DAMSEL - A Data Model Storage Library for Exascale Science (API and Use cases)

(This work is supported by Office of Advanced Scientific Computing Research under the program of X-stack Software Research)

Saba Sehrish
CScADS 2012
July 31, 2012

NORTHWESTERN UNIVERSITY

Outline

- Project Team
- Motivation
- Damsel I/O Library
- Usecases: FLASH, GCRM
- Data layout (In Progress)

NORTHWESTERN UNIVERSITY

Project Team

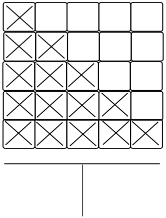
- **Northwestern University:** Alok Choudhary, Wei-keng Liao, Saba Sehrish, Sueng Woo Son
- **Argonne National Laboratory:** Rob Ross, Rob Latham, Tim Tautges
- **The HDF Group:** Quincey Koziol, Ben Clifford, Peter Cao
- **NC State University:** Nagiza Samatova, Sriram Lakshminarasimhan

1 Motivation
- Existing I/O Libraries
- Goals

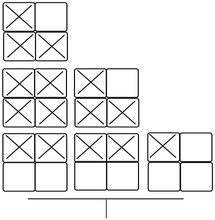
Existing I/O Libraries

- Storage data models developed in the 1990s; Network Common Data Format (netCDF) and Hierarchical Data Format (HDF)
- I/O library interfaces still based on low-level vectors of variables
- Lack of support for sophisticated data models, e.g. AMR, unstructured Grids, Geodesic grid, etc
- Require too much work at application level to achieve close to peak I/O performance

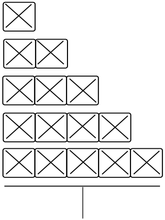
Example: Lower Triangle Matrix



netCDF: fixed dimensions

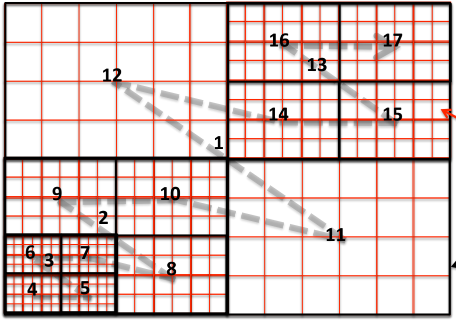


HDF5: Potential for odd interactions between application data layout and chunk allocation



Lower-triangular aware storage mode and layout

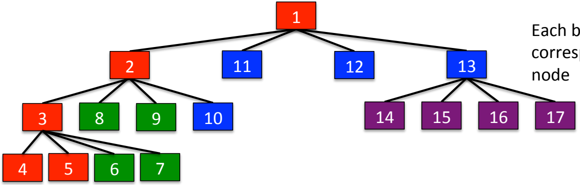
Example: FLASH



FLASH - AMR Grid

- Red boxes are cells
- Black boxes are blocks

Morton order



Each block in AMR grid corresponds to a tree node

Example: FLASH

- Parallel adaptive-mesh refinement (AMR) code; Block structured - a block is the unit of computation
- **Tree information:** FLASH uses tree data structure for storing grid blocks and relationships among blocks, including lrefine, which_child, nodetype and gid.
- **Per-block metadata:** FLASH stores the size and coordinates of each block in three different arrays: coord, bsize and bnd_box
- **Solution Data:** Physical variables i.e. located on actual grid are stored in a multi-dimensional (5D) array e.g. UNK

NORTHWESTERN UNIVERSITY

Goals

- Provide higher-level data model API to describe more sophisticated data models, e.g. structured AMR, geodesic grid, etc
- Enable exascale computational science applications to interact conveniently and efficiently with storage through the data model API
- Develop a data model storage library to support these data models, provide efficient storage data layouts
- Productizing Damsel and working with computational scientists to encourage adoption of this library by the scientific community

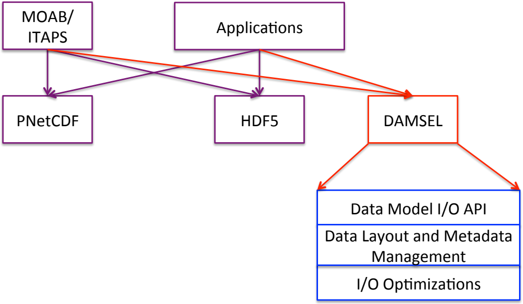
2 Damsel I/O Library
- Data Model
- API

Proposed Approach

- A set of data models I/O APIs relevant to computational science applications
- A data layout component that maps these data models onto storage efficiently,
- A rich metadata representation and management layer that handles both internal metadata and that generated by users and external tools,
- I/O optimizations: adaptive collective I/O, request aggregation, and virtual filing,

NORTHWESTERN UNIVERSITY

Damsel Big Picture

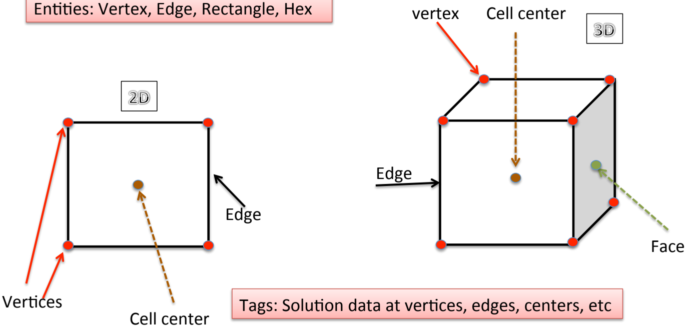


Data Model Components

- Describe structural/(hierarchical) and solution information through API
- To describe the structural information, i.e. Grid data Entity, Collections, Structured Blocks
- To describe the solution variable, i.e. Solution data Tags on Entities, Collections, Structured Blocks

Example: Entity and Tags

Entities: Vertex, Edge, Rectangle, Hex

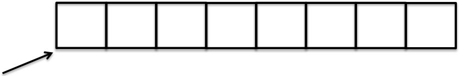


Tags: Solution data at vertices, edges, centers, etc

Example: Sequence of entities and Tags

Step 1: Create a sequence of entities (QUADS)

Step 2: Define an entity by specifying vertices



start_coord[2] = {0.0, 0.0}

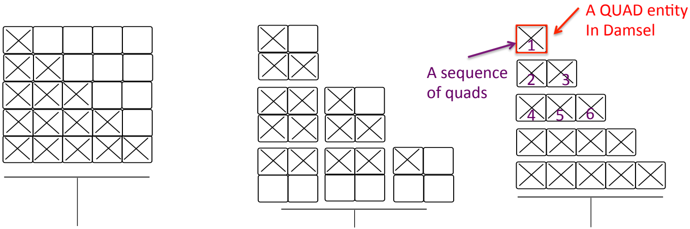
Step 3: Set coordinates of vertices

Step 4: Define tags with name (temp) and type (float)

Step 5: Map tags to the entities

Step 6: Iterate through all tags and write to file

Example: Lower Triangle Matrix



netCDF: fixed dimensions

HDF5: Potential for odd interactions between application data layout and chunk allocation

Lower-triangular aware storage mode and layout

Damsel Program Flow

- damsel_library lib = DMSLlib_Init();
- Create a model
  `DMSLmodel_create(DAMSEL_TYPE_HANDLE_64);`
- Fill in the application specific model details e.g. number of entities, types of entities, etc
  1) `damsel_handle my_handle = {12, 45, 67, 89 };`
  2) `damsel_container my_container = DMSLcontainer_create_vector(model, my_handle, 4);`
  3) `damsel_collection my_coll = DMSLcoll_create(model, my_handle, my_container, DAMSEL_HANDLE_COLLECTION_TYPE_VECTOR);`

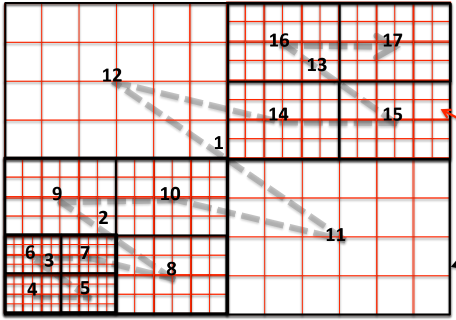
Damsel Program Flow

- Fill in the application specific variables and solution data e.g. tags (coordinates, solution data)
  1) `damsel_handle tag_handle = 10001;`
  2) `DMSLtag_define(model, "temperature", DAMSEL_TYPE_FLOAT);`
  3) `DMSLmodel_map_tag(data, my_coll, &tag_handle);`
- DMSLexecute(model);
- DMSLlib_finalize(lib);

3 Usecases

- Usecase I: FLASH
- Usecase II: GCRM

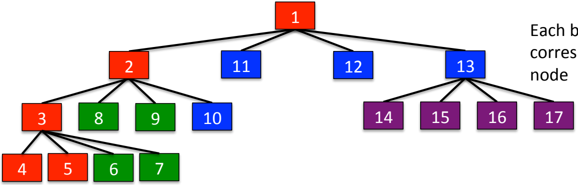
Introduction



FLASH - AMR Grid

- Red boxes are cells
- Black boxes are blocks

Morton order



Each block in AMR grid corresponds to a tree node

Introduction

- The FLASH is a modular, parallel multi-physics simulation code capable of handling general compressible flow problems found in many astrophysical environments.
- Parallel adaptive-mesh refinement (AMR) code; Block structured - a block is the unit of computation
- **Tree information:** FLASH uses tree data structure for storing grid blocks and relationships among blocks, including lrefine, which_child, nodetype and gid.
- **Per-block metadata:** FLASH stores the size and coordinates of each block in three different arrays: coord, bsize and bnd_box
- **Solution Data:** Physical variables i.e. located on actual grid are stored in a multi-dimensional (5D) array e.g. UNK

FLASH using existing I/O Libraries

FLASH in PnetCDF

```
/*Step 1: Create data set*/
ncmpi_create_data()

/*Step 2: Define dimension*/
status = ncmpi_def_dim(ncid, "dim_tot_blocks", (MPI_Offset)
(*total_blocks), &dim_tot_blocks);

/*Step 3: Define variables*/
Status = ncmpi_def_var (ncid, "runtime_parameters", NC_INT, rank,
dimids, &varid[id]);
status = ncmpi_def_var (ncid, "lrefine", NC_INT, rank, dimids,
&varid[id]);

/*Step 4: Create attributes for some variables*/
status = ncmpi_put_att_int(ncid, 1, intScalarNames[i], NC_INT, 1,
&intScalarValues[i]);

/*Step 5: Write structural & solution data*/
/* Write data from memory to file */
    err = ncmpi_put_vara_all(fileID, varID, diskStart, diskCount,
pData, memCountScalar, memType);

/*Step 6: Close the dataset/file*/
ncmpi_close(fileID);
```

FLASH using DAMSEL data model

- Goal: to describe hierarchical/structural and solution information through API
- Entity
  - FLASH blocks as a sequence of entities
- Collections
  - Blocks assigned to collections to define hierarchical/structural information
- Tags
  - coordinates, size, bounding box
  - UNK (temprature, pressure, etc)

NORTHWESTERN UNIVERSITY

FLASH using DAMSEL API

Step 1: Define sequence of block entities

```
1. damsel_handle block_id [17]={1, 2, 3, 4, 5,
   6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17};
2. damsel_container block_collection_id =
   DMSLcontainer_create_vector(model, block_id,
   17);
3. Damsel_collection DMSLcoll_create();
4. DMSLentity_define(block_collection_id, , ,);
```

Step 2: Defining block metadata using tags

```
1. damsel_handle coord_tag_handle = 10004;
2. DMSLtag_define(model, &coord_tag_handle,
   coords_array_type, "coordinates");
3. DMSLmodel_map_tag(block_coords,
   block_collection_id, &coord_tag_handle);

// Same procedure for bounding box, size, etc
```


NORTHWESTERN UNIVERSITY

FLASH using DAMSEL API

Step 3: Define hierarchy through collections

```
1. damsel_handle temp_cont[5] = {3, 4, 5, 6, 7};
2. damsel_container c31 =
   DMSLcontainer_create_vector(model, temp_cont, 5);
3. damsel_handle parent_tag_handle = 10023;
4. DMSLtag_define(model, &parent_tag_handle, TYPE_HANDLE,
   ”Parent_b3");
5. DMSLmodel_map_tag(2, c31, &parent_tag_handle);
```

Step 4: Defining Solution data using tags

```
1. damsel_handle unk_tag_handle = 10004;
2. DMSLtag_define(model, &unkd_tag_handle, unk_array_type,
   ”UNK");
3. DMSLmodel_map_tag(unk_data, block_collection_id,
   &unk_tag_handle);
```

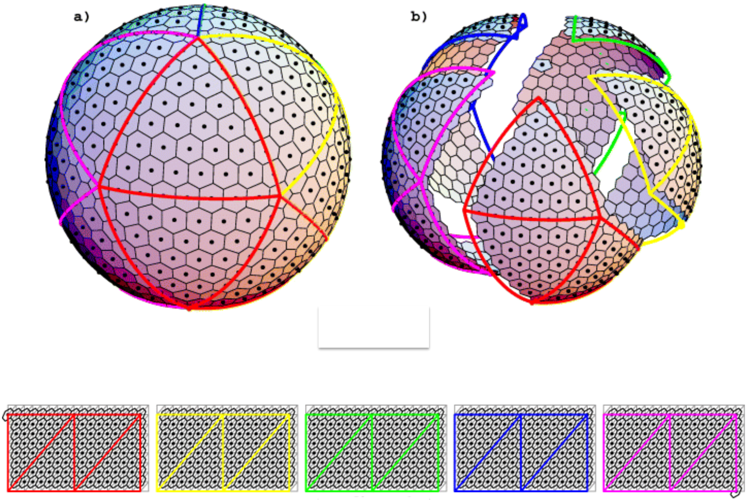

NORTHWESTERN UNIVERSITY

FLASH using DAMSEL API

Step 5: Mapping to file handles

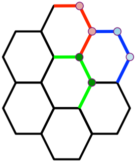
```
1. DMSLmodel_attach(model, "test-flash.h5",
   MPI_COMM_WORLD, NULL);
2. DMSLmodel_map_handles_inventing_file_handles(block_c
   ollection_id);
3. DMSLmodel_map_handles_inventing_file_handles(unk_tag
   _handle);
4. …
5. DMSLmodel_transfer_async(model,
   DAMSEL_TRANSFER_TYPE_WRITE, &req);
6. Finalize lib instance
```

Introduction

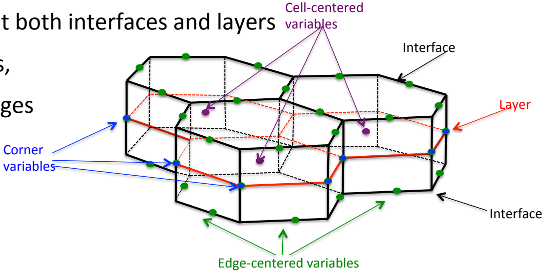


Introduction

- Grid data
  - Cell corners (2/cell)
  - Cell edges (3/cell)
  - Layers and interfaces



- Solution data at both interfaces and layers
  - Cell centers,
  - corners, edges



GCRM using existing I/O Libraries

PNetCDF

- Grid Data:
  - Dimensions: Cells, edges, interfaces, etc
  - Variables: grid_center_lat(cells), grid_corner_lat(corners), cell_corners(cells, cellcorners)
- Solution Data:
  - float pressure(time, cells, layers)
  - float u(time, corners, layers)
  - float wind(time, edges, layers)

NORTHWESTERN UNIVERSITY

GCRM using DAMSEL

- A Hexagonal Prism entity to describe a cell
- An unstructured mesh to describe GCRM grid (no hierarchical information)
- Or a structured mesh to describe GCRM grid

NORTHWESTERN UNIVERSITY

Summary

- Motivation
- DAMSEL Data Model
- API Implementation
- Usecases: FLASH and GCRM
- Data layout work is in progress

NORTHWESTERN UNIVERSITY