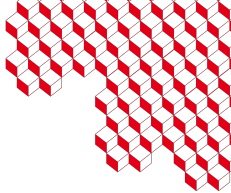


MEDCoupling Introduction and overview

08-03-2024

Aymeric SONOLET, Guillaume BROOKING



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Agenda

- Overview of MEDCoupling
- Notebooks 1 and 2 about DataArray, Mesh and Field
- Presentation of MEDLoader
- Notebooks 3, 4, and 5 about MEDLoader
- Presentation of Remapper
- Notebook 6 about Remapper
- Notebooks of ExempleComplet/

Objectives



- Get an overview of the library features
- Understand of main objects: `dataArray`, `Mesh`, `Field`
- Master simple and representative cases

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Mesh and Fields

A typical scientific simulation requires:

- **Meshes**, spatial discretization of a geometric domain
- **Fields**, physical data on mesh entities

main input/output of a numerical solver: (*spatial descr., initial conditions, boundary conditions, etc.*)

Creating or modifying meshes and fields is difficult



Why using MEDCoupling ?

Custom Meshes and Fields for each code

- well suited
- hard to develop
- hard to interact with other codes and tools (e.g. post-processing)

Using MEDCoupling in several codes

- may have limitations
- inherit from all MEDCoupling features
- share development effort
- easy to interact with other codes and tools

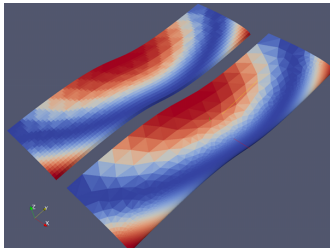
Differences with SMESH

- field manipulation
- highly scriptable creation of simple meshes
- an **interface** between simulation codes and tools



MEDCoupling Features

- Mesh
 - Build from scratch
 - Refine and split
 - Intersect
- Fields
 - Projection from one mesh to another
 - Projection taking into account physical nature of the field
 - Parallel projections
- Almost everything available in **Python**





Misc. features

- Convex hull computation
- Duplicate nodes identification
- Degenerated cells reduction, typically a flat triangle
- Point localization
- Algebraic volume, area, length computation
- Mesh concatenation
- Eigen values computation
- Gauss points management
- And many more



What does MED means ?

Modèle d'Échange de Données

- Core structures (arrays, meshes and algorithms)
- Projection (interpolation and field projection)
- Parallelism (DEC - Data Exchange Channel)
- File I/O (MEDFiles)
- MEDReader, Paraview plugin to visualize MEDFiles
- MED GUI (aka Fields)



Historical context

1996

ÉdF R&D, data exchange between simulation codes
standardization effort

2001

MED-file library (ÉdF/CEA), for data exchange, integrated to the
SALOME platform

2010

First version of MEDCoupling
Almost 15 years of development

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DataArrays (1/2)

- To do all this, surely, we need
 - Arrays of points (mesh nodes coordinates, centers of mass, ...)
 - Arrays of “data” (fields, etc ...)
- First building block: DataArray
 - “Similar” to a list with several columns
 - Usually much more rows than columns!
 - Example: array of 2D points = DataArrayDouble
 - `coo = mc.DataArrayDouble([(1.0,2.0), (2.0,3.5), (1.5,3.4)])`
 - Array of 3 tuples and 2 components
- Main sub-types: DataArray’s of int or double
- All indices start at zero
- In Python, DataArray-s are manipulated very much like NumPy arrays
- Important point for I/O: DataArray-s have a name, and so have their components



DataArrays (2/2)

- All standard operators directly accessible using operators:
 - `da = mc.DataArrayInt([1,2,3])`
 - `da *= 2`
 - `da = (1-da)`
 - Similarity with NumPy: by default, operations are done at the tuple level (no matrix-like operations)
- Advanced operations: intersection (for DAInt), min/max extraction, ...
- Link with NumPy (need to have a MED compiled with NumPy support!)
 - `DataArrayInt` and `DataArrayDouble` can be converted to NumPy array
 - Efficient in both ways (no copy, just ownership transfer)
 - Advantages
 - mmap, serialize/deserialize with multiprocessing
 - Usage with arrays of bool (`where()` clauses)
 - Syntactic sugar for dimension management (translate, `newaxis`, ...)
 - Link with SciPy for linear algebra
 - Link with pyCUDA
 - Restrictions
 - Some services missing: `getMinMaxPerComponent()`, `findCommonTuples()`, ... or to be invoked with another approach
 - No names associated to arrays/components



Renumbering, Easy index manipulation

- indexing methods like `numpy`:
 - `da[:, 0]` : extract the first component of all tuples (i.e. first column of the array)
 - `da[[1,0,2]]` : reorganize the array
- Many MEDCoupling functions work with (or return) arrays in the format above.
- See Array Renumbering section of the documentation.

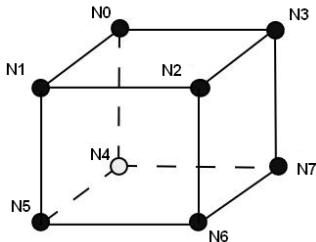


Meshes

- In the MED world, a mesh is
 - The spatial discretization of a continuous geometrical domain
 - Associated to only one array of underlying point coordinates (a `dataArrayDouble`, called the nodes of the mesh)
 - With only one single mesh dimension
 - You can NOT mix a mesh representing 3D volumes (say cubes) with 2D areas (triangles)
 - A mesh also has a name (important for I/O) and a time-step ID
- Do not confuse
 - Mesh dimension: dimension of the cells
 - Spatial dimension: number of components in the array of coordinates
 - Example: an helix-shaped curve (= a wire shaped like a corkscrew) has
 - Mesh dim = 1 (this is a simple wire made of segment cells)
 - Spatial dimension = 3
 - A curved surface has mesh dimension = 2, space dimension = 3
- A mesh is made of cells: segments in 1D, surfaces in 2D, volumes in 3D.
- Main types of mesh in MEDCoupling: structured, unstructured and extruded

Cell representation (unstructured meshes)

- A cell is described by the list of its **nodes' indices** (not coordinates)
 - e.g. [0, 1, 2, 3, 4, 5, 6, 7]
 - “cell” can be a segment in 1D
- Need for convention: there is more than one way to index a cube's vertices:
- No explicit notion of “edges” (resp. “faces”) for a 2D (resp. 3D) cell
- Only points. Other entities can be computed on the spot, with `buildDescendingConnectivity()`





About cells

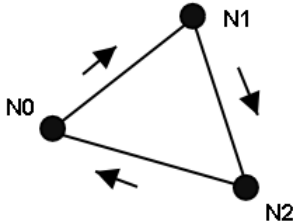
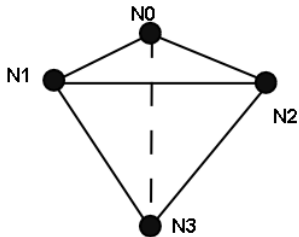
Label of cell types

- HEXA8: a hexahedron with 8 points (i.e. a linear cube)
- HEXA20: g. hexahedron with 20 points (can represent a “quadratic” element, a “cube with curved faces”).
- TETRA4, TETRA10, etc.

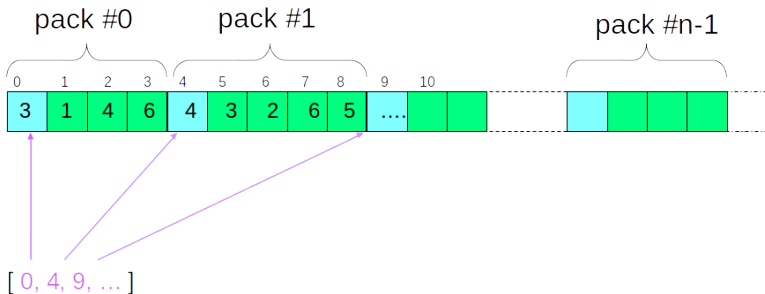
See the MED-file documentation, for more information.

Numbering order

- In 2D, reverse trigonometric convention is used



Indirect indexing format



Notably, used for representation of cells' connectivity



Fields, more than an array of values

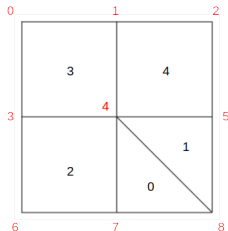


- represents some physical quantity associated with a spatial domain
 - No continuous description of the physical quantity over the domain
 - A finite set of values, associated to some constituents of the mesh
 - At a low level, a DataArray associated to a given mesh
 - Can have more than one component!
- A field can be supported by nodes (vertices) `ON_NODES`, cells (elements) of the mesh `ON_CELLS`, or more complex items
- A field has a temporal discretization
 - `NO_TIME`
 - `ONE_TIME`
 - `CONST_ON_TIME_INTERVAL`
- For some operations (interpolation), one need to define the physical nature of the field (extensive field or intensive field)
- More on all this with interpolation . . .
- Examples
 - Magnetic field: tensor field of double values: 3 components (B_x , B_y , B_z)
 - Temperature field: scalar field of double values: 1 component

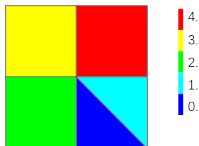


Illustration

- Unstructured 2D mesh, of QUAD4 and TRI3
- The cell 2 has the connectivity [3, 4, 7, 6] (clockwise)



- A P0 (i.e. 0N_CELLS field on this mesh), with 5 values



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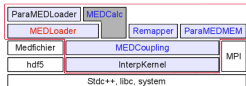
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Dependency Structure



- Several sub-parts each dedicated to a specific task
 - MEDCoupling: memory model and general processing
 - MEDLoader: persistence
 - ParaMEDMEM: parallelism
- A big effort to have little dependencies
- Parts are:
 - Swigged
 - Swigged and wrapped with CORBA
 - System dependencies

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Note for C++ developers

A few words about the code

- source code
 - 150k lines of C++
 - 40k lines of Python
- tests
 - ~1600 unit tests
 - memory leak check for each unit tests (valgrind)
- build
 - cmake



Base classes

RefCountObject abstract class

- Similarities with VTK code structure
 - Ease the interaction with VTK (ParaView plugins)
 - Historically, there's been a reflection about using VTK directly
- All (significant) MEDCoupling classes inherit from
 - RefCountObject
 - A pointer and a counter
 - Memory management philosophy: someone owns the object after its creation
 - incrRef() to take ownership of the object / decrRef() to release it
 - Template class MCAuto is here to help
 - Smart pointer behavior (no Boost dependency)
 - No need to decrRef() if used
 - valgrind is your friend
 - Careful, some MEDCoupling functions
 - give you pointer ownership: e.g. mergeNodes()
 - Some don't: getCoords()