

Documentation - draft

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Part I

Some programming practices

- Use .hpp for header files and .cpp for source files
- Use `std::cout`, do not use `printf` for output.
- If a function must be performed by only one processor (processor 0), then write an `ifproc` INSIDE the FUNCTION (not outside).
- Divide the includes in FEMuS includes, C++ includes, other external libraries' includes.
 - Always put include guards in header files.
 - Try to put the includes EXPLICITLY WHERE THEY HAVE TO BE, and not thinking that somewhere some include will lead me to the file i need...
 - In the SCRIPTS, almost all the variables have a `FM_` or `FEMUS_` prefix. The variables without this prefix are like this because they are defined for external packages. For instance, `PETSC_DIR` and `PETSC_ARCH` are used to COMPILE PETSC.
 - when you create a NEW HEADER, make sure you change the INCLUDE GUARD. Then, make sure you add the new files to git.
 - when you change the name of a file, header or source, recompile all the applications and make sure that everything compiles correctly.
 - when you start a file, put the source code among the "namespace femus"
 - data encapsulation, please

Chapter 1

Debugging, parallel

Put yourself in the simplest case

First of all, check that the coarse mesh has enough elements: if the coarse mesh only has 1 element, then Metis does not work

Then, try to only run Mesh and Printing, by commenting the solution of your System. See how the Metis partitions are printed.

Fine, it works.

1.0.0.1 Use valgrind!!!

1.0.0.2 Command

```
mpiexec -n 1 femus-dbg -start_in_debugger
```

1.0.0.3 Segfaults

If you use -info it tells you a lot of things about PETSC calls. -log_trace, -info, -log_summary

Finding a segmentation fault shouldn't be too difficult with valgrind or gdb (see also this link: <http://www.cprogramming.com/debugging/segfaults.html>)

Di solito guardi uno dei puntatori nella riga in cui si blocca e magari e' un puntatore non inizializzato, oppure e' un puntatore a NULL, oppure e' un puntatore che e' stato deallocato, oppure sto dereferenziando un puntatore al di fuori del suo range, oppure qualcosa altro ma poco...

Per quanto riguarda le PETSC puo' essere molto lungo riuscire a trovare un segmentation fault, perche' dovresti andare a vedere DENTRO LE STRUTTURE (Mat, Vec sono strutture di C) e guardare di quegli elementi qual e' quello che causa il segmentation fault.

Per fare questo conviene USARE LE PETSC in DEBUG MODE e vedere quale output ti danno; cosi' vedi le chiamate all'interno della libreria petsc.

Part II

Application

1.1 How to SETUP a NEW APPLICATION of the LIBRARY (will do a script probably)

- Create a folder in the Applications directory with your main function and your src/header files - Write the Cmakelists.txt file for it - Add the reference to the application in the Cmakelists.txt of the package library - open cmake-gui and run configure and generate - NOW PAY ATTENTION TO WHAT HAPPENS WHEN YOU ADD SOURCE FILES to the LIBRARY (not to the application)! You have to update the LIST in the src/ cmake file!!! (use ls -l) - now go to the binary directory and type make to generate the library - then enter your application folder and run make to generate your executable

1.2 How to IMPLEMENT A NEW APPLICATION

- Follow the examples

1.3 How to change the mesh file of an application

- Put the mesh file in the input/ directory - Set the filename in the main file

1.4 How to run in parallel with threads instead of cores

"nproc" gives the number of threads. If your CPU has 2 threads per core, "mpirun -n " works up to nproc/2

To overcome this, do

"mpirun -map-by socket:OVERSUBSCRIBE -n ..."

1.5 How to schedule a suite of runs

- Script

1.6 When you change the input file in the repo folder (NOT IN THE BINARY FOLDER) then you have to RERUN CMAKE !!!

1.7 How to RESTART a run of an application

- THE WHOLE RUN is in a single "time" DIRECTORY... so to restart we will EXCLUSIVELY READ from THAT DIRECTORY

- Set the folder from which to restart in the file `run_to_restart_from` - set the ITERATION NUMBER in the "initial_step" variable in the configuration file IN THE FOLDER OF THE CONSIDERED RUN! - set the other parameters like "nsteps"

- We must be very careful. - We must change ALMOST NOTHING - Do not change NUMBER OF PROCESSORS - Do not change NUMBER OF LEVELS - Do not change the OUTPUT FOLDERNAME (of course...)

Part III

Application: main stages

Chapter 2

Main blocks

- Mesh generation
 - Mesh Partitioning for parallel (Metis)
 - Solution on a Mesh
 - Problem with Solution unknown (certain unknowns, certain not)
 - Solution: Boundary conditions
 - Solution: Initial conditions
 - Space discretization (and quadrature)
 - Time discretization (i.e. quadrature in time)
 - System of a Problem (Nonlinear loop, Linear Solver, Preconditioner, etc.)
 - Final output
 - MultilevelMesh
 - MultilevelSolution(MultilevelMesh)
 - MultilevelProblem(MultilevelSolution)
 - System
 - MultilevelProblem.add(System)
 - System.solve() –, with this process, the MultilevelSolution (which is accessed by System through MultilevelProblem) is updated

Chapter 3

Init

3.1 Parallel initialization

3.2 Input parser

Chapter 4

Mesh

If you choose `LINEAR` for the `MESH DISCRETIZATION`, it only works in `SERIAL`! It could actually work if the `MESH` was `LINEAR`...

For now, the Mesh must be `BI/TRI-QUADRATIC`. Could it be `Tri7`, or does it have to be `Tri6`??? We have to test.

4.1 MultilevelMesh

`EraseCoarseLevels`: it shifts the level vector, so if you start with 5 levels and you want to remove the first 3, it shifts 4 and 5 to the 1st and 2nd position

4.2 Mesh

4.2.1 Boundary mesh

Whenever you want to retrieve the Boundary of a Mesh, you need to loop over each mesh element and then loop over its *faces*.

If the `FaceElementIndex` is < 0 , then it is a *boundary* face.

When the `FaceElementIndex` is stored, the flag that is on the mesh file is made `NEGATIVE` and then we subtract 1

4.2.2 Interface mesh

If I wanted some **interface** faces, not on the boundary, I should set their `FaceElementIndex` to be > 0 . How does this affect the rest of the code?

4.3 Elem

The `Elem` class contains the **list** of all elements

```

//      7-----14-----6
//      /|              /|
//      / |            / |
//      15 |      25    13 |
//      / 19      22  / 18
//      /  |            /  |
//      4-----12-----5
//      | 23 |      26  | 21 |
//      |   3-----10-|-----2
//      | /           | /
// 16 / 20           17 /
// | 11      24 | 9
// | /         | /
// | /         | /
// 0-----8-----1

```

```

//      3
//      /\
//      /\
//      /\
//      9 | 8
//      /\
//      /\
//      2-----5-----1
//      /\
//      /\
//      6 | 4
//      /\
//      /\
//      0

```

```

//      5
//      /\
//      /\
//      /\
//      11 | 10
//      /\
//      /\
//      3-----9-----4

```



```

//      | 17      | 16      |
//      |      2      |
//      |      / \      |
//      |     /   \      |
// 12    |  / 15  \ 13
//      | 8       7      |
//      | /       \      |
//      | /       \      |
//      | /       \      |
//      | /       \      |
//      0-----6-----1

```

```

//      3-----6-----2
//      |           |
//      |           |
//      7       8       5
//      |           |
//      |           |
//      0-----4-----1

```

```

//      2
//      | \
//      |  \
//      5   4
//      |   6 \
//      |   \
//      0-----3-----1

```

```

//
// 0-----2-----1
//

```

4.4 Geometric Elements

4.5 MeshInput

These mesh files also set FLAGS to faces

4.5.1 From function (MeshGeneration)

4.5.2 Gambit IO

4.5.3 MED IO

4.6 MeshPartitioning

4.6.0.1 Elem and Node splitting

In a FE code you have you must do a partition of Elements and Nodes among the processes.

Elements only belong to one process

Nodes belong to one process but then they are also Ghosted (for the other processes that “own” them)

4.6.1 MeshMetisPartitioning

The Metis library is responsible for that

The Elements are reordered, so that

the 1st range goes to proc 0, the 2nd range goes to proc 1, and so on...

4.6.2 MeshASMPartitioning

4.7 MeshRefinement

Chapter 5

Solution (Quantities, Equations, Operators)

5.1 MultilevelSolution

Only MultilevelSolution has a Writer object. This writer will write from the FINEST level available.

Solution does not have a Writer.

Similarly, MultilevelMesh has a Writer, but not Mesh.

However, currently the Writer in MultilevelMesh does not work.

- The values of variables are taken from the MultilevelSolution object..

That's where the absolute values are stored, otherwise it is only about delta x in the nonlinear loops

5.2 MultilevelSolution: Boundary conditions

They are set through a function pointer.

They are associated to the Solution and not to the Equation.

In this way you can set BCs also for Solutions that are not Unknowns of an Equation

5.2.1 Dirichlet

- Dirichlet boundary conditions are set AFTER the ASSEMBLY process, by setting a Dirichlet row to zero and putting 1 in the diagonal, and by setting the corresponding Residual to ZERO at those rows

5.2.2 Neumann

They are set by implementing a boundary integral

5.3 MultilevelSolution: Initial conditions

5.3.0.1 Check that boundary values and initial values at the boundary are CONSISTENT

5.4 Output: Writer

Chapter 6

Problem

6.1 MultilevelProblem

Everything in the Assemble function (and in other parts too) is accessed through this class

Il problema deve essere dotato dei dati CONDIVISIBILI tra tutte le EQUAZIONI:
- parametri fisici / di visualizzazione - puntatori alle equazioni - puntatori ai punti di gauss per l'integrazione - puntatore al MESH - NUMERO DI LIVELLI del multigriglia

Io ci aggiungerei anche - MGpar, parametri del MG disponibili per tutte le equazioni.

6.2 Quadrature

You put it here so that many systems can share it

Clearly, if you have terms with different polynomial degrees, you pick for the quadrature the ones that guarantees exactness for the highest-degree polynomial

6.3 FE Abstract Families (with precomputed Quadrature evaluations)

Chapter 7

System(s) (of a Problem)

After the MGSolve or MLSolve or solve function is called, the MultilevelSolution vector is updated and ready to be printed to file...

But where exactly is it updated? Also, the print routines only print at the FINE level, so is MultilevelSolution updated only at the FINE level or at ALL levels???

Ok, what happens is that the MultilevelSolution object contains a VECTOR (based on number of levels) of Solution objects, and THIS is the vector that the Writer uses need to access if I want to retrieve my values!!!

System: the System class has a
std::vector of Mesh pointers and a
std::vector of Solution pointers,

and it also has pointers to MultilevelSolution and MultilevelMesh...

MultilevelMesh, in turn, has a std::vector of Mesh pointers in it;

MultilevelSolution, in turn, has a std::vector of Solution pointers in it

- Every Mesh should be SINGLE-LEVEL, but it has a _ProjCoarseToFine object, so it is not really single-level...

Chapter 8

Solvers and preconditioners

8.1 Linear Equation Solver (child of Linear Equation)

This is to handle $Ae = -r$

The LinearImplicitSystem has a vector of LinearEquationSolver objects (one for each mesh level)

Every LinearEquationSolver has a Solver (which somehow tends to be called Smoother often times) and a Preconditioner

8.2 ML vs. MG solver

In MG you pass the Smoother, while in ML you don't.

Part IV

Git Cheat Sheet

8.3. WORKFLOW FOR UPDATING THE MASTER IN THE FORK FROM THE MASTER IN THE MAIN REPOS

- First golden rule: using the manual never hurts.
- Set name and email in your computer:
git config --global user.name "Name Surname" git config --global user.email "name.surname@example.com"
- To check what configuration you obtained, do
git config --list
(this shows you more than you see with "git config -e" because it also reads other git configuration files, such as \$HOME/.gitconfig)
- To contribute: Create a personal github account Create a fork of the femus repository in your github account Clone your fork in your computer Work in your computer (do branches, commit changes, ...) Push your branches back to your fork Send a pull request to the main femus repository The maintainers will decide what to do with the pull request and possibly it will be merged to master Periodically, sync the master in the fork with the master in the main femus repository

8.3 WORKFLOW for updating the master in the FORK from the master in the MAIN REPO

In github:

Go in the MAIN REPO

Click on "Pull requests" (on the right) Click on "New pull request" (green button) Click on "compare across forks" The "base fork" is going to be the FORK master branch The "head fork" is going to be the MAIN master branch Click on "create pull request" Add some title for it Make sure that the branches can be AUTOMATICALLY MERGED (otherwise you have to solve the conflicts using command line...) Click on "Merge pull request" (you find it by scrolling towards the bottom of the page) Click on "Confirm merge"

From command line:

To be added

Part V

Salome

Chapter 9

SHAPER Module

This is a new module that in the long run is supposed to replace the role of the GEOM module. In the meantime, you can: - perform drawing operations in the Shaper module - do "Export to Geom" if you want to then do the meshing.

At the beginning you start with a "Partset" that contains 7 elements (Origin, axes, ...) that cannot be deleted To draw stuff in Shaper, first create a Part with "New Part".

Notice: things that are exported to Geom are those that appear under the "Results" of a Part. If you have no object in the Results, nothing will be exported to Geometry.

Then, it's not so clear how to start setting points... Should I use Construction, or Sketch... or Build...

Ok, it seems like: - Sketch is for drawing things "imprecisely", as if it was a real sketch, without specifying precise coordinates and so on. - Construction allows to put precise information

When you do a Sketch, remove the Interaction Style Switch (white mouse icon)

- If you built a Point as a Construction in the Partset and you want to REMOVE it, you have to click on "Partset" and say "Activate". Then you can right-click and finally "Delete" is active. Then, Deactivate again to continue drawing

- Pay attention sometimes when you Dump study, it seems like you may lose the Shaper part!!!

Chapter 10

GEOMETRY Module

10.1 ROTATIONS

If you have to rotate, do not do that in the Geometry, because then the Mesh will not follow. If you do it in the Mesh, the Geometry does not follow either.

10.2 SPLIT EDGES/FACES

The tool for this is: Partition then Explode. At first it seems like with Partition no split happens, but then if you do Explode you will get all the pieces It seems like Cut is not the right tool for splitting

Pay attention to the difference between Common and Intersection

Chapter 11

MESH Module

11.1 Basic procedure

Use the NoteBook tab to define variables and parametrize your operations!

11.1.1 Geometry

Create faces (Draw points and lines if needed, or create Faces directly) – Extract edges from a face (Explode)

11.1.2 Mesh

Create Mesh object (only initialize) Create SubMesh of Mesh over the wanted SubGeometry – Hypothesis: Propagation of 1D Hypothesis

In Mesh: – 2D: Quadrangle Mapping 1D: Wire Discretization, or another SubMesh with Propagation in the other direction (this would overwrite Wire Discretization)

– Convert EACH mesh to the order you need (linear/quadratic/biquadratic) You have to do this operation BEFORE creating a CompoundMesh, because the compound mesh does not have an underlying geometry to use

You have to do ONE BY ONE, you cannot do by selecting all meshes at once!!!

– Build CompoundMesh to merge the meshes – Check the Boundary of the CompoundMesh!!! – When you do a Compound, the double nodes are MERGED, but the inner edges or inner faces are not REMOVED! So, you have to remove them manually!!! – You need to remove the boundary elements of the previous separate pieces that are now inside the new domain! To do so you do "Remove elements" and you set a filter "Free borders - Not": inner boundary elements are non-free borders Unfortunately you don't see this operation as a new object in the Mesh menu – Rename it to "Mesh" + something!!!

11.1.3 Groups of Mesh elements

(must be named `Group_X_Y`, where X is the flag given to the object and Y is the type of boundary condition (0 = Dirichlet, 1 = Neumann). What about the groups that are not for boundary conditions?)

In order to enforce Boundary Conditions, Material Properties, and potentially other things too, we have to define Groups of Edges, or Faces, or Volumes (Groups of Nodes for the extremes of a 1d domain)

The flexible way to define these groups is NOT by selecting the IDs but by doing either "Group on geometry" or "Group on filter"

- AAA: I think I found how to do the "quadrangle-mapping" mesh of a face where one side has multiple edges coming from Explode!!! I just do the same, but I specify "Composite wire discretization" instead of "Wire discretization"!!!

- You can use Filters to define Groups of Mesh Elements

11.2 QUADRILATERAL MESH of a CIRCLE/SEMISPHERE

Divided Disk or Divided Cylinder do exactly what you are looking for!!!

Partition a semisphere using a Divided Disk!

Beware: it is essential that a vertex of the inner square is aligned with the "meridian arc" that is intrinsic in the generation of a Sphere surface!

For a circle, just do a square in the middle, then divide the circumference into four parts, join the angles of the squares with the vertices of these parts and you are done.

For the semisphere, if you try the same it doesn't work, because the faces that are constructed do not belong to the original semisphere...

So the idea seems to be NOT the following: - make curved edges on the semisphere - use them to create curved faces So, try to avoid starting from the Edges and instead keep yourself at the level of Faces. Then only at the end you will Explode to get the Edges (that you may need later for submeshes)

Also, try not to cut too much, because if you do so you may have multiple edges on one side and then it is not so easy to mesh...

The other way to go is to directly create subfaces by Partition of the semisphere!

First you split, then you join...

Now:

- Fuse doesn't work with non-planar faces... - Glue Edges is to put together coincident edges, but not to remove them - It seems like the right option is Sewing, then Union faces, then Explode to get the edges for the submeshes - The only problem is that now one face does not have 4 edges, but one side can be made of multiple edges, and that creates problems in the mapping algorithm. So, it's all about making 1 edge

11.3. WHEN YOU DO A 3D MESH, NOT ONLY WILL YOU HAVE VOLUMES AND FACES, BUT ALSO THE EDGES

11.3 When you do a 3d mesh, not only will you have Volumes and Faces, but also the Edges of the “Bounding Box”

You can leave the edges where they are, because in 3d only Volumes and Faces will be read from the code

11.4 Basic procedure - 3D

- If I want to create a mesh of a Box with 3 arbitrary mesh discretizations in the 3 directions, what is the best way to do that?

I cannot create a Submesh of a Submesh

- Geometry Create Volumes — Extract Faces from a Volume — Extract Edges from 2 faces in order to do Submesh of 3 edges in the x,y,z directions - Mesh I'd say I'll treat a Face like I do in 2D, and then do a Mapping to opposite Faces... You don't want to do Automatic Hexahedralization or Tetrahedralization...

- Another method could perhaps be to create 1d meshes and Propagate their Hypothesis on opposite edges! Global Algorithms: 3d: Hexahedron (i,j,k) 2d: Quadrangle mapping 1d: Wire discretization - Here sometimes it gives trouble if you don't specify any "Number of Segments"...

Do 3 submeshes on 3 Edges, and on each of them establish a "Propagate hypothesis on opposite edges"

11.4.1 MESH EXTRUSION

- If your mesh can be thought of as an Extrusion of a 2D mesh, one way to do this is simply to do your 2D mesh and then extrude it

- Do extrusion only of faces to avoid generation of extra edges

- "Scale factors" refer to the TRANSVERSAL direction, not the orthogonal one

11.5 HOW TO SHARE SUBMESHES ON CONTIGUOUS FACES

When you explode adjacent faces, the edges are called differently... we should identify them

11.6 Change the Geometry in the Mesh with “Move node”

There is a command called ”Move node”, perhaps it helps avoiding to remesh everything if I go back and change the Geometry instead...

-

11.7 Translate Mesh

Copy Mesh of course does not do the trick, you need “Translation”

“Offset” of a mesh does not work for Quadratic mesh

“Translation” of a mesh works with “Create a new mesh” and “Copy groups” creates a translated copy

11.8 Stretch elements

“Scale transform” does the trick

11.9 BOUNDARY CONDITIONS

I think it’s best if I do the groups on the initial meshes (before doing the Compound) because there I can do ”Group on geometry”, while a Compound does not have an associated Geometry to it (alternatively, one could do Group on Filter maybe)

11.10 Mesh controls

You want to check that there are

- no Free Nodes or Orphan Nodes (nodes that don’t belong to any element)
- no Double Nodes
- no Inner Edges (only Free Borders, i.e., edges that are at the boundary of the domain)

Chapter 12

Questions

- When I remove a Group, can I ask to remove also the elements of that group from the Mesh???

- When you do Extrusion, it also generates the Groups of Volumes from Groups of Faces! It puts a suffix **_extruded**

- When you remove inner edges in a compound mesh and then you dump the script and reload it, the mesh is corrupted! On the other hand, if instead of dumping the script I save the study it is NOT corrupted! So, I will stick with saving the study for now.

- Other times, you dump the script and the Shaper is gone!! It is a current bug! Up to now, you need to activate Shaper before any dumping. Sorry.

- Operations in the Mesh such as "Convert to/from quadratic", "Remove elements" and others are not shown as stages in the Mesh menu in Object Browser

- Intersection vs. Common: the first does it with Edges, the second does it with Volumes, basically...

- To remove Extra Edges on a Face, you first have to create an auxiliary volume, and then do Repair-¿ Remove extra edges from that volume, then that face will be fixed! Another trick is to put the Face in a Compound. There it works!

- When you convert a mesh to quadratic/biquadratic, do it on a Mesh that is ATTACHED to a Geometry, because it is with the geometry that new nodes are added! Otherwise nothing happens!

- What is the difference between Regular Faces and Free Faces in the Mesh algorithms? For instance, the Disk only shows algorithms for Free faces...

- Is it possible to merge items obtained by Explode command? If I have 5 edges exploding from a quadrangular face, where 2 of them form one of the actual 4 edges, can I merge them so that the face looks to have 4 items instead?

Possible answer: I think the way to go in these cases is to do, after Explode, a "Create Group" in the Geometry. That group should appear as a "child" of the Geometry object you will then mesh. I can try this to double check.

Part VI

Hdfview

Follow the instruction in the HDFVIEW website

At the end of the build process, you should have an `hdfview.sh` script inside the `bin` directory of your build. You must open that script and change the `INSTALLDIR` variable with the path of this build (by default, `/usr/local` is in it)

Another alternative to view the content of an HDF5 file is to use the `'h5dump'` utility shipped with HDF5 (installed through PETSc, for instance)