TRUST ICoCo Tutorial V1.8.2

CEA Saclay

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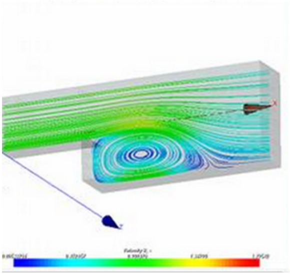
1. Introduction to code coupling and ICoCo
2. TRUST and ICoCo initialization
3. Basic test case
4. Coupled problem with ICoCo

Why code coupling?

Code coupling ... what for ?

- Traditionnaly *numerical simulation codes* focus on a single physics
  - One code for thermics
  - Another code for mechanics,
  - Etc...
- Real life studies require the simulation of different physics
  - E.g. nuclear reactor simulations require a blend of: thermics, neutronics, mechanics...
- Solution? Code coupling!
  - Have different codes communicating one with another...
  - while each code deals with its own area of expertise



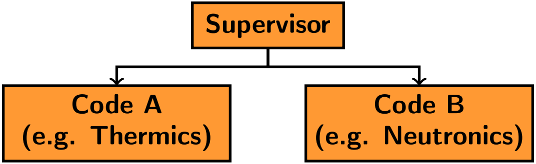
Code coupling

First approach

- An entity driving the complete computation is needed: the **supervisor**
    - Initializes code A and code B
    - Loop through code A and code B
    - Centralize exchanges and conversions between A and B

  Supervisor is usually written from scratch as a C++ program, Python script, ...

- In a dummy approach : supervisor needs to know *both* A and B API. It becomes cumbersome if :
    - more than 2 codes to couple ...
    - single supervisor is meant to run with different pairs of codes (code C, D, E ...)



Code coupling

Better: common interface!

Idea: define a unique *interface* to which each code must comply

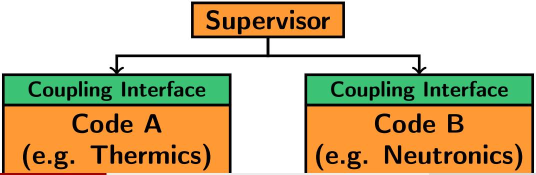
- Only an *interface*, i.e. a contract (=an API) that each code fulfills
- *Implementation* (=plugging wires) of this interface is tightly linked to the details of the code...

Advantages:

- All codes implementing the (unique) interface can be passed to the supervisor (almost) without modifying it! **Versatility**

Constraints:

- Need to implement the interface for each code to be coupled



ICoCo, **I**nterface for **Co**de **Co**upling

ICoCo is such a coupling interface:

- Stands for **I**nterface for **Co**de **Co**upling
- Written in C++
- Initially designed for simulation codes exhibiting **iterative time loops**
- Presents a set of standard methods whose signature is fixed, with no default implementation:
  - initializeTimeStep()
  - validateTimeStep()
  - abortTimeStep()
  - ...
- Uses the notion of field for data exchange between codes
  - A field is a set of values supported by a mesh
  - A possible implementation: **MEDCouplingFieldDouble**, from SALOME's MEDCoupling library

Further reading

Meaningful documentation

- ICOCO presentation in TRUST documentation:
  "An Interface for Code Coupling ICoCo v1.2"

```
load TRUST environnement
$ evince $TRUST_ROOT/doc/Kernel/ICoCo_V1.2.pdf &
```

- Ask the "APIProblem.pdf" note to trust@cea.fr

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- ICoCo: two way coupling

Initialization of TRUST environment

- Before starting this Tutorial,
  it is highly recommended to know some TRUST commands and hints.
- Source the TRUST environment:
  - On CEA Saclay PCs and callisto cluster, TRUST versions are available with (e.g. X.Y.Z=1.8.0):
    source /home/triou/env_TRUST_X.Y.Z.sh
  - On your own computer, download and install the latest version of TRUST in your local folder $MyPathToTRUSTversion (unless this was already performed), then write on the terminal:
    source $MyPathToTRUSTversion/env_TRUST.sh
- To check if the configuration is well and to locate sources:
  `$ echo $TRUST_ROOT`

Initialization of ICoCo environment

- Source the ICoCo environment:

```
$ source $TRUST_ROOT/Outils/ICoCo/ICoCo_src/full_env_MEDICoCo.sh
```

- check if ICoCo is compiled:

```
$ ls $exec
```

- If you obtain "ls: cannot access **/Outils/ICoCo/ICoCo_src/ICoCo_opt: No such file or directory", then compile ICoCo_src:

```
$ cd $TRUST_ROOT/Outils/ICoCo/ICoCo_src
$ baltik_build_configure -execute
$ make optim debug
$ source full_env_MEDICoCo.sh
```

- If you do not have rights to compile ICoCo (Typically if TRUST install is made by someone else):

```
$ mkdir -p ICoCo
$ cp -r $TRUST_ROOT/Outils/ICoCo/ICoCo_src ICoCo/ICoCo_src
$ cd ICoCo/ICoCo_src
$ baltik_build_configure -execute ; make optim debug
$ source full_env_MEDICoCo.sh
```

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Goal of this first exercise

The idea here is to:

1. Create a reference test case
   - To be launched with TRUST executable.
2. Update the test case in order to:
   - Launch it sequentially with ICoCo without information exchange.
   - Ensure that obtained results are identical to those obtained in step 1.
3. Realize your first information exchange between the supervisor and datafile
   - Impose a boundary condition from the supervisor and launch the calculation sequentially with ICoCo
   - Compare the results with those obtained with TRUST executable.
4. Make the test case running with ICoCo in parallel:
   - Launch the computation with ICoCo on 2 processes
   - Compare obtained results with those with TRUST executable.

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TRUST: test case creation

We will copy a reference test case from TRUST tests database that we launch with TRUST.

- Copy Vahl_Davis_hexa test case in your repository:
  ```
  $ mkdir ICoCo_exercises
  $ cd ICoCo_exercises
  $ trust -copy Vahl_Davis_hexa
  ```
- Rename the folder to distinguish your tests:
  ```
  $ mv Vahl_Davis_hexa Vahl_Davis_hexa_trust
  $ cd Vahl_Davis_hexa_trust
  ```
- Rename the datafile to be consistent with the folder's name:
  ```
  $ mv Vahl_Davis_hexa.data Vahl_Davis_hexa_trust.data
  ```
- Launch calculation:
  ```
  $ trust Vahl_Davis_hexa_trust
  ```
- You obtained a Vahl_Davis_hexa_trust.lml file. We will need it in the following part.

ICoCo: without exchange

Adjusting the datafile

- Now let's do the same thing with ICoCo:
  `$ cd ..`
- You are now in the folder "ICoCo_exercises", create a new directory in order to launch your test case with ICoCo:
  `$ trust -copy Vahl_Davis_hexa`
  `$ mv Vahl_Davis_hexa Vahl_Davis_hexa_ICoCo`
- Rename the datafile to be consistent with the folder's name:
  `$ cd Vahl_Davis_hexa_ICoCo`
  `$ mv Vahl_Davis_hexa.data Vahl_Davis_hexa_ICoCo.data`
- Edit the datafile and add to it ICoCo instructions:
  - *Add* the following line after "*dimension*" definition:
    `Nom ICoCoProblemName Lire ICoCoProblemName pb`
  - *Comment* the "*solve pb*" instruction at the end of the datafile.

ICoCo: without exchange

Creation of the main.cpp file

- Create the main.cpp which will launch the calculation:
  ```
  $ file="main_Vahl_Davis_hexa_ICoCo.cpp"
  $ cp $TRUST_ROOT/doc/TRUST/exercices/ICoCo/$file main.cpp
  ```
- Open main.cpp file and see the main method which creates the objects and launches computation.
- You can use ICoCo with 1 or more processors, but in this part we use only one processor to solve the problem.

Creation of the makefile

- Create a makefile for your calculation:
  ```
  $ cp $project_directory/share/bin/create_Makefile .
  $ sh create_Makefile
  ```
- Compile it:
  ```
  $ make
  ```
- This creates an executable "couplage" and a datafile "couplage.data".

ICoCo: without exchange

Launch calculation

- Execute it:
  `$./couplage`
- You should obtain the same results as with TRUST executable. Compare TRUST and ICoCo results with:
  `$ compare_lata Vahl_Davis_hexa_ICoCo.lml ../Vahl_Davis_hexa_trust/Vahl_Davis_hexa_trust.lml`
- Both lml files are identical!

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   - ICoCo: two way coupling

ICoCo: first input

Adjusting the main.cpp file

- Copy the following test case in your repository:

```
$ cd ..
$ cp -r Vahl_Davis_hexa_ICoCo Vahl_Davis_hexa_ICoCo_exchange
$ cd Vahl_Davis_hexa_ICoCo_exchange
```

- Clean the repository and rename the datafile:

```
$ trust -clean
$ mv Vahl_Davis_hexa_ICoCo.data
Vahl_Davis_hexa_ICoCo_exchange.data
```

- We will add a block in the main.cpp file to exchange values.
- Copy the following file in your folder:

```
$ file="main_Vahl_Davis_hexa_ICoCo_exchange.cpp"
$ cp $TRUST_ROOT/doc/TRUST/exercices/ICoCo/$file main.cpp
```

ICoCo: first input

Adjusting the datafile

- Then modify the datafile Vahl_Davis_hexa_ICoCo_exchange.data to make the input:
  - Change the line:
    "Gauche Paroi_temperature_imposee Champ_Front_Uniforme 1 10."
    to
    "Gauche Paroi_temperature_imposee ch_front_input { nb_comp 1 nom TEMPERATURE_IN_DOM probleme pb }"
  - You can see that the field "TEMPERATURE_IN_DOM" is the one employed in the main.cpp file.

ICoCo: first input

Launch calculation

- Now we can compile and launch the calculation:

```
$ make
$ ./couplage
```

- You may obtain the same results as with TRUST executable.
- Compare it:

```
$ compare_lata Vahl_Davis_hexa_ICoCo_exchange.lml
../Vahl_Davis_hexa_trust/Vahl_Davis_hexa_trust.lml
```

- The files are the same! **(but not for the first time step!!!!!)**

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ICoCo: on 2 processes

Adjusting the main.cpp file

- Copy the following test case in your repository:
  ```
  $ cd ..
  $ cp -r Vahl_Davis_hexa_ICoCo_exchange
  Vahl_Davis_hexa_ICoCo_para
  $ cd Vahl_Davis_hexa_ICoCo_para
  ```
- Clean the repository and rename the datafile:
  ```
  $ make clean
  $ rm main.cpp Vahl_Davis_hexa_ICoCo_exchange.lml
  $ mv Vahl_Davis_hexa_ICoCo_exchange.data
  Vahl_Davis_hexa_ICoCo_para.data
  ```
- Partition the domaine and create a parallel datafile:
  ```
  $ trust -partition Vahl_Davis_hexa_ICoCo_para
  ```
- Copy the following file in your folder:
  ```
  $ file="main_Vahl_Davis_hexa_ICoCo_para.cpp"
  $ cp $TRUST_ROOT/doc/TRUST/exercices/ICoCo/$file main.cpp
  ```

ICoCo: on 2 processes

Adjusting the main.cpp file

- Open the main.cpp file and search for the MPI command lines.
- Open this file and look where:
  - the processors are added: search for "dom_ids"
  - the names of the datafiles: search for "data_file"
- Create the makefile and coompile your new file:

```
$ sh create_Makefile
$ make
```

- To run parallel, you have to use the following mpirun command:

```
$ mpirun -np 2 ./couplage
```

- Compare your results with the sequential ones:

```
$ compare_lata PAR_Vahl_Davis_hexa_ICoCo_para.lml
../Vahl_Davis_hexa_exchange/Vahl_Davis_hexa_exchage.lml
```

- Sequential and parallel computation yield the same results!!

Goal of this second exercise

The idea here is to:

1. Create a reference test case treating a coupled problem
    - To be launched with TRUST executable in sequential and parallel.
2. Create two datafiles, each one for a problem:
    - Launch it with TRUST first to ensure that datafiles do not contain errors
    - Launch it with ICoCo without any information exchange after updating datafiles.
3. Realize a one way coupling with ICoCo:
    - One way coupling means that one problem runs alone while some inputs of the second problem are provided by the first one
    - Launch the calculation sequentially with ICoCo
    - Compare the results with those obtained with TRUST executable.
4. Realize a two-way coupling with ICoCo:
    - Two-way means that each problem will have inputs provided by the other one.
    - Launch the computation with ICoCo.

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First with TRUST

Copy a coupled problem test case and launch it with TRUST

- Copy the coupled problem docond_VEF_3D from TRUST tests database:
  ```
  $ cd ICoCo_exercises
  $ trust -copy docond_VEF_3D
  $ mv docond_VEF_3D docond_VEF_3D_trust
  ```
- Launch calculation:
  ```
  $ cd docond_VEF_3D_trust
  $ trust docond_VEF_3D
  ```
- Now, run the calculation in parallel also:
  ```
  $ trust -partition docond_VEF_3D
  $ trust PAR_docond_VEF_3D 2
  ```
- Compare the sequential & parallel results:
  ```
  $ compare_lata docond_VEF_3D.lml PAR_docond_VEF_3D.lml
  ```
  The results are the same. Differences are below the threshold: 10^{-5}!

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ICoCo: without exchange

Separate the meshes of the coupled problem

- Create your ICoCo test case:

  ```
  $ cd ICoCo_exercises
  $ trust -copy docond_VEF_3D
  $ mv docond_VEF_3D docond_VEF_3D_ICoCo
  $ cd docond_VEF_3D_ICoCo
  ```

- Create separate mesh and calculation datafiles from docond_VEF_3D:

  ```
  $ cp docond_VEF_3D.data docond_VEF_3D_mesh1.data
  ```

- Edit the file docond_VEF_3D_mesh1.data, and:
  - Add a line containing "End" instruction after the partitionning block.
  - Remove all the lines below the added "End"
  - Remove the time scheme and the problems definition
  - Uncomment the partition block

  Now, docond_VEF_3D_mesh1.data datafile defines geometry, mesh and paritionning for both domains (solide and fluid).

ICoCo: without exchange

Separate the meshes of the coupled problem

- Create a datafile for each domain:
  `$ cp docond_VEF_3D_mesh1.data docond_VEF_3D_mesh2.data`
- In the file docond_VEF_3D_mesh1.data, keep only the information of the solid domain.
- In the file docond_VEF_3D_mesh2.data, keep only the information of the fluid domain.
- Run these datafiles to partition domains:
  `$ trust docond_VEF_3D_mesh1`
  `$ trust docond_VEF_3D_mesh2`
  You must these four .Zones files:
  DOM1_0000.Zones DOM2_0001.Zones
  DOM1_0001.Zones DOM2_0000.Zones

ICoCo: without exchange

Run with separated meshes

- In docond_VEF_3D.data datafile:
  - delete the mesh and partitionning blocks (which are now in the mesh datafiles)
  - Uncomment the 'scatter' block
- Launch the calculation in parallel:
  `$ trust docond_VEF_3D 2`
- Compare these results with previous parallel results:
  `$ compare_lata docond_VEF_3D.lml ../docond_VEF_3D_trust/PAR_docond_VEF_3D.lml`
  The results are identical!
- Separate results in two lml files:
  - add "fichier pb1" in the "Post_processing" block of the solid's problem,
  - add "fichier pb2" in the "Post_processing" block of the fluid's problem,
- Run calculation to create these two files:
  `$ trust docond_VEF_3D 2`

ICoCo: without exchange

Separate the coupled problem into two new problems

- Create a datafile for the solid domain's problem:
  `$ cp docond_VEF_3D.data docond_VEF_3D_dom1.data`
- In docond_VEF_3D_dom1.data datafile, remove the lines:
  - Probleme_Couple pbc
  - Associate pbc pb1
  - Associate pbc pb2
  - "fichier pb1" and "fichier pb2"
- Change the following lines:
  - Associate pbc sch → Associate pb sch
  - Discretize pbc dis → Discretize pb dis
  - Solve pbc → Solve pb
- Create a datafile for the fluid domain's problem:
  `$ cp docond_VEF_3D_dom1.data docond_VEF_3D_dom2.data`
- In docond_VEF_3D_dom1.data, keep only the information about the solid domain (pb1, dom_solide) and subtitute pb1 → pb in the whole datafile

Separate the coupled problem into two new problems

Separate datafiles

- In docond_VEF_3D_dom2.data, keep only the information about the fluid domain (pb2, dom_fluide) and subtitute pb2 → pb in the whole datafile.
- Note that the coupling between solid and fluid problems is concretized by heat exchange between both domains. This coupling concerns the "Paroi_echange1" boundary of solid domain and "Paroi_echange2" boundary for of fluid domain.
- Modify docond_VEF_3D_dom1.data datafile to have:
  Paroi_echange1 paroi_contact pb Paroi_echange2
  →
  Paroi_echange1 paroi_temperature_imposee Champ_Front_Uniforme 1 50.
- Modify docond_VEF_3D_dom2.data datafile to have:
  Paroi_echange2 paroi_contact pb Paroi_echange1
  →
  Paroi_echange2 paroi_temperature_imposee Champ_Front_Uniforme 1 50.

Separate the coupled problem into two new problems

Running separately datafiles using trust

- Run docond_VEF_3D_dom1.data and docond_VEF_3D_dom2.data in parallel:
  `$ trust docond_VEF_3D_dom1 2`
  `$ trust docond_VEF_3D_dom2 2`
  The two problems must run.
- Notice that there is no coupling at all for the moment.

Adjusting datafiles for ICoCo

- To create the ICoCo problem, just after 'dimension 3', add in docond_VEF_3D_dom1.data and docond_VEF_3D_dom2.data:
  `Nom ICoCoProblemName Lire ICoCoProblemName pb`
- Remove 'Solve pb' because the solving step will be made by ICoCo.

Run with ICoCo

Creation of the main.cpp file

- We have to create a new executable which will use our datafiles.
- Copy the following main.cpp file in your repository:
  ```
  $ file="main_docond_VEF_3D_ICoCo.cpp"
  $ cp $TRUST_ROOT/doc/TRUST/exercices/ICoCo/$file main.cpp
  ```
- Open this file and look where:
  - the processors are added: search for "dom_ids"
  - the names of the datafiles: search for "data_file"
  - the loop to iterate on time steps: search for "while"

Run with ICoCo

Compiling and launching

- Create a makefile to compile your main.cpp file:
  `$ sh $project_directory/share/bin/create_Makefile 4`
- Compile the main.cpp file:
  `$ make`
- Launch calculation:
  `$ mpirun -np 4 ./couplage`
- Compare the results to the results of the coupled problem:
  `$ compare_lata pb1.lml docond_VEF_3D_dom1.lml`
  `$ compare_lata pb2.lml docond_VEF_3D_dom2.lml`
- As expected, there are differences between the results because there is no coupling here, we impose the temperature in the datafiles!

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Run with ICoCo

Adjusting datafiles

- Now, we want to send the temperature from the "Paroi_echange2" boundary of the fluid domain to the Paroi_echange1 boundary of the solid domain.
- Create a new directory:

```
$ cd ICoCo_exercises
$ cp -r docond_VEF_3D_ICoCo docond_VEF_3D_ICoCo_coupling1
$ cd docond_VEF_3D_ICoCo_coupling1
```

- In the docond_VEF_3D_dom2.data datafile, add in the "Definition_champs" block of the post-processings:

```
TEMPERATURE_OUT_DOM2 Interpolation {
  localisation elem
  domaine dom_fluide_boundaries_Paroi_echange2
  source refChamp { Pb_Champ pb temperature }
}
```

  where "dom_fluide_boundaries_Paroi_echange2" is a predefined name for the boundary Paroi_echange2 of the fluid's domain.

Run with ICoCo

Adjusting datafile

- In the docond_VEF_3D_dom1.data datafile, change the boundary condition on the 'Paroi_echange1' boundary to:
  Paroi_echange1 paroi_temperature_imposee ch_front_input {
  nb_comp 1 nom TEMPERATURE_IN_DOM1 probleme pb }
- Copy the main.cpp file for this exchange:
  `$ file="main_docond_VEF_3D_ICoCo_coupling1.cpp"`
  `$ cp $TRUST_ROOT/doc/TRUST/exercices/ICoCo/$file main.cpp`
- Compare this main.cpp file with the previous one (use tkdiff, meld or diff):
  `$ tkdiff main.cpp ../docond_VEF_3D_ICoCo/main.cpp`
- You can find where the added fields in datafiles TEMPERATURE_IN_DOM1 and TEMPERATURE_OUT_DOM2 are used in a new part for exchanges.
- Notice that we use two new objects: one TrioDEC object and one TrioField object.
- Some comments are written to help you.

Run with ICoCo

Adjusting datafile

- Compile the main.cpp file:
  `$ make`
- Launch calculation:
  `$ mpirun -np 4 ./couplage`
- Compare results with those without coupling:
  `$ compare_lata docond_VEF_3D_dom1.lml ../docond_VEF_3D_ICoCo/docond_VEF_3D_dom1.lml`
  `$ compare_lata docond_VEF_3D_dom2.lml ../docond_VEF_3D_ICoCo/docond_VEF_3D_dom2.lml`
  - The results on the domain dom2 are the same as this calculation made only one more postprocessing (TEMPERATURE_OUT_DOM2).
  - But, we can see that the coupling works well because the results on the domain dom1 changes.

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Run with ICoCo

Adjusting datafile

- Two way coupling for thermal problems should use Dirichlet and Neumann's boundary conditions (using only Dirichlet boundary conditions for coupling both sides would not work).
- So we want to send the heat flux from the Paroi_echange1 boundary of the solid domain's problem to the Paroi_echange2 boundary of the fluid domain's problem.
- Create a new directory for this part:

```
$ cd ICoCo_exercises
$ cp -r docond_VEF_3D_ICoCo_coupling1
docond_VEF_3D_ICoCo_coupling2
$ cd docond_VEF_3D_ICoCo_coupling2
```

- Inspire you from the previous part to make a Neumann boundary condition (heat flux imposed).

Run with ICoCo

Adjusting datafile

- In the docond_VEF_3D_dom1.data datafile, add a "Definition_champs" block in the post-processings:

```
FLUX_SURFACIQUE_OUT_DOM1 Interpolation {
  localisation elem
  domaine dom_fluide_boundaries_Paroi_echange1
  source Morceau_equation {
   type operateur numero 0 option flux_surfacique_bords
   source refChamp { Pb_Champ pb temperature }
  }
}
```

  where "dom_solide_boundaries_Paroi_echange1" is a predefined name for the boundary Paroi_echange1 of the solid domain.
- In the docond_VEF_3D_dom2.data datafile, switch the boundary condition on the 'Paroi_echange2' boundary to:
  Paroi_echange2 paroi_flux_impose ch_front_input {
  nb_comp 1 nom FLUX_SURFACIQUE_IN_DOM2 probleme pb }

Run with ICoCo

Adjusting datafile

- Modify the main.cpp file to add a new exchange:
  - Create a new TrioDEC object to do information exchange from domain dom2 to domain dom1:
    TrioDEC dec_flux(dom2_ids, dom1_ids);
  - Create a new TrioField object:
    TrioField field_flux;
  - Add code lines into the while loop to do information exchange.
- You can have a look at the main_docond_VEF_3D_ICoCo_coupling2.cpp file for this exchange:

```
$ file="main_docond_VEF_3D_ICoCo_coupling2.cpp"
$ cp $TRUST_ROOT/doc/TRUST/exercices/ICoCo/$file .
```

- Compare it to the previous one using tkdiff (you can use meld, tkdiff or diff depending on which software is installed on your computer):

```
$ tkdiff main_docond_VEF_3D_ICoCo_coupling2.cpp
../docond_VEF_3D_ICoCo_coupling1/main.cpp
```

Run with ICoCo

Adjusting datafile

- You can find the usage and synchronization of the new fields FLUX_SURFACIQUE_IN_DOM2 and FLUX_SURFACIQUE_OUT_DOM1.
- Compile your main.cpp file:
  `$ make`
- Launch calculation:
  `$ mpirun -np 4 ./couplage`
- Compare results with the first ones:
  `$ compare_lata docond_VEF_3D_dom1.lml ../docond_VEF_3D_ICoCo/pb1.lml`
  `$ compare_lata docond_VEF_3D_dom2.lml ../docond_VEF_3D_ICoCo/docond_VEF_3D_dom2.lml`

Run with ICoCo

Adjusting datafile

- As you can see, the results are not the same because ICoCo coupling is different from coupled problem in TRUST. If this problem reaches convergence, results would be the same at least at the final time.
- For further learning, you can read the pdf report of "CouplageFluideSolide" validation form.
  You can visualize this report by:
  ```
  $ cd $project_directory/share/Validation
  $ cd Rapports_automatiques/CouplageFluideSolide
  $ Run_fiche -xpdf
  ```