TRUST/TrioCFD 1.7.2
user's training session

TRUST/TrioCFD 1.7.2 user's training session

- Presentations
  - TRUST/TrioCFD   (1st day)
  - Automated test case with TRUST   (2nd day AM)
  - Mesh with tools (Xprepro, Salomé or Gmsh) (2nd day PM)

- Practice:
  - TRUST/TrioCFD   (1st day PM/2nd day AM)
  - Automated test case with TRUST   (2nd day AM)
  - Xprepro/Salomé/Gmsh   (2nd day PM)

- We provide also:
  - Advanced TRUST/TrioCFD user sessions   (optional, 3rd day)
  - TRUST/TrioCFD developer sessions   (optional, 4th and 5th days)

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La force de l'innovation

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- Examples of data files

TRUST/TrioCFD historic (1/4)

- Trio_U code: CFD code for incompressible monophasic / diphasic flow
- Developed at the CEA/DEN/DANS/DM2S/STMF service
  - LMSF lab's chief: anne.burbeau@cea.fr
  - TRUST project leader : gauthier.fauchet@cea.fr
  - TrioCFD project leader: mathieu.peybernes@cea.fr
- Trio_U, a software brick used by other CEA applications:
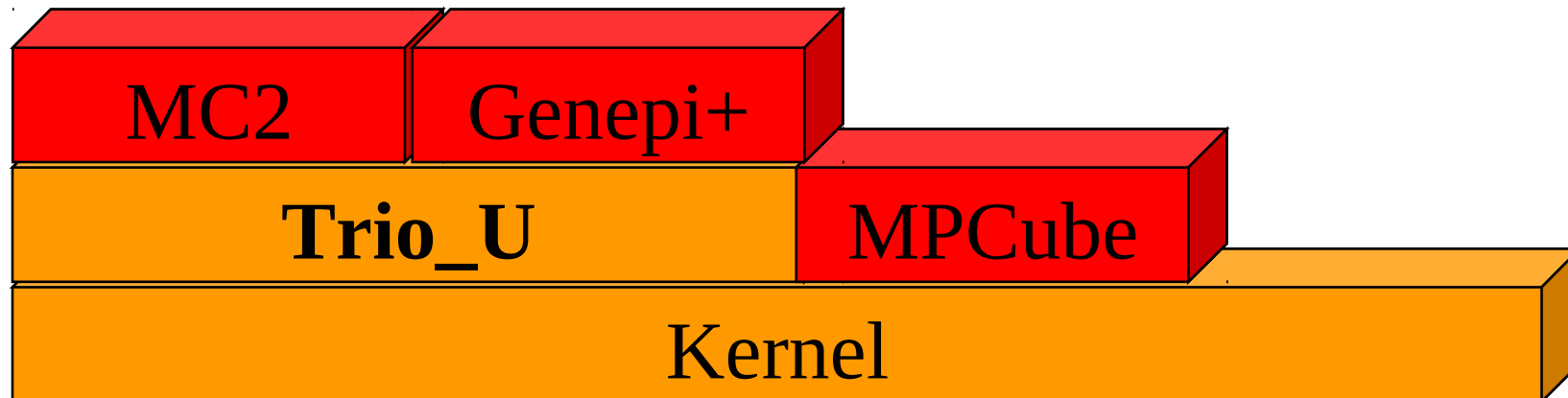
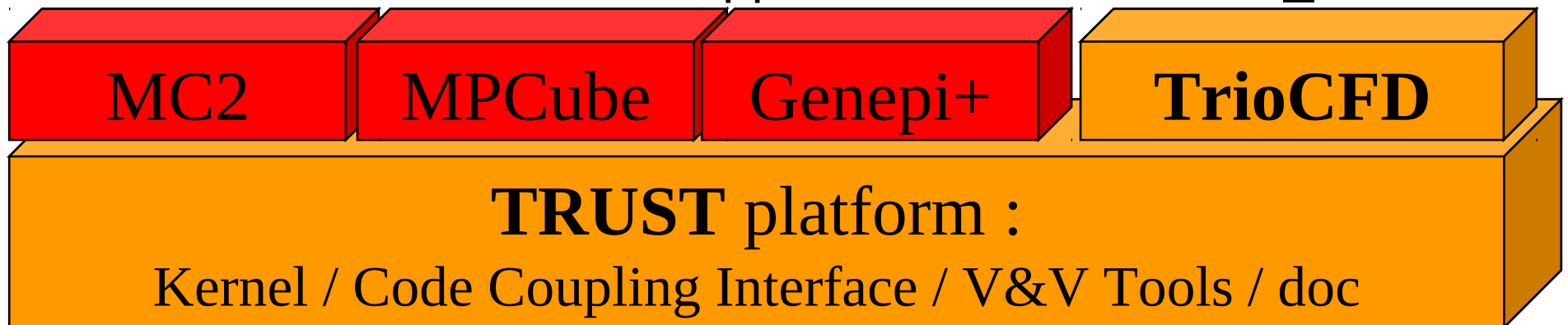# TRUST/TrioCFD historic (2/4)

- 1994: start of the project Trio_U
- 01/1997 : v1.0 (VDF only)
- 06/1998 : v1.1 (VEF version)
- 04/2000 : v1.2 (parallel version)
- 07/2001 : v1.3 (compressible version)
- 11/2002 : v1.4 (new LES turbulence models)
- 02/2006 : v1.5 (VDF/VEF Front Tracking)
- 10/2009 : v1.6 (data structure revamped)
- 06/2015 : v1.7 (cut into TRUST and TrioCFD
  + switch to open source)

TRUST/TrioCFD historic (3/4)

Recently, Trio_U was divided in two parts:

- a **BALTIK** project named **TrioCFD** based on new platform named **TRUST,**

  Trio_U = TRUST + TrioCFD (FT, Radiation, LES, zoom)

- where :

  – **TRUST**: "**TR**io_**U S**oftware for **T**hermohydraulics",

  – **BALTIK**: "**B**uild an **A**pplication **L**inked to **T**rio_U **K**ernel".

MC2	MPCube	Genepi+	**TrioCFD**

TRUST platform :
Kernel / Code Coupling Interface / V&V Tools / doc

- The kernel contains the equations, space discretizations, numerical schemes, parallelism...

TRUST/TrioCFD historic (4/4)

- Main CEA goals:

  - R&D platform for fluid mechanics

  - To advocate LES turbulence models or RANS-LES coupling for nuclear safety studies

  - Codes coupling (fluid, structure, neutronic…)

  - Alternative to commercial CFD software

  - To base on advanced technology (C++, COO, //…)

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Modeling flow with TRUST/TrioCFD (1/7)

- Incompressible single phase flow
  - Laminar or Turbulent flow

  - Navier Stokes with or without energy equation

  - Incompressible fluid or with low variation for volumic mass
    - Boussinesq hypothesis:

      $\rho = \rho(T) \sim \rho_0 - \beta(T-T0)$

    - Quasi-compressible model:

      $\rho = \rho(P,T)$ for low mach numbers

$$Div\left(\vec{u}\right) = 0$$

$$\frac{\partial \vec{u}}{\partial t} + \vec{u}\nabla\vec{u} = -\nabla P^* + Div\left(v\nabla\vec{u}\right)$$

$$P^* = \frac{P}{\rho} + gz$$

$$\frac{\partial T}{\partial t} + \vec{u}\nabla T = Div\left(\alpha\nabla T\right)$$

Modeling flow with TRUST/TrioCFD (2/7)

Description of the Quasi Compressible model used

- Accounts for space and time variations of density due to high changes of temperature:

$$Ideal\,gas\,law : \rho(\vec{x},t) = \frac{P_0(t)}{RT(\vec{x},t)}$$

- Filters acoustic waves in order to avoid too small time-step:

$$Total\,pressure : P(\vec{x},t) = P_0(t) + P_1(\vec{x},t)$$

Thermodynamic pressure : $P_0(t)$

Hydrodynamic pressure : $P_1(x,t)$

$$with\ P_1 \approx M^2 P_0\ and\ M = Mach \ll 1$$

- Set of equations solved:

$$\frac{\partial \rho}{\partial t} + div(\rho \vec{u}) = 0$$

$$\frac{\partial}{\partial t}(\rho u_i) + div(\rho u u_i) - \sum_{j=1}^{N} \frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right] + \frac{\partial P_1^*}{\partial x_i} = -\rho g_i$$

$$P_1^* = P_1 + \frac{2}{3}\mu\,div(\vec{u})$$

$$P_0 = \rho RT$$

$$\rho C_p \frac{dT}{dt} - \sum_{j=1}^{N} \frac{\partial}{\partial x_j}\left(K\frac{\partial T}{\partial x_j}\right) = Q + \frac{dP_0}{dt}$$

Modeling flow with TRUST/TrioCFD (3/7)

- Heat exchange
    - Conduction
    - Radiation in transparent medium
    - Radiation in semi-transparent medium

- Transport of passive scalars $\quad \dfrac{\partial C_i}{\partial t} + \vec{u}\, \nabla C_i = Div\left(D_i\, \nabla C_i \right)$

- Porous Media
    - Surface or volume porosities
   - Singular or regular pressure loss

Modeling flow with TRUST/TrioCFD (4/7)

- Particles transport model:

  - One way coupling
    - Particle motion affected by the flow

  - Two way coupling
    - As above but particle disturbances also affect the flow

  - Possible to convert droplet/bubble below a given size into particles during a Front Tracking calculation

Modeling flow with TRUST/TrioCFD (5/7)

Two phases flow (Front tracking model)

- Eulerian mesh where Navier Stokes equations are solved

- Lagrangian moving mesh for the interface locations

- Coalescence or breakup models for bubbles and drops
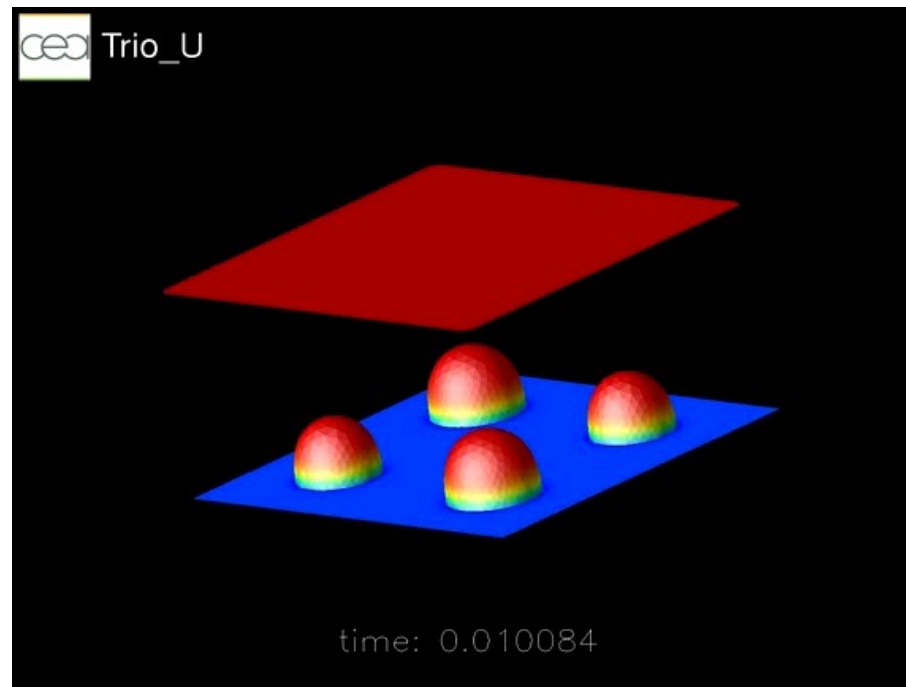
Boiling bubbles

Modeling flow with TRUST/TrioCFD (6/7)

Front tracking model

- Can be declined in TrioCFD to use an Immersed Boundary Method using IBC (Immersed Boundary Conditions)
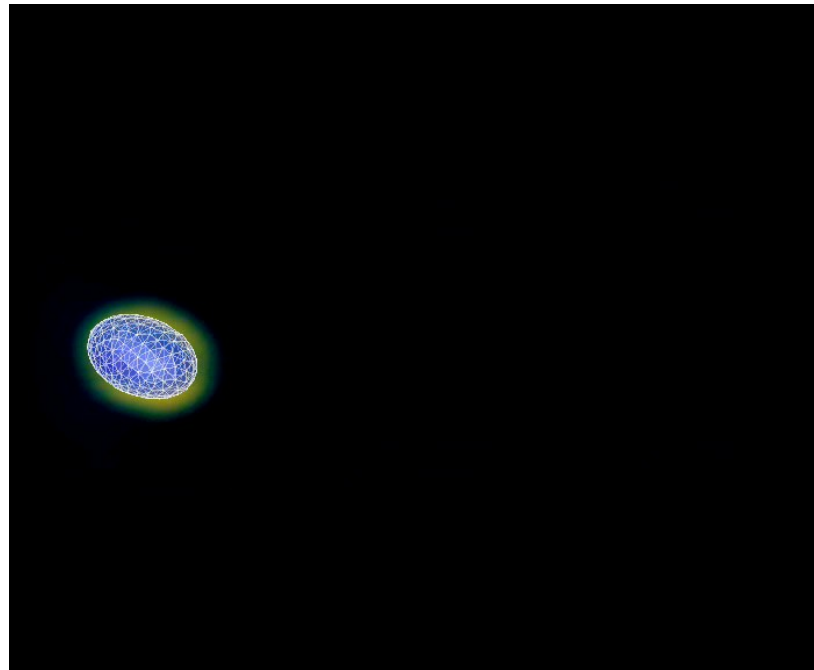
Example of a flow around a rotating body defined by an IBC

Modeling flow with TRUST/TrioCFD (7/7)

- **2D calculation**
  - Plane, Cartesian coordinates (x,y)
  - Axi-symmetric, coordinates (r,z) (VDF only)

- **3D calculation**
  - Cartesian coordinates (x,y,z)
  - Cylindrical coordinates (r,θ,z) (VDF only)

- **Transient flow calculation calculated by:**
  - Explicit, semi-implicit or implicit time schemes

- **Steady state calculation obtained:**
  - By convergence of the transient flow

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Examples of performed calculations (1/2)

- Academic calculations
  - Plane channel with conduction coupling at the wall
  - Flow around obstacle
  - Pipe flow
  - Impinging jet
  - Isotropic turbulence

Examples of performed calculations (2/2)

- **Industrial calculations**
  - Various studies about the core of a reactor
  - Thermal stress in a T-shaped mixing pipe
  - Natural convection in a storage room of waste
  - Atmospheric dispersion (polluting or radio-nucleid)
  - Compressor blades in GFR (Gas Fast Reactor)
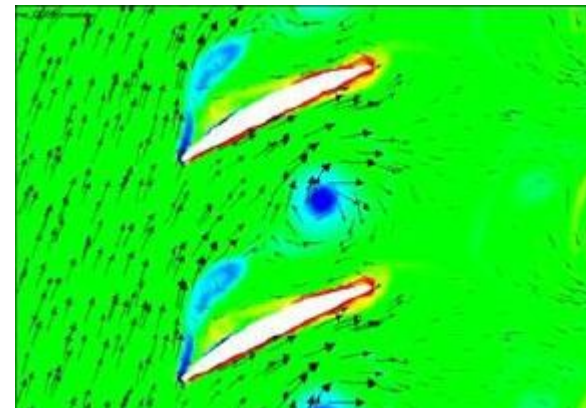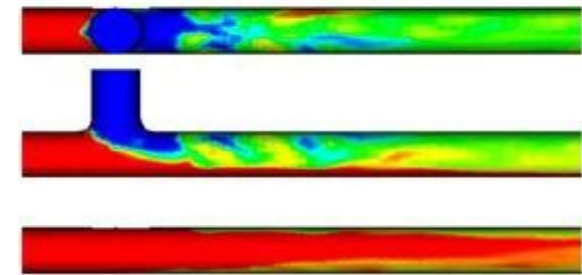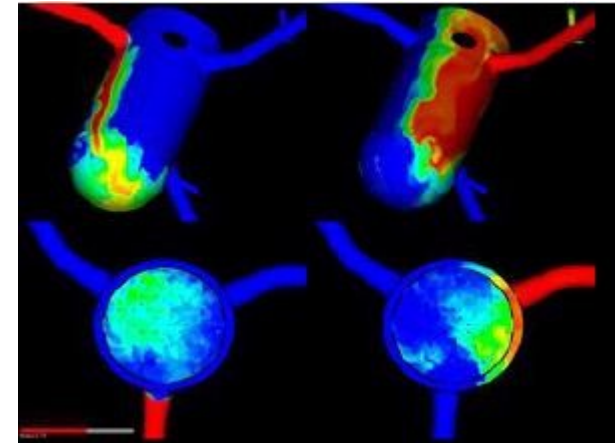
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La force de l'innovation

Models, schemes, numerical methods (1/6)

Discretizations (1/5)

- **F**inite **D**ifferences **V**olumes (**VDF**)
  - Structured meshing ; velocity and pressure are shifted
  - Scalar unknown is mesh centred
  - Velocity is normal at the face

$$\vec{V} . \vec{n}$$

$$P \\ T \\ k \\ \varepsilon \; ...$$
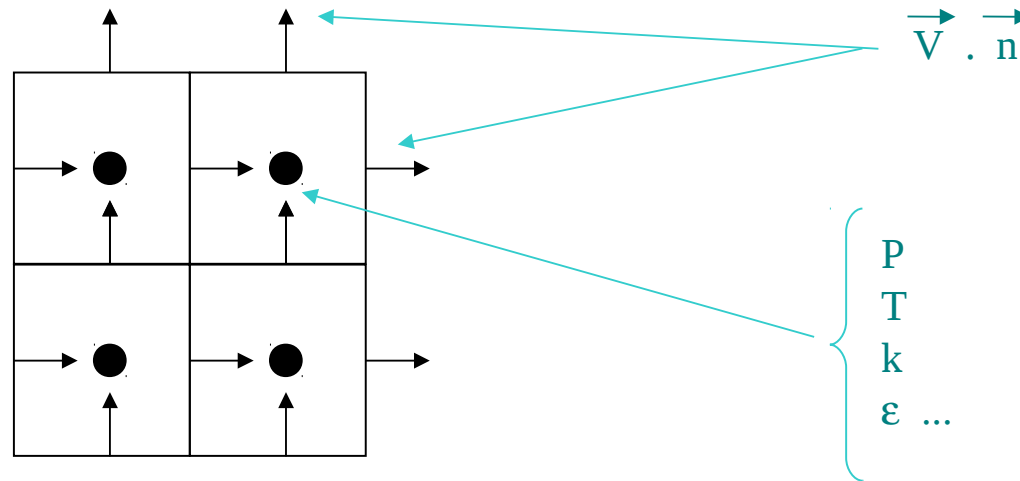
Discretizations (2/5)

- **F**inite **E**lements **V**olumes (**VEF**)
  - Unstructured meshing triangles (2D) or tetrahedrons (3D)
  - Unknown fields are face centered (P1NC)
  - Physical characteristics are cell centered
  - Pressure :
    - Mesh centered and at the vertex (P0+P1)

$$\vec{V_x}$$
$$\vec{V_y}$$
$$V_z$$
$$T$$
$$k$$
$$\varepsilon...$$
$$P$$
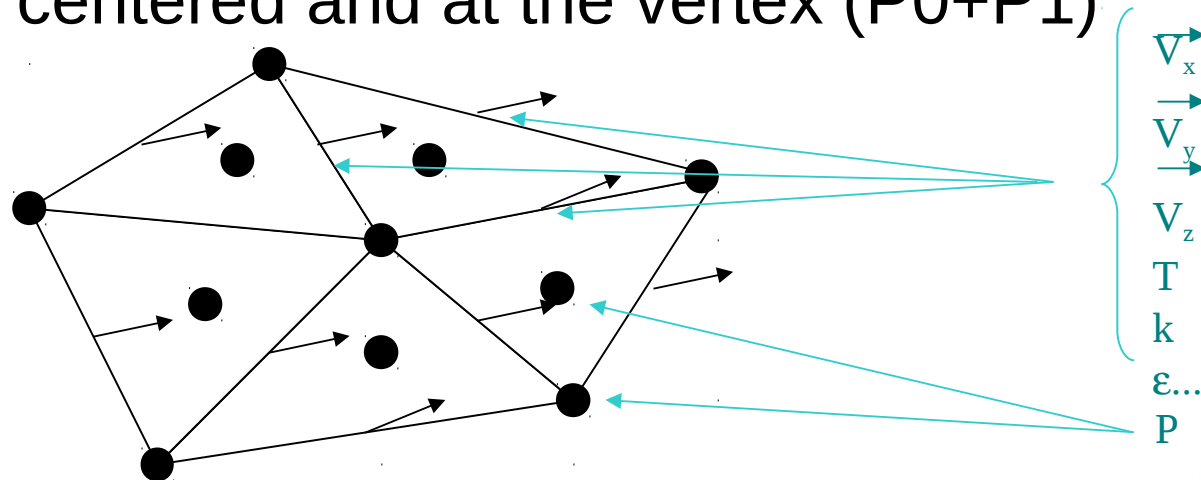
Discretizations (3/5)

- **F**inite **E**lements **V**olumes (**VEF**)

  - By default, P0+P1 for pressure but less/more pressure nodes is possible:
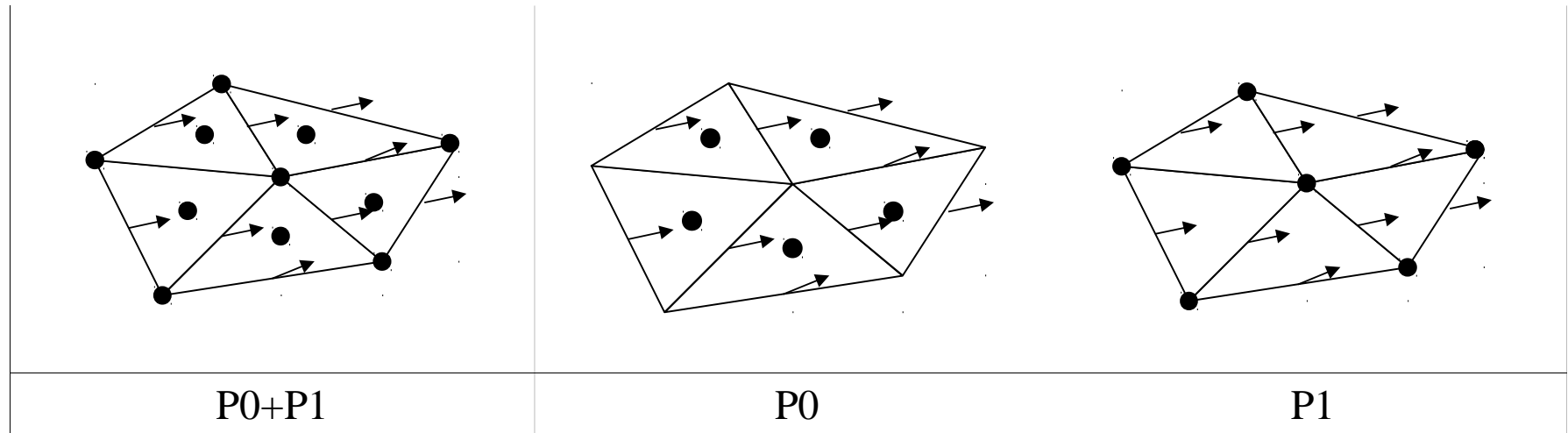
P0+P1	P0	P1

Plus in 3D: P0+P1+Pa
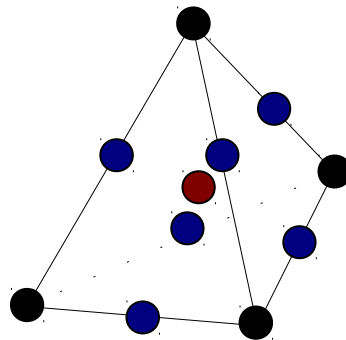
11 pressure nodes per tetra:

-1 in center (P0)

-4 on vertexes (P1)

-6 on edges (Pa)

-> **Useful** for flow with a strong source term & a low velocity field where P0+P1 pressure gradient P0+P1 has trouble to match the source term

La force de l'innovation

Discretizations (4/5)

- ## Kind of mesh permitted
  - ### Quadrangular or triangular meshing for 2D cases
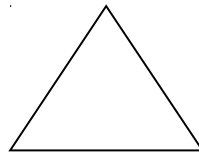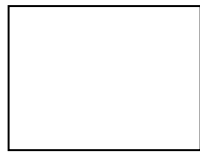
  - ### Hexahedral or tetrahedral meshing for 3D cases
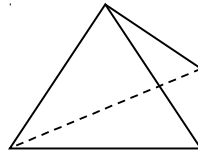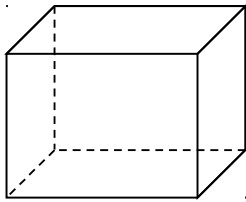
  - ### Non standard or hybrid meshing not supported
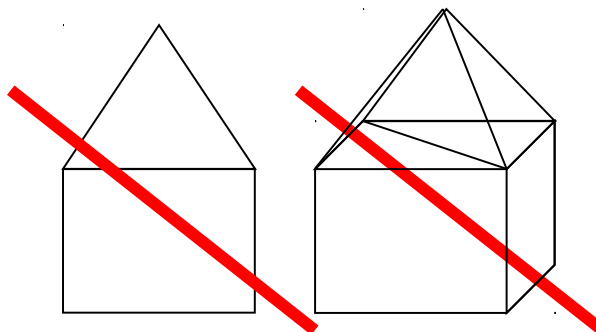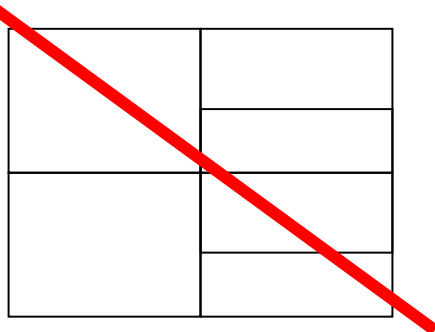
Discretizations (5/5)

- **Kind of mesh permitted**
  - Internal boundaries partially supported
    - with ICEM, spit faces in two and define boundaries
    - TRUST will differentiate the two faces
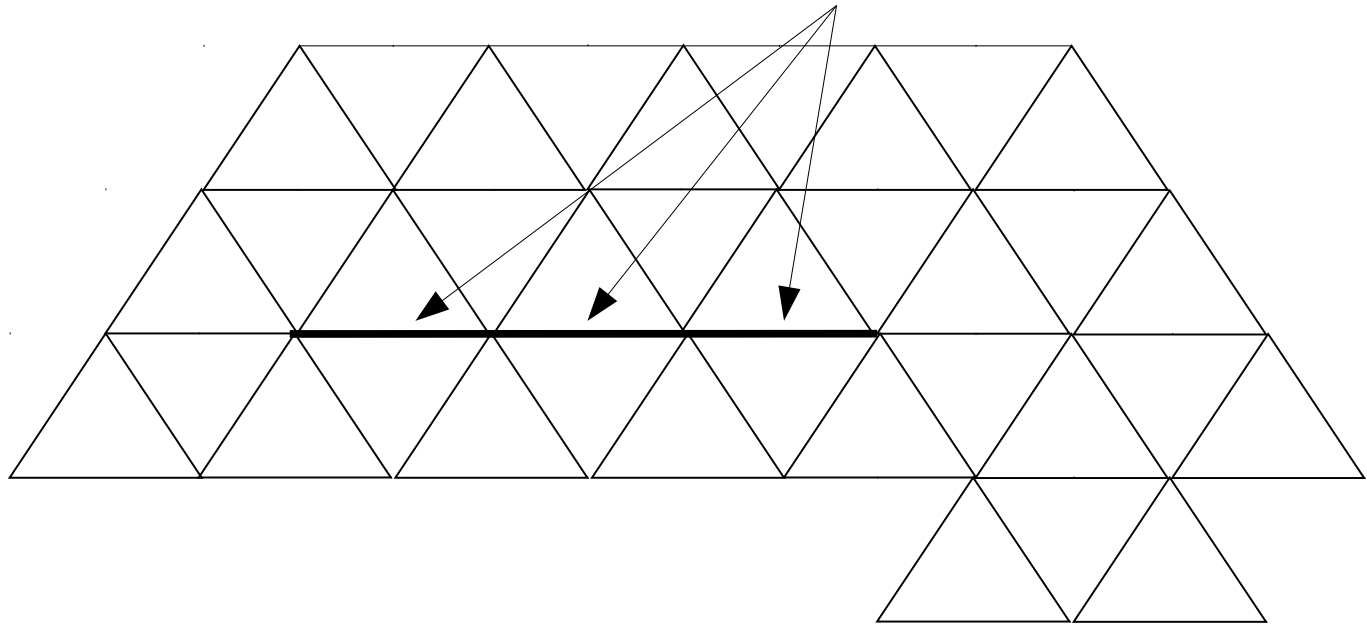
Models, schemes, numerical methods (2/6)

- Discretizations (VDF/VEF)
- **Time and space schemes**
- Boundaries conditions
- Source terms
- Solvers for linear systems
- Turbulence models

Time and space schemes (1/2)

- Explicit time schemes:

$$\frac{\partial I}{\partial t}^{n+1} + \vec{u}^n \nabla I^n = Div\left(\alpha \nabla I^n\right)$$

  - Euler explicit (order 1)
  - Runge Kutta (order 2 or 3)

- Semi-implicit time scheme:

$$\frac{\partial I}{\partial t}^{n+1} + \vec{u}^n \nabla I^n = Div\left(\alpha \nabla I^{n+1}\right)$$

  - Euler semi-implicit (diffusion implicited)

- Implicit time schemes (not unconditionally stable):

$$\frac{\partial I}{\partial t}^{n+1} + \vec{u}^{n+1} \nabla I^{n+1} = Div\left(\alpha \nabla I^{n+1}\right)$$

  - Implicite, Piso, Simple (dynamic time step)

Time and space schemes (2/2)

- convection schemes with VDF discretization
  - Quick (order 2-3)
  - Centre (order 2 or 4) « centered »
  - Amont (order 1) « upwind »

- convection schemes with VEF discretization
  - EF_stab (order 2) « centered stabilized »
  - Muscl (order 2) « quick like »
  - Amont (order 1) « upwind »

Models, schemes, numerical methods (3/6)

- Discretizations (VDF/VEF)
- Time and space schemes
- **Boundaries conditions**
- Source terms
- Solvers for linear systems
- Turbulence models

Boundaries conditions (1/3)

Available BC for momentum equation

- Wall:
  - No slip (u=0)
  - Slipping at the wall (u.n=0)
  - Imposed tangential velocity

- Fluid boundary:
  - Imposed velocity
  - Imposed pressure or pressure gradient
  - Free outlet (Orlanski)
  - Periodic

Boundaries conditions (2/3)

Available BC for energy equation

- Wall:
    - Imposed temperature
    - Adiabatic or imposed flux
    - Imposed exchange (coefficient)
    - Contact resistance possible between two walls

- Fluid boundary:
    - Imposed temperature
    - No flux
    - Periodic

Boundaries conditions (3/3)

- Boundary condition values may be:
  - Uniform on the boundary
  - Space dependent
  - Time dependent
  - Read in a file

Models, schemes, numerical methods (4/6)

- Discretizations (VDF/VEF)
- Time and space schemes
- Boundaries conditions
- **Source terms**
- Solvers for linear systems
- Turbulence models

Source terms (1/3)

- ## Navier Stokes equation:
  - ### Boussinesq $\qquad\qquad S=\boldsymbol{\rho}_0 g\boldsymbol{\beta}(T-T_0)$
    - Useful for small variation of volumic mass

  - ### Flow rate $\qquad\qquad\qquad S=Q_m$

  - ### Pressure loss $\qquad\qquad S=-0.5\boldsymbol{\rho}C_f U|U|/D$
    - Regular pressure loss (Blasius or Cf given by the user)

  - ### Periodic channel $\qquad\qquad S=Q_m$
    - Useful to keep constant flow rate into a periodic channel

  - ### …

Source terms (2/3)

- ## Navier Stokes equation:

  Calculation into a non Galilean referential R'. Coriolis and inertial forces, the user specifies:

  - Acceleration and velocity of R' referential into the Galilean referential R

  - Ω, dΩ/dt : rotation and its derivative term into the R' referential

  - A centre of the rotation of R' into R with the coordinates given into the R' referential

$$\vec{F}_{ie} = -m\,\vec{a}_e = -m\,(\vec{a}(A)_{(R)} + \left(\frac{d\vec{\Omega}_{(R'/R)}}{dt}\right)_{(R)} \wedge \vec{AM} + \vec{\Omega}_{(R'/R)} \wedge (\vec{\Omega}_{(R'/R)} \wedge \vec{AM}))$$

$$\vec{F}_{ic} = -m\,\vec{a}_c = -m\,2\vec{\Omega}_{(R'/R)} \wedge \vec{v}_r$$

Source terms (3/3)

- ## Energy equation:
  - ### Volumic heat power $\qquad$ S=P
    - For example into a solid media

  - ### ....

- ## Concentration equation:
  - ### Boussinesq $\qquad$ $S=\rho_0 g\beta(C-C_0)$
    - Useful to build a two miscible fluids calculation (if the volume mass is similar). Concentration C will be equal to the fraction fluid

- Discretizations (VDF/VEF)
- Time and space schemes
- Boundaries conditions
- Source terms
- **Solvers for linear systems**
- Turbulence models

Solvers for linear systems (1/3)

Linear systems	Sparse	Symmetric	Constant
Pressure linear system for incompressible flow	✖	✖	✖
Pressure linear system for quasi compressible flow	✖	✖	✖
Pressure linear system for diphasic flow	✖	✖	
Use of an implicit scheme	✖		
Radiation in transparent medium			✖
Radiation in semi transparent medium	✖	✖	✖

Solvers for linear systems (2/3)

- TRUST solvers (default choice):
  - Symmetric matrix (e.g. pressure solver)
    - GCP (Conjugate gradient with SSOR preconditioning)
  - Non symmetric matrix (e.g. implicit solver)
    - GMRES or Bi-CGSTAB with diagonal preconditioning

- Integrated PETSc solvers (advanced choice):
  - Symmetric matrix
    - Parallelized Cholesky:
      - If enough memory available AND matrix is constant, generally the best choice under 500 cores (max 1000 cores on 10e6 cells, ~2s/timestep to solve Ax=B)
    - BI-CGSTAB with block jacobi ICC(1):
      - The fastest if high scalability needed (>1000 cores), use GCP with block jacobi ICC(1) if BI-CGSTAB diverges. RCM ordering of the local matrix may accelerate also.
  - Non symmetric matrix
    - GMRES or BI-CGSTAB with diagonal preconditioning:
      - Generally faster than previous TRUST versions

Solvers for linear systems (3/3)

- **Iterative solvers (GC, GMRES,…)**
  - Need a tolerance ε to be defined : $||Ax\text{-}B||<\varepsilon$
  - Possible pitfall because it is an absolute (not a relative) value in TRUST
  - So, check the balances!
    - Exemple: Solving pressure system for an incompressible flow $\Leftrightarrow$ Div(u)=0
      - So, check the flow rate error in .out file

- **Direct solvers (PETSc Cholesky)**
  - Use it if possible

Models, schemes, numerical methods (6/6)

- Discretizations (VDF/VEF)
- Time and space schemes
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- Solvers for linear systems
- **Turbulence models**

La force de l'innovation

Turbulence models (1/1)

- DNS (Direct numerical simulation)
  - No model

- RANS (Reynolds averaged Navier Stokes equations)
  - 0 equation
    - Mixing length
  - 2 equations
    - Standard k-ε

- LES (Large eddy simulation)
  - Wale http://www.cfd-online.com/Wiki/Wall-adapting_local_eddy-viscosity_(WALE)_model
  - Smagorinsky http://www.cfd-online.com/Wiki/Smagorinsky-Lilly_model

- Wall laws
  - Standard (logarithmic law)
  - TBLE (Turbulent Boundary Layer Equations)

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Data files & calculation (1/5)

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- Data file description....................p47
- Operations on meshes.................p55
- Post processing description..........p58
- Output files description.................p66

TRUST and interfaces between tools (1/1)

ICEM

I-DEAS

Salomé

Ansys

Gmsh

Xprepro

TRUST/TrioCFD code

Sources

Tests

Manuals

Salomé

Tecplot

VisIt

Gnuplot

Xmgr
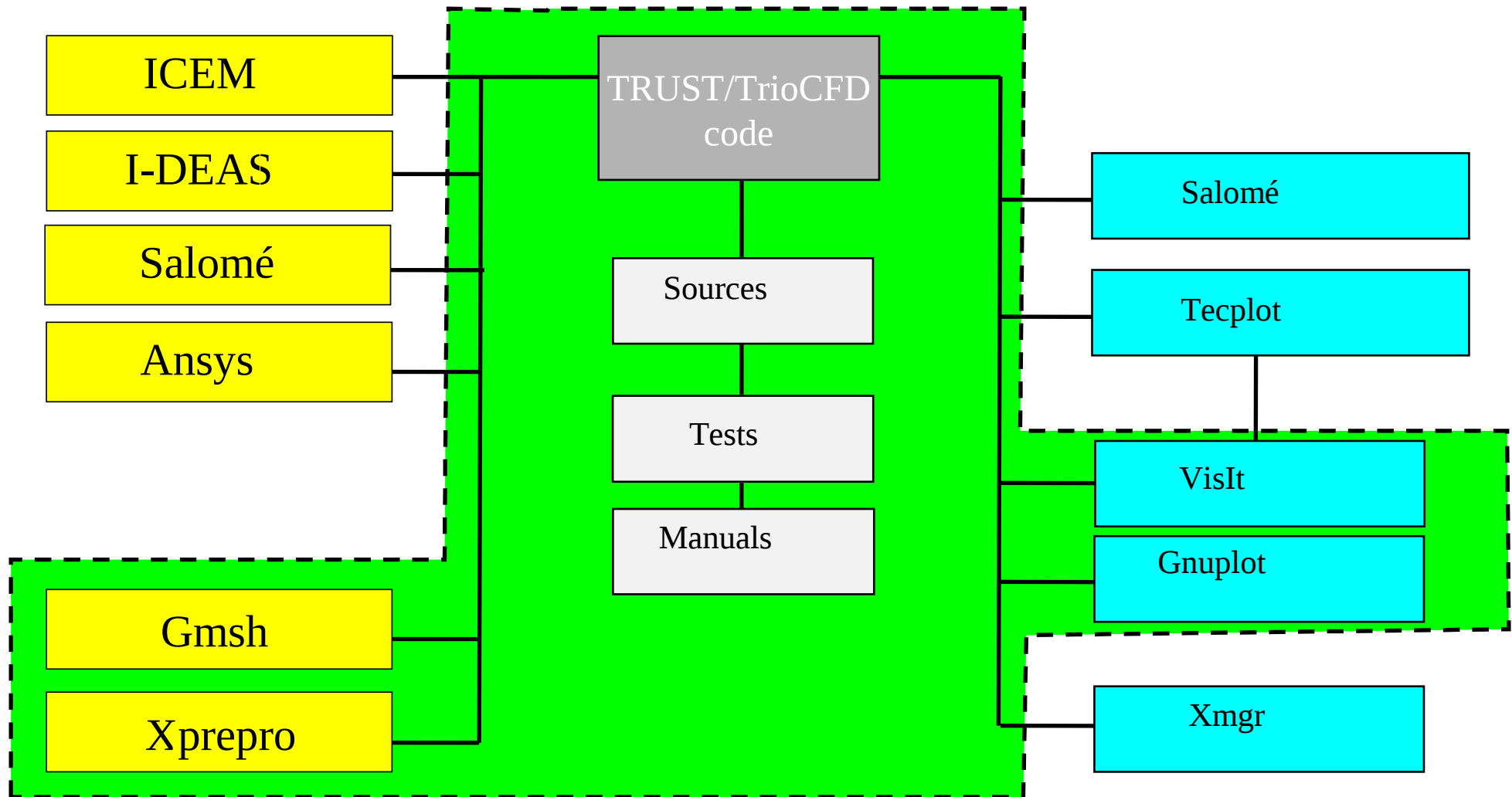
TRUST/TrioCFD package released and supported

Data files & calculation (2/5)

- TRUST and tools interfaces
- **Data file description**
- Operations on meshes
- Post processing description
- Output files description

Data file description (1/7)

- Objects creation with keywords (Domain, Time scheme, Problem, Fluid, …) :

Data file objects definition

Domaine my_domain

Pb_Thermohydraulique my_problem

Schema_Euler_Explicite my_scheme

…

Data file description (2/7)

- Action on these objects with keywords:

Read_file my_domain *meshing.geom # Read a mesh file #*

Read_file *file.geo ; # Read external instructions #*

Read my_scheme {

    tinit 0.

    dt_min 0.001

    dt_max 0.002

    dt_impr 0.001

    …. }

Associate my_problem my_scheme # Association #

Read my_problem { …. } # Read (define) the problem #

Data file description (3/7)

```
# Hydraulique 2D laminar flow with Quick scheme #
dimension 2

Pb_hydraulique pb
Domaine dom

# BEGIN MESH #
Read_file Obstacle.geo ;
# END MESH #

# BEGIN PARTITION
Partition dom
{
        Partitionneur  tranche { tranches 2 1 }
        Larg_joint 2
        Nom_Zones DOM
}
Fin
END PARTITION #

# BEGIN SCATTER
Scatter DOM.Zones dom
END SCATTER #

# A discretization is selected #
VDF ma_discretisation

Schema_Euler_explicite mon_schema
Read mon_schema
{
        tinit 0
        tmax 5.0
        nb_pas_dt_max 1000
        dt_min 5.e-3  # Trio_U stops if dt_stab<dt_min #
        dt_max 5.e-3
        dt_impr 5.e-3
        dt_sauv 1.
        facsec 0.5
        seuil_statio 1.e-8
}
# Calculation timestep dt=min(dt_stab,dt_max)*facsec #
# dt_stab=1/(1/dt(convection)+1/dt(diffusion)) #
# 1D : dt(convection)=dx/max(U) dt(diffusion)=dx^2/(2D) #
```

```
# A media is defined #
Fluide_Incompressible milieu
Read milieu
{
        mu Champ_Uniforme 1 3.7e-05    # Dynamic viscosity #
        rho Champ_Uniforme 1 2         # Volumic mass #
}
# Create links between objects #
Associate pb dom
Associate pb mon_schema
Associate pb milieu
Discretize pb ma_discretisation
Read pb
{
        Navier_Stokes_standard
        {
                convection { quick }
                diffusion { }   # By default, 2nd order scheme #
                conditions_initiales { vitesse Champ_Uniforme 2 0. 0. }
                boundary_conditions {
                        Square paroi_fixe # Wall U= 0 #
                        Upper  symetrie
                        Lower  symetrie
                        # Neumann boundary condition P=0 #
                        Outlet frontiere_ouverte_pression_imposee
                           Champ_front_Uniforme 1 0.
                        # Dirichlet boundary condition U=(1,0) #
                        Inlet  frontiere_ouverte_vitesse_imposee
                           Champ_front_Uniforme 2 1. 0.
                }
                solveur_pression GCP {
                        # Parameter of SSOR #
                        precond ssor { omega 1.5 }
                        # Convergence threshold which impacts flow mass rate #
                        # Warning: not a dimensionless number so the flow mass #
                        # rate should be checked during the first time-steps #
                        seuil 1.0e-06
                        impr # Print the residual error  ||Ax-B|| #
                }
        }
}
```

Data file description (4/7)

List of possible keywords to define a field:

- Volume fields, keyword **Champ_TYPE** where TYPE may be:
  - **uniforme** (uniform field)
  - **uniforme_par_morceaux** (uniform field per sub-zone)
  - **fonc_t** (uniform time dependent field)
  - **fonc_xyz** (space dependent field)
  - **fonc_txyz** (space and time dependent field)
  - **fonc_fonction** (depends on another field, analytic function)
  - **fonc_tabule** (depends on another field, tabulated function)
  - **fonc_MED** (read a MED field)
  - **don_lu** (field read in a file)

- Surface fields, keyword **Champ_front_TYPE** where TYPE:
  - As volume fields plus:
  - **lu** (field read in a file)
  - **recyclage** (field extracted from a plane or a boundary of another problem)
  - …

Data file description (5/7)

Formulas for a field in a data file:

Champ_front_fonc_txyz 2 **cos**(y+x^2) t+**ln**(y)
Champ_fonc_xyz domain_name 2 **tanh**(4*y)*(0.95+0.1***rnd**(1)) 0.

The variables which can be used are:

      x,y,z   : coordinates
      t   : time

Constant or mathematical functions available:

      PI, ABS, COS, SIN, TAN, ATAN, EXP, LN, SQRT, INT, ERF, RND(x), COSH, SINH, TANH
      NOT(x), _AND_, _OR_, _GT_, _GE_, _LT_, _LE_

You can also use the following operations:

      +   : addition
      -      : substracte
      /   : division
      *   : multiplication
      %   : modulo
      $: max
      ^   : power
      <   : lesser than
      >   : greater than
      [: less or equal to
      ]   : greater of equal to
      ( )   : test if

Example of Champ_Fonc_MED

First calculation on a VDF mesh:

Postraitement { **fichier** *VDF_field* **format med Champs dt_post** 0.1 { **vitesse elem** } }

Second calculation on a different refined VEF mesh with initial condition from the VDF field:

conditions_initiales { **vitesse Champ_Fonc_MED last_time** *VDF_field.med* domain **vitesse elem** 0 }
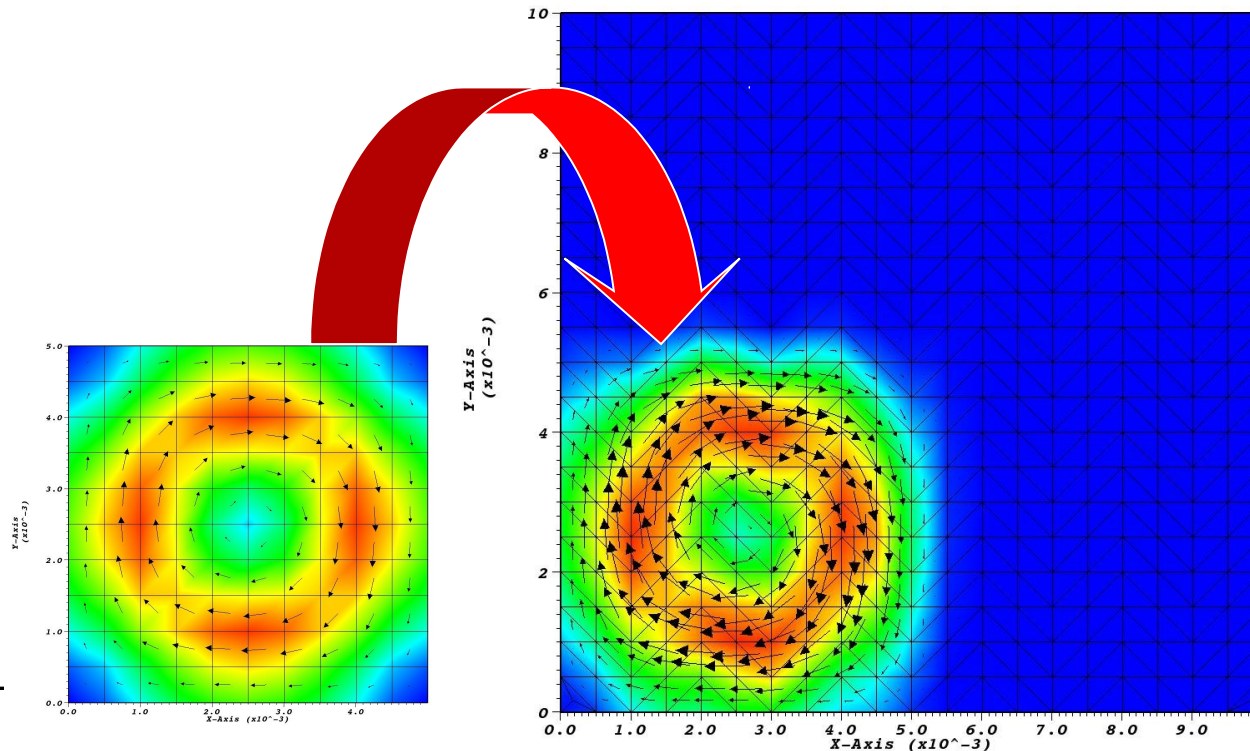
Data file description (7/7)

Example of TrioCFD coupled problems

Periodic box to provide a fully developed turbulent flow inlet for the T-shaped domain:

- Thermalhydraulic problem solved in the T-shaped domain.

- Hydraulic problem solved in the periodic box.

- Coupling problem which solves sequentially each problem.

Periodic boundary condition

Dirichlet condition with **Champ_front_recyclage** field keyword
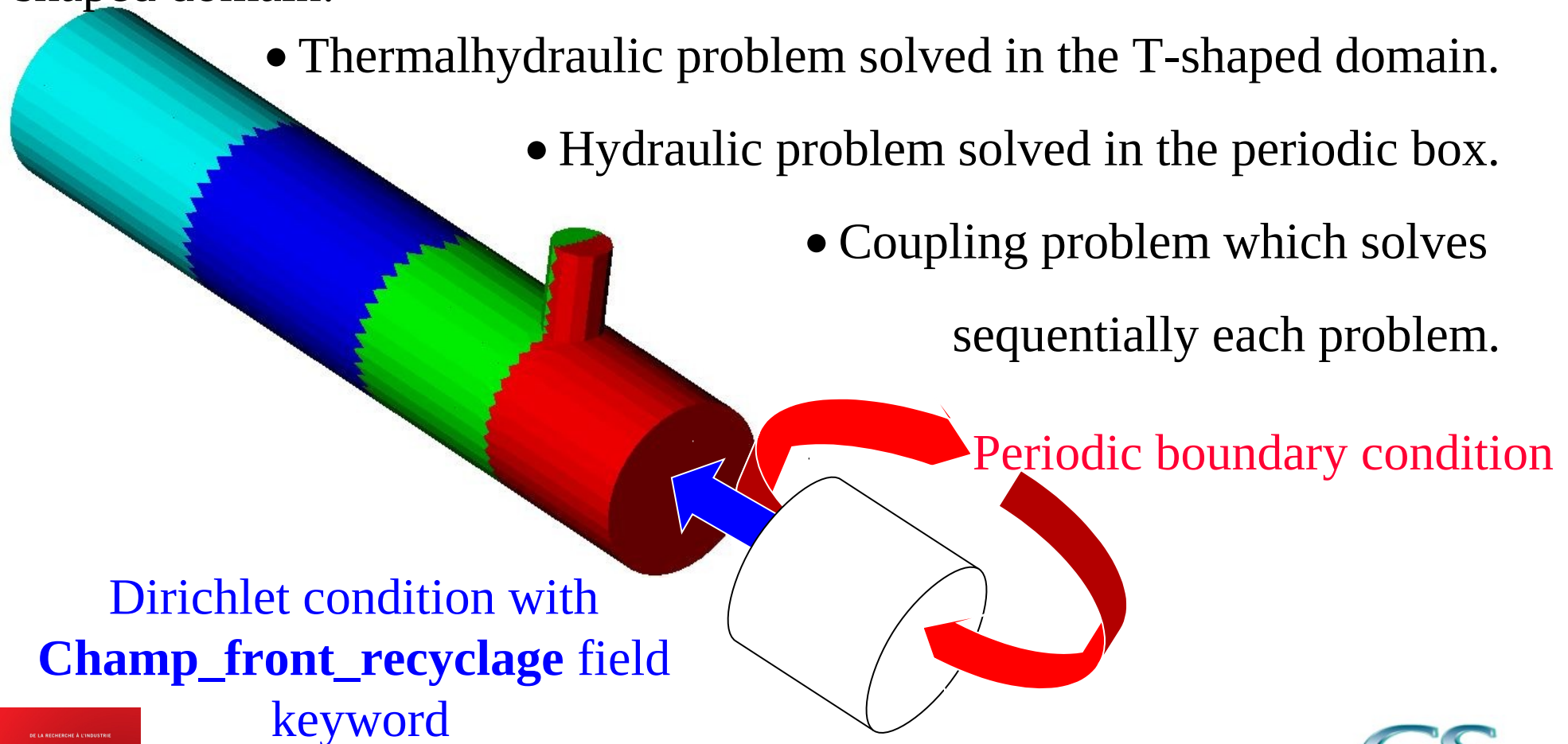
Data files & calculation (3/5)

- TRUST and tools interfaces
- Data file description
- **Operations on meshes**
- Post processing description
- Output files description

Operations on meshes (1/2)

Mesh dom {
Pave Left

```
{
Origine 0. 0.
Nombre_de_Noeuds 6 23
Longueurs 0.1 0.22
}
{
bord Inlet X = 0. 0. <= Y <= 0.22
bord Upper Y = 0.22 0. <= X <= 0.1
bord Lower Y = 0. 0. <= X <= 0.1
bord Square X = 0.1 0.1 <= Y <= 0.12
} ,
```

Pave Up

```
{
Origine 0.1 0.12
Nombre_de_Noeuds 2 11
Longueurs 0.02 0.1
}
{
bord Upper Y = 0.22 0.1 <= X <= 0.12
bord Square Y = 0.12 0.1 <= X <= 0.12
} ,
```

Pave Bottom

```
{
Origine 0.1 0.
Nombre_de_Noeuds 2 11
Longueurs 0.02 0.1
}
{
bord Lower Y = 0. 0.1 <= X <= 0.12
bord Square Y = 0.1 0.1 <= X <= 0.12
} ,
```

Pave Right

```
{
Origine 0.12 0.
Nombre_de_Noeuds 41 23
Longueurs 0.8 0.22
}
{
bord Outlet X = 0.92 0. <= Y <= 0.22
bord Lower Y = 0. 0.12 <= X <= 0.92
bord Upper Y = 0.22 0.12 <= X <= 0.92
bord Square X = 0.12 0.1 <= Y <= 0.12
}
}
```
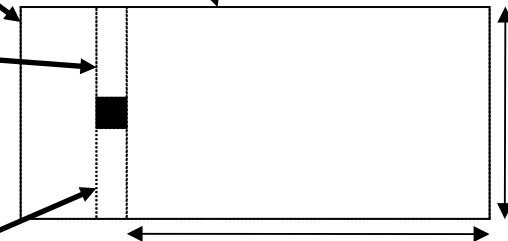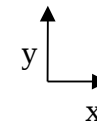
Origine: Block origin Ox Oy [Oz]

Nombre_de_noeuds: Nodes number Nx Ny [Nz]

Longueurs: Lengths Lx Ly [Lz]

Bord: Boundary

Operations on meshes (2/2)

- List of possible keywords to adjust a mesh:

    - **Dilate** (to change the size of a mesh)
    - **Mesh** (to mesh a block or merge several meshes)
    - **Transformer** (to transform a mesh with a function)
    - **Rotation** (to rotate a mesh according to an axis)
    - **Extruder** (to extrude a 2D mesh into a 3D mesh)
    - **Trianguler**/**Tetraedriser** (to triangulate, to tetraedrise)
    - **Raffiner_**(**an**)**isotrope** (to refine a mesh)
    - **RegroupeBord** (to merge or rename boundaries)
    - **Supprime_Bord** (to suppress boundaries)
    - **Remove_Elem** (to create holes in a VDF mesh)
    - …

Data files & calculation (4/5)

- TRUST and tools interfaces
- Data file description
- Operations on meshes
- **Post processing description**
- Output files description

Post processing description (1/7)

```
        Postraitement
        {
                # Definition of probes for 1D plot #
                Sondes
                {
                        sonde_pression          pression            periode 0.005       points 2    0.13 0.105    0.13 0.115
                        sonde_vitesse           vitesse             periode 0.005       points 2    0.14 0.105    0.14 0.115
                        sonde_vit        nodes  vitesse             periode 0.005       segment 22  0.14 0.0      0.14 0.22
                        sonde_Pmoy              Moyenne_pression    periode 0.005       points 2    0.13 0.105    0.13 0.115
                        sonde_Pect              Ecart_type_pression periode 0.005       points 2    0.13 0.105    0.13 0.115
                }
                format lata    fichier results  # Instantaneous fields and time averaged fields written into a LATA format results.lata file #
                # Definition of 2D/3D instantaneous fields for post-processing #
                Champs dt_post 1.
                {
                        # Fields location #
                        pression elem
                        pression som
                        vitesse elem
                        vitesse                 # By default, location is som (vertexes) #
                        vitesse faces
                }
                # Definition of 2D/3D statistical (time averaged) fields for post-processing #
                Statistiques dt_post 1.
                {
                        t_deb 1. t_fin 5.
                        moyenne vitesse elem
                        ecart_type vitesse som
                        moyenne pression elem
                        ecart_type pression som
                }
        }
}
Solve pb                # Solve the problem : Start the time scheme loop #
End                     # Optional keyword end #
```

Post processing description (2/7)

Probes : "Nodes" option

"**Nodes**" option moves the probes to the nearest faces, but take care of stretched meshes!

sonde_vit **nodes vitesse periode** 0.005 **segment** 22 0.14 0.0 0.14 0.22

In the following 2D example, the initial probes in **red** are defined along a segment from boundary to boundary, but when applying option "**nodes**" it moves the probes (in **blue**) to the nearest face and sometimes near the boundary the nearest face **IS NOT** a boundary face.

Since several version it is possible to visualize the .son files containing the probes in Visit. It provides you a point MESH which is the localization of the probes. We will try in the 1.6.9 version to help user by improving the messages in the .err file when probes are moved according to the "nodes" option and also to run VisIt on .son files directly from the triou script.
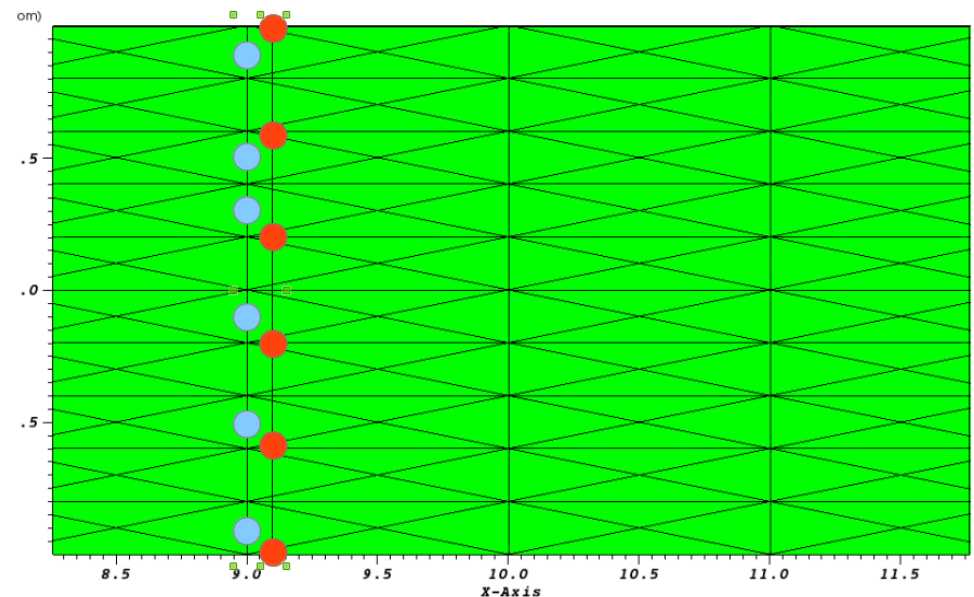
So, if you want extreme probes of the segment on the boundaries, <u>try to move slightly the segment</u>.

Post processing description (3/7)

TRUST results export

2D/3D results files are readable:

- Either directly by :
  - VisIt (use *lata* format <u>in the data file</u> "**format lata**")*
  - Salomé (use *med* format <u>in the data file</u> "**format med**", to post-process use "ParaVis" in Salomé and open med file with "builtin")

- Or after read then export by VisIt (VTK format):
  - Paraview, Tecplot

1D results files by :
- Gnuplot, XmGrace, Excel

*: VisIt, thanks to a new plugin released with Trio_U 1.6.9 reads also the MED format

Post processing description (4/7)

- **Possible basic post processed fields**
  - Equation unknowns (velocity, pressure, temperature,…)
  - Physical characteristics (dynamic viscosity, thermal conductivity,…)
  - Model fields (turbulent viscosity, friction velocity,…)

  The complete list of keywords for fields which could be post processed for the current calculation is printed into the .err file :

Reading of fields to be postprocessed

Milieu_base : 1 **masse_volumique**

Fluide_Incompressible : 2 **viscosite_cinematique viscosite_dynamique**

Equation_base : 1 **volume_maille**

Operateur_base : 0

Navier_Stokes_std : 16 **divergence_U gradient_pressionY gradient_pressionX gradient_pression pression_pa pression vitesseY vitesseX vitesse taux_cisaillement courant_maille reynolds_maille y_plus porosite_volumique critere_Q vorticite**

- **Possible advanced post processing fields**
  - Can be created in the data file with the keyword **Definition_champs**
  - 3 examples given:
    - Monitoring extreme values of a field
    - Averaging a field on a boundary
    - Error between Trio_U and an analytical solution

Post processing description (5/7)

Maximal value of a field

```
Read pb {

 ….

 Postraitement {

            Definition_champs {

                        # Creation of the 0D field: maximal temperature of the domain #

                        temperature_max Reduction_0D {

                                    methode max

                                    source refChamp { Pb_champ pb temperature }

                        }

            }

            Sondes {

                        # Print max(temperature) into the datafile_TMAX.son file #

                        tmax temperature_max periode 0.01 point 1 0. 0.  0.

            }

            Champs dt_post 1.0 { … }

    }

 }
```

Post processing description (6/7)

Averaging a field on a boundary

Domaine dom # 3D domain with a boundary named wall #

….

Domaine surface # 2D domain object created for use by the Extraction keyword #

Read problem {

  …

 Postraitement {

      Definition_champs {

            # Creation of the 0D field: mean temperature on the boundary wall #

            wall_mean_temperature **Reduction_0D** {

                methode moyenne

                source Extraction {

                    domaine surface **nom_frontiere** wall **methode trace**

                    source refChamp { **Pb_champ** problem **temperature** }

                }

            }

      }

      # Print into the datafile_TWALL.son file #

      Sondes { twall wall_mean_temperature **periode** 0.01 **point** 1 0. 0. 0. }

      Champs dt_post 1.0 { … }

    }

}

Post processing description (7/7)

Calculating an error between fields

```
Postraitement {

        Definition_champs { # Creation of the 3D  field: error #

                error Transformation {

                        methode formule expression 1 velocity-solution

                        sources {

                                refChamp { Pb_champ problem vitesse nom_source velocity } ,

                                Transformation {

                                        methode vecteur expression  3  x*y  x+y  z

                                         nom_source solution

                                }

                        }

                }

                # Calculate the L2 norm of the error as 0D field #

                error_norm Reduction_0D { methode norme_L2  source_reference error }

        } # Print into the datafile_ERROR_NORM.son file #

        Sondes { sonde_error_norm error_norm  periode 0.01 point 1 0. 0.  0.  }

        format LATA Champs dt_post 1.0 {

                error           # Post process the error field #

                vitesse

                }
}
```

Data files & calculation (5/5)

- TRUST and tools interfaces
- Data file description
- Operations on meshes
- Post processing description
- **Output files description**

Output files description (1/6)

Saving process

- Unknowns (velocity, temperature,…) are saved in:

  - one *.xyz* file

  - one or several (parallel calculation) *.sauv* files

- By default, saving process in *.sauv* happens during the calculation:

  - At the start and at the end

  - Periodically (each 23 hours of CPU with **tcpumax** keyword)

  - But, user may also specify a time physical period (**dt_sauv** keyword)

- By default, saving process in *.xyz* file happens during the calculation:

  - At the end

  - But, user may enable it with a specific keyword

- By default, there is a default name for the *.sauv* files (testcase_000n.sauv), the format is binary, and the files are appended during successive saves but user can change the behaviour with the keywords:

sauvegarde|sauvegarde_simple binaire|formatte|xyz *filename.sauv|filename.xyz*

with: - **sauvegarde_simple** : the file is deleted before the save

                 - **formatte** : the format of the file ASCII instead of binary

                 - **xyz**: the *.xyz* file is written instead of the *.sauv* files

Output files description (2/6)

Restarting process

Restarting the calculation is possible :

 - Either from *.sauv* file(s) (one file per process)

-> Necessary to restart the calculation with the <u>same</u> number of equations on the <u>same</u> number of processes

- Or from a *.xyz* file

-> Possible to restart a calculation by changing the number of equations solved

-> Possible to restart with a <u>different</u> number of processes

The mandatory syntax in the data file is:

reprise binaire|formatte|xyz *filename.sauv|filename.xyz*

Output files description (3/6)

TRUST files summary

- Input:
  - Data file: .data
  - Meshing: .geom (or .bin)
  - Instructions file: .geo
  - Sub zones: .ssz
  - Sub domains: .Zones
- Output :
  - 2D/3D results: .lata (or .med)
  - 1D results: .son
  - Saving-restart: .sauv ou .xyz
  - Listing (physical infos): .out
  - Listing (warnings&errors&domain infos): .err
  - Listing of boundary fluxes: *.out
  - CPU performances: .TU
  - Time steps, facsec, equation residuals: .dt_ev
  - Stop file (0 or 1): .stop

Output files description (4/6)

TRUST with VisIt
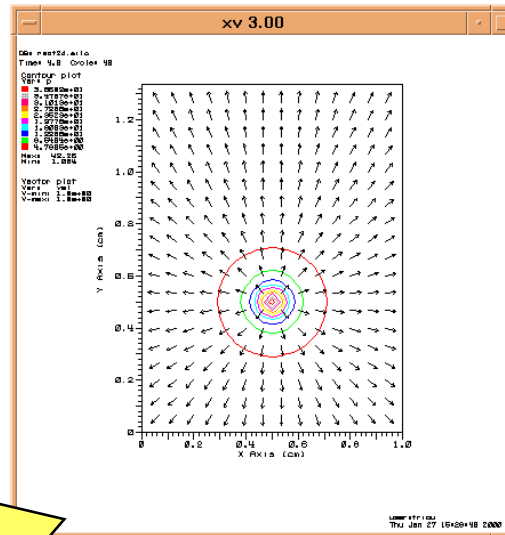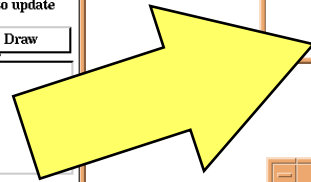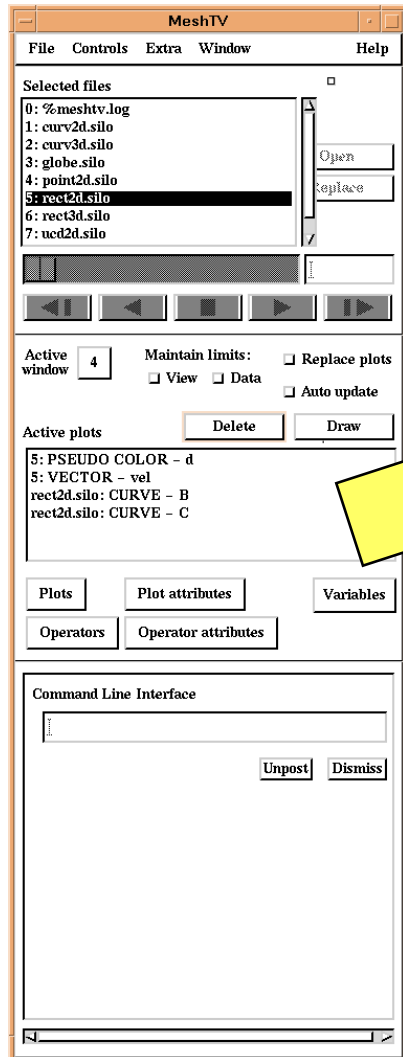
Vectors/Scalars
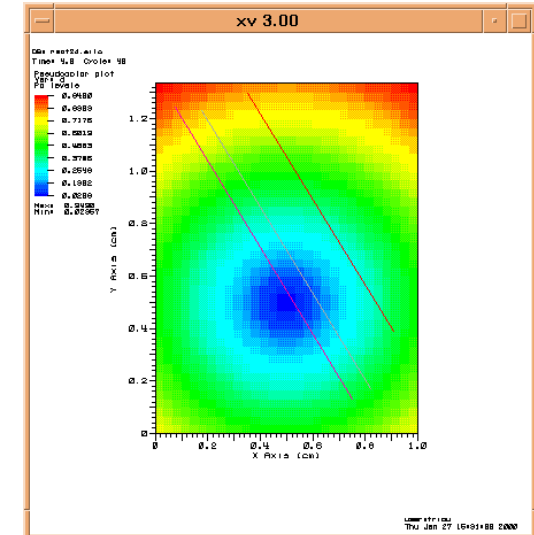
2D Slice
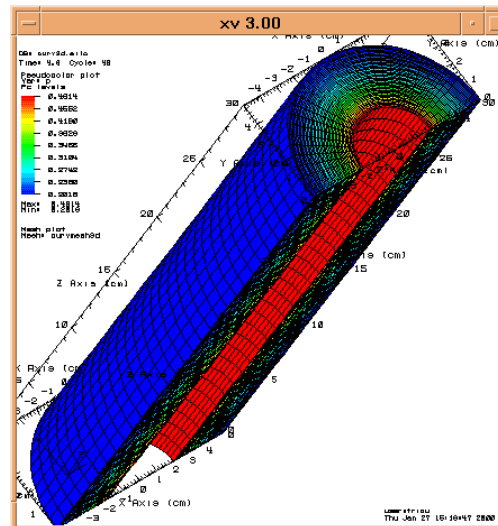
3D View
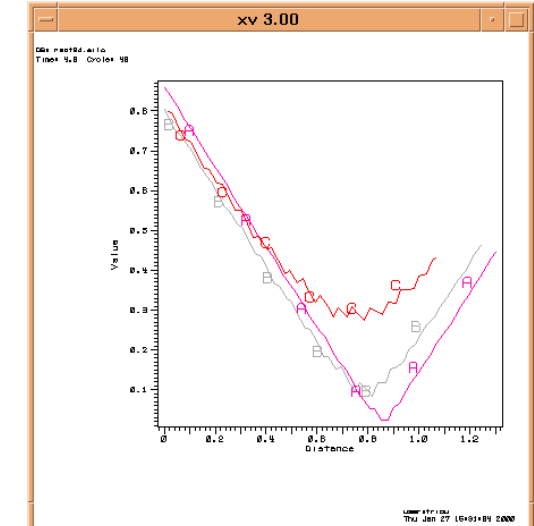
1D Cut

Output files description (5/6)

TRUST with VisIt

Visualize boundaries

Visualize partition
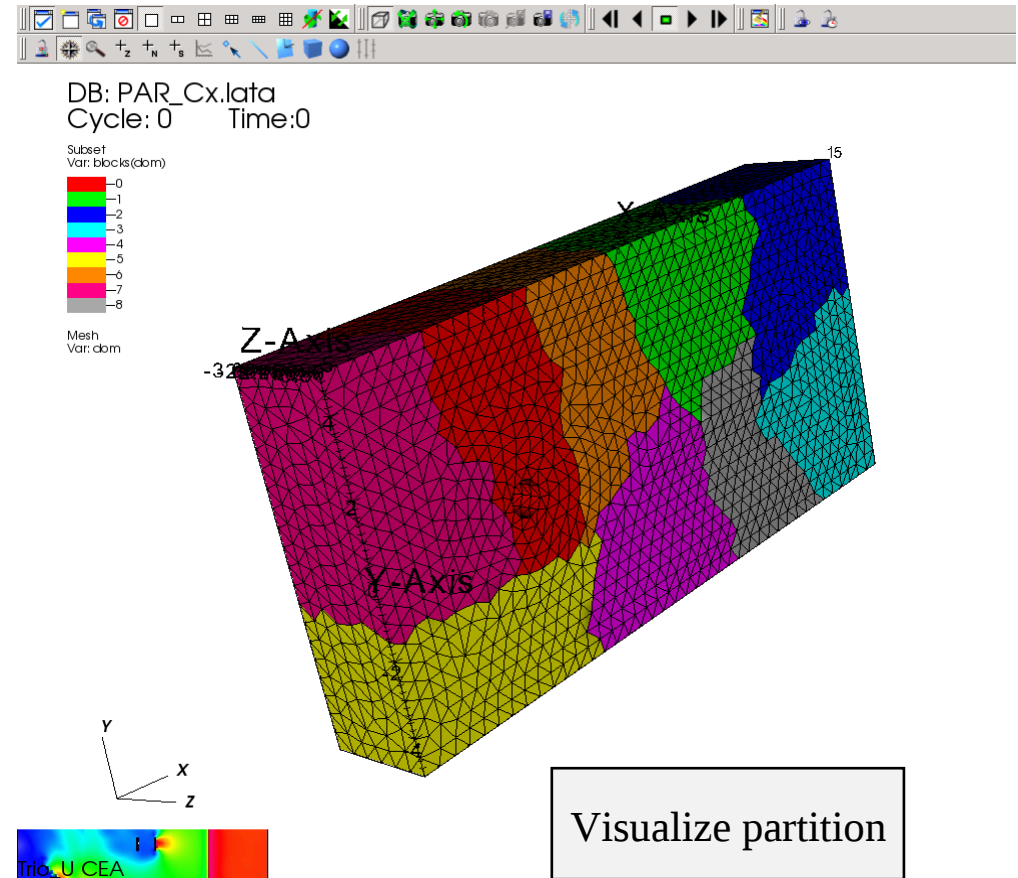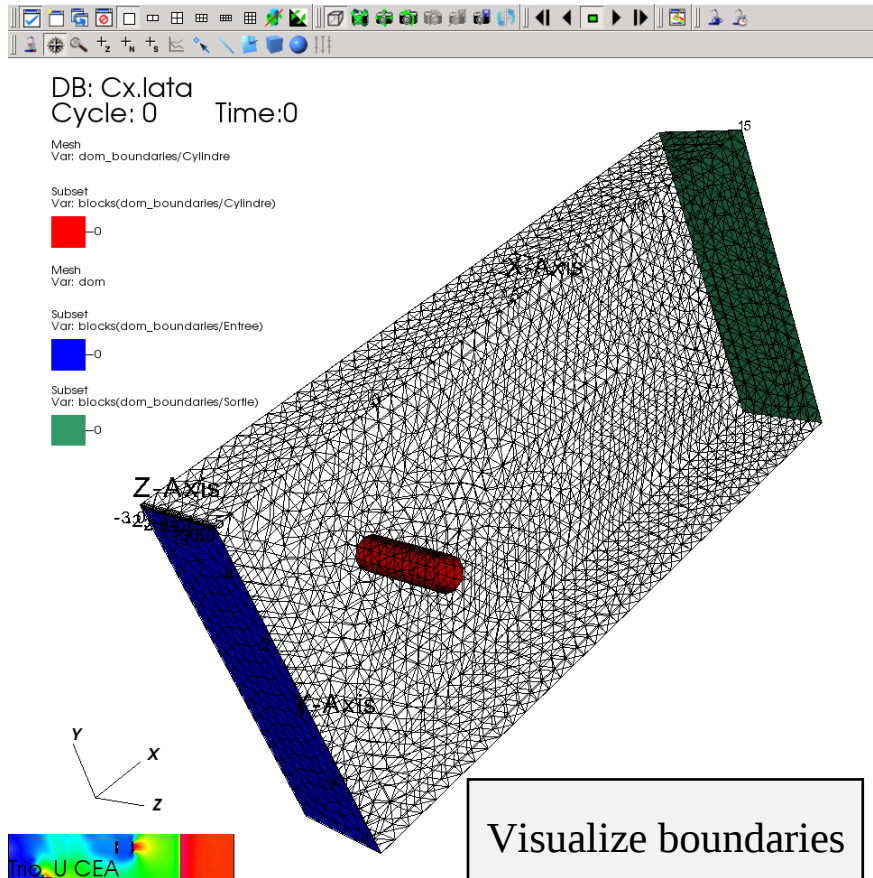
For more informations and to download manuals see :

https://wci.llnl.gov/codes/visit/manuals.html

Output files description (6/6)

TRUST with gnuplot

Real-time display of calculated quantities:
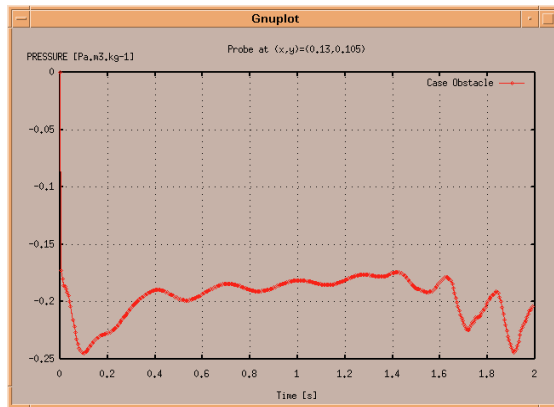
One point probe
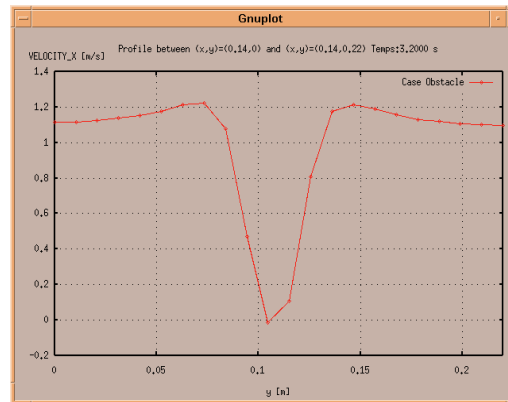
Probes segment
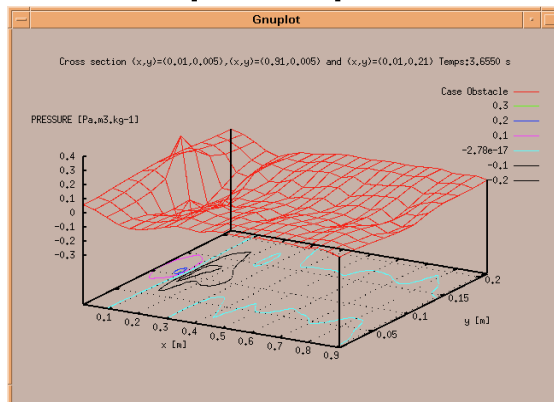
Probes plane
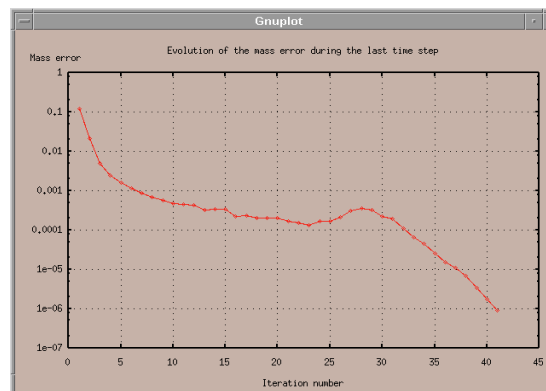
Convergence

Instantaneous or averaged value and also, flux balance at the boundaries like:

-flow rate

-pressure forces

-viscous forces

-heat flux

…

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- Automating validation test case
- Mesh generators: Xprepro/Salomé/Gmsh
- TRUST/TrioCFD support
- Examples of data files

Command lines (1/3)

- TRUST environment initialization:

  source $TRUST_ROOT/env_TRUST.sh

- To run a TRUST calculation with the trust script:
    - Sequential run:

      trust *datafile*

    - Parallel run on N CPUs:
        - Partitioned mesh partitioned should be created sequentially, then interactively:

          trust *datafile N*

        - Or to run on a batch-queuing system, add this line into the submission file :

          mpirun –np *N **$exec** datafile N*

- To redirect into output and error files, after the command line, add:

  trust *…. 1>datafile.out 2>datafile.err*

Command lines (2/3)

- To copy a data file from the test database:
  trust -copy datafile

- To edit interactively (change/add schemes, solvers...) a data file with:
  EditData datafile.data

- Check a data file without running TRUST:
  VerifData datafile.data

- To visualize the mesh and its boundaries used by a data file:
  trust -mesh datafile[.data]

- To run and follow probes during your calculation (used of "Run_sonde" script):
  trust -monitor datafile[.data]

- To monitor only your calculation:
  trust -probes [datafile[.data]]

Command lines (3/3)

- To run VisIt with a LATA results file:
  visit -o datafile.lata

- To clean your calcul directory:
  trust -clean

- To open the PDF documentation (User's manual):
  trust -doc

- To browse some useful resources (PDF manuals, test cases, keywords, C++ classes,…) :
  trust -index

- In all cases, the TRUST binary may be changed by the **$exec** variable and by default, exec=$TRUST_ROOT/exec/TRUST_mpi_opt

Practice

Exercise 1: Obstacle.data + VisIt

(incompressible 2D flow)

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Parallel calculation (1/3)

- **Parallel calculation description..** p79
- Parallel calculation on clusters..... p85
- Visualization with VisIt................. p93

Parallel calculation description (1/5)

- SPMD model (Single Program Multiple Data)

- Messages exchange by MPI (Message Passing Interface)

- From PC to massively // computer, with shared or distributed memory

Parallel calculation description (2/5)

- Domain partitioning tools :
  - Metis
  - Tranche "band partitioning"

- Performances are partition dependent :
  - Same number of cells by sub-domain
  - To minimize the joints length (boundaries between sub-domains)

- Some rules of thumb for performance
  - If possible, use 20000-30000 cells per process
  - Look at cluster specificities:
    - L2 size cache
    - Latency network
    - ...
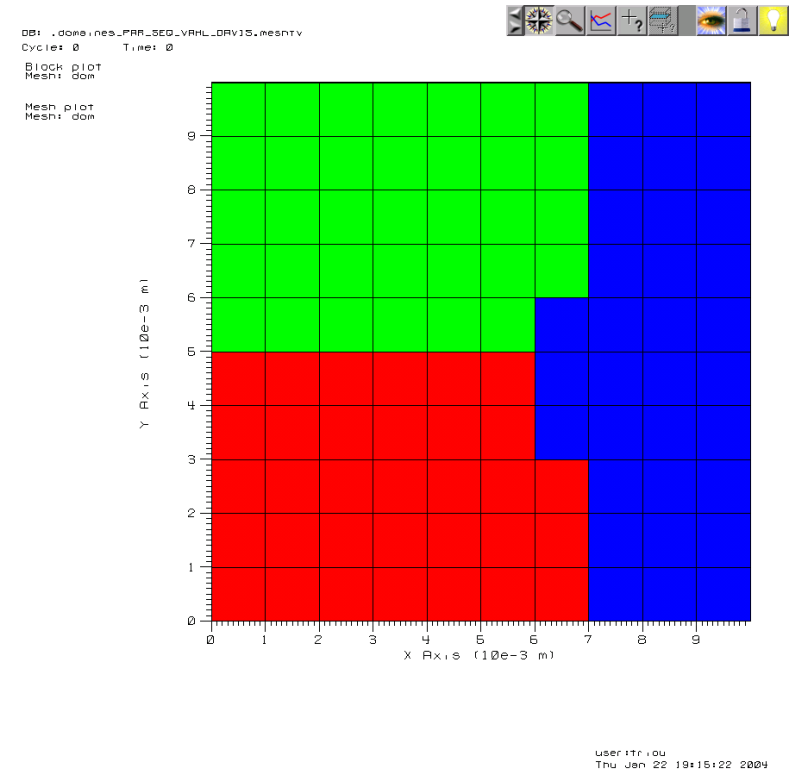
Parallel calculation description (3/5)

- **Definition of overlapping width value**
  - Number of vertexes or elements on the remote sub-domain known by the local sub-domain
  - Specified by the users during partitioning task
  - This value depends on the space scheme orders:
    - 1 if 1-2nd order
    - 2 if 3-4th order
  - In practice, use 2 except if you use **only** upwind schemes

Overlapping width : 1

Boundary between 2 sub-domains

Overlapping width : 2
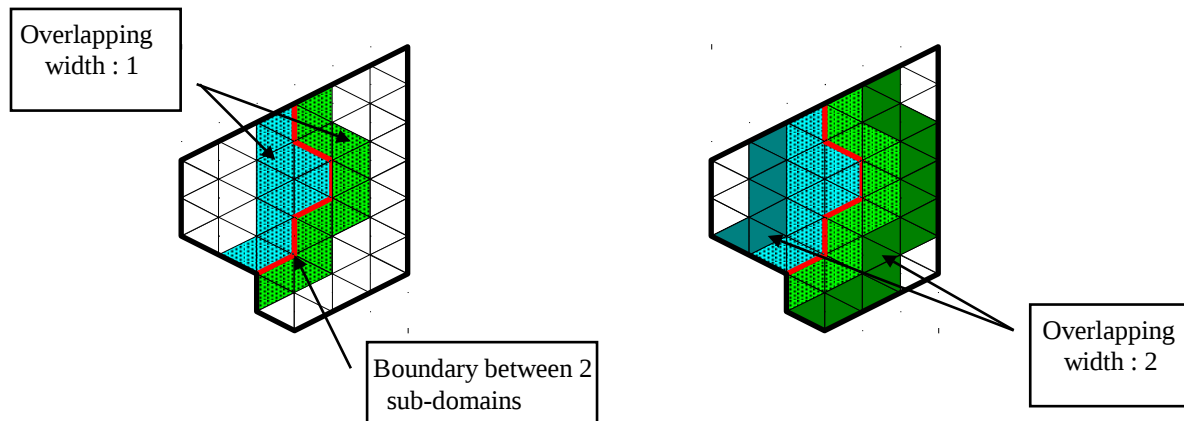
Parallel calculation description (4/5)

- ## Performance examples :
  - ### PC linux cluster (Scali network):

Processors	Speed Up	Efficiency
1	1	1
2	1.7	0.86
4	3.2	0.80
8	5.5	0.69
16	7.5	0.47
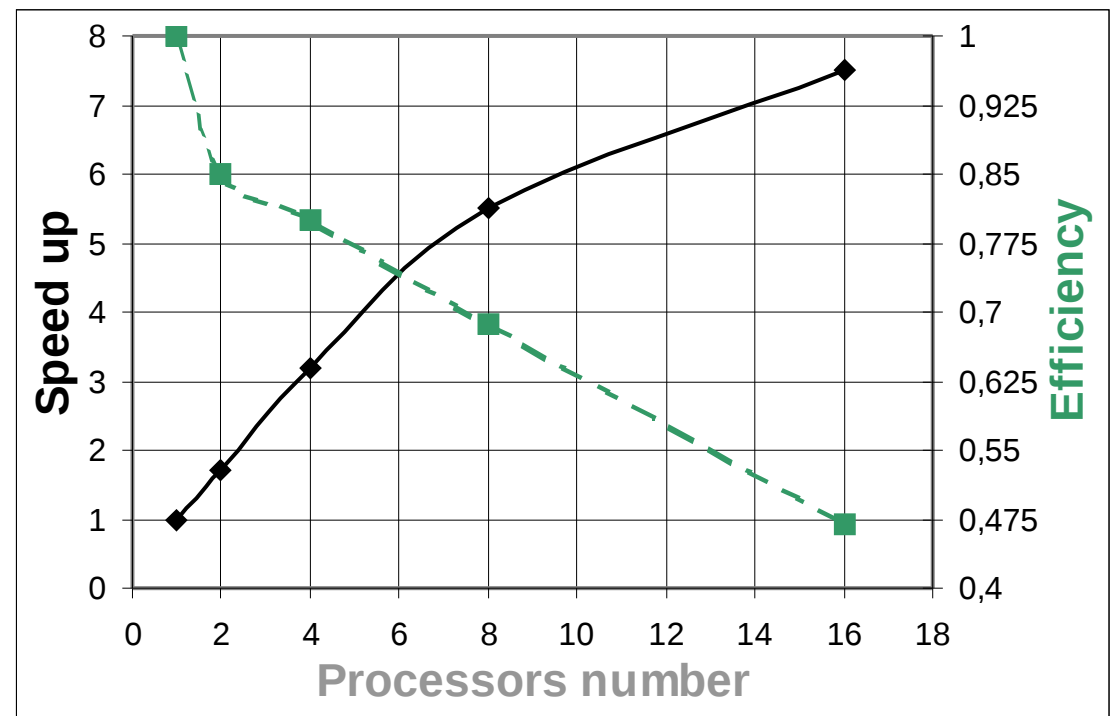
Parallel calculation description (5/5)

Some advices:

- Choose a number of elements per process between 20000 and 30000 for optimal performances. Below 20000 elements/process, TRUST parallel efficiency may dramatically decreases. Example on curie:
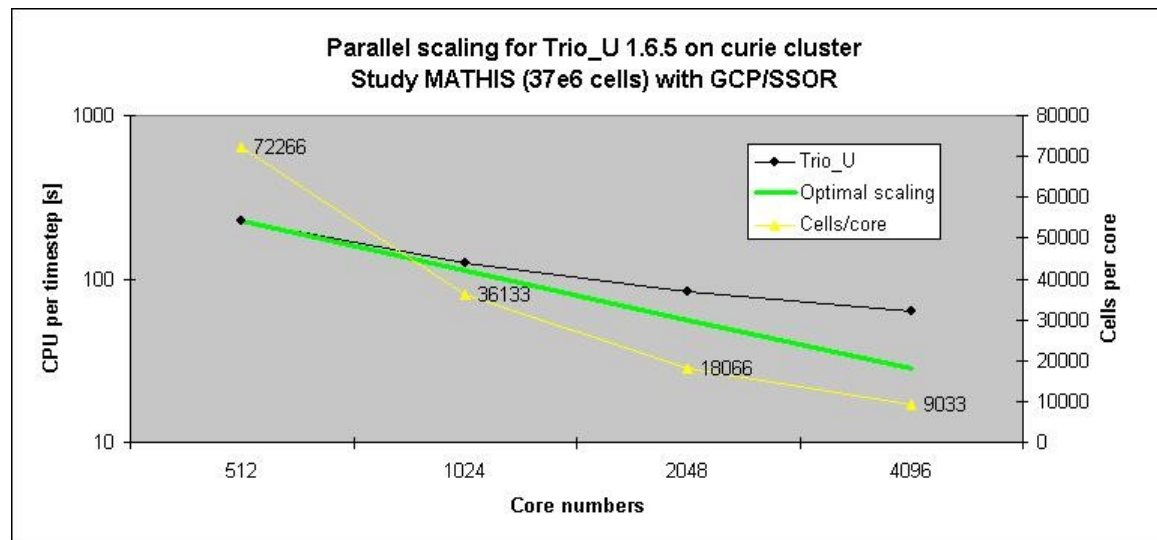
Scaling of curie from 72000 cells/core to 9000 cells/core

Parallel calculation (2/3)

- Parallel calculation description
- **Parallel calculation on clusters**
- Visualization with VisIt

Parallel calculation on clusters (1/7)

- To connect to:
  - CEA/DM2S service cluster: callisto (1168 cores)
  - CEA/CCRT cluster: airain (~10000 cores)
  - CEA/TGCC cluster: curie (~92000 cores)
  - CINES cluster: occigen (~50 000 cores)
  - CEA/Cadarache cluster: mezel2 (~600 cores)

- Ask for a login:
  - callisto (access for CEA only)
  - CCRT http://www-ccrt.cea.fr
  - TGCC http://www-hpc.cea.fr/fr/complexe/tgcc.htm
  - occigen https://www.cines.fr/occigen-le-nouveau-supercalculateur/
  - mezel https://www-linuxcad.intra.cea.fr/dokuwiki/doku.php/cluster

- Once you have the login, connect from your PC to:
  - ssh –X login@name.intra.cea.fr (name=callisto-login1 | callisto-login2)
  - ssh –X login@name.ccc.cea.fr (name=curie-ccrt-gw | airain-gw)
  - ssh –X login@occigen.cines.fr
  - Ssh -X login@mezel

La force de l'innovation

Parallel calculation on clusters (2/7)

- **TRUST/TrioCFD versions located on:**
  - callisto   ROOT=/panfs/ixion/home/triou/
  - CCRT/TGCC   ROOT=/ccc/scratch/cont002/den/triou/
  - occigen   ROOT=/opt/software/applications/trio_u/

  with stable versions:
  - $ROOT/TRUST/TRUST_X.Y.Z
  - $ROOT/TrioCFD/TrioCFD_X.Y.Z

  and versions in development (if exists):
  - $ROOT/Version_beta_clustername/TRUST   -> future X.Y.Z+1 version
  - $ROOT/Version_beta_clustername/Composants/TrioCFD

- For **TRUST** configuration, you can add in your ~/.profile (or ~/.bashrc) file, the lines:

  # Example of TRUST environment on callisto:
  source /panfs/ixion/home/triou/TRUST/TRUST_1.7.2/env_TRUST.sh 1>/dev/null 2>&1

- **Check your environment**, after you reconnect to the cluster, look at TRUST_ROOT variable:
  echo $TRUST_ROOT

Parallel calculation on clusters (3/7)

- Space discs on callisto:
  - /home (limited space but there is backup)
  - /panfs/ixion/home (local space backup)
  - /panfs/ixion/scratch (local space no backup)

- Space discs and quotas on CCRT/TGCC:
  - /ccc/cont002/home (3 GB, slow I/O, backup)   -> Data shared by all clusters
  - /ccc/work (1 TB, fast I/O, no backup)   -> Source code, binary (also shared)
  - /ccc/scratch (20 TB, fastest I/O, no backup)   -> Data, code output
  - /ccc/store (infinite size, backup, but data are slow to access)   -> Data archiving

- Space discs on occigen:
  - /home (40 GB/user, backup)
  - /store (200 GB/group, backup, limited to 100 000 files/group)
  - /scratch (4 TB/group, no backup)

Parallel calculation on clusters (4/7)

- Sequential interactive run (but very time-limited), for example to run a datafile to partition a mesh:

  trust datafile

- Parallel interactive run (but very time-limited), for example to check your datafile:

  trust datafile nb_processes

- To use the batch queuing system (for a long time-limited run), you need to create first a submission file (named sub_file):

  trust –create_sub_file datafile nb_processes

- Then, you submit the job:

callisto:	**sbatch**	sub_file
CCRT/TGCC:	**ccc_msub**	sub_file
occigen:	**sbatch**	sub_file
mezel:	**sbatch**	sub_file

Parallel calculation on clusters (5/7)

- Before you submit the job, you can edit and change the values of the submission file sub_file

- The submission file describes:
  - The job name
  - The number of cores required
  - The default output files
  - The CPU time required (the CPU value selects implicitly a queue)
  - The location of the TRUST study
  - The TRUST parallel command line

Parallel calculation on clusters (6/7)

- Example on callisto

```
#SBATCH  -J name_of_the_job
#SBATCH  -p slim
#SBATCH --qos=normal_slim
#SBATCH -t 2880
#SBATCH -n 2
cd /panfs/ixion/home/login/study
mpirun -np  nbprocs $exec datafile nbprocs 1>jdd.out 2>jdd.err
```

- Example on CCRT/TGCC

```
#MSUB –r job_name
#MSUB –n nb_procs
#MSUB –o out.%J
#MSUB –e err.%J
#MSUB –T 86400
# On cluster curie, add also your project (e.g. genden):
#MSUB –A genden
cd /ccc/scratch/cont002/den/login/study
mpirun -np nb_procs ./Trio_U_mpi_opt datafile nb_procs 1>datafile.out 2>datafile.err
```

- Example on occigen

```
#SBATCH  -J name_of_the_job
#SBATCH -t 24
#SBATCH -n 2
#SBATCH -N 1
cd directory_of_my_study
srun --mpi=pmi2 -K1 --resv-ports -n $SLURM_NTASKS $exec datafile $SLURM_NTASKS1>jdd.out 2>jdd.err
```

Parallel calculation on clusters (7/7)

- Description of partition/queues/classes for each cluster:

  callisto: **slim** (no limit of CPU, limited to 800 cores, 6.4GB/core)

  large (no limit of CPU, limited to 320 cores, 12.8GB/core)

  fat (no limit of CPU, limited to 48 cores, 21.3GB/core)

  CCRT/TGCC: **test** (30 minutes of CPU, limited to 256 cores)

  prod (24 hours of CPU)

  More class informations with the command **class**

  occigen: **all** (24 hours of CPU)

- List of jobs and their state:

  callisto: **squeue**

  CCRT/TGCC: **ccc_mpp**

  occigen: **squeue -u** your_login or **squeue -j** job_number

- Kill a job (the job_number is given by the previous command):

  callisto: **scancel** job_number

  CCRT/TGCC: **ccc_mdel** job_number

  occigen: **scancel** job_number**train**

La force de l'innovation

Parallel calculation (3/3)

- Parallel calculation description
- Parallel calculation on clusters
- **Visualization with VisIt**

Visualization with VisIt (1/2)

On clusters

- If available, use a **HPCDrive** deported session on CCRT/TGCC clusters to run VisIt without network slowness

  - Available on curie cluster: https://visu-tgcc.ccc.cea.fr/HPCDrive/home
  - Available on airain cluster: https://visu-airain.ccc.cea.fr/HPCDrive/home
  - Ask us the HPCDrive user manual

- Or the client/server mode
  - See the following description VisIt (**callisto)**
  - Unhappily, this mode DOES NOT work with CCRT/TGCC clusters
  - Fine tuning of a critical option: Rendering->Advanced->Auto (2000KPolys)

- Or local mode
  - Copy the LATA results from the cluster to your PC and run the parallel version of VisIt

Visualization with VisIt (2/2)

Recent features with VisIt

-The TRUST install builds a parallel version of VisIt:

> visit –np 8 –o results.lata

-Client/server mode available by default for some clusters (callisto)

> • You run the TRUST calculation on the cluster

> • You visualize with VisIt your results from your Linux/Windows PC without data copy and/or network slowness

File->Open file…

Select the host (remote host or localhost)

then browse the files to your study.
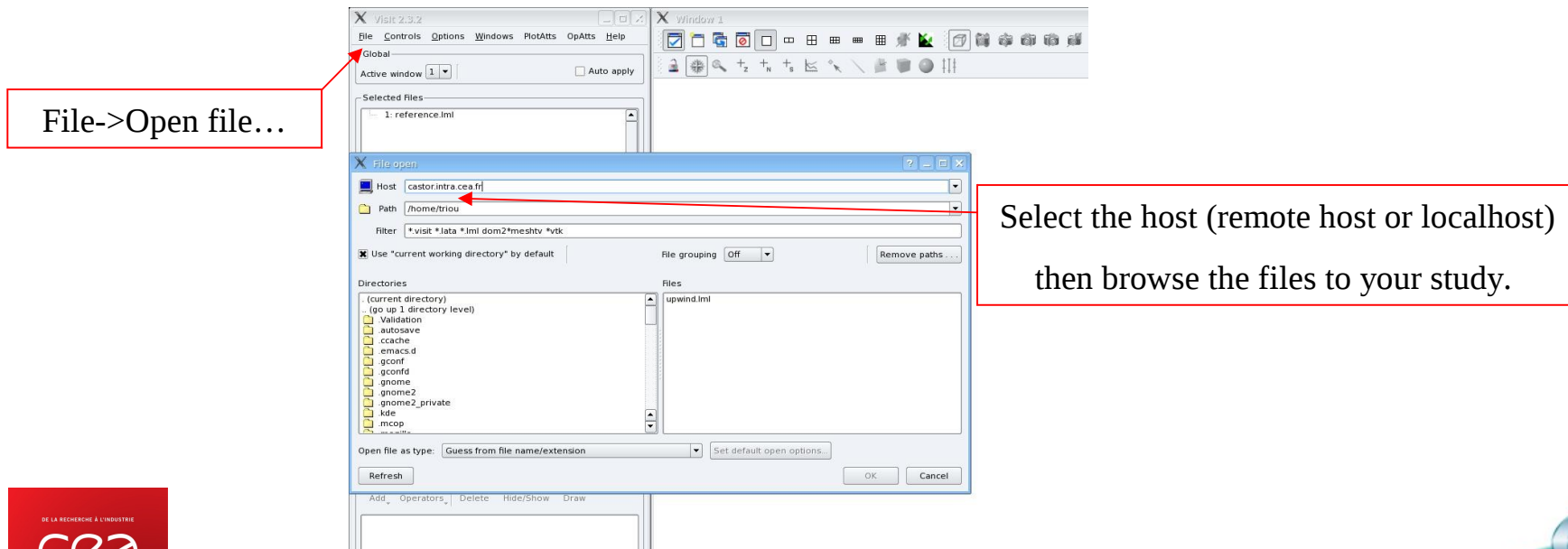
Practice

Exercise 2: Obstacle.data //

Exercise 3: Calculation on callisto

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Recommendations (1/6)

- **For VEF meshing**.........................
- For conditions................................
- For schemes...................................
- For turbulence................................
- For post processing........................
- What if?...

Recommendations for VEF meshing (1/2)

- **Mesh refinement**
  - Minimum of 10 points between two walls
  - To avoid very small time steps, do not create small cells in high velocity regions

- **Boundary layers**
  - Quality of the mesh near boundary layer will be improved if 2 or 3 layers of regular cells is used near the wall

- **Tetra general mesh recommendations**
  - Avoid significant changes in the mesh size of two adjacent tetras. A propagation factor of 20% seems to be the upper limit (5% recommended)

Recommendations for VEF meshing (2/2)

- Tetra general mesh recommendations:

  - Avoid the use of a great amount of obtuse cells (angles between faces greater than 90°). In the contrary, non physical phenomena are observed to the diffusion operator.

    - Use any optimization tools of mesh generators to reduce too large angles
    - Check in the .err file of TRUST, the angles histogram of the mesh
    - Visualize the field (mesh quality) named LargestAngle_elem

  - Use isotropic cells in all directions as mush as possible for a 3D flow. In the case of a flow in a given direction (1D flow), the stretching of a mesh up to a hundred times in the preferred direction nevertheless doesn't much degrade the results

  - Look the Meshing paragraph of the Best Practice Guide for more advices

Recommendations (2/6)

- For VEF meshing
- **For conditions**
- For schemes
- For turbulence
- For post processing
- What if?

La force de l'innovation

Recommendations for conditions (1/1)

- Boundary conditions
  - Wall conditions for RANS model (no rule for the LES model):
    - The first discretization point should be in the logarithmic layer (30<y+<500). y+ field may be post-processed to check this condition.
  - Look for paragraph "Boundary conditions" in Best Practice Guide

- Initial conditions
  - Look for paragraph "Initial conditions" of the Best Practice Guide to optimize the flow initialization in order to improve/reach faster the convergence

Recommendations (3/6)

- For VEF meshing
- For conditions
- **For schemes**
- For turbulence
- For post processing
- What if?

Recommendations for schemes (1/6)

Space scheme

- Convection schemes with VEF discretization
  - EF_stab
    - Use it for Navier Stokes and scalar equations (temperature, concentration)
    - Option α is a compromise between:
      - robustness (α near 1, the default value)
      - accuracy (smaller value for α)
    - α=0.2 gives the better results. When the mesh is stretched in one direction, this scheme may have some convergence issues.
    - α= 1 insures the stability and gives the same results for a lot of cases when the forced convection flow has a preferred direction.
  - Muscl
    - Use it for very perturbed or mixing flows
- Convection schemes with VDF discretization
  - Quick

Recommendations for schemes (2/6)

Explicit time scheme

Time step dt = facsec * dt(CFL condition: Courant-Fiedrichs-Lewy)

- Euler explicit scheme:

    facsec<=1

- Runge Kutta schemes (facsec limit may be increased):

    facsec=2 if RK2
    facsec=3 if RK3
    facsec=4 if RK4

Recommendations for schemes (3/6)

Implicit time scheme

When to use it?

- To solve a steady state calculation (e.g. k-ε simulation)
- To reduce the time of the transient state of a calculation before switching to an explicit time scheme

WARNING: An unsteady calculation solved with an implicit scheme may give non physical results !

How to use it?

- Define upper and lower limits of the dynamic time step algorithm
- Define a solver (**GMRES**, **BiCGSTAB**,…)
- Define the convergence criterias

Recommendations for schemes (4/6)

Implicit time scheme

- Dynamic time step algorithm:

    Time step dt = facsec(t) * dt(CFL condition)

    with :

    facsec(0) = **facsec**   (lower limit keyword)
    facsec(t^{n+1}) = a * facsec(t^n)
    facsec(t) <= **facsec_max**   (upper limit keyword)

    The algorithm uses a=1.2 and reduces it if necessary

Recommendations for schemes (5/6)

- In a first approach, use **facsec**=**facsec_max** with:
  - **facsec_max**=20-30 for:
    - hydraulic calculation only
    - thermal hydraulic with forced convection and no or low coupling between velocity and temperature

  - **facsec_max**=90-100 for:
    - thermal hydraulic with forced convection and a strong coupling between velocity and temperature

  - **facsec_max**=300 for:
    - thermal hydraulic with natural convection

  - much higher value is possible for:
    - conduction calculation

- In a second approach (no convergence):
  - keep **facsec_max** and reduce **facsec** to 5 or 10

Recommendations for schemes (6/6)

- It is possible to specify a solver for each equation:
  - Momentum equations
    - **GMRES** solver generally works well
  - Scalar equations
    - **BICGSTAB/ILU** if **GMRES** converges slowly or not at all
  - Transport k-ε equations
    - **GMRES** solver and if no convergence (rare), solve these equations with an explicit scheme

- Convergence criteria's
  - Threshold convergence (keyword **seuil**) of the iterative solver (to have at least 3 iterations)
  - A maximal number of iterations may be specified with **nb_it_max** keyword (5 is a good value)
  - For coupled problems, another parameter:
    - keyword **seuil_convergence_implicite** should be set to 0.001(or less) for strongly coupled problems to guarantee the correct coupling of various equations as e.g. hydraulic and thermal phenomena

Recommendations (4/6)

- For VEF meshing
- For conditions
- For schemes
- **For turbulence**
- For post processing
- What if?

Recommendations for turbulence (1/5)

Which turbulence models?

Interested in averaged quantities

- k-ε standard model
    - Low cost but lack of generality

Interested in fluctuating quantities

- LES model
    - Involves a refined 3D mesh
    - Recommended in the following cases

Recommendations for turbulence (2/5)

Which turbulence models?

LES model if:

- Strongly non stationary flow
    - Access to mechanical or thermal fluctuations
    - Mixing phenomena
    - Free and impinging jets

- Flow with important secondary structures
    - Tube bends
    - Rectangular channels at reduced Reynolds numbers

- Flow with detachment and/or reattachment
    - Backward facing steps
    - Obstacles

- Flow at slow regimes
    - Natural convection

Recommendations for turbulence (3/5)

RANS calculation

- Model adapted to high Reynolds number

- First discretization point of the mesh should be located in the logarithmic zone (y+~30)

- Taking care to the initial and boundary conditions for k and ε will avoid some issues and dramatically improve convergence
    - In a first approach (for example 10% turbulence rate), you can use (U, bulk velocity and L, a relevant dimension, example a pipe diameter):
        - k ~ 3/2*(turbulence_rate*U)^2
        - ε ~ k$^{1.5}$/L

- Use EF_stab scheme for the Navier Stokes equation

- Use upwind scheme for k-ε equation

Recommendations for turbulence (4/5)

LES calculation

- Time schemes:
  - High order explicit schemes like:
    – Runge Kutta order 3 (ut facsec 1.0 for LES)
    – Adams Bashforth order 2

- Convection schemes:
  - VEF:

    -EF_stab with α=0.2 for Navier Stokes equation (do not use first order scheme for a LES, so if you need to set α=1.0 to insure convergence, then something is wrong with your mesh)

  - VDF:

    -Centre (order 4) and if unstable use facsec=0.2

Recommendations for turbulence (5/5)

LES calculation

- Use a periodic box to provide a turbulent velocity field (see page 54):
    - The length of the periodic box should be at least 8*Dh
      (Dh: hydraulic diameter)

    - Do not stretch the mesh in the axial direction of the box

- Models
    - First approach, use Wale model, then check the turbulent energy spectra

    - If Wale is unable to dissipate sufficiently the high frequencies, use the Smagorinsky model (see "Post processing" paragraph of the Best Practice Guide)

Recommendations (5/6)

- For VEF meshing
- For conditions
- For schemes
- For turbulence
- **For post processing**
- What if?

Recommendations for post processing (1/1)

- Fields can be visualized at:
  - element, vertex, or face
- Prefer visualization without linear interpolation
- The fields visualized without linear interpolation are :
  - At elements (keyword elem)
    - pressure, turbulent viscosity, y+, physical properties and for VDF only, temperature, concentration, k, ε
  - At vertexes (keyword som)
    - pressure
  - At faces (keyword faces)
    - velocity and for VEF only, temperature, concentration, k, ε
- Prefer the LATA format which can be converted to any other TRUST format

Recommendations (6/6)

- For VEF meshing
- For conditions
- For schemes
- For turbulence
- For post processing
- **What if?**

Recommendations : What if? (1/1)

The calculation does not converge…

- Symptoms:
    - Time-step decreases to the **dt_min** lower limit
    - wall law does not converge (error message)
    - implicit diffusion algorithm does not converge (warning message)
    - …

- Try:
    - Reduce the time-step (use **facsec** value 0.5 or 0.2) if using an **explicit** scheme
    - Reduce the upper limit of the time-step (reduce **facsec_max**) if using an **implicit** scheme
    - If using the **EF_stab** scheme, try to increase α value incrementally (0.2 to 0.3 or 0.5 or 1.0) to recover stability or reduce the **facsec** (if no change, switch to muscl scheme)
    - If using the **centre** scheme, reduce the **facsec** or change your scheme (**quick** scheme)
    - Contact Trio_U support

Practice

Exercise 4: Turbulent flow on a 3D step

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- Mesh generators: Xprepro/Salomé/Gmsh
- TRUST/TrioCFD support
- Examples of data files

Automating validation test case (1/11)

- What is an automated test case ?

- How to generate an automated test case?

- How to run an automated test case?

Automating validation test case (2/11)

- **What is an automated test case ?**

  - Tool to compare TRUST results and experimental data and/or analytical solutions

    -> As final result a report PDF file containing

    » figures (images or gnuplot plots)

    » tables with results

    » visualizations (built by VisIt tool)

    » etc…

  - Useful to quickly validate a new TRUST/TrioCFD version or to compare different versions of the code

Automating validation test case (3/11)

- **How to generate an automated test case?**

  - Create a directory for example Test_case_name and under:
  - src directory will contain the elements to build the test case
  - build directory will contain the results of the building run
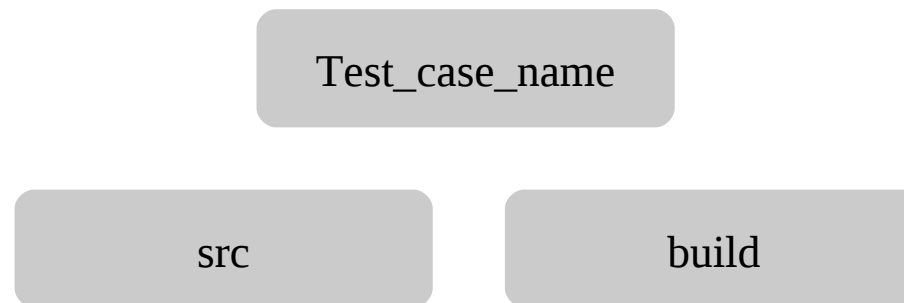
Automating validation test case (4/11)

- **How to generate an automated test case?**

  - In the src directory, you will create a:
    - **.prm** file (mandatory)
      - It contains the automated test case description
    - **prepare** script (optional)
      - It will build one (several) data file(s) in the build sub-directories
    - **pre_run** script (optional)
      - It will do operations BEFORE calculations begin, for example the mesh partition before a parallel calculation
    - **post_run** script (optional)
      - It will extract relevant information from the raw result files AFTER the calculation finishes (run python scripts,...)
    - other optional files/directories necessary to build the test case
      - data file, mesh file, experimental data, images,…

Automating validation test case (5/11)

- Example of a **prm** file (and final PDF result):

Several data files will be run by TRUST/TrioCFD

Parametres {

    Titre "2D Channel flow with imposed Twall and volumetric power"

    Description "2D Channel flow with imposed wall temperature"

    Auteur "Simone Vandroux"

    CasTest dir1 Canal_2D_grossier.data

    CasTest dir2 Canal_2D_semi_grossier.data 4

}

Chapitre {

    Titre " Test Description "

    Description " \latex_(\textbf{Tested options}\latex_)"

    Description " Type of flow: Thermohydraulic laminar 2D"

    Description " Time scheme: Euler explicite"

    Description " Convection schemes: Amont, muscl, EF_stab {volumes_etendus}"

    Description " Discretization: VEFPreP1b"

    Description " Type of boundary conditions: Momentum: periodic and symetry"

    Description "   Energy: periodic and imposed temperature"

    Description " Type of fluid: properties of helium gas at 700°C

    Description " "

    Description "\latex_(\textbf{Physical properties}\latex_)"

    Description " The physical properties correspond to the properties of Helium at 700°C"

    Description "\latex_($\rho = 4.40684\: kg.m^{-3}$\latex_)"

    Description "\latex_(μ\latex_) = 4.46437e-05 Pa.s"

    Description "\latex_($\lambda = 0.344964 \: W.m^{-1}.K^{-1}$\latex_)"

    Description "Cp = 5193 J/kg/K"

    Description "\latex_($\beta = 0.0014285714\: K^{-1}$\latex_)"

    Description "Pr = 0.67 "

Latex format can be integrated

---

2   Test Description

Tested options
Type of flow: Thermohydraulic laminar 2D
Time scheme: Euler explicite
Convection schemes: Amont, muscl, EF_stab {volumes_etendus}
Discretization: VEFPreP1b
Type of boundary conditions: Momentum: periodic and symetry
Energy: periodic and imposed temperature
Type of fluid: properties of helium gas at 700°C
Physical properties
The physical properties correspond to the properties of Helium at 700°C
$\rho = 4.40684\ kg.m^{-3}$
$\mu = 4.46437e\text{-}05\ Pa.s$
$\lambda = 0.344964\ W.m^{-1}.K^{-1}$
Cp = 5193 J/kg/K
$\beta = 0.0014285714\ K^{-1}$
Pr = 0.67
Boundary limits
Hydraulic: symetry at walls
Energy: imposed temperature T=0 at walls, imposed volumetric power=1 in the calculation domain
Initial conditions:
For this periodic calculation, the exact temperature solution is a parabolic profile:
$T(y) = \frac{P}{\lambda} \cdot \frac{y}{2} \cdot (y - H)$
It is imposed as an initial temperature profile.
Solving of equations:
Equation Navier_Stockes_standard:
Pressure solver: solveur_pression Gcp { precond ssor { omega 1.5 } seuil 1.e-10

Imposed wall temperature

Periodic BC   Imposed volumetric power   Periodic BC   H=2m

L=5m

2D Channel flow with imposed Twall and volumetric power   2

Automating validation test case (6/11)

```
Figure {
    Titre " geometry"
    Image cas_test_3.jpg
}
Visu {
            titre "Coarse mesh"
            Width 6 cm
            mesh ./Canal_2D_grossier.lata dom_pb2
            pseudocolor ./Canal_2D_grossier.lata dom_pb2 TEMPERATURE ELEM
            blackvector ./Canal_2D_grossier.lata dom_pb2 VITESSE ELEM

}
Figure {

    Titre "Heat flux as a function of time for various meshings"
    Dimension 2
    Description "The graph below shows the heat flux"
    Description "The calculation stops when the calculation has reached a stationary
sate."

    LabelX "time (in s)"
    LabelY "Heat flux at the wall (in W)"
    InclureDescCourbes 0
    Legende below title "légende"
    Courbe {
            Legende "-Flux bord coarse mesh"
            Origine "Trio_U"
            Version "1.5.4"
            fichier ./Canal_2D_grossier_pb2_Diffusion_chaleur.out
            Style linespoints
            colonnes ($1) (-$2)

    }
```

An image (jpg format for example) will be included to describe the geometry

An image with temperature and vector velocity from VisIt will be included
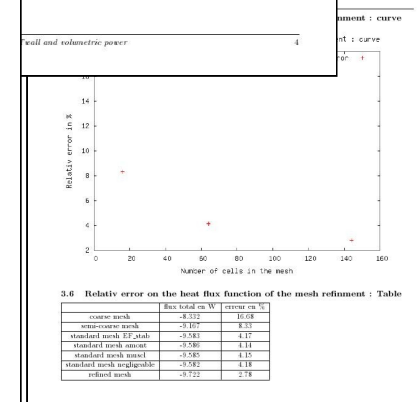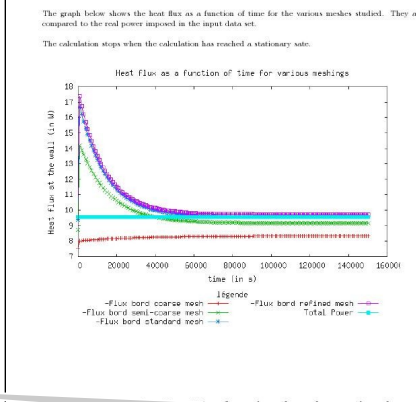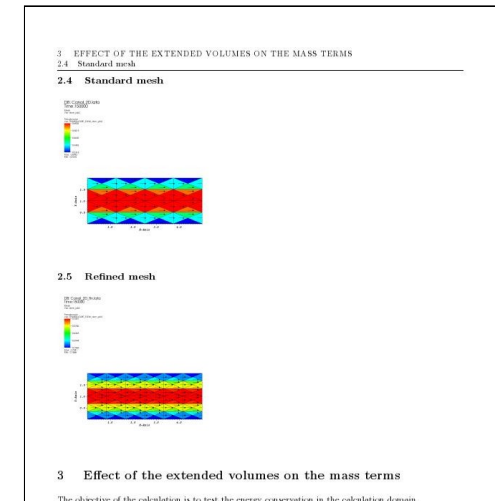
Example of figures plotted by gnuplot

Automating validation test case (7/11)

- **Example** of a **prepare** script:

```bash
#!/bin/bash

# Loop on several convection schemes:

for scheme in "muscl ef_stab upwind"

do

    # Create a sub directory into the build directory

    mkdir  $scheme

    # Go into the sub directory

    cd $scheme

    # Copy the flow.data into a new file named flow.data

    cp ../flow.data flow.data

    # Substitute into the the data file the SCHEME string by  the the value of  the  $scheme variable

    echo –e "1,$ s?SCHEME?$scheme?g\nw" | ed flow.data

    # Create a link with pre_run and post_run script

    ln –s –f ../pre_run .

    ln –s –f ../post_run .

    # Come back to the build directory

    cd ..

done
```

Automating validation test case (8/11)

- Example of a **pre_run** script:

```
#!/bin/bash

# Uncompress the mesh file

gunzip –c ../Channel.msh.gz  >  Channel.msh

# Partition the mesh with the make_PAR.data tool:

make_PAR.data flow.data
```

Automating validation test case (9/11)

- Example of **post_run** script:

```bash
#!/bin/bash
# The first parameter is the name of the data file:
datafile=$1
file=${datafile%.data}
# Read the pressure drag on the 5th column of the last line (final time) of
# the pressure force file:
fp=`tail -1 $file"_pb_Force_pression.out" | awk '{print $5}'`
# Read the viscous drag:
fv=`tail -1 $file"_pb_Contrainte_visqueuse.out" | awk '{print $5}'`
# Calculate the total drag:
Drag='echo $fp $fv | awk '{print $1+$2}''
#Drag=`echo "$fp+$fv" | bc –l`
# Write the total drag into a file to be included into a table of the PDF file
echo $Drag > drag.dat
```

Automating validation test case (10/11)

- **How to run an automated test case?**

  – "**Run_fiche**" command should be run either from the root directory of the test case, either in the src directory
  – All operations made by **Run_fiche** are in the build directory:

  » First, it runs the **prepare** script

  » Then for each calculation:

  Test_case_name

  -runs the **pre_run** script

  -runs the calculation

  src   build

  -runs the **post_run** script

  » Then builds the PDF report file

Automating validation test case (11/11)

- User guide:
  - $TRUST_ROOT/doc/TRUST/HowTo_Validation.pdf

- .prm syntax documented in:
  - $TRUST_ROOT/Validation/Outils/Genere_courbe/doc/manuel.xhtml

- Examples of automated verification test case:
  - $TRUST_ROOT/Validation/Rapports_automatiques/Verification/Verification_codage

Practice

Exercise 5: Validation form

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Mesh generators (1/4)

Possible meshing tools (1/3)

- **TRUST internal mesh tool**

  - Used by keywords in the data file

  - Limited to simple geometry (assembling of rectangle in 2D or blocks in 3D)

- **Xprepro**

  - External tool

  - To create a complex geometry but with a regular hexahedral mesh

- **Or use of a mesh generator tool linked with TRUST:**

  - Salomé

  - Gmsh

Possible meshing tools (2/3)

- ## Mesh generator tools :
  - ICEM (Ansys) generates a file at Trio_U format
  - TRUST reads .unv files from I-DEAS*
  - TRUST reads 2D/3D meshes from old tools of Fluent (Gambit/TGrid)
  - TRUST reads « .med » meshes from Salomé or Gmsh

- ## Form factors (view factors for the radiation model):
  - Link between Ansys and TRUST

*:tetrahedral meshing only

Possible meshing tools (3/3)

- Presentation of 3 mesh generators: **Xprepro**, **Salomé**, **Gmsh**

- Exercise with 1 mesh generator according to your needs

Mesh generator	Xprepro	Salomé	Gmsh	Other (ICEM,...)
Availability	Free	Free	Free	License
TRUST discretization	VDF	VEF	VEF	VEF
TRUST package	Yes	No	Yes	No
TRUST tutorial	Yes	Yes	Yes	No
Support	triou@cea.fr	support-salome@cea.fr	gmsh@geuz.org	

Mesh generators (2/4)

- Possible meshing tools
- **Xprepro**
- Salomé
- Gmsh

Xprepro (1/6)

Modeling/mesh tool created by the TRUST team
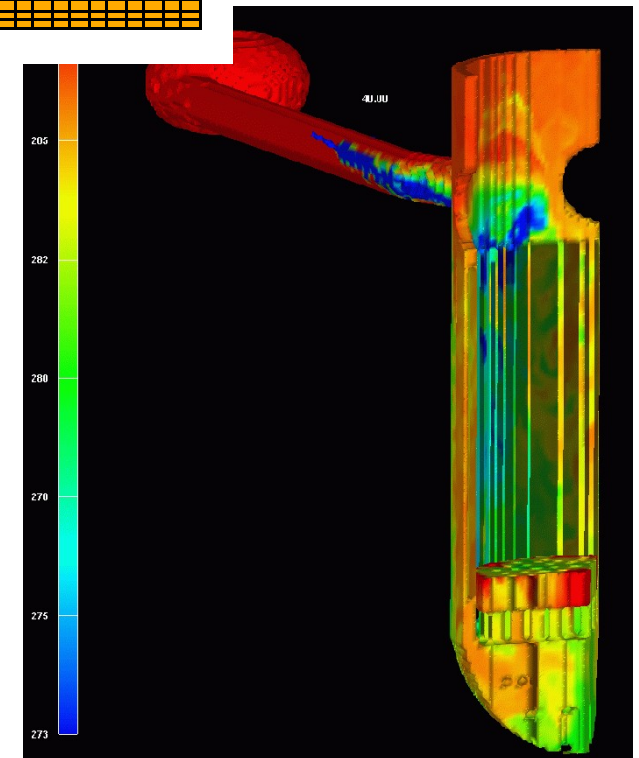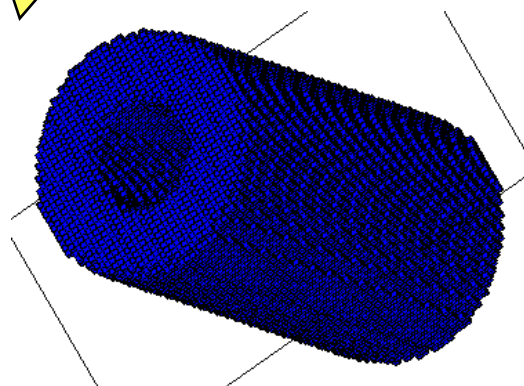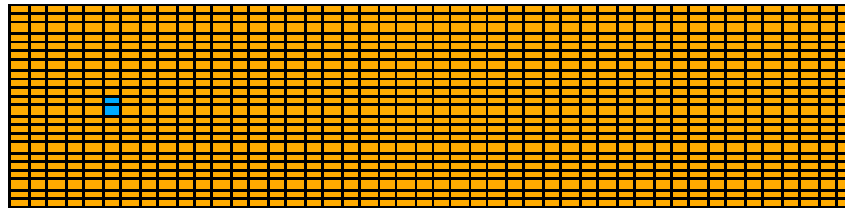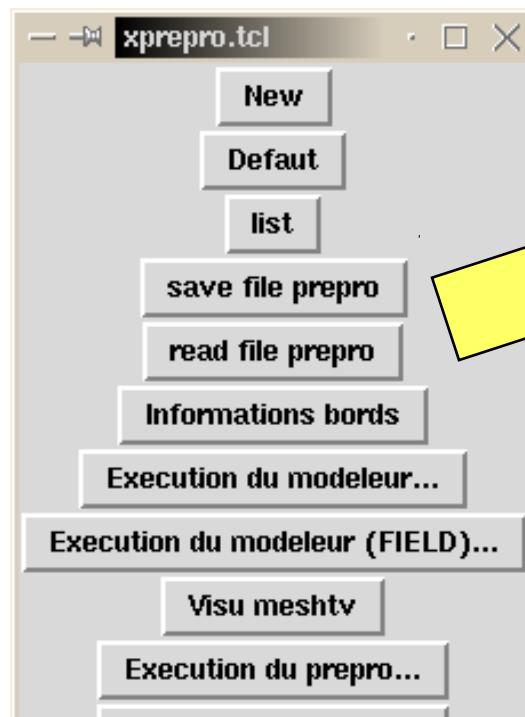
Xprepro (2/6)

- 3 ways to start with the GUI :
  - New : Begin from scratch
  - Default : Start from a parallelepiped
  - Examples :
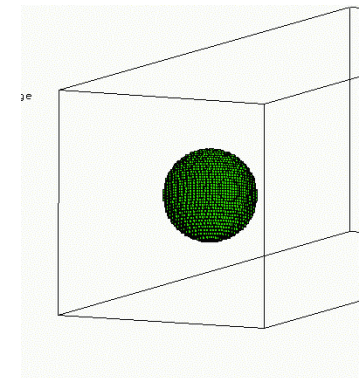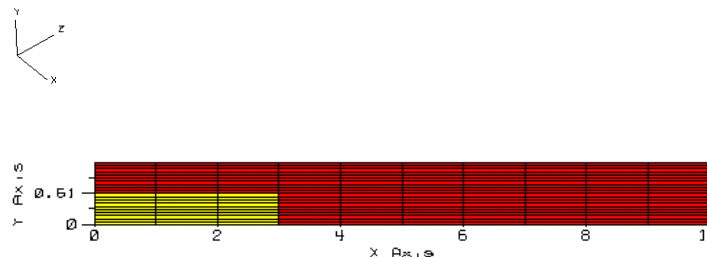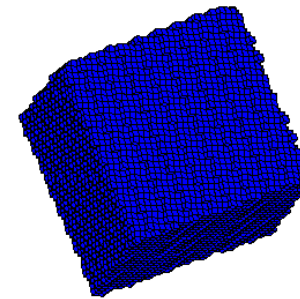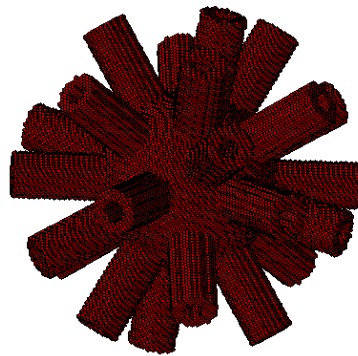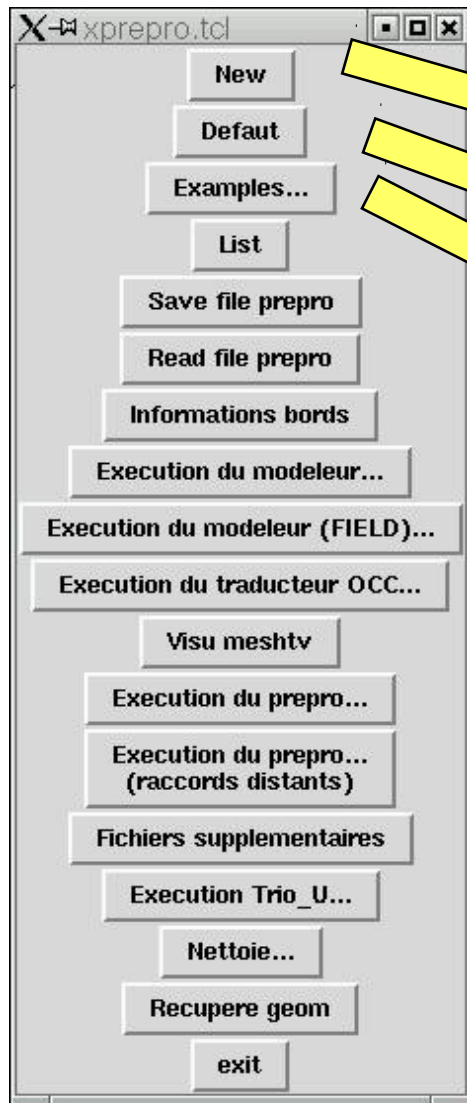
Xprepro (3/6)

- **GUI typical working sequence:**
  - Choice of the initial geometry
  - Edit the dimensions file
  - Work into in the view-list
  - Build the model
  - Visualize the pre-mesh
  - Build the final mesh
  - Test the .geom mesh with TRUST
  - Move files into your study
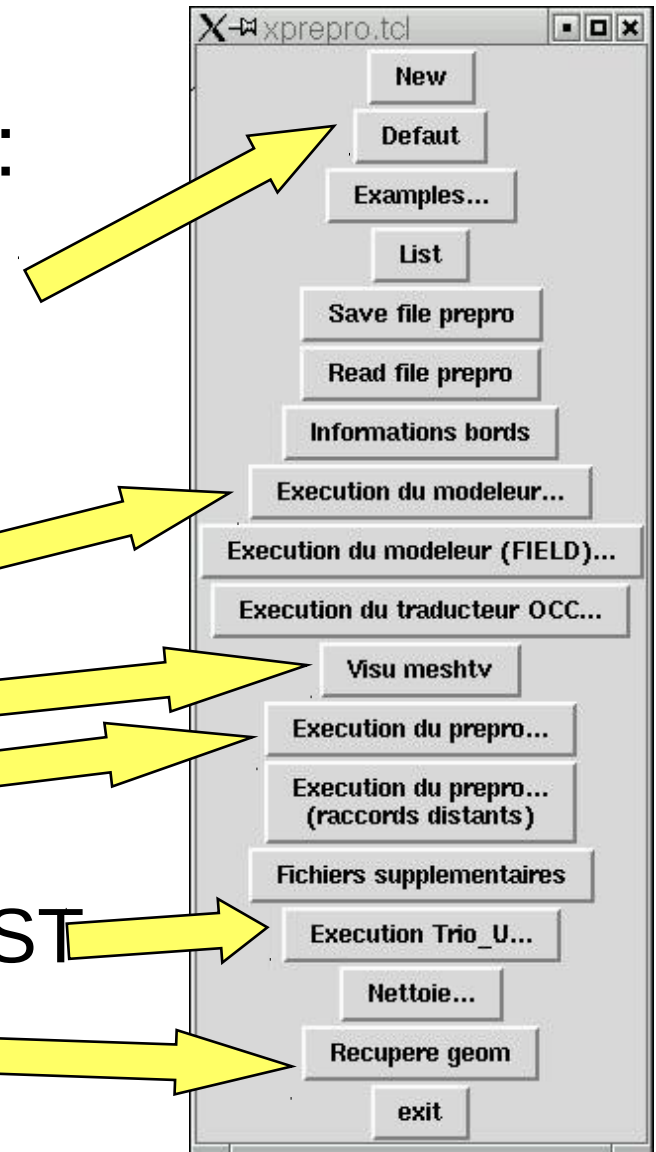
Xprepro (4/6)

- **The GUI Viewlist contains:**
  - **The pre-mesh**
    - The grids according X,Y,Z
    - The number of pts Nx, Ny, Nz
  - **Shapes definition**
    - The name
    - The coordinates
    - Take care of the definition order (read from top to bottom)
  - **Some comments (COMM)**

The GUI window "viewlist" contains:

```
-1 "" tailles nx = 4  ny = 4  nz = 4    Modify

0 "maillage" (Comm)
1 "dx" Maillage_x_regulier XMIN = xomin  XMAX =
2 "dy" Maillage_y_regulier YMIN = yomin  YMAX =
3 "dz" Maillage_z_regulier ZMIN = zomin  ZMAX =
4 "remplissage du domaine" (Comm)
5 "remplissage du domaine" Pave XMIN = xomin
6 "definition des bords du doamine" (Comm)
7 "Bord arriere" Pave XMIN = xomin-eps  XMAX =
8 "Bord avant" Pave XMIN = xomin-eps  XMAX =
9 "bord gauche" Pave XMIN = xomin-eps  XMAX =

add    edit    copy    move    delete    exit
```

Xprepro (5/6)

Main features:

- Tool to create the geometric model of the domain to mesh

- This model does not depend of the mesh

- Model can be parameterized (variables can be used to define the dimensions of the model)

- A language can be used to modify/duplicate several parts of the model

- Tool to create a 2D or 3D structured mesh of the domain for a VDF calculation

Xprepro (6/6)

- **Other features:**
  - Once the model is finished, visualization of a pre-mesh
  - We can create sub-zones (group of several cells)
  - We can partition the domain with Xprepro for // calculation (obsolete feature)

- **Xprepro is made of:**
  - A GUI written in Tcl/Tk
  - A fortran program
    - Built and compiled during model and mesh phases

Mesh generators (3/4)

- Possible meshing tools
- Xprepro
- **Salomé**
- Gmsh

Salomé (1/2)
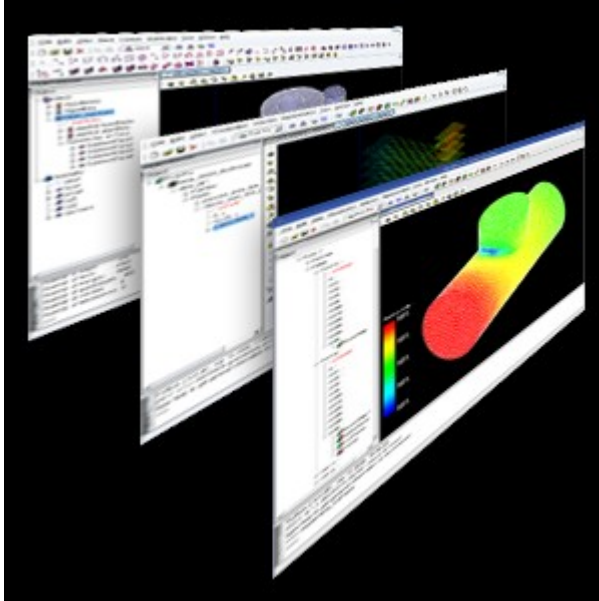
Salomé: An OpenSource platform (CEA, EDF, OpenCascade,...) which provides a 2D/3D element mesh generator. It is available here for download:

http://www.salome-platform.org

-> **Salomé** is not provided in the TRUST package

-> To have a full training session, or receive support for install or use, see:

http://www.salome-platform.org/service-and-support

support-salome@cea.fr

Short description soon to use the Geometry and Mesh modules....

Salomé (2/2)

NB: Xprepro → Salomé

- Geometric model
  - Import the Xprepro CAD (python file) or build the CAD in Salomé
- Boundary definition
  - Create a geometric group
  - Work with the OCC viewer
- Mesh phase
  - Define the surface mesh then the volume mesh (ex: Netgen)
  - Detect/suppress the duplicated nodes
- Mesh files
  - MED export from Salomé
  - Read the mesh in TRUST data file (**Lire_MED** keyword)

Mesh generators (4/4)

- Possible meshing tools
- Xprepro
- Salomé
- **Gmsh**

Gmsh (1/3)
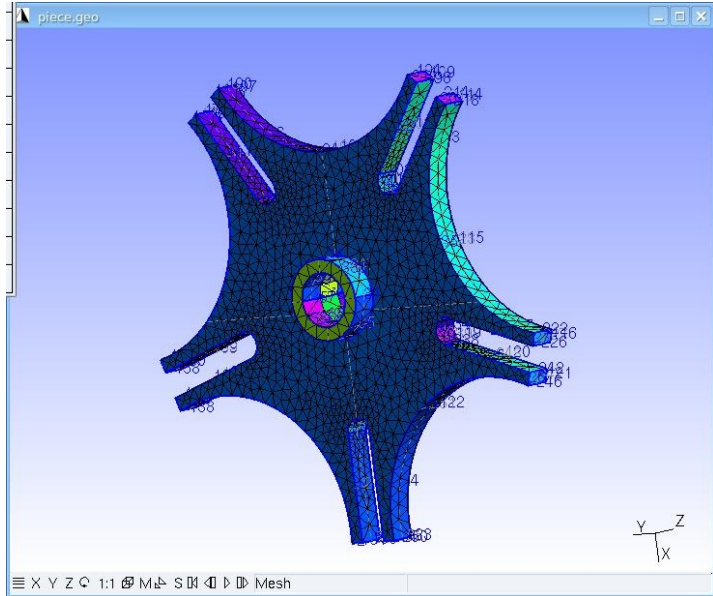
Gmsh: A 2D/3D finite element mesh generator available here:

http://www.geuz.org/gmsh

-> The documentation is here:

http://geuz.org/gmsh/doc/texinfo/gmsh.html

-> Gmsh is downloaded and built during the TRUST install. There are tutorials and examples under:

$TRUST_ROOT/exec/gmsh/share/doc/gmsh/tutorial

$TRUST_ROOT/exec/gmsh/share/doc/gmsh/demos

-> Support on Gmsh at gmsh@geuz.org

Best is to start from a .geo file of one of the previous examples. Run Gmsh with:

    gmsh *file.geo*

Edit and change your .geo file and use the **Reload** button to update the geometry visualization.

Gmsh (2/3)

Example of .geo file

// Variables definition

lc = 0.02;

// First cell size (used when points

// are defined):

lc1 = lc * 8;

// Second cell size

lc2 = lc / 2;

// Circle diameter

D = 0.14 ;

E = D ;

param = 1;

H = param * 10 * D ;

X = param * 5 * D ;
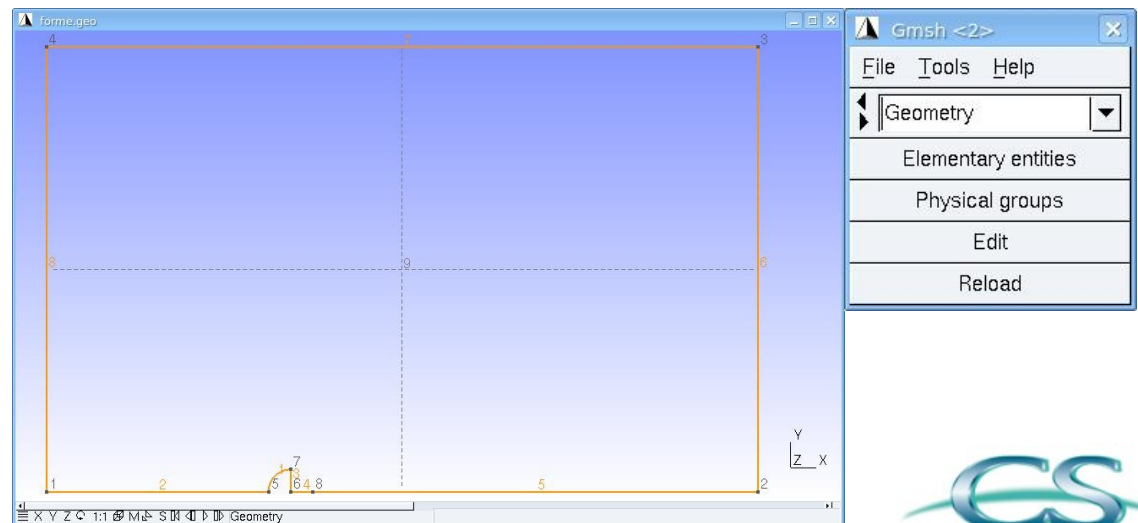
L = param * 10 * D + X + E;

// Points definition

Point(1) = {0,0,0,lc1};

Point(2) = {L,0,0,lc1};

Point(3) = {L,H,0,lc1};

Point(4) = {0,H,0,lc1};

Point(5) = {X,0,0,lc2};

Point(8) = {X+E,0,0,lc2};

// Lines definition

Line(2) = {1,5}; // 2 points

Line(5) = {8,2};

Line(6) = {3,2};

Line(7) = {3,4};

Line(8) = {4,1};

// 1/4 Circle definition

Point(6) = {X+D/2,0,0,lc2}; // Center

Point(7) = {X+D/2,D/2,0,lc2};

// 3 points for the circle arc (P1,Center,P2):

Circle(1) = {5,6,7};

Line(3) = {7,6};

Line(4) = {6,8};

// A circle arc is STRICTLY smaller than Pi

// Naming the boundaries is MANDATORY

// and it is thanks to the

// Physical Line (use Lines or Circle to define it)

// DO NOT USE LINE LOOPS !!!!

Physical Line("Shape") = {1,3};

Physical Line("Axis") = {2,4,5};

Physical Line("Outlet") = {6};

Physical Line("Top") = {7};

Physical Line("Inlet") = {8};

// A lineloop is a loop on several lines

// for defining/orienting a surface

// Use negative lines to reverse the

// orientation of the line

Line Loop(1) = {2,1,3,4,5,**-6**,7,8};

// The surface will use the lineloop

Plane Surface(1) = {1};

// Naming the domain is MANDATORY

Physical Surface("domain") = {1};

Gmsh (3/3)

Mesh and import

Switch from Geometry to Mesh
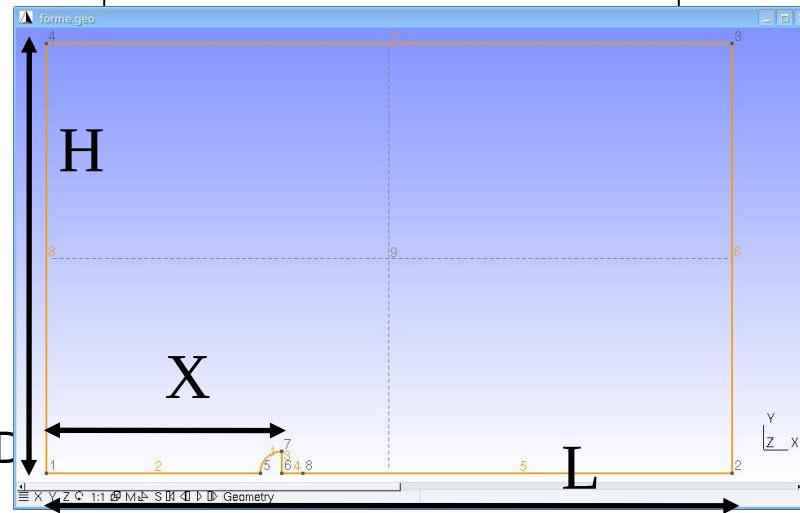
2D mesh (in 3D, 3D mesh AND do not forget to optimize 3D after that)
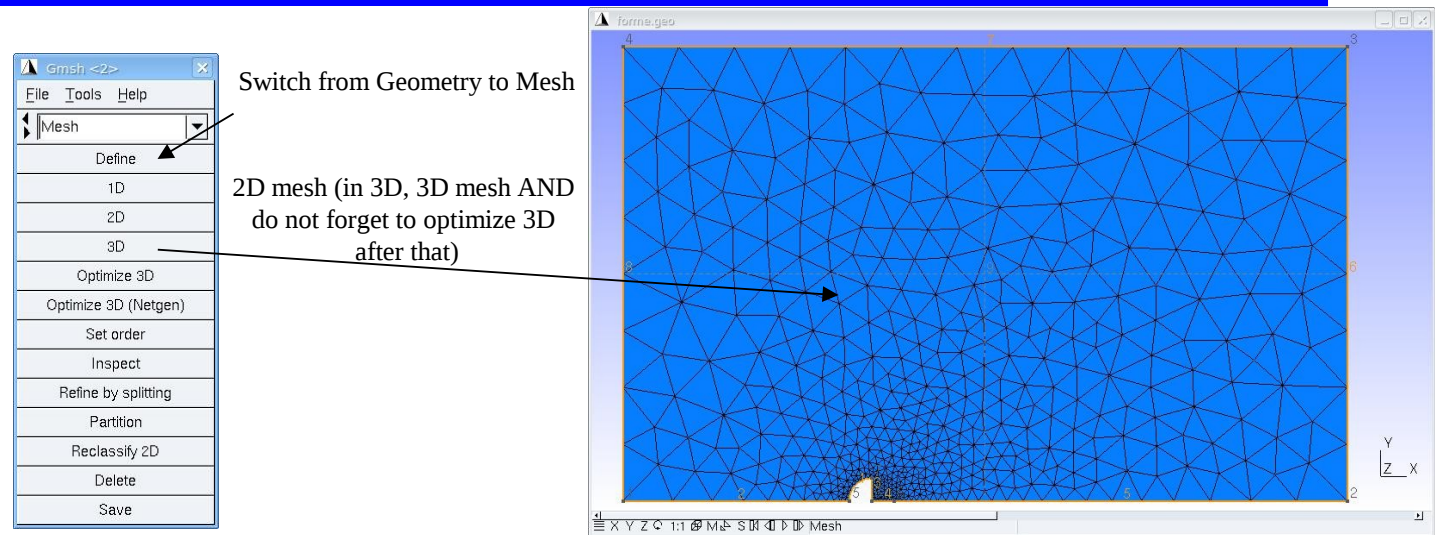
Then, export the mesh to a MED format file (File->Save As, format MED) and <u>DO NOT</u> select "Save All" because points could be saved. <u>Important:</u> Check that your mesh is created with the command (if nothing appears, you forgot to name boundaries and/or the domain with the Physical keywords):

gmsh *file.med*

To import the mesh, add in the TRUST datafile:

Dimension 2

Domaine dom

Lire_MED family_names_from_group_names dom mesh_name *file.med # By default, the mesh name is the name of the file, so there mesh_name=file #*

If you have created several domains into the same Gmsh mesh, you will add cause the different domains in the Gmsh mesh file are seen as subzones.

Domain second_dom

Create_domain_from_sous_zone { **domain_final** second_domain **par_sous_zone** sub_zone_name **domaine_init** dom }

Practice

Exercise 6: Meshing tools

VEF calculation with TRUST

- Run Salomé exercise in the tutorial
- Run Gmsh exercise in the tutorial

Run Xprepro exercise in the tutorial if one is interested by a VDF calculation with TRUST

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TRUST/TrioCFD support (1/2)

Subscribe to the TrioCFD newsletters (diffusion list):

- Users (1 mail/trimester) http://saxifrage:3500/wws/info/trio_u_annonces
- Developers (1 mail/week) http://saxifrage:3500/wws/info/trio_u_dev

Download new versions from sourceforge site:

- TRUST: http://sourceforge.net/projects/trust-platform/files/
- TrioCFD: http://sourceforge.net/projects/triocfd/files/

See recent research publications related to TrioCFD project:

- Web site: http://www-trio-u.cea.fr

Hot line

- **triou@cea.fr**
- Céline CAPITAINE   01 69 08 42 68 (Saclay bât 451 pièce 50)
- Marthe ROUX   01 69 08 00 02 (Saclay bât 451 pièce 50)

TRUST/TrioCFD support (2/2)

- A release every 6 months:

  - Linux version only
  - Installed on several CEA clusters, TGCC/CCRT and CINES
  - Installation by users or TRUST/TrioCFD support

- Documentation available under $TRUST_ROOT/doc/TRUST directory else ask it to CEA project leaders:

  - **TRUST_and_TrioCFD_presentation.pdf** (these slides)
  - **TRUST_tutorial.pdf**   TRUST/TrioCFD/Meshing exercises
  - **Models_Equations_TRUST.pdf**   "Methodology for incompressible single phase flow"
  - **Best_Practice_TRUST.pdf**   "Validation of Trio_U code"
  - **User_Manual_TRUST.pdf**   "User Manual TRUST/TrioCFD"
  - **HowTo_Validation.pdf**   "Organisation of TrioCFD validation data base"
  - **Manuel_Xprepro.pdf**   "User Manual Xprepro"
  - **Developer_TRUST_presentation.pdf**   TRUST development Presentation

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- **Examples of data files**

Examples of data files (1/3)

```
#  Front Tracking calculation #
dimension 3

# Generic problem used for Front Tracking calculation #
Probleme_FT_Disc_gen pb
Domaine DOM
# BEGIN MESH #
Mesh DOM
{
        Pave pave1
        {
                        origine 0. 0. 0.
                        longueurs 0.04 0.04 0.06
                        nombre_de_noeuds 11 11 16

        }
        {

                        bord paroi X = 0.   0. <= Y <= 0.04 0. <= Z <= 0.06
                        bord paroi X = 0.04 0. <= Y <= 0.04 0. <= Z <= 0.06
                        bord paroi Y = 0.   0. <= X <= 0.04 0. <= Z <= 0.06
                        bord paroi Y = 0.04 0. <= X <= 0.04 0. <= Z <= 0.06
                        bord bas   Z = 0.   0. <= X <= 0.04 0. <= Y <= 0.04
                        bord haut  Z = 0.06 0. <= X <= 0.04 0. <= Y <= 0.04

        }
}
# END MESH #
# BEGIN PARTITION
Partition DOM
{
        Partitionneur tranche { tranches 2 1 1 }
        Larg_joint 2
        Nom_Zones DOM
}
End
END PARTITION #
# BEGIN READ
Scatter DOM.Zones dom
END SCATTER #
```

```
VDF dis
Schema_Euler_explicite  sch
Read sch
{
        tinit 0.
        tmax  0.1
        dt_min 1.e-7
        dt_max 0.5e-2
        dt_impr 10.
        dt_sauv 100
        seuil_statio -1
}
# First phase: liquid #
Fluide_Incompressible liquide
Read liquide
{
        mu  Champ_Uniforme 1 0.282e-3
        rho Champ_Uniforme 1 1000.
}
# Second phase: gas #
Fluide_Incompressible gaz
Read gaz
{
        mu  Champ_Uniforme 1 0.282e-3
        rho Champ_Uniforme 1 100.
}
```


session   159
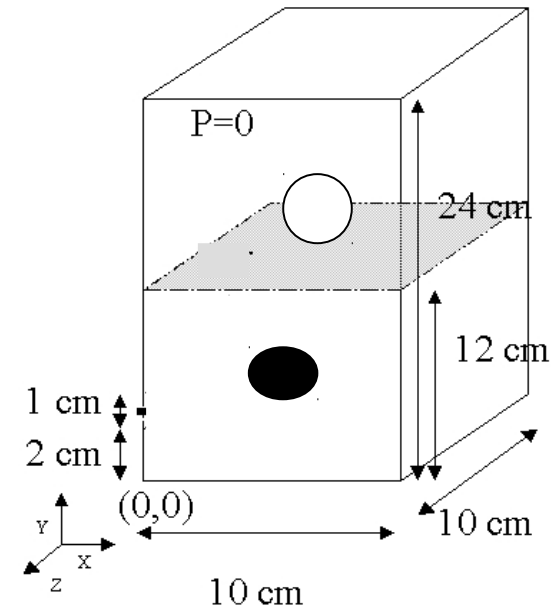
Front Tracking calculation (2/4)

 # Definition of the two phase media #
Fluide_Diphasique fluide
Read fluide
{
    # Give a number for each phase #
    fluide0 liquide
    fluide1 gaz
    # Surface tension #
    sigma champ_uniforme 1 0.05
}
 # Add a constituent #
Constituant constituant
Read constituant
{
    diffusivite Champ_Uniforme 1 1e-6
}
 # Gravity field #
Champ_Uniforme gravite
Read gravite 3 0. 0. -9.81
Associate fluide gravite

 # Navier Stokes equation #
Navier_Stokes_FT_Disc   hydraulique
 # One equation for the two phase flow interface #
Transport_Interfaces_FT_Disc   interf
 # One equation for a moving body #
Transport_Interfaces_FT_Disc   body
 # One equation for the constituent #
Convection_Diffusion_Concentration concentration

Associate pb hydraulique
Associate pb interf
Associate pb body
Associate pb concentration
Associate pb DOM
Associate pb sch

Associate pb fluide
Associate pb constituant
Discretize pb dis
 # Define the front tracking problem #
Read pb
{
    hydraulique
    {
        # Turbulence model needed and zeroed for laminar flow #
        modele_turbulence sous_maille_wale {
            Cw 0 **turbulence_paroi negligeable**
        }
        # Iterative method to solve the pressure linear system with a non-constant matrix #
        solveur_pression GCP { **precond ssor** { **omega** 1.5 } **seuil** 1e-12 **impr** }
        convection { **quick** }
        diffusion { }
        conditions_initiales { **vitesse champ_uniforme** 3 0. 0. 0. }
        # Relation beetween Navier Stokes equation and interface equations #
        equation_interfaces_proprietes_fluide interf *# The velocity field moves the gas-liquid interface #*
        equation_interfaces_vitesse_imposee body *# The body has an imposed velocity field, so moves the fluid #*
        boundary_conditions
        {
         haut **Sortie_libre_rho_variable champ_front_uniforme** 1 0. *# Outlet boundary condition for FT model #*
         paroi **paroi_fixe**
         bas **Frontiere_ouverte_vitesse_imposee champ_front_uniforme** 3 0.0 0.0 0.001
        }
    }

Front Tracking calculation (3/4)

```
interf
{
    # Definition of the transport method of the interface: velocity from the
    Navier Stokes equation #
    methode_transport vitesse_interpolee hydraulique
    # Initial position of the water-gas interface and a drop of water #
    conditions_initiales {
        fonction z-0.03-((x-0.02)^2+(y-0.02)^2)*10 ,
        fonction ajout_phase0 (x-0.02)^2+(y-0.02)^2+(z-0.045)^2-(0.01)^2
    }
    # Options for the meshing algorithm #
    iterations_correction_volume 1
    n_iterations_distance 2
    remaillage {
                pas 0.000001 nb_iter_remaillage 1
                critere_arete 0.35 critere_remaillage 0.2
                pas_lissage 0.000001 lissage_courbure_iterations 3
                lissage_courbure_coeff -0.1 nb_iter_barycentrage 3
                relax_barycentrage 1 facteur_longueur_ideale 0.85
                nb_iter_correction_volume 3
                seuil_dvolume_residuel 1e-12
    }
    # Algorithm for the collision algorithm between interfaces #
    collisions
    {
        active  juric_pour_tout
        type_remaillage Juric { source_isovaleur indicatrice }
    }
    # Boundary condition, variable contact angle is possible #
    boundary_conditions
    {
                paroi Paroi_FT_disc symetrie
                haut  Paroi_FT_disc symetrie
                bas   Paroi_FT_disc symetrie
    }
}
```

```
body
{
        # Initial position of the moving body #
        conditions_initiales { fonction -(((x-0.02))^2+((y-0.02)/0.6)^2+((z-
        0.02)/0.6)^2-(0.015^2)) }
        remaillage {  pas 1e8  }
        boundary_conditions
        {
                        haut  Paroi_FT_disc symetrie
                        paroi Paroi_FT_disc symetrie
                        bas   Paroi_FT_disc symetrie
        }
        # 2 methods to move the body: velocity(x,y,z)=f(x,y,z) or
        x(t),y(t),z(t)=f(t),g(t),h(t) #
        methode_transport vitesse_imposee
            -(y-0.02)*10    (x-0.02)*10  0.
}
# Constituent equation #
concentration
{
        diffusion { negligeable }
        convection { quick }
        conditions_initiales { concentration champ_fonc_xyz DOM 1 EXP(-((x-
        0.02)^2+(y-0.02)^2+(z-0.03)^2)/0.03^2) }
        boundary_conditions {
          haut  frontiere_ouverte C_ext Champ_Front_Uniforme 1 0.
          paroi paroi  # Concentration flux = 0 #
          bas   paroi
        }
}
```

Front Tracking calculation (4/4)

```
Postraitement
{
        Sondes {
                    vitesse vitesse periode 1.e-7 point 1 0.02 0.02 0.03
                    pression pression periode 1.e-7 point 1 0.02 0.02 0.03
                    indicatrice_interf indicatrice_interf periode 1.e-7 point 1 0.02 0.02 0.03
        }
        Champs dt_post 0.05
        {
                    indicatrice_interf
                    concentration
        }
}
liste_postraitements
{
        # Another keywords to post process FT results #
        Postraitement_ft_lata liquid_gas
        {
                    dt_post 0.05 nom_fichier liquid_gas
                    format binaire print
                    champs sommets { vitesse }
                    champs elements
                    {
                                distance_interface_elem_interf
                                distance_interface_elem_body
                                indicatrice_interf
                                pression
                                concentration
                                vitesse
                    }
                    # Post process the moving grid of the interface #
                    interfaces interf {
                        champs sommets { courbure vitesse }
                    }
```

```
        }
        Postraitement_ft_lata body
        {
                    dt_post 0.05
                    nom_fichier body
                    format binaire
                    print
                    interfaces body {
                        champs sommets { courbure }
                    }
        }
    }
}
Solve pb
End
```

Practice

Exercise 7: Tank Filling 3D

Examples of data files (2/3)

- Front Tracking calculation
- **Quasi compressible example**
- Genepi+ data file

Quasi compressible example (1/5)

```
dimension 2
Domaine dom_fluid
Mesh dom_fluid {

Pave Entree1              {

        Origine 0. 0.

        Nombre_de_Noeuds 4 3

        Longueurs 0.6  0.4

        }

        {

        Bord inlet1  Y  =  0.      0. <= X <= 0.6

        Bord wall    X  =  0.      0. <= Y <= 0.4

        Bord wall    X  =  0.6     0. <= Y <= 0.4

        } ,

Pave Sortie1              {

        Origine 0. 5.4

        Nombre_de_Noeuds 4 3

        Longueurs 0.6  0.4

        }

        {

        Bord outlet1 Y  =  5.8     0. <= X <= 0.6

        Bord wall    X  =  0.      5.4 <= Y <= 5.6

        Bord wall    X  =  0.6     5.4 <= Y <= 5.8

        Bord P_imp   X  =  0.      5.6 <= Y <= 5.8

        } ,

Pave Entree2              {

        Origine 1. 0.

        Nombre_de_Noeuds 4 3

        Longueurs 0.6  0.4

        }
```

```
        {

        Bord inlet2  Y  =  0.       1. <= X <= 1.6

        Bord wall    X  =  1.       0. <= Y <= 0.4

        Bord wall    X  =  1.6      0. <= Y <= 0.4

        } ,

Pave Sortie2            {

        Origine 1. 5.4

        Nombre_de_Noeuds 4 3

        Longueurs 0.6  0.4

        }

        {

        Bord outlet2 Y  =  5.8      1.  <= X <= 1.6

        Bord wall    X  =  1.       5.4 <= Y <= 5.8

        Bord wall    X  =  1.6      5.4 <= Y <= 5.6

        Bord P_imp   X  =  1.6      5.6 <= Y <= 5.8

        } ,

Pave Enceinte          {

        Origine 0. 0.4

        Nombre_de_Noeuds 9 26

        Longueurs 1.6  5.

        }

        {

        Bord wall    Y  =  0.4        0.6 <= X <= 1.

        Bord wall    Y  =  5.4        0.6 <= X <= 1.

        Bord wall    X  =  0.         0.4 <= Y <= 5.4

        Bord wall    X  =  1.6        0.4 <= Y <= 5.4

        }

}

Trianguler_fin dom_fluid  # Triangulate the mesh #
```

TRUST coupled with Cathare via ICoCo

Quasi compressible example (2/5)

```
Schema_Euler_implicite sch
Read sch
{
        tinit 0.
        tmax 10.
        dt_min 1.e-6
        dt_max 0.01
        dt_impr 0.01
        dt_sauv 1000.0
        seuil_statio 1.e-6
        # Options related to implicit scheme #
        facsec 20
        facsec_max 500
        Solveur Piso
        {
            # Convergence threshold for the iterative method
#
          # (by default GMRES) to solve the unsymmetric #
          # linear system #
            seuil_convergence_solveur 1.e-6
        }
}

# Definition of the a thermalhydraulic problem #
# using the Quasi-compressible model #
Pb_thermohydraulique_QC pb1

# VEF discretization selected #
VEFPreP1B dis

# Gravity defined as a uniform field #
Champ_Uniforme gravite
Read gravite 2 0 -9.81
```

```
# Define the media, helium gas #
Fluide_Quasi_Compressible helium
Read helium
{
        # Pressure in Pa #
        pression 7000000.

        # Sutherland law for viscosity and conductivity #
        Sutherland mu0 1.6E-5 T0 273.15 Slambda 235. C 235.

        # Ideal gas law #
        loi_etat gaz_parfait {
            Prandtl 1.
            # Specific heat at constant pressure #
            Cp 5193.
            # Cv, specific heat at constant volume given by gamma=Cp/Cv #
             gamma 1.666
        }

        # Keyword for open flow (Neuman condition ), total pressure is constant #
        traitement_pth constant
}

# Create link between objects #
Associate helium gravite
Associate pb1 dom_fluid
Associate pb1 sch
Associate pb1 helium
Discretize pb1 dis
```

6

La force de l'innovation

Quasi compressible example (3/5)

```
# Definition of four surface domains #
# each extracted from a boundary of the problem #
domaine entree1
extraire_surface
{
        domaine entree1
        probleme pb1
        avec_certains_bords 1 inlet1
}

domaine entree2
extraire_surface
{
        domaine entree2
        probleme pb1
        avec_certains_bords 1 inlet2
}

domaine sortie1
extraire_surface
{
        domaine sortie1
        probleme pb1
        avec_certains_bords 1 outlet1
}

domaine sortie2
extraire_surface
{
        domaine sortie2
        probleme pb1
        avec_certains_bords 1 outlet2
}
```

```
Read pb1
{
        Navier_Stokes_QC
        {
                solveur_pression petsc cholesky { } # Direct solver, pressure matrix is constant #
                convection { muscl }
                diffusion { }
                conditions_initiales { vitesse Champ_Uniforme 2  47.  0. }
                boundary_conditions {
                                # Dirichlet boundary condition mass flow rate #
                                # Ch_front_input : ICOCO coupling field #
                                inlet1  frontiere_ouverte_rho_u_impose ch_front_input {
                                    nb_comp 2 nom rho_u_entree1 probleme pb1
                                }
                                inlet2  frontiere_ouverte_rho_u_impose ch_front_input {
                                    nb_comp 2 nom rho_u_entree2 probleme pb1
                                }
                                outlet1 frontiere_ouverte_rho_u_impose ch_front_input {
                                    nb_comp 2 nom rho_u_sortie1 probleme pb1
                                }
                                outlet2 frontiere_ouverte_rho_u_impose ch_front_input {
                                    nb_comp 2 nom rho_u_sortie2 probleme pb1
                                }
                                P_imp   Frontiere_ouverte_pression_imposee
                                                Champ_front_Uniforme 1 70.e5
                                wall    paroi_fixe
                }
                # Definition of a source term (pressure loss) #
                sources {
                  Perte_Charge_isotrope {
                    diam_hydr champ_fonc_txyz dom_fluid  1 1.4-1.3908*(y]1.4)*(y[4.4)
                    lambda 4*((16/Re)$(0.079/(Re^0.25))$0.003)
                  }
                }
        }
```

Quasi compressible exemple (4/5)

```
Convection_Diffusion_chaleur_QC
{
        diffusion { }
        convection { muscl }
        conditions_initiales { Temperature Champ_Uniforme 1 673. }
        boundary_conditions {

        # Boundary conditions for temperature #
        # ch_front_input coupling keyword #
        inlet1 frontiere_ouverte t_ext ch_front_input {
            nb_comp 1 nom temperature_entree1 probleme pb1
        }
        inlet2 frontiere_ouverte t_ext ch_front_input {
            nb_comp 1 nom temperature_entree2 probleme pb1
        }
        outlet1 frontiere_ouverte t_ext ch_front_input {
            nb_comp 1 nom temperature_sortie1 probleme pb1
        }
        outlet2 frontiere_ouverte t_ext ch_front_input {
            nb_comp 1 nom temperature_sortie2 probleme pb
        }
        # Outlet boundary condition for temperature #
        P_imp Frontiere_ouverte T_ext champ_front_uniforme 1 700.
        # Zero heat flux #
        wall paroi_adiabatique
        }
        # Heat source term #
        sources
        {
            Puissance_thermique champ_fonc_xyz dom_fluid 1
2400e6*2/3./10./(3*3.1416*0.7*0.7)*0.6/1.8*1.53*(y]1.4)*(y<4.4)
        }
}
```

```
Postraitement
{
            # As usual, just notice the masse_volumique keyword
            for the volume mass field #
            Sondes
            {
            sonde_pression1 pression periode 0.05 segment 31
0.1 0   0.1 5.8
            sonde_pression2 pression periode 0.05 segment 31
1.5 0   0.1 5.8
            sonde_vitesse1 vitesse periode 0.05 segment 31   0.1
0   0.1 5.8
            sonde_vitesse2 vitesse periode 0.05 segment 31   1.5
0   0.1 5.8
            sonde_temperature1 temperature periode 0.05 segment
31   0.1 0   0.1 5.8
            sonde_temperature2 temperature periode 0.05 segment
31   1.5 0   0.1 5.8
            sonde_rho1 masse_volumique periode 0.05 segment
31   0.1 0   0.1 5.8
            sonde_rho2 masse_volumique periode 0.05 segment
31   1.5 0   0.1 5.8

            }

            format lata
            Champs dt_post 0.05
            {
                        pression elem
                        pression som
                        vitesse elem
                        temperature elem
                        temperature faces
                        masse_volumique elem

            }
}
```

Quasi compressible example (5/5)

```
Postraitements        # List of postprocessing blocks #
{
entree1 {
        # Restrict postprocessing on surface meshes previousluy defined #
        domaine entree1
        # Keyword to create new postprocessing fields #
        Definition_champs
        {
                    # Define a pressure surface field by Interpolating pressure #
                    # volume field on the elements of the surface mesh #
                    pressure_entree1 champ_post_interpolation
                    {
                                localisation elem
                                domaine entree1
                                source champ_post_refchamp {
                                   pb_champ  pb1 pression
                                }
                    }
                    # Define a temperature surface field #
                    temperature_entree1 champ_post_interpolation
                    {
                                localisation elem
                                domaine entree1
                                source champ_post_refchamp {
                                   pb_champ  pb1 temperature
                                }
                    }
        }
    }
}
# Same tasks for each surface meshes #
entree2 { … }
sortie1 { … }
sortie2 { … }
}
Solve pb1        # Solve the problem #
End
```

session

La force de l'innovation

Practice

Exercise 8: Low Mach number flow

Examples of data files (3/3)

- Front Tracking calculation
- Quasi compressible example
- **Genepi+ data file**

Genepi+ data file (1/4)

```
dimension 3
ecriturelecturespecial 1 # Keyword to not save .xyz file #

# Create domains #
domaine dom
domaine MAILLAGE_GENEPI
# Read a MED file (may be composed of several meshes, a
given mesh name is necessary) #
lire_med dom MAILLAGE_GENEPI tface.med
lire_med MAILLAGE_GENEPI MAILLAGE_GENEPI maigro.med

# The keyword is used to rename boundary #
regroupebord dom Wall   { WALL_01   }
regroupebord dom Entree_branche_chaude   { INLET_03   }
regroupebord dom Entree_branche_froide   { INLET_02   }
regroupebord dom Sortie   { OUTLET_04   }

ef dis  # Define the specific discretization for Genepi+ #

schema_euler_implicite sch2 # Define an implicit scheme #
Lire sch2 {
   tinit 0.0  tmax 55.0
   dt_min 0.02439 dt_max 0.02439
   dt_start dt_fixe 0.02439   # To insure the first time step is imposed #
   facsec 50000
   nb_pas_dt_max 40000
   dt_sauv 1.0  dt_impr 0.5
   seuil_statio 1e-05
   solveur implicite  {
      solveur gmres  # Iterative solver for the implicit linear system #
      {
       impr seuil 1e-08  # Threshold convergence for the solver #
       diag     # Diagonal pre-conditioning #
      }
   }
}
```

```
# Define the gravity field #
champ_uniforme gravite
Lire gravite 3 0.0 0.0 -9.80665

# Specific Genepi+ keywords: #
fluide_melange freon
Lire freon {
   type_fluide fr_114_9_12b
   init_file dump.all
}
pb_melange pb

# Link objects #
Associer freon gravite
Associer pb dom
Associer pb sch2
Associer pb freon
discretiser pb dis

# Keyword to write the domain in a LATA file to visualization purpose #
postraiter_domaine  { format lata fichier geom domaine dom }

# Keyword to define a volume porosity field and a surface porosity field #
# Here the fields are read from a MED file #
porosites_champ pb champ_fonc_med last_time betan_betae.med MAILLAGE_GENEPI
        POROSITE_2 elem 0.0
```

Old data file

Genepi+ data file (2/4)

```
Lire pb {
    # Genepi+ keywords #
    navier_stokes_melange {
     # Usual keywords for Navier Stokes #
     solveur_pression gcp
      {
        precond ssor { omega 1.5 } seuil 1e-08
      }
     convection   { generic amont }
     diffusion   { option { grad_u_transpose_partout 1 } }
     conditions_initiales {  vitesse champ_fonc_xyz dom 3 0 0 0 }
     conditions_limites
      {
        Wall symetrie
        Sortie frontiere_ouverte_pression_imposee champ_front_uniforme  1 880000.0
        # Boundary condition can also be read in MED files, here velocity profiles: #
        Entree_branche_chaude frontiere_ouverte_vitesse_imposee champ_front_med_test champ_fonc_med last_time maigro.med MAILLAGE_GENEPI VITESSE_3 som
        0.0
        Entree_branche_froide frontiere_ouverte_vitesse_imposee champ_front_med_test champ_fonc_med last_time maigro.med MAILLAGE_GENEPI VITESSE_3 som 0.0
      }
     modelisation {
        diffusion_turbulente 1
        prandtl 0.5
        faisceau
        {
           champ_rotation champ_fonc_med last_time     rotation_faisceau.med            MAILLAGE_GENEPI champ_vectoriel_1 elem 0.0
           champ_presence champ_fonc_med last_time   rotation_faisceau.med            MAILLAGE_GENEPI champ_scalaire_2 elem 0.0
           transpose_rotation
        }
        plaques_in_file plaques.data  # Definition in an external data file #
        init_file dump.all
      }
     pression_initiale champ_uniforme  1 880000
     # List of source terms : separated by comma #
     sources { source_derive , source_frottement , source_pesanteur }
    }
```

Genepi+ data file (3/4)

```
enthalpie_melange # Energy equation definition #
    {
      convection   { generic amont }
      diffusion   {  option  { grad_u_transpose_partout 1  } }
      conditions_initiales { enthalpie champ_uniforme  1 140000.0 }
      conditions_limites  {
         Wall symetrie
         Sortie frontiere_ouverte T_ext champ_front_fonc_txyz  1 1.193e5
         # An example of space dependant boundary condition, hear an Heaviside function for enthalpy: #
         Entree_branche_chaude frontiere_ouverte_enthalpie_imposee champ_front_fonc_txyz 1 1.193e5-400*(x_gt_0.31)*(x_lt_0.32)
         Entree_branche_froide frontiere_ouverte_enthalpie_imposee champ_front_fonc_txyz  1 1.185e5+400*(x_gt_0.31)*(x_lt_0.32)
       }
     # Source terms and an example of a source term read in a file #
      sources { source_derive , source_scalaire  champ_fonc_med  last_time sourceHgros.med MAILLAGE_GENEPI scalar_1 elem 0.0 }
     # It is possible to change the default parameters of the implicit scheme in case of slow convergence of one equation #
      parametre_equation parametre_implicite  {
        solveur gmres {  impr  seuil 0.0001 diag controle_residu 1 } # controle_residu is a parameter to check the residual do not increase suddenly #
       }
    }
  postraitement
   {
    # Probes to monitor some fields, here on the cell 0 of the master process #
     sondes {
        sonde_hsat enthalpie_saturation_liquide periode 1e-06 numero_elem_sur_maitre 0
        sonde_L chaleur_latente_melange periode 1e-06 numero_elem_sur_maitre 0
      }
     format lata champs  binaire dt_post 1e-0 # binaire is useless cause it is now the default for LATA output format #
      {
        pression elem
        vitesse som
        enthalpie som
        taux_de_vide_melange elem
      }
    }
  }
Resoudre pb
```

Genepi+ data file (4/4)

```
# File plaques.data #
{
    {
                description OBSTACLE1
                champ_aire champ_fonc_med last_time          frt-singulier.med  MAILLAGE_GENEPI          AIRE_OBSTACLE_1 elem 0.
                transpose_rotation champ_rotation champ_uniforme 9
                 -1. 0. 0.
                0. 1. 0.
                0. 0. -1.
    }
    ,
    {
                description OBSTACLE2
                champ_aire champ_fonc_med last_time frt-singulier.med          MAILLAGE_GENEPI          AIRE_OBSTACLE_2 elem 0.
                transpose_rotation champ_rotation champ_uniforme 9
                1. -0. 0.
                0. 1. -0.
                0. 0. 1.
    }
    ,
    {
                description OBSTACLE3
                champ_aire champ_fonc_med last_time frt-singulier.med          MAILLAGE_GENEPI     AIRE_OBSTACLE_3 elem 0.
                transpose_rotation champ_rotation champ_uniforme 9
                0. -1. 0.
                1. 0. -0.
                0. 0. 1.
    }
}
```