,:,:)**
  - gridDataStruct=CENTER*
- Use SPECIES ssss in Config for unk(SSSS_SPEC,:,:,:,:)
  - gridDataStruct=CENTER
- Use MASS_SCALAR mmmm for unk(MMMM_MSCALAR,:,:,:,:)
  - gridDataStruct=CENTER
- Use FACEVAR ffff in Config for facevarx(FFFF_FACE_VAR,:,:,:,:), facevary(FFFF_FACE_VAR,...), & facevarz(FFFF_FACE_VAR,...)
  - gridDataStruct=FACEX/FACEY/FACEZ *(or for some calls:* FACES*)*
- Use GRIDVAR ggg for scratch(:,:,:,GGG_SCRATCH_GRID_VAR,:)
  - gridDataStruct=SCRATCH

* Many Grid interfaces have a gridDataStruct argument to specify what kind of data to act on. Examples: Grid_getBlkPointer, Grid_putBlkData, Grid_getBlkIndexLimits, Grid_fillGuardCells. See API documentation of these interface for details.

** The internal organization (order of array indices) is important for code working with block pointers as returned by Grid_getBlkPointer.

Configuring Variables for Grid Data Structures II

- Use VARIABLE vvvv in Config for unk(VVV_VAR,:,:,:,:)
  - gridDataStruct=CENTER
- Use SPECIES ssss in Config for unk(SSSS_SPEC,:,:,:,:)
  - gridDataStruct=CENTER
- Use MASS_SCALAR mmmm for unk(MMMM_MSCALAR,:,:,:,:)
  - gridDataStruct=CENTER

Cell-centered variables from VARIABLE, SPECIES, MASS_SCALAR become parts of the same large array:

- unk(1:NPROP_VARS,:,:,:,:) holds *NPROP_VARS* VARIABLEs
- unk(SPECIES_BEGIN:SPECIES_END,:,:,:,:) holds *NSPECIES* SPECIES
  - Note: often *NSPECIES=0,* in that case SPECIES_END=SPECIES_BEGIN-1
- unk(MASS_SCALARS_BEGIN:NUNK_VARS,:,:,:,:) holds *NMASS_SCALARS* MASS_SCALARs
  - Often *NMASS_SCALARS=0,* in that case MASS_SCALARS_BEGIN = NUNK_VARS+1

More On Variables for Grid Data Structures

- The "VARIABLE" part of unk represents most solution variables
  - VARIABLE dens TYPE: PER_VOLUME – conserved variable per volume-unit
  - VARIABLE ener TYPE: PER_MASS – energy in mass-specific form
  - VARIABLE temp TYPE: GENERIC – not a conserved entity in any form

  Specify the TYPE correctly to ensure correct treatment in Grid interpolation.

  See Config files in existing code Units for examples: *Hydro, Eos,* ...
- The SPECIES part of unk represents mass fractions
  - Get automatically advected by *Hydro*
  - Should probably be used with *Multispecies* Unit and *Multigamma* EOS
  - Should always add up to 1.0, code may enforce this
  - Treated as a per-mass variable for purposes of interpolation
- The MASS_SCALAR part of unk represents additional variables
  - Get automatically advected by *Hydro*
  - Treated as a per-mass variable for purposes of interpolation

Dimensions and Geometries

Geometry Support

The FLASH4 *Grid* supports these geometries:

- Cartesian - 1D, 2D, 3D
- Cylindrical - 2D, (3D)
- Spherical - 1D, (2D), (3D)
- Polar - (2D)

Combinations in bold have been extensively used & tested at the FLASH Center.

(Note: for a specific application, geometry support may be limited by available solvers!)

The *Grid* Implementation:

- Makes used of Paramesh4 support of geometries
- Centralized support by *Grid* unit, provides routines for cell volumes, face areas, etc.
- *Grid* uses geometry-aware conservative interpolation at refinement boundaries
  - This is thr default interpolation, internally called “monotonic”.
  - we provide a way to use an alternative Grid implementation's native methods instead:

    ./setup ... -gridinterpolation=native
- Use setup -3d -geometry= and/or runtime parameter *geometry* in flash.par to specify.

What the Grid Code Unit Actually Does

Note: the following focuses on AMR Grids; UG is simpler.

The Grid unit is responsible for

- Keeping account of the spatial domain as a whole:
  - Extent and size, outer boundaries
- Keeping and maintaining block structure:
  - Which blocks exist?
  - Where are they?
  - Sizes and other properties of blocks
  - Neighbors
  - Parent / child links for AMR
- Initializing block structure:
  - Initialize the metadata and links mentioned above
  - Keep Grid structure valid:
    - Consistent (if A is child of B, then B must be parent of A, etc. etc.)
    - For PARAMESH: no refinement jumps by more than 1 level

What the Grid Unit Actually Does - Cont.

Note: the previous slide was mostly about metadata; now the stuff actually wanted by users...

The *Grid* unit is also responsible for

- Keeping data ("User data", "Solution data", "payload"):
  - Provide storage
    - UNK, FACEVAR{X,Y,Z}, SCRATCH, (WORK)
    - FLUXes and other more temporary arrays
- **Initializing** solution data:
  - Actually **left to the user**, who provides a subroutine *Simulation_initBlock()*
  - *Grid* **invokes** user function, applies **refinement criteria**, repeat as necessary
- maintaining and keeping track of data during refinement changes:
  - Apply refinement criteria as requested
  - Copy data within processor, and/or communicate between procs
  - Involves prolongation (interpolation)
  - Involves restriction (valid data in PARENT blocks)

What the Grid Unit Actually Does - Cont..

Note: the previous slide was about data and mesh changes; now what's left to do between those changes?

- The *Grid* unit is **also** responsible for
- Operations that communicate user data between blocks:
  - Prolong (interpolate) data
    - After new leaf blocks are created
  - Restrict (summarize) data
    - PARENT blocks usually get summarized data as part of guard cell filling
  - Flux correction (special operation invoked from *Hydro*)
  - Edge averaging (special operation invoked from MHD *Hydro*)

And finally...

  - Guard cell filling
    - The most important form of data communication on an established mesh configuration.
    - Called frequently, by various code units
    - May move a lot of data between procs, efficiency is important!

Guard Cell Filling – When

Note: the following is focused on Paramesh4, but the high-level calls apply to all grid implementations

- When are guard cells filled?
  - **Directly**: High-level call to *Grid_fillGuardCells* (or maybe *amr_guardcell*)
    - Always a global operation involving all processors
    - Usually fills guard cells of LEAF blocks and their parents – but don't count on it for PARENT blocks.
  - Indirectly: internally as part of some other Grid operation
    - As part of *amr_prolong* (filling new leaf blocks)
  - Indirectly during global direct filling:
    - Auxiliary filling of a PARENT block's guard cells in order to provide input for interpolation to this PARENT's child, a finer-resolution LEAF node.

Guard Cell Filling - Usage

When should **you** fill guard cells?

- Before a subroutine that you have written uses guard cells, you need to make sure they are filled with valid and current data.
- FLASH4 does not guarantee that guard cells are valid on entry to a solver, source term code unit, etc.!

- How should you fill guard cells?
  - Only worry about direct filling of LEAF guard cells – that is nearly always what is needed.
  - Basic high-level call:

    ```
    Call Grid_fillGuardCells(CENTER_FACES,ALLDIR)
    ```

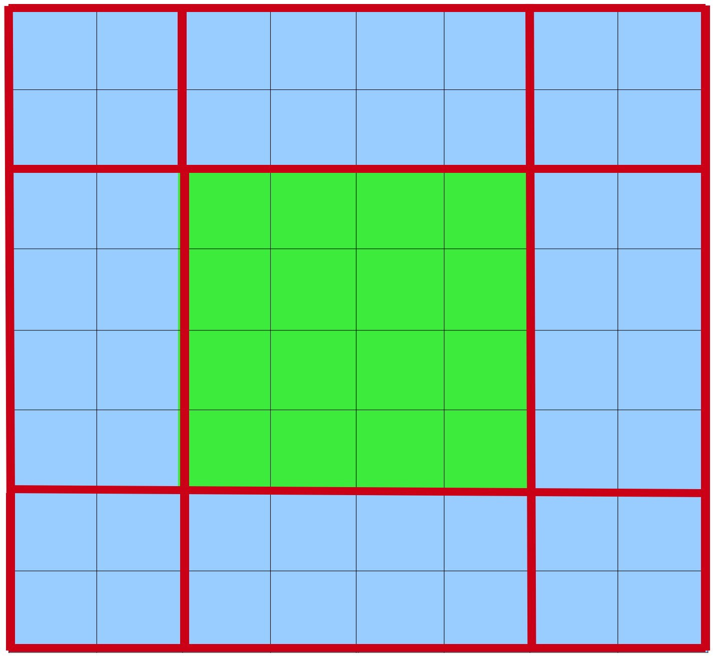
  - High-level call with automatic Eos call on guard cells:

    ```
    Call Grid_fillGuardCells(CENTER_FACES,ALLDIR,doEos=.true.)
    ```

    - Eos often needs to be called to get cells at refinement boundaries, where data was interpolated, into thermodynamic balance.
  - There are many additional optional arguments, see API docs. They are for increasing performance, and can all be initially ignored.

GC Overview: blocks, cells, regions

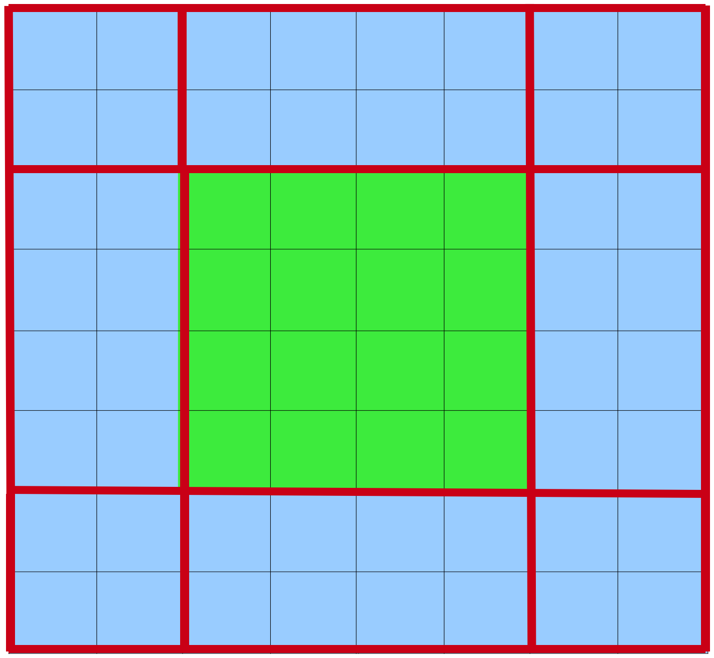
- Blocks consist of cells: guard cells and interior cells.
- For purposes of guard cell filling, guard cells are organized into guard cell regions.



- During guard cell filling, each guard cell region may get filled from a different data source:
  - A local **neighbor block**
  - A remote **neighbor block**
  - **A boundary condition**
    - using data from adjacent interior cells
    - Using fixed or coordinate-based data
  - **Interpolation** from parent (if the block touches a fine/coarse boundary)
- In PARAMESH4, diagonal regions are treated just like “face neighbor” regions.

Filling guard cells I

- For purposes of guard cell filling, guard cells are organized into guard cell regions.



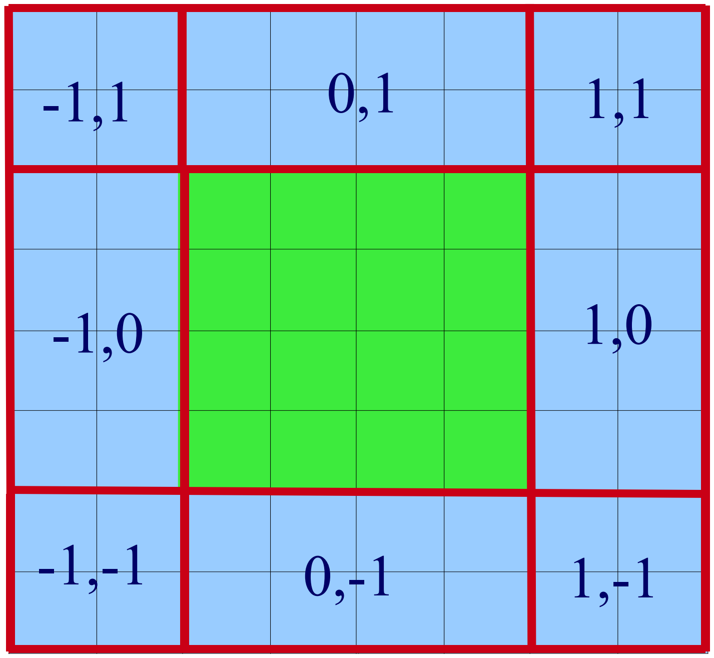
- During guard cell filling, each guard cell region may get filled from a different data source:
  - A local neighbor block
  - A remote neighbor block
  - A boundary condition
    - using data from adjacent interior cells
    - Using fixed or coordinate-based data
  - Interpolation from parent (if the block touches a fine/coarse boundary)

Filling guard cells Ia

- For purposes of guard cell filling, guard cells are organized into guard cell regions.

In 2D, a block has 8 guard cell regions.

In 3D, a block has 26 guard cell regions!



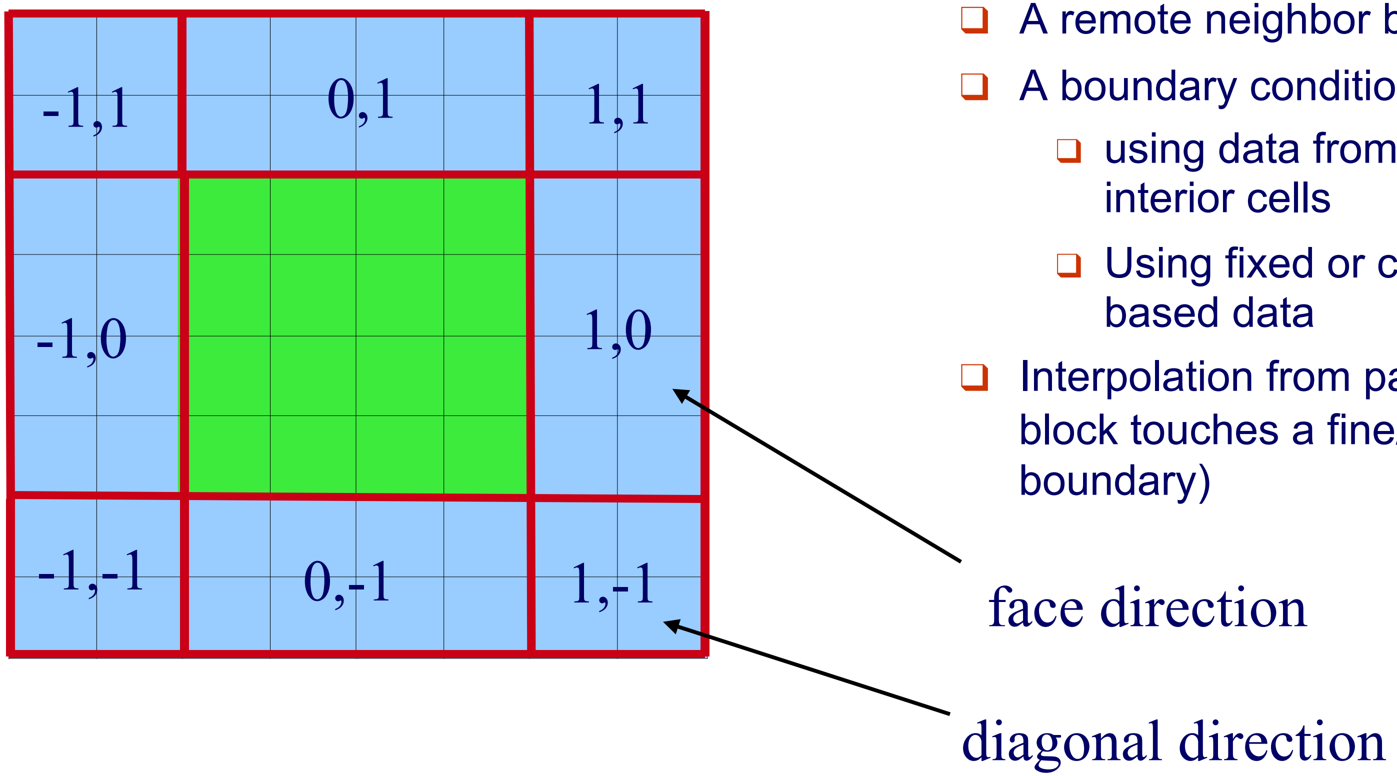
- During guard cell filling, each guard cell region may get filled from a different data source:
  - A local neighbor block
  - A remote neighbor block
  - A boundary condition
    - using data from adjacent interior cells
    - Using fixed or coordinate-based data
  - Interpolation from parent (if the block touches a fine/coarse boundary)

Filling guard cells Ib

- For purposes of guard cell filling, guard cells are organized into guard cell regions.

In 2D, a block has 8 guard cell regions.

In 3D, a block has 26 guard cell regions!



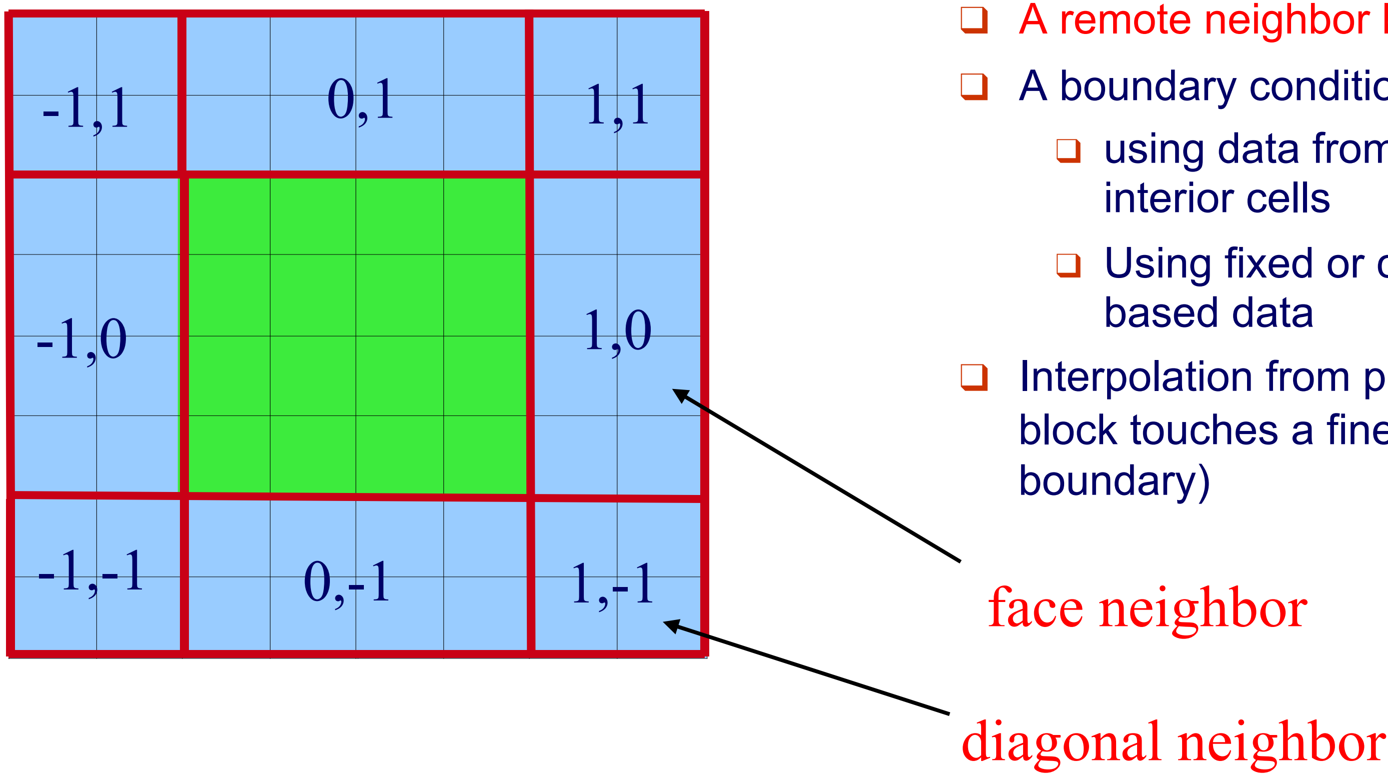
- During guard cell filling, each guard cell region may get filled from a different data source:
  - A local neighbor block
  - A remote neighbor block
  - A boundary condition
    - using data from adjacent interior cells
    - Using fixed or coordinate-based data
  - Interpolation from parent (if the block touches a fine/coarse boundary)

Filling guard cells Ic

- For purposes of guard cell filling, guard cells are organized into guard cell regions.

In 2D, a block has 8 guard cell regions.

In 3D, a block has 26 guard cell regions!

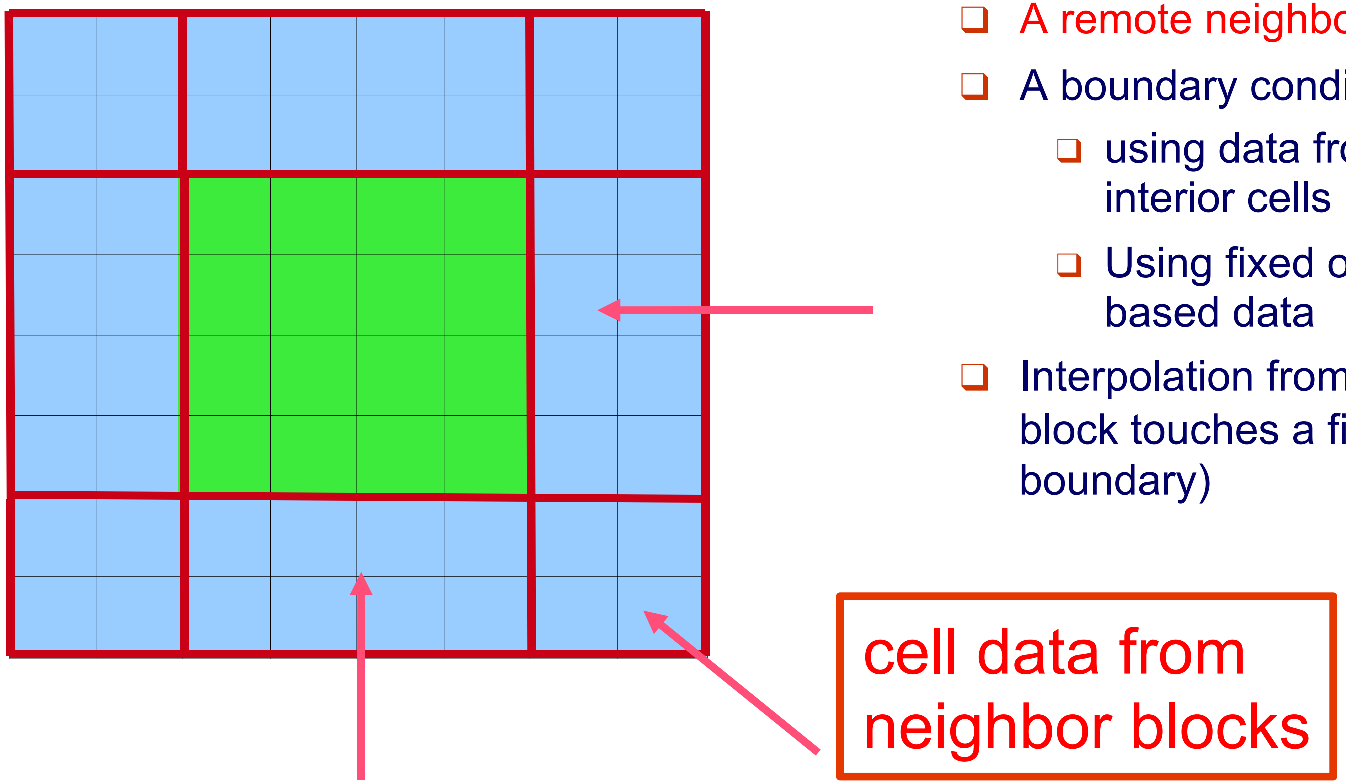


- During guard cell filling, each guard cell region may get filled from a different data source:
  - A local neighbor block
  - A remote neighbor block
  - A boundary condition
    - using data from adjacent interior cells
    - Using fixed or coordinate-based data
  - Interpolation from parent (if the block touches a fine/coarse boundary)

Filling guard cells from neighbors I

- For purposes of guard cell filling, guard cells are organized into guard cell regions.

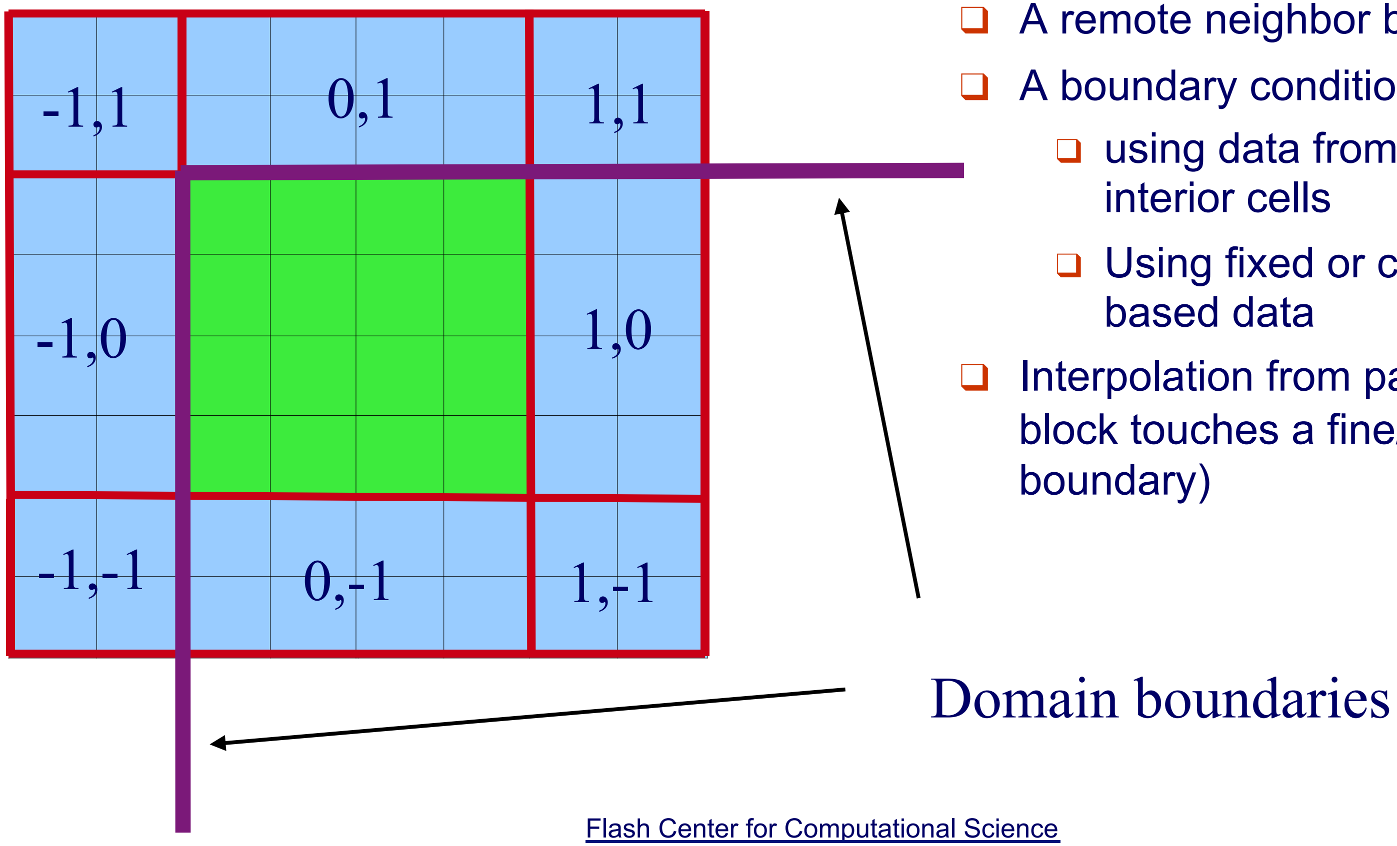
- During guard cell filling, each guard cell region may get filled from a different data source:
  - A local neighbor block
  - A remote neighbor block
  - A boundary condition
    - using data from adjacent interior cells
    - Using fixed or coordinate-based data
  - Interpolation from parent (if the block touches a fine/coarse boundary)



Filling guard cells at Boundary I

- For purposes of guard cell filling, guard cells are organized into guard cell regions.

Now assume a block at the **corner of the domain**:

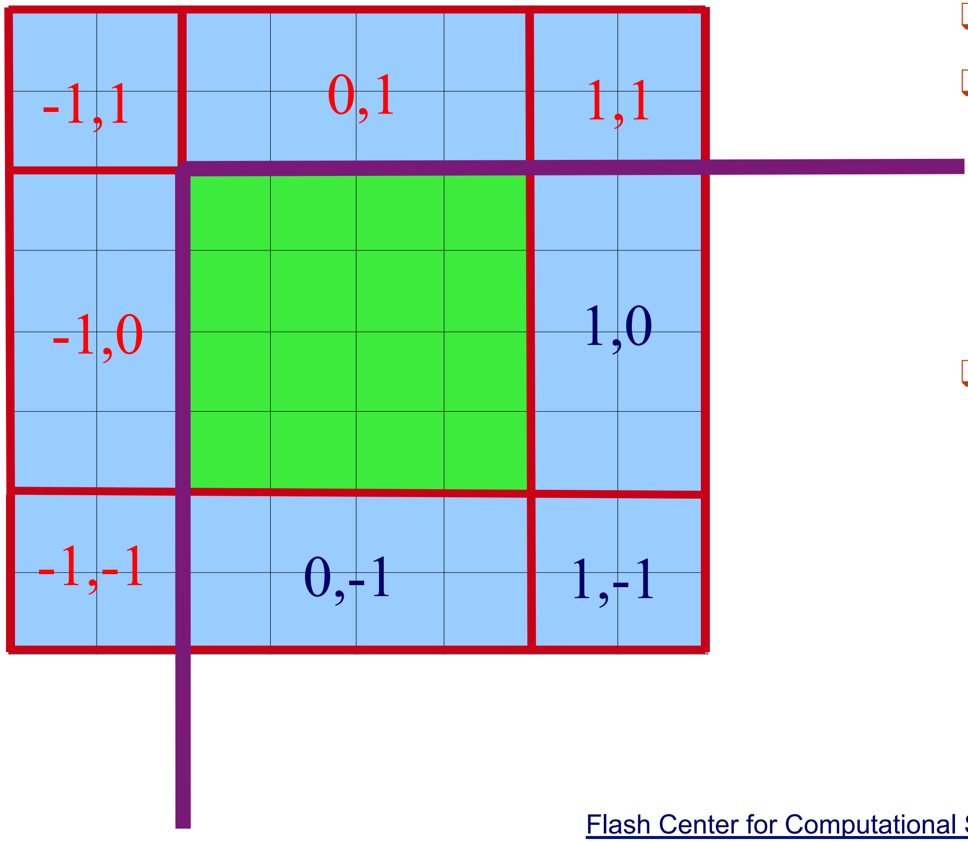


- During guard cell filling, each guard cell region may get filled from a different data source:
  - A local neighbor block
  - A remote neighbor block
  - A boundary condition
    - using data from adjacent interior cells
    - Using fixed or coordinate-based data
  - Interpolation from parent (if the block touches a fine/coarse boundary)

Filling guard cells at Boundary II

- For purposes of guard cell filling, guard cells are organized into guard cell regions.

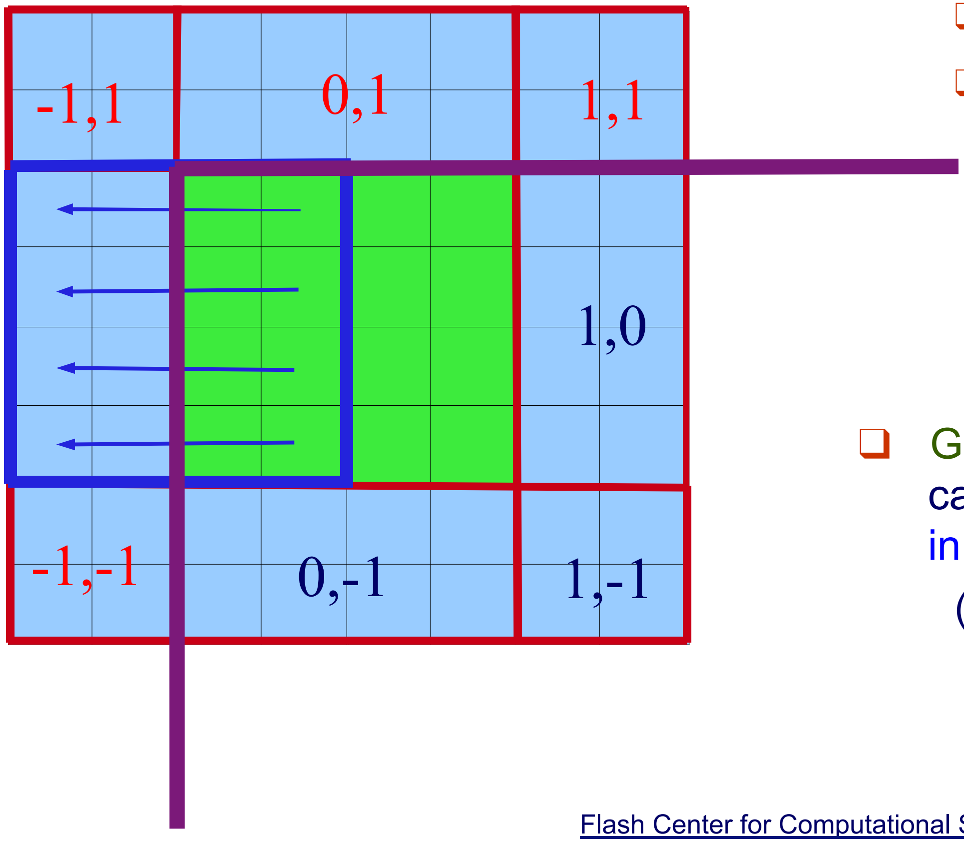
The guard cell regions in red represent locations **outside of the domain**:



- During guard cell filling, each guard cell region may get filled from a different data source:
  - A local neighbor block
  - A remote neighbor block
  - A boundary condition
    - using data from adjacent interior cells
    - Using fixed or coordinate-based data
  - Interpolation from parent (if the block touches a fine/coarse boundary)

Filling guard cells at Boundary III

- For purposes of guard cell filling, guard cells are organized into guard cell regions.

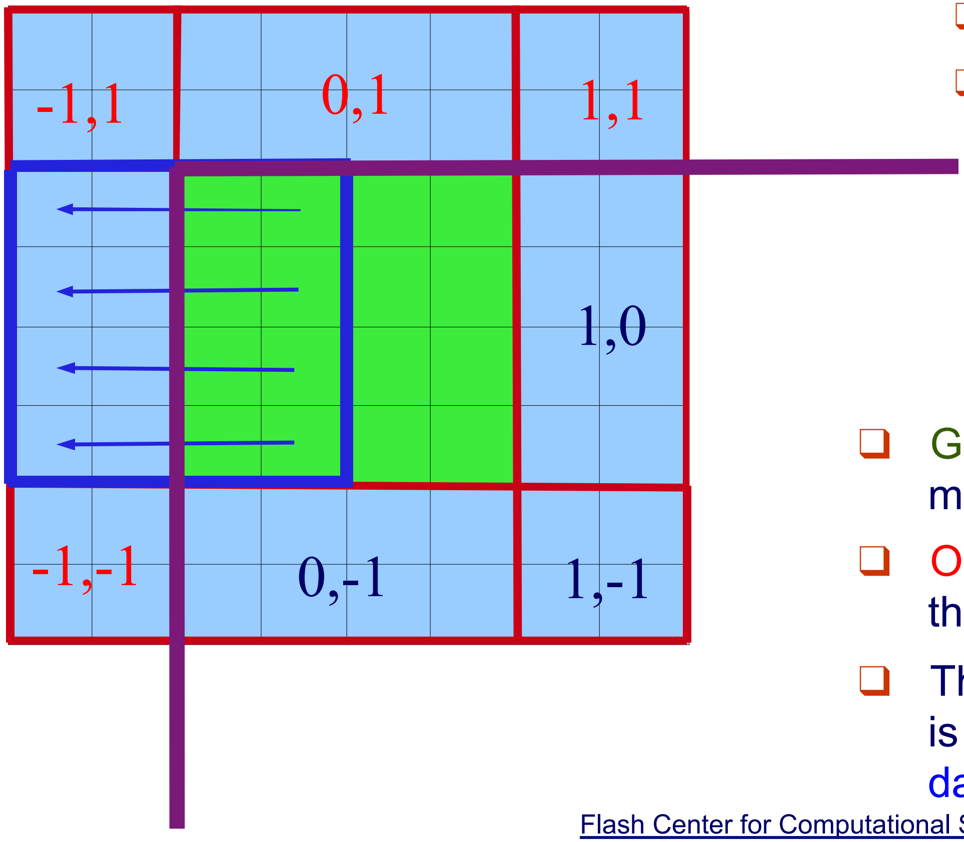


- During guard cell filling, each guard cell region may get filled from a different data source:
  - A local neighbor block
  - A remote neighbor block
  - A boundary condition
    - using data from adjacent interior cells
    - Using fixed or coordinate-based data
- Grid_bcApplyToRegionSpecialized is called and passed a pointer to the data in the blue region.

  (actually, to a copy of the block data)

Filling guard cells at Boundary IV

- For purposes of guard cell filling, guard cells are organized into guard cell regions.



- During guard cell filling, each guard cell region may get filled from a different data source:
  - A local neighbor block
  - A remote neighbor block
  - A boundary condition
    - using data from adjacent interior cells
    - Using fixed or coordinate-based data
- Grid_bcApplyToRegionSpecialized may fill in the guard cell region.
- OR it may decline to handle this, and then:
- The subroutine Grid_bcApplyToRegion is called and passed a pointer to the data in the blue region.

Implementing Boundary Conditions

- *Grid_bcApplyToRegionSpecialized* gets called first
  - This is normally a no-op stub
  - This is the preferred place to users to hook in **customized implementations**.
  - May decide to handle the call, based on BC type, direction, ...
  - Before returning, sets “applied” flag to signal that the BC was handled.

- *Grid_bcApplyToRegion* gets called if *Grid_bcApplyToRegionSpecialized* did not handle the case.
  - The standard implementation of *Grid_bcApplyToRegion* in source/Grid/GridBoundaryConditions provides the standard simple BC types: REFLECTING, OUTFLOW, DIODE, ...
  - It is a good place to start if you need to write your own!

- Both interfaces provide information that an implementation, can use to fill guard cells at boundaries, including:
  - A block handle (usually, block ID) identifying the block being filled
  - Location of the data region within the Grid block

BCs – Complications

- Grid_bcApplyToRegion* may be called on a non-LEAF block.
- Grid_bcApplyToRegion* may be called on a block that is not even local!
  - This can happen if a parent block needs to be filled to provide input data for interpolation, and the parent resides on a different PE from the leaf.
  - Simple BC methods don't have to be aware of this.
  - But if your method depends on coodinate information, or needs to access the block by its ID, beware!
  - See source/Grid/GridBoundaryConditions/README and Users Guide in those cases.
- The data region passed to Grid_bcApplyToRegion* is in transposed form:

  Reference it like regionData(I,J,k,ivar), where
  - I counts cells in the normal direction (NOT always: x direction!),
  - J,K cont cells in the other directions
  - Ivar counts variables

  This is convenient for implementing simple BC where location does not matter, but complicates things if you need to know where a cell is within the block.
  - Use provided examples!

BCs – Simplifications

- If you prefer a simpler interface:
  - Handle one data row at a time (vector of data in normal direction)
  - Powerful enough to implement hydrostatic boundaries
  - REQUIRES Grid/GridBoundaryConditions/OneRow (see source files there!)
  - Implements a version of Grid_bcApplyToRegionSpecialized
  - Provides functions Grid_applyBCEdge, Grid_applyBCEdgeAllUnkVars
  - Too customize, user should provide own implementation of Grid_applyBCEdge.F90 (or Grid_applyBCEdgeAllUnkVars.F90)

IO Unit

- The *IO* unit is responsible for
  - Writing checkpoint files
    - For restarting, …
  - Writing "plot files"
    - For visualization
    - For further analysis
  - Writing particle data files
    - For visualization and further processing

- binary output files are writing in a structured format: **HDF5**, pnetcdf
- Various tools can process FLASH files, including **Visit**

Grid and other Infrastructure Code

- Questions?