Lecture 4b

Design of SAMR Systems, Advanced Parallelization, Usage

Course *Block-structured Adaptive Mesh Refinement Methods for Conservation Laws*
Theory, Implementation and Application

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Outline

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Simplified structured designs

Distributed memory parallelization fully supported if not otherwise states.

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- DAGH/Grace [Parashar and Browne, 1997]
  - Just C++ data structures but no methods
  - All grids are aligned to bases mesh coarsened by factor 2
  - http://userweb.cs.utexas.edu/users/dagh

Systems that support general SAMR

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- SAMRAI - Structured Adaptive Mesh Refinement Application Infrastructure
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- Chombo
  - Redesign and extension of BoxLib by P. Colella et al.
  - Both multigrid and explicit algorithms demonstrated
  - Some embedded boundary support
  - https://seesar.lbl.gov/anag/chombo

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- Overture (Object-oriented tools for solving PDEs in complex geometries)
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- Cell-based Cartesian AMR: RAGE
  - Embedded boundary method
  - Explicit and implicit algorithms
  - [Gittings et al., 2008]

AMROC

- "Adaptive Mesh Refinement in Object-oriented C++"
- $\sim 46,000$ LOC for C++ SAMR kernel, $\sim 140,000$ total C++, C, Fortran-77
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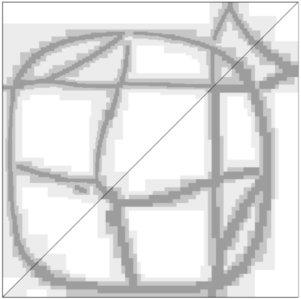

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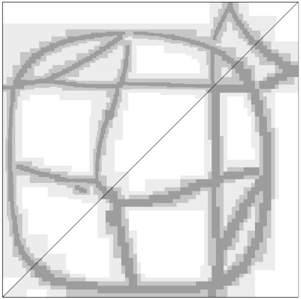
- V1.0: http://amroc.sourceforge.net



	l_{max}	Level 0	Level 1	Level 2	Level 3	Level 4
AMROC's DAGH grids/cells	1	43/22500	145/38696			
	2	42/22500	110/48708	283/83688		
	3	36/22500	78/54796	245/109476	582/165784	
	4	41/22500	88/56404	233/123756	476/220540	1017/294828
Original DAGH grids/cells	1	238/22500	125/41312			
	2	494/22500	435/48832	190/105216		
	3	695/22500	650/55088	462/133696	185/297984	
	4	875/22500	822/57296	677/149952	428/349184	196/897024

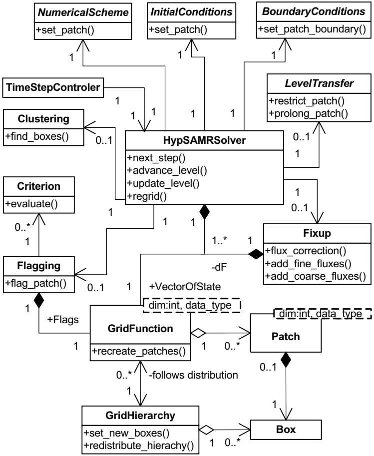
Comparison of number of cells and grids in DAGH and AMROC

The Virtual Test Facility

- Implements all described algorithms beside multigrid methods
- AMROC V2.0 plus solid mechanics solvers
- Implements explicit SAMR with different finite volume solvers
- Embedded boundary method, FSI coupling
- $\sim 430,000$ lines of code total in C++, C, Fortran-77, Fortran-90
- autoconf / automake environment with support for typical parallel high-performance system
- http://www.cacr.caltech.edu/asc
- [Deiterding et al., 2006][Deiterding et al., 2007]

UML design of AMROC

- Classical framework approach with generic main program in C++



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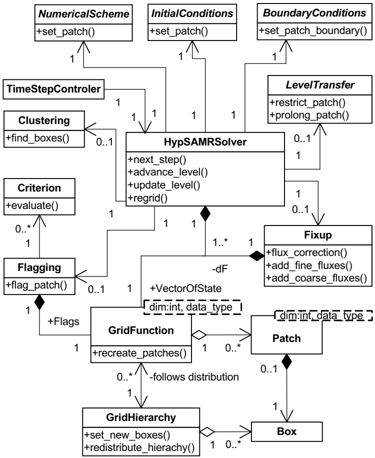

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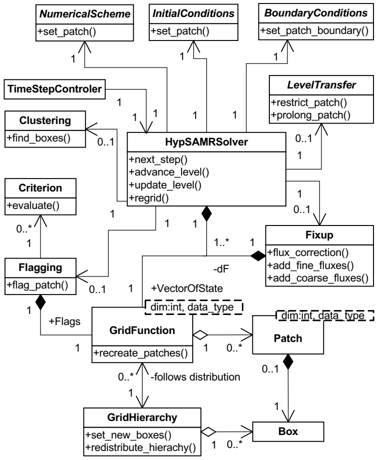

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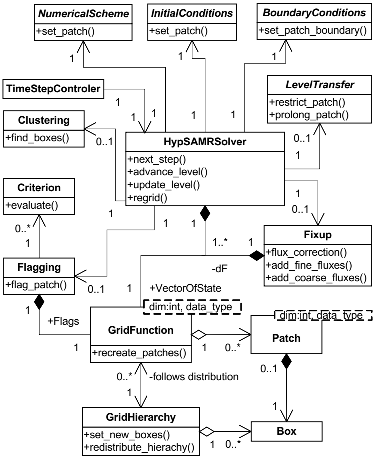

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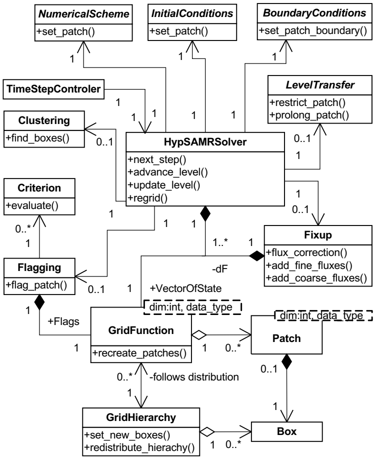

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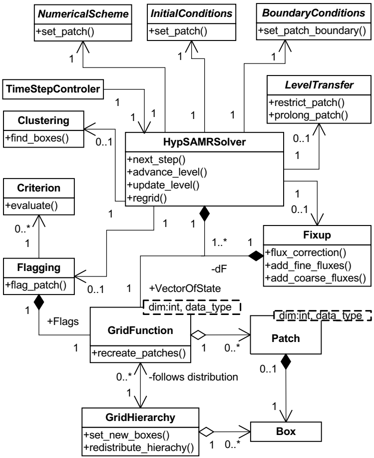
- Expert usage (algorithm modification, advanced output, etc.) in C++



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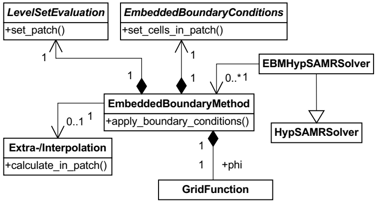
- Hierarchical parallel data structures are typically C++, routines on patches often Fortran

Embedded boundary method / FSI coupling

- Multiple independent EmbeddedBoundaryMethod objects possible
- Specialization of GFM boundary conditions, level set description in scheme-specific F77 interface classes



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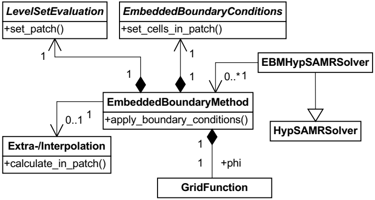
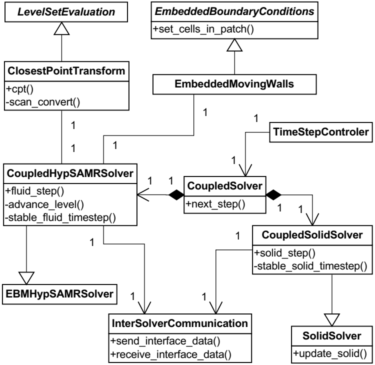




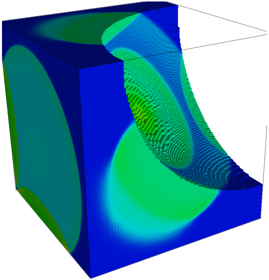
- Coupling algorithm implemented in further derived HypSAMRSolver class
- Level set evaluation always with CPT algorithm
- Parallel communication through efficient non-blocking communication module
- Time step selection for both solvers through CoupledSolver class

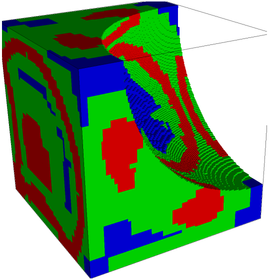
Performance assessment

- Test run on 2.2 GHz AMD Opteron quad-core cluster connected with Infiniband
- Cartesian test configuration
- Spherical blast wave, Euler equations, 3rd order WENO scheme, 3-step Runge-Kutta update
- AMR base grid 64^3, $r_{1,2} = 2$, 89 time steps on coarsest level
- With embedded boundary method: 96 time steps on coarsest level
- Redistribute in parallel every 2nd base level step
- Uniform grid $256^3 = 16.8 \cdot 10^6$ cells

Level	Grids	Cells
0	115	262,144
1	373	1,589,808
2	2282	5,907,064

Grid and cells used on 16 CPUs





Cost of SAMR (AMROC V2.0)

- Flux correction is negligible

CPUs	16	32	64
Time per step	32.44s	18.63s	11.87s
Uniform	59.65s	29.70s	15.15s
Integration	73.46%	64.69%	50.44%
Flux Correction	1.30%	1.49%	2.03%
Boundary Setting	13.72%	16.60%	20.44%
Regridding	10.43%	15.68%	24.25%
Clustering	0.34%	0.32%	0.26%
Output	0.29%	0.53%	0.92%
Misc.	0.46%	0.44%	0.47%

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Time per step	43.97s	25.24s	16.21s
Uniform	69.09s	35.94s	18.24s
Integration	59.09%	49.93%	40.20%
Flux Correction	0.82%	0.80%	1.14%
Boundary Setting	19.22%	25.58%	28.98%
Regridding	7.21%	9.15%	13.46%
Clustering	0.25%	0.23%	0.21%
GFM Find Cells	2.04%	1.73%	1.38%
GFM Interpolation	6.01%	10.39%	7.92%
GFM Overhead	0.54%	0.47%	0.37%
GFM Calculate	0.70%	0.60%	0.48%
Output	0.23%	0.52%	0.74%
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- Main costs: `Regrid(l)` operation and ghost cell synchronization

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AMROC scalability tests

Basic test configuration

- Spherical blast wave, Euler equations, 3D wave propagation method
- AMR base grid 32^3 with $r_{1,2} = 2, 4$. 5 time steps on coarsest level
- Uniform grid $256^3 = 16.8 \cdot 10^6$ cells, 19 time steps
- Flux correction deactivated
- No volume I/O operations
- Tests run IBM BG/P (mode VN)

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Weak scalability test

- Reproduction of configuration each 64 CPUs
- On 1024 CPUs: $128 \times 64 \times 64$ base grid, $> 33,500$ Grids, $\sim 61 \cdot 10^6$ cells, uniform $1024 \times 512 \times 512 = 268 \cdot 10^6$ cells

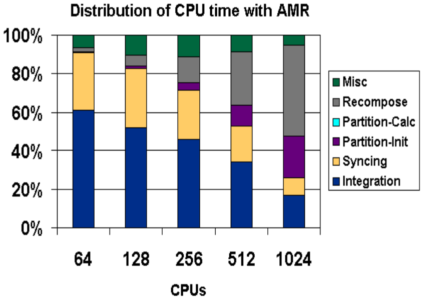
Level	Grids	Cells
0	606	32,768
1	575	135,312
2	910	3,639,040

Strong scalability test

- $64 \times 32 \times 32$ base grid, uniform $512 \times 256 \times 256 = 33.6 \cdot 10^6$ cells

Level	Grids	Cells
0	1709	65,536
1	1735	271,048
2	2210	7,190,208

Scalability tests AMROC V2.0



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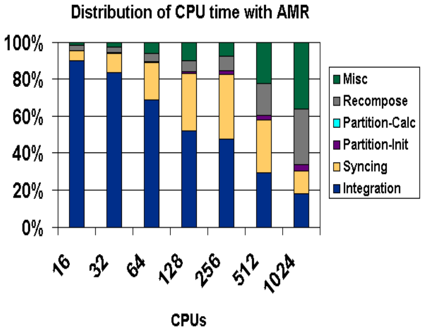

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- Recompose: topological list operations, construction of boundary info, redistribution of data blocks
- Partition-Init, Partition-Calc: construction of space filling curve

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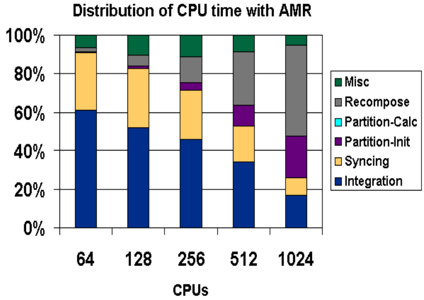

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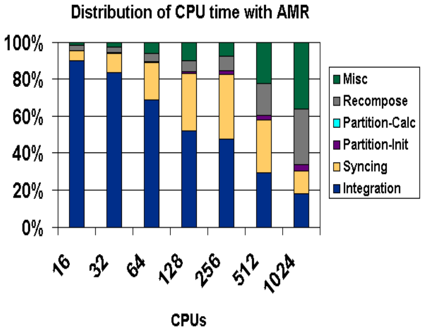

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- Costs for Partition-Init and Recompose increase dramatically for large problem size

Topological list operations

Weak scalability problems are due to non-parallel sub-algorithms!

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- Operations $\cap$, $\setminus$ on two box lists have complexity $O(NM)$
- Costs of operations in `Recompose(l)`, that use global box lists G_l, increase quadratically, cf. [Wissink et al., 2003]

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- Operations $\cap$, $\setminus$ on two box lists have complexity $O(NM)$
- Costs of operations in `Recompose(l)`, that use global box lists G_l, increase quadratically, cf. [Wissink et al., 2003]
- Solution
  - Clip G_l with properly chosen quadratic bounding box around G_l^p before using $\cap$, $\setminus$

Topological list operations

Weak scalability problems are due to non-parallel sub-algorithms!

- Operations $\cap$, $\setminus$ on two box lists have complexity $O(NM)$
- Costs of operations in `Recompose(l)`, that use global box lists G_l, increase quadratically, cf. [Wissink et al., 2003]
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  - Clip G_l with properly chosen quadratic bounding box around G_l^p before using $\cap$, $\setminus$
- All topological operations in `Recompose(l)` involving global lists can be reduced to local ones
- Present code V2.1β still uses `MPI_allgather()` to communicate global lists to all nodes
- Global view is particularly useful to evaluate new local portion of hierarchy and for data redistribution

Construction of space-filling curve

Computation of space filling curve

- Partition-Init

Construction of space-filling curve

Computation of space filling curve

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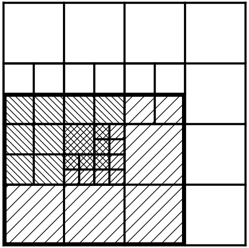
  1. Compute aggregated workload for new grid hierarchy G_l and project result onto level 0



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- Partition-Init
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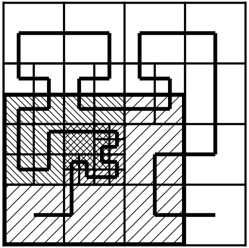

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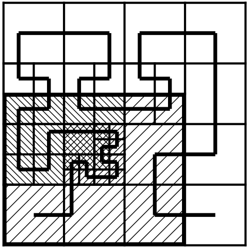

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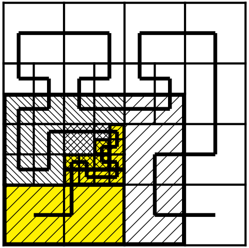

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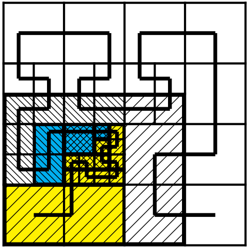

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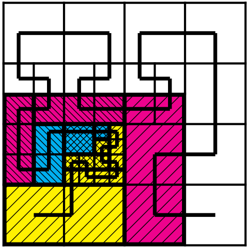

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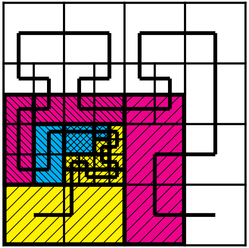

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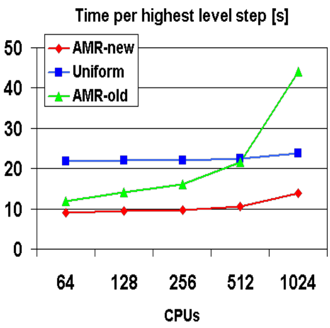
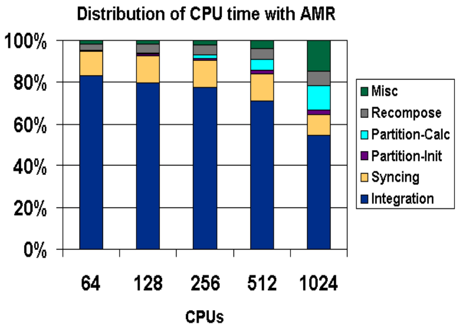
  1. Compute entire workload and new work for each processor
  2. Go sequentially through SFC-ordered list of partitioning units and assign units to processors, refine partition if necessary and possible
- Ensure scalability of Partition-Init by creating SFC-units strictly local
- Currently still use of `MPI_allgather()` to create globally identical input for Partition-Calc

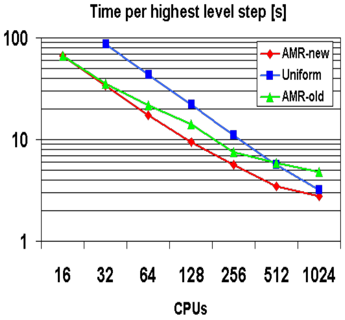
Weak scalability test V2.1β

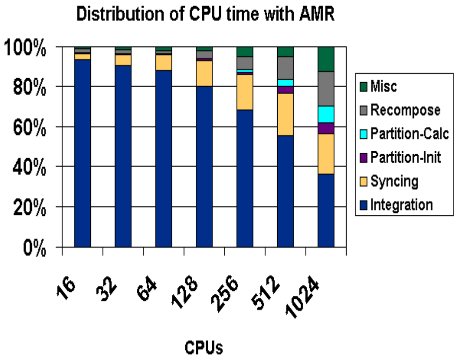




- Overall performance improvement for 1024 CPUs by $\sim 69\,\%$
- Absolute costs for Syncing are almost constant
- 1024 required usage of -DUAL option due to usage of global lists data structures in Partition-Calc and Recompose

Strong scalability test V2.1β





- Overall performance improvement for 1024 CPUs by 43 %

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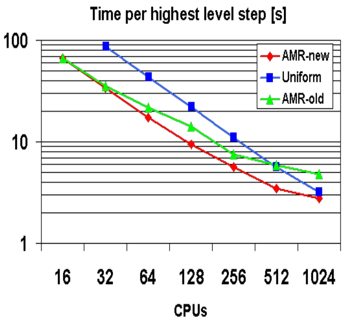

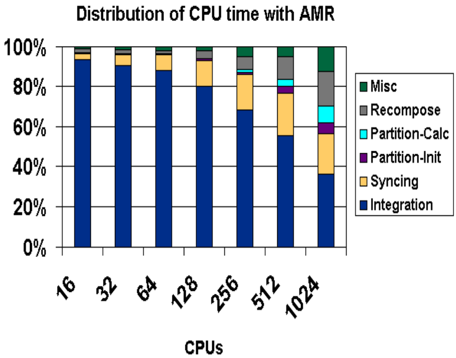

- Overall performance improvement for 1024 CPUs by 43 %
- Improved partitioning algorithm allowed usage of GuCFactor=1 instead of 2 before and full parallel data redistribution in every `Regrid(l)` instead of every 2nd level-0 step

To-Do

Comments

- Scalability of V2.1β for finite volume methods is comparable to results reported from Chombo and SAMRAI

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- Significantly better scalability has so far only been reported for shallow hierarchies [Greenough et al., 2005] and/or tailored parameters choices

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Next step

- Eliminate aggregation of global box list data (that currently uses simply `MPI_allgather()`)

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Next step

- Eliminate aggregation of global box list data (that currently uses simply `MPI_allgather()`)
  - Partition-Calc: assignment of SFC-ordered sequence and refinement could be executed sequentially on each node

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- Eliminate aggregation of global box list data (that currently uses simply `MPI_allgather()`)
  - Partition-Calc: assignment of SFC-ordered sequence and refinement could be executed sequentially on each node
  - Global topology lists: assemble only those portions of global lists on each node that are relevant for the subsequent operations. Use Cartesian bounding box information to construct irregular point-to-point communication pattern for list data between nodes

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Future work

- Large-scale hierarchical I/O

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Future work

- Large-scale hierarchical I/O
- Hybrid parallelization (considering accelerators), cf. [Schive et al., 2010], [Jourdon, 2005]

Quick start with AMROC V2.0 I

Standard Linux development system assumed! See install_vtf.pdf for details.

1. Unpack hdf4_src.tgz into home directory: cd; tar -xvzf hdf4_src.tgz
2. cd asc; ./build_hdf4.sh
3. If last step successful libdf.a, libjpeg.a, libmfhdf.a, libsz.a, libz.a are in $HOME/asc/hdf4/lib.
4. Unpack AMROC-Clawpack-1.0.tgz into $HOME/asc:
   cd $HOME/asc; tar -xvzf AMROC-Clawpack-1.0.tgz
5. With mpicc, mpicxx commands
   5.1 cd vtf
   5.2 ./configure -C --enable-opt=yes --enable-mpi=yes HDF4_DIR=$HOME/asc/hdf4
       If autoconf, automake are available add --enable-maintainer-mode to last line
   5.3 cd gnu-opt-mpi

Quick start with AMROC V2.0 II

5.4 `make`

5.5 `source ../ac/paths.sh`

5.6 Optional unit test

  5.6.1 `../amroc/testrun.sh -m make -r 4 -s`

  5.6.2 `../amroc/testrun.sh -c`

6. Without MPI

6.1 `cd vtf`

6.2 `./configure -C --enable-opt=yes --enable-mpi=no HDF4_DIR=$HOME/asc/hdf4`
If `autoconf`, `automake` are available add
`--enable-maintainer-mode` to last line

6.3 `cd gnu-opt`

6.4 `make`

6.5 `source ../ac/paths.sh`

6.6 Optional unit test

  6.6.1 `../amroc/testrun.sh -m make -r 0 -s`

  6.6.2 `../amroc/testrun.sh -c`

Quick start with AMROC V2.0 III

7. Realistic example
   - 7.1 Change to compilation directory `gnu-opt/gnu-opt-mpi`: `cd amroc/clawpack/applications/euler/2d/SphereLiftOff`
   - 7.2 `make`
   - 7.3 Change to corresponding directory with solver.in: `cd vtf/amroc/clawpack/applications/euler/2d/SphereLiftOff`
   - 7.4 `./run.py` or `./run.py 2` (if you have compiled with MPI on a dual-core system)
   - 7.5 `gnuplot Density.gnu` shows density evolution of lower boundary
   - 7.6 Create binary VTK files for Paraview or VisIt: `hdf2tab.sh "-f display_file_visit.in"`
   - 7.7 Execute VisIt or Paraview and load the VTK files for visualization.

Quick start with AMROC V2.0 IV

8. FSI example (requires MPI)
   - 8.1 `cd $HOME/asc/gnu-opt-mpi/vtf/fsi/beam-amroc/VibratingBeam`
   - 8.2 `make`
   - 8.3 `cd $HOME/asc/vtf/fsi/beam-amroc/VibratingBeam`
   - 8.4 `./run.py 4`
     Change `LastNode` entry in `solver.in` for different processor number.
   - 8.5 `hdf2tab.sh`
   - 8.6 Execute VisIt or Paraview and load the VTK files for visualization.
9. For further documentation see http://www.cacr.caltech.edu/asc

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