Trio_U 1.7.0 user's training session





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Presentations

Trio_U (1st day AM)
 Mesh with tools (Xprepro, Salomé or Gmsh) (2nd day AM)

Automated test case with Trio U

(2nd day AM)



Practice:

• Trio U (1st day PM/2nd day PM)

Tyrepro/Salomé/Gmsh (2[™] day AM)

We provide also:

Advanced Trio_U user sessions (optional, 3rd day)

• Trio_U developer sessions (optional, 4th and 5th days)

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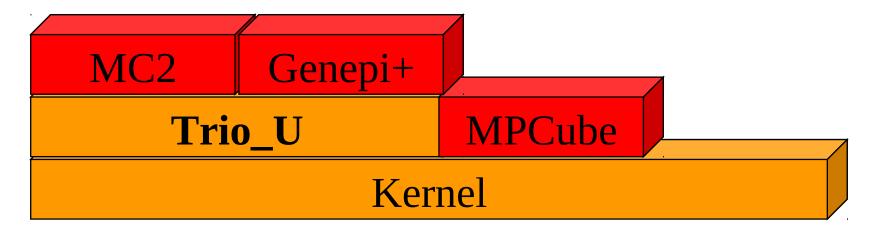
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Trio U

- CFD code for incompressible monophasic/diphasic flow
- Developed at the CEA/DEN/DANS/DM2S/STMF/LMSF laboratory
 - Lab's chief: anne.burbeau@cea.fr
 - Project leader: gauthier.fauchet@cea.fr
 - Trio_U, a software brick used by other CEA apps:







Trio_U project

- 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, //...)





Trio_U project

- 1994: start of the project
- 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)
- 12/2014 : v1.7





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Trio_U: Modeling flow (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:
 ρ=ρ(T)~ ρ,-β(T-T0)
 - Quasi-compressible model: $\rho=\rho(P,T)$ for low mach numbers

$$\begin{aligned}
&Div(\vec{u}) = 0 \\
&\frac{\partial \vec{u}}{\partial t} + \vec{u} \nabla \vec{u} = -\nabla P^* + Div(v \nabla \vec{u}) \\
&P^* = \frac{P}{\rho} + gz \\
&\frac{\partial T}{\partial t} + \vec{u} \nabla T = Div(\alpha \nabla T)
\end{aligned}$$



Trio_U: Modeling flow (2/7)

Description of the Quasi Compressible model used

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

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

• 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 $M = Mach << 1$

Set of equations solved:

$$\begin{split} \frac{\partial \rho}{\partial t} + div(\rho \vec{u}) &= 0 \\ \frac{\partial}{\partial t} (\rho u_i) + div(\rho u u_i) - \sum_{j=1}^N \frac{\partial}{\partial x_j} \left[\mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] + \frac{\partial P_1^*}{\partial x_i} &= -\rho g_i \\ P_1^* &= P_1 + \frac{2}{3} \mu div(\vec{u}) \\ P_0 &= \rho RT \\ \rho C_p \frac{dT}{dt} - \sum_{j=1}^N \frac{\partial}{\partial x_j} \left(K \frac{\partial T}{\partial x_j} \right) &= Q + \frac{dP_0}{dt} \end{split}$$

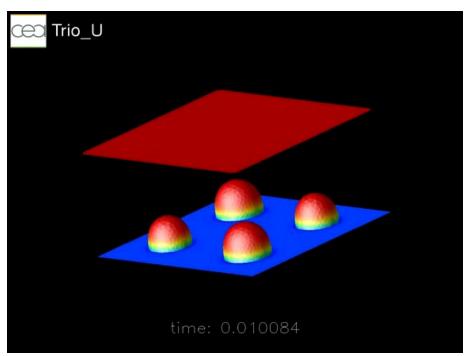




Trio_U: Modeling flow (3/7)

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

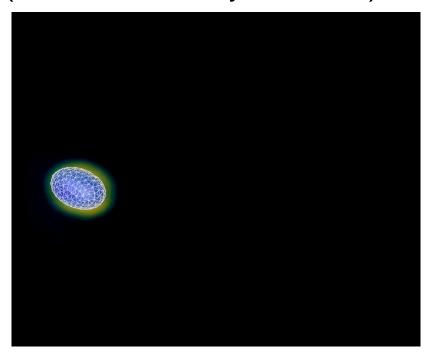




Trio_U: Modeling flow (4/7)

Front tracking model

 Can be declined in Trio_U to use an Immersed Boundary Method using IBC (Immersed Boundary Conditions)



Example of a flow around a rotating body defined by an IBC





Trio_U: Modeling flow (5/7)

- 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





Trio_U: Modeling flow (6/7)

- Heat exchange
 - Conduction
 - Radiation in transparent medium
 - Radiation in semi-transparent medium
- Transport of passive scalars $\frac{\partial C_i}{\partial t} + \vec{u} \nabla C_i = Div(D_i \nabla C_i)$
- Porous Media
 - Surface or volume porosities
 - Singular or regular pressure loss



Trio_U: Modeling flow (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 or semi implicit time schemes
- Steady state calculation obtained:
 - Either by convergence of the transient flow
 - Or by using an implicit time scheme





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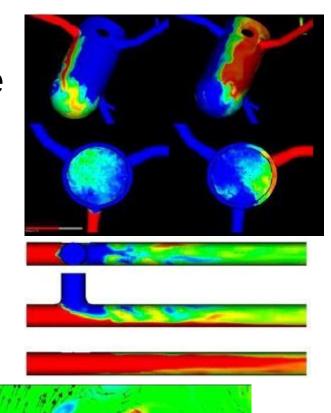
Examples of performed calculations (1/2)

- 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)



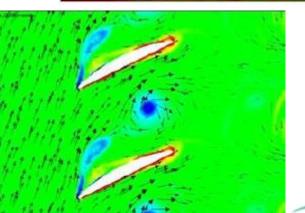




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Trio_U description

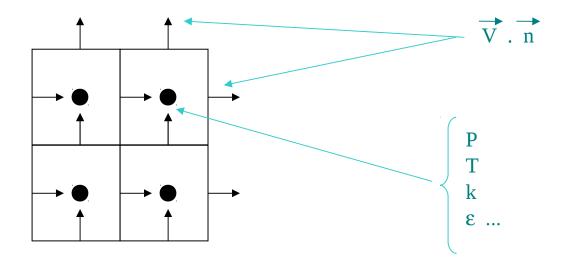
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Discretizations (1/3)

- Finite Differences Volumes (VDF)
 - Structured meshing; velocity and pressure are shifted
 - Scalar unknown is mesh centred
 - Velocity is normal at the face

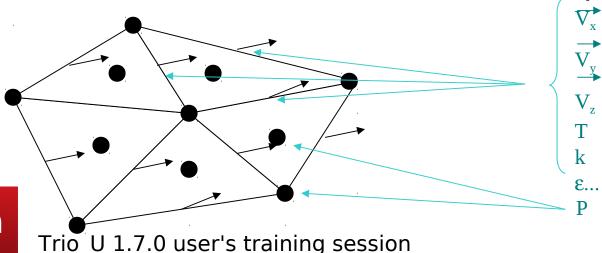






Discretizations (2/3)

- Finite Elements Volumes (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)

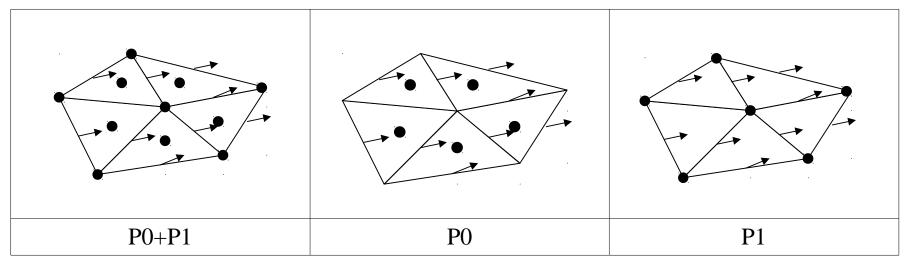




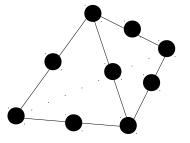
Discretizations (3/3)

Finite Elements Volumes (VEF)

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



Plus in 3D: P0+P1+Pa



11 pressure nodes per tetra:

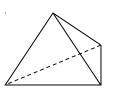
- -1 in center (P0)
- -4 on vertexes (P1)
- -6 on edges (Pa)
- -> **Useful** for flow with a strong source term & a low velocity field where P0+P1 pressure gradient P0+P1 has trouble to match the source term

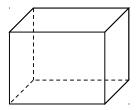


La force de l'innovation

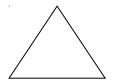
Kind of mesh permitted

Tetrahedral or hexahedral meshing for 3D cases



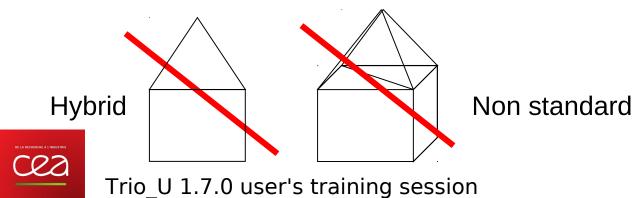


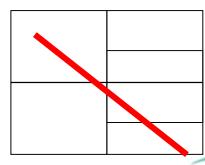
Triangular or quadrangular meshing for 2D cases





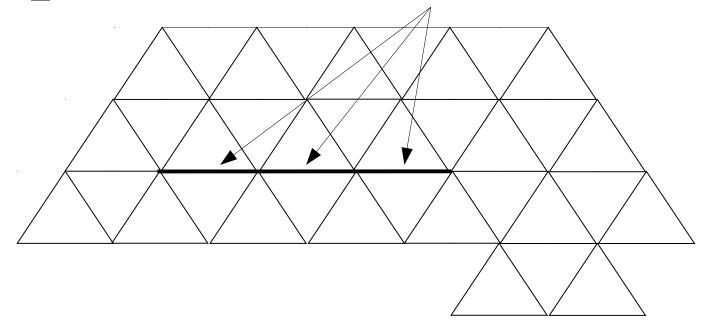
Hybrid or non standard not supported





Kind of mesh permitted

- Internal boundaries partially supported :
 - With ICEM, split faces in two and define boundaries
 - Trio_U will differentiate the two faces



Trio_U description

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





Time schemes

Explicit schemes:

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

- Euler explicit (order 1)
- Runge Kutta (order 2 or 3)
- Semi-implicit scheme:

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

- Euler semi-implicit (diffusion implicited)
- Implicit schemes (not unconditionally stable):

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

• Implicite, Piso, Simple (dynamic time step)



Convection schemes

VDF

- Quick (order 2-3)
- Centre (order 2 or 4) « centered »
- Amont (order 1) « upwind »
- VEF
 - EF_stab (order 2) « centered stabilized »
 - Muscl (order 2) « quick like »
 - Amont (order 1) « upwind »





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Available boundary conditions (Momentum)

• 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



Available boundary conditions (Energy)

• Wall:

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

• Fluid boundary:

- Imposed temperature
- No flux
- Periodic



Available boundary conditions

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



Trio_U description

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Source terms

Navier Stokes equation:

Boussinesq

$$S = \rho_0 g \beta (T - T_0)$$

Useful for small variation of volumic mass

Flow rate

$$S=Q_m$$

Pressure loss

$$S=-0.5\rho C_1U|U|/D$$

Regular pressure loss (Blasius or Cf given by the user)

Periodic channel

$$S=Q_m$$

Useful to keep constant flow rate into a periodic channel

• ...



Source terms

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 , d Ω /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

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

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



Source terms

- Energy equation:
 - Volumic heat power

S=P

- For example into a solid media
-

- Concentration equation:
 - Boussinesq

$$S = \rho_0 g \beta (C - C_0)$$

 Useful to build a two miscible fluids calculation (if the volume mass is similar). Concentration C will be equal to the fraction fluid



Trio_U description

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Trio_U linear systems

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



Solvers for linear systems

- Trio_U 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 Trio_U versions





Solvers for linear systems

- Iterative solvers (GC, GMRES,...)
 - Need a tolerance ε to be defined : $||Ax-B|| < \varepsilon$
 - Possible pitfall because it is an absolute (not a relative) value in Trio_U
 - So, check the balances!
 - Exemple: Solving pressure system for an incompressible flow Div(u)=0
 - -So, check the flow rate error in .out file
- Direct solvers (PETSc Cholesky)
 - Use it if possible





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Turbulence models

- 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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Trio_U data file description

 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
...
```



Trio_U data file description

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 example (Incompressible flow)

```
# 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 { } # Bv default, 2<sup>nd</sup> 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|| #
```

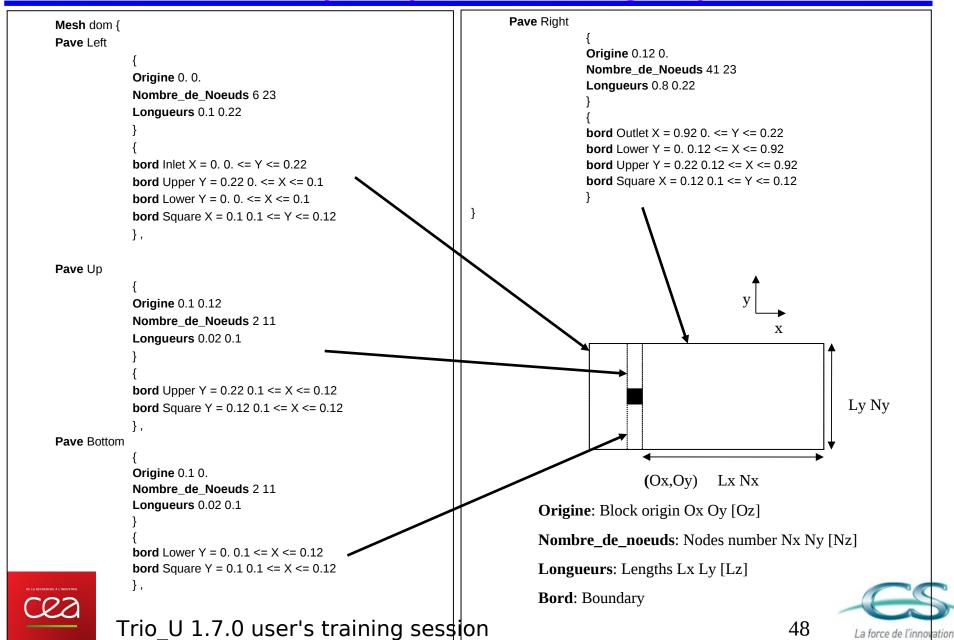
Data file example (Incompressible flow)

```
Postraitement
             # Definition of probes for 1D plot #
             Sondes
                          sonde pression
                                                     pression
                                                                                periode 0.005
                                                                                                           points 2
                                                                                                                        0.13 0.105
                                                                                                                                     0.13 0.115
                                                     vitesse
                                                                                                           points 2
                                                                                                                                      0.14 0.115
                          sonde_vitesse
                                                                                periode 0.005
                                                                                                                        0.14 0.105
                          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
                                                                                                                                     0.13 0.115
                                                     Ecart type pression
                                                                                periode 0.005
                                                                                                           points 2
                                                                                                                        0.13 0.105
             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
                                                     # By default, location is som (vertexes) #
                          vitesse
                          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 #
```

Optional keyword end

End

Data file example (Obstacle.geo)



Operations on meshes

Trio_U keywords:

- **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)
- ...



Probes: "Nodes" option

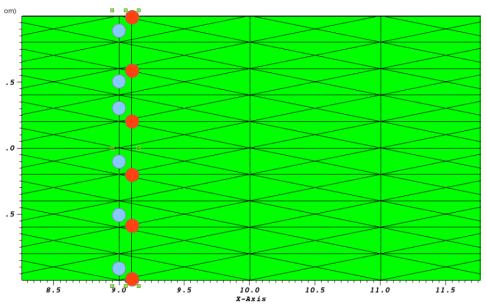
"**Nodes**" option moves the probes to the nearest faces, but take care of stretched meshes!

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, try to move slightly the segment.



Possible post processed fields

Basic 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

Advanced 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





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 { ... }
```





Averaging a field on a boundary

```
Dimension 3
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 { ... }
```



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 {
                                         # Post process the error field #
                           error
                           vitesse
```

Trio_U data file description

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)

don_lu (field read in a file)

fonc_MED (read a MED field)

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)





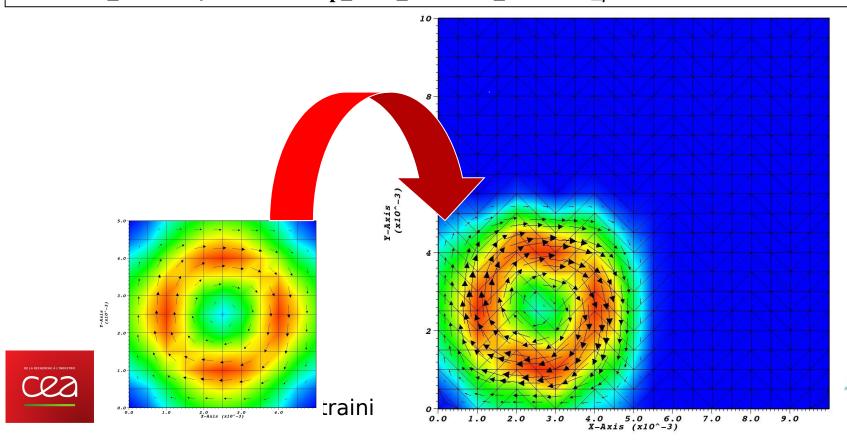
Example of Champ_Fonc_MED

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:

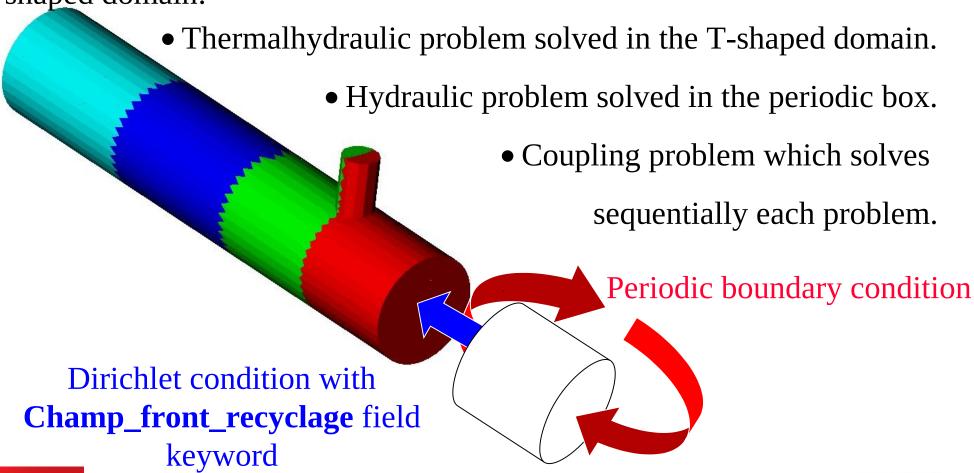
conditions_initiales { **vitesse Champ_Fonc_MED last_time** *VDF_field.med* domain **vitesse elem** 0 }





Example of Trio_U coupled problems

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



Trio_U data file description

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:
      : coordinates
X,Y,Z
       : 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
```



Trio_U 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)
 - 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





Trio_U 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



Trio_U files summary

• Input:

• Data file : .data

Meshing : .geom

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):



Trio_U results export

2D/3D results files are readable:

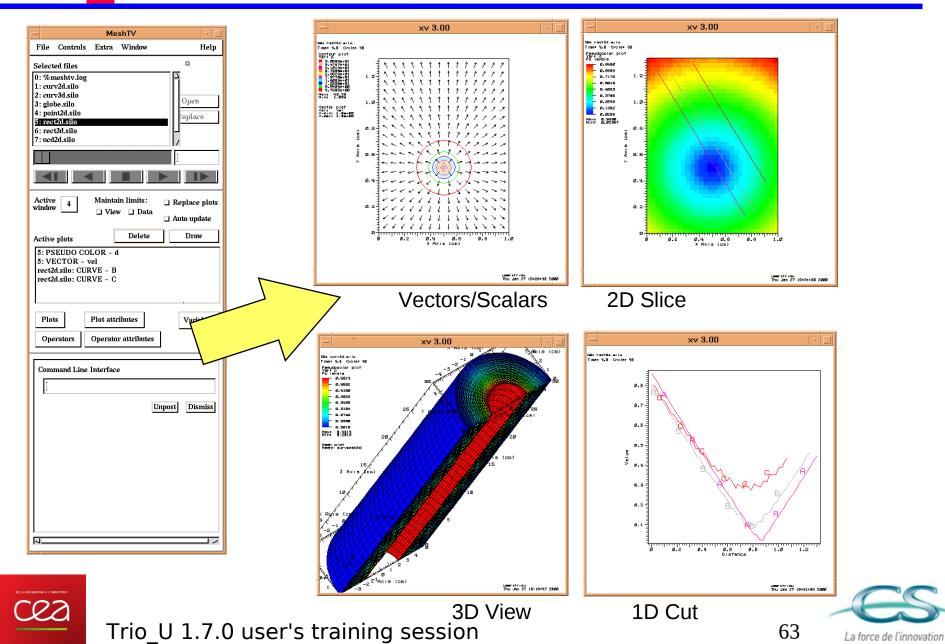
- Either directly by :
 - VisIt (use lata format in the data file "format lata")*
 - Salomé (use med format in the data file "format med", to post-process use "ParaVis" in Salomé and open med file with "builtin")
- Or after read then export by VisIt (VTK format):
 - Paraview, Tecplot

1D results files by:

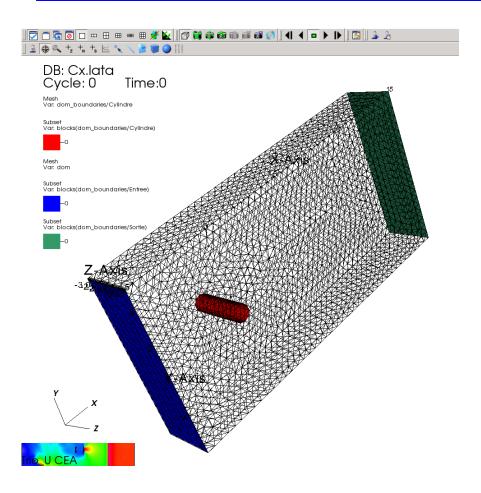
Gnuplot, XmGrace, Excel

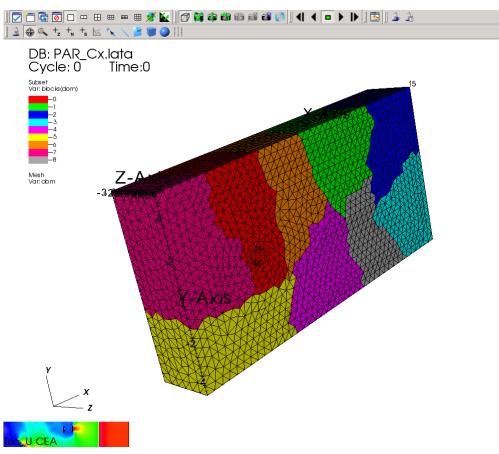


Trio U with VisIt



Trio_U with VisIt





Visualize boundaries

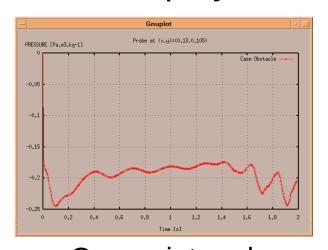
Visualize partition

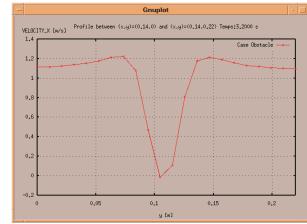


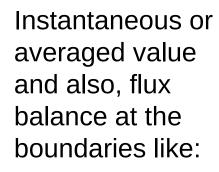


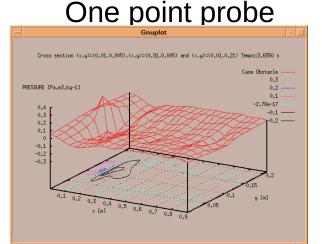
Trio_U with Gnuplot

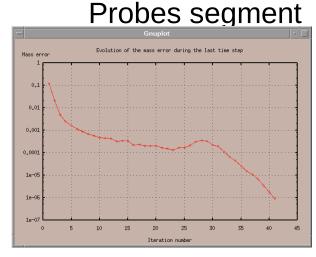
Real-time display of calculated quantities:











-flow rate

-pressure forces

-viscous forces

-heat flux

. .

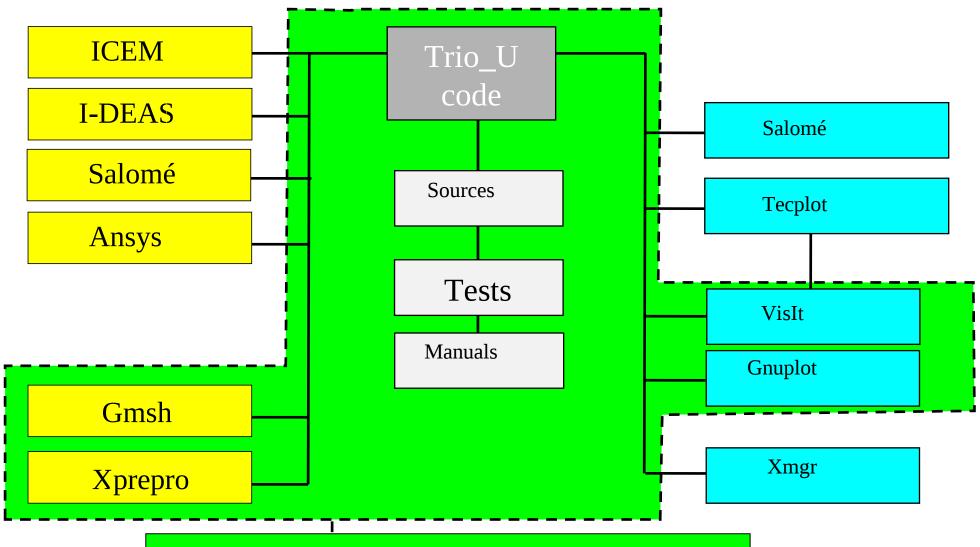


Probes plane

Convergence



Trio_U and interfaces between tools





Trio_U package released and supported



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Trio_U command lines

Trio_U environment initialization:

source \$TRIO_U_ROOT/bin/Init_Trio_U

- To run a Trio_U calculation with the triou script:
 - Sequential run:

triou datafile

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

triou 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:

triou 1>datafile.out 2>datafile.err



Trio_U command lines

- To copy a data file from the test database:
 triou -copy datafile
- To edit interactively (change/add schemes, solvers...) a data file with:
 EditData datafile.data
- Check a data file without running Trio_U:
 VerifData datafile.data
- To visualize the mesh and its boundaries used by a data file: triou -mesh datafile[.data]
- To run and follow probes during your calculation (used of "Run_sonde" script):
 triou -monitor datafile[.data]
- To monitor only your calculation:
 triou -probes [datafile[.data]]





Trio_U command lines

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

• To clean your calcul directory:

triou -clean

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

triou -doc

To browse some useful resources (PDF manuals, test cases, keywords, C++ classes,...):

firefox \$TRIO U ROOT/index.html

In all cases, the Trio_U binary may be changed by the \$exec variable and by default, exec=\$TRIO_U_ROOT/exec/Trio_U_mpi_opt



VisIt demonstration

Demonstration of the Vislt tool.

For more informations and to download manuals see :

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

Practice

Exercise 1 : Incompressible 2D flow

→ Obstacle.data



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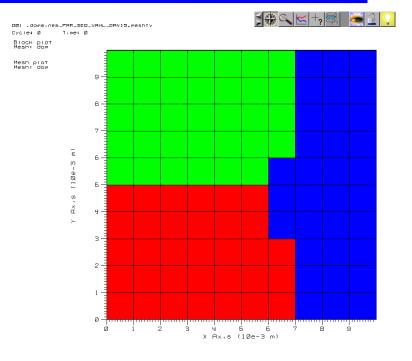


Parallel calculations with Trio_U (1/4)

- SPMD model (Single Program Multiple Data)
- Messages exchange by MPI (Message Passing Interface)
- From PC to massively // computer, with shared or distributed memory

Parallel calculations with Trio_U (2/4)

- 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)



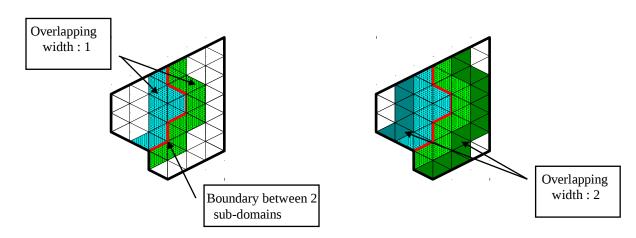
user:tr:ou Thu Jan 22 19:15:22 2004

- Some rules of thumb for performance
 - If possible, use 20000-30000 cells per process
 - Look at cluster specificities:
 - L2 size cache
 - Latency network
 - ...



Parallel calculations with Trio_U (3/4)

- Definition of overlapping width value
 - Number of vertexes or elements on the remote subdomain 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



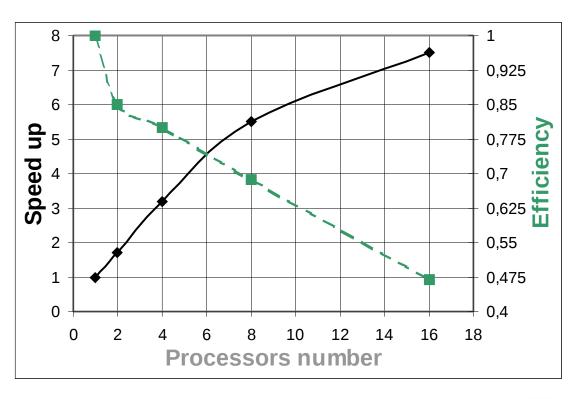




Parallel calculations with Trio_U (4/4)

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

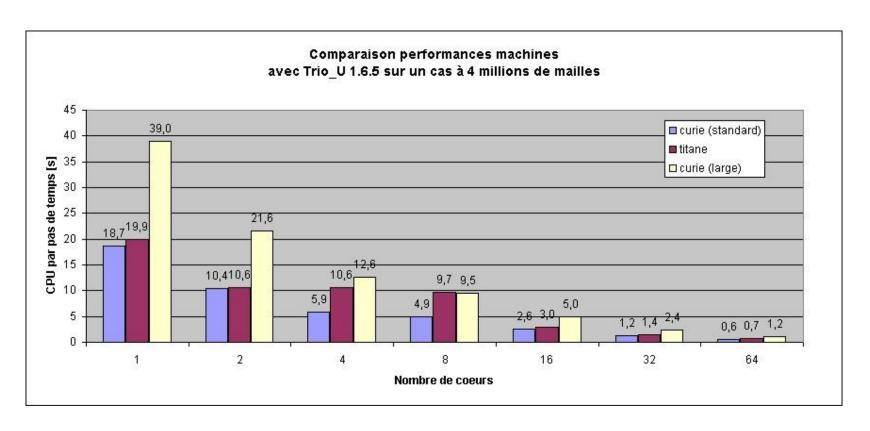
Processors	Speed Up	Efficiency
1	1	1
2	1.7	0.86
4	3.2	0.80
8	5.5	0.69
16	7.5	0.47





- To connect to:
 - CEA/DM2S service cluster: callisto (1168 cores)
 - CEA/CCRT clusters: airain (~10000 cores)
 - CEA/TGCC cluster: curie (~92000 cores)
 - CEA/Cadarache cluster: mezel2 (~600 cores)
 - CINES cluster: occigen (~50 000 cores)
 - PRACE LRZ cluster : supermuc (~155000 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
 - jade http://www.cines.fr/spip.php?article524
 - occigen https://www.cines.fr/occigen-le-nouveau-supercalculateur/
- 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 | airain)
 - ssh –X login@occigen.cines.fr





Performance of the new CEA cluster curie compared to previous cluster titane

curie (large): 5040 nodes of 2 eight cores @ 2.27Gh curie (standard): 360 nodes of 4 eight cores @ 2.3Ghz





Trio_U versions located on:

callisto
 ROOT=/panfs/ixion/home/triou

CCRT/TGCC ROOT=/ccc/scratch/cont002/den/triou

occigen
 ROOT=\$HOMEDIR (home de l'utilisateur)

With Trio_U stable versions:

\$ROOT/Trio U-X.Y.Z/Trio U

\$ROOT/Trio_U-X.Y.Z_patch/Trio_U -> X.Y.Z version plus important patchs

And Trio_U version in development:

\$ROOT/Version_test_clustername/Trio_U
 -> future X.Y.Z+1 version

For Trio_U configuration, add in your ~/.profile (or ~/.bashrc) file, the lines:

Example of Trio_U environment on callisto: source /panfs/ixion/home/triou/Trio_U-1.6.9/Trio_U/bin/Init_Trio_U 1>/dev/null 2>&1

• **Check your environment**, after you reconnect to the cluster, look at TRIO_U_ROOT variable: echo \$TRIO_U_ROOT



- Space discs on callisto:
 - /home (limited space but there is backup)
 - /panfs/ixion/home (local space)
 - /data/tmpdm2s or /data/tmplepp (shared spaces)
- Space discs and quotas on CCRT/TGCC:
 - /ccc/cont002/home (3 GB, slow I/O, backup)
 - /ccc/work (1 TB, fast I/O, no backup)
 - /ccc/scratch (20 TB, fastest I/O, no backup)
 - /ccc/store (infinite size, backup, but data are slow to access)
- -> Data shared by all clusters
- -> Source code, binary (also shared)
- -> Data, code output
- -> 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)



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

triou datafile

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

triou 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):

triou -create_sub_file datafile nb_processes

Then, you submit the job:

mezel2: qsub sub_file callisto: sbatch sub_file CCRT/TGCC: ccc_msub sub_file occigen: sbatch sub_file



- 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 Trio_U study
 - The Trio_U parallel command line



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

exec=absolute_path_to_the_Trio_U_binary

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
exec=absolute_path_to_the_Trio_U_binary
srun --mpi=pmi2 -K1 --resv-ports -n $SLURM_NTASKS $exec datafile $SLURM_NTASKS1>jdd.out 2>jdd.err
```





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)

• <u>List of jobs and their state:</u>

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_numbertrain



Another useful Trio_U script (not on occigen for the moment):

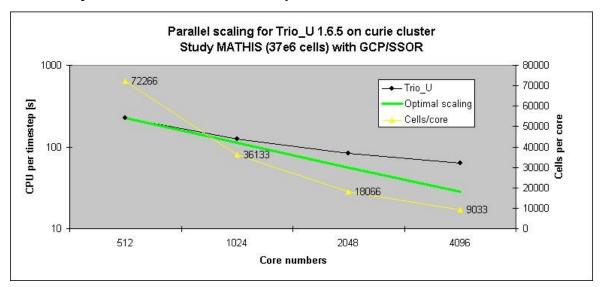
reprise_auto [-test]

- Submits a job in the current directory (a correct submission file should created before)
- Submits periodically new jobs in a way that the Trio_U calculation will restart automatically as soon as possible after the end of the previous job
- This script also backups the main files of the calculation into a dedicated directory
- The –test option will test (into a sub-directory named test_reprise_auto) this script for a
 first calculation restarted after 15 minutes.



Some advices:

-Choose a number of elements per process between 20000 and 30000 for optimal performances. Below 20000 elements/process, Trio_U parallel efficiency may dramatically decreases. Example on curie:



Scaling of curie from 72000 cells/core to 9000 cells/core



Visualization on clusters with VisIt

- If available, use a VisuPortal deported session on CCRT/TGCC clusters to run Vislt without network slowness
 - Available on curie cluster: https://visu-tgcc.ccc.cea.fr/VisuPortal/home
 - Available on airain cluster: https://visu-airain.ccc.cea.fr/VisuPortal/home
 - Ask us the VisuPortal user manual
- Or the Client/server mode
 - See the previous description here with VisIt (callisto, jade, eris, ...)
 - 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

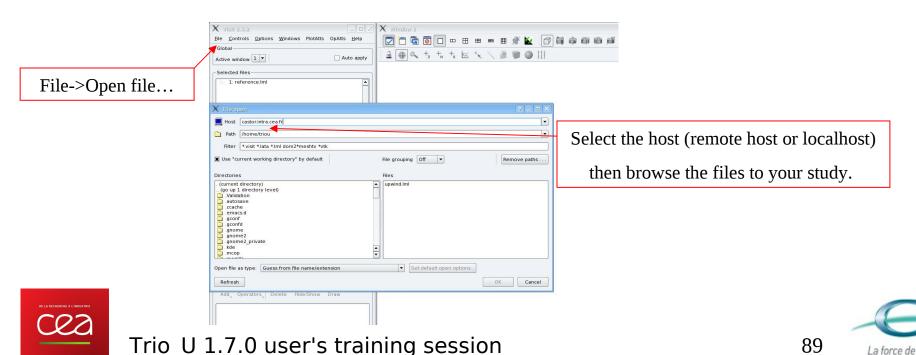


Recent features with VisIt

-The Trio_U install builds a parallel version of VisIt:

visit –np 8 –o results.lata

- -Client/server mode available by default for some clusters (callisto, eris, jade)
 - You run the Trio_U calculation on the cluster
- You visualize with VisIt your results from your Linux/Windows PC without data copy and/or network slowness



La force de l'innovation

Practice

Exercise 2 : Obstacle.data //

Exercise 3: Calculation on callisto

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Recommendations for use of models

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 use of 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 VEF meshing

- 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

- 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 Trio_U, 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 for conditions

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 for convection

- VEF Schemes
 - 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
- VDF schemes



Quick



When to use it?

- To solve a steady state calculation (e.g. $k-\varepsilon$ 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



Dynamic time step algorithm:

```
Time step dt = dt(Courant-Fiedrichs-Lewy condition) * facsec(t)
```

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



- 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





- 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



Time step dt = facsec * dt(CFL condition)

• 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



Specific recommendations for LES

- Time schemes:
 - High order explicit schemes like:
 - -Runge Kutta order 3 (but 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



Specific recommendations for LES

- Use a periodic box to provide a turbulent velocity field (see page 56):
 - 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 precessing paragraph of the Best Practice Guide)



Recommendations for 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 \sim 3/2*(turbulence\_rate*U)^2

\epsilon \sim k^{15}/L
```

- Use EF_stab scheme for the Navier Stokes equation
- Use upwind scheme for k-ε equation



Recommendations for post processing

- 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 Trio_U format (thanks to lata2dx tool)



What if?

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



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Meshing tools released with Trio_U

- Trio_U 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 Trio_U:
 - Salomé
 - Gmsh



Meshing with Trio_U

- Mesh generator tools :
 - ICEM (Ansys) generates a file at Trio_U format
 - Trio U reads .unv files from I-DEAS*
 - Trio_U reads 2D/3D meshes from old tools of Fluent (Gambit/TGrid)
 - Trio_U reads « .med » meshes from Salomé or Gmsh
- Form factors (view factors for the radiation model):
 - Link between Ansys and Trio_U

*:tetrahedral meshing only



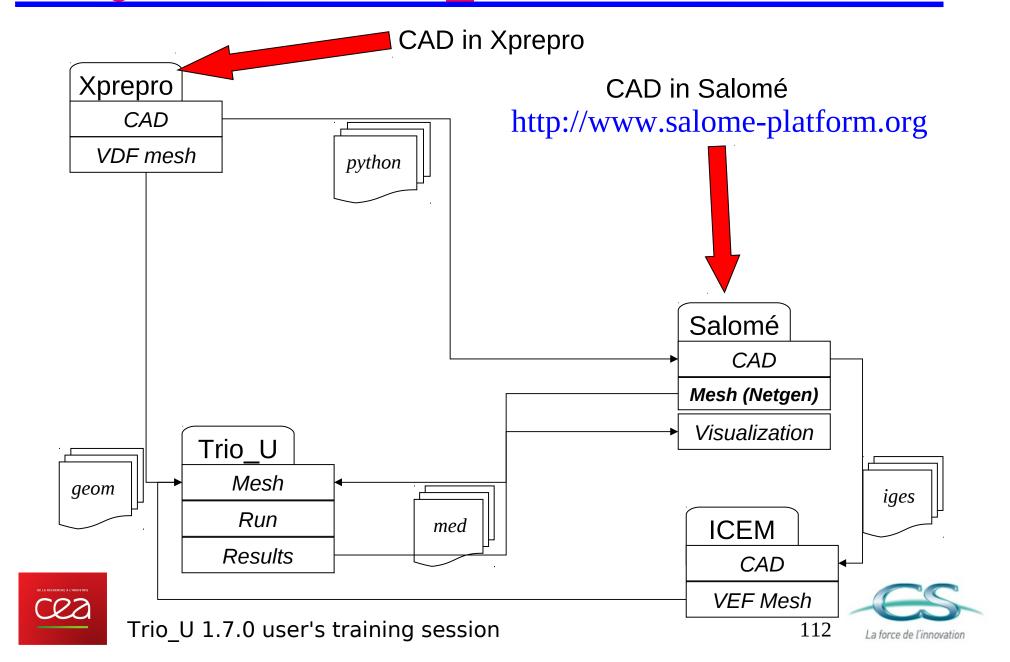
Meshing tools presented

- 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
Trio_U discretization	VDF	VEF	VEF	VEF
Trio_U package	Yes	No	Yes	No
Trio_U tutorial	Yes	Yes	Yes	No
Support	triou@cea.fr	support-salome@cea.fr	gmsh@geuz.org	



Integration with Trio_U & Salomé

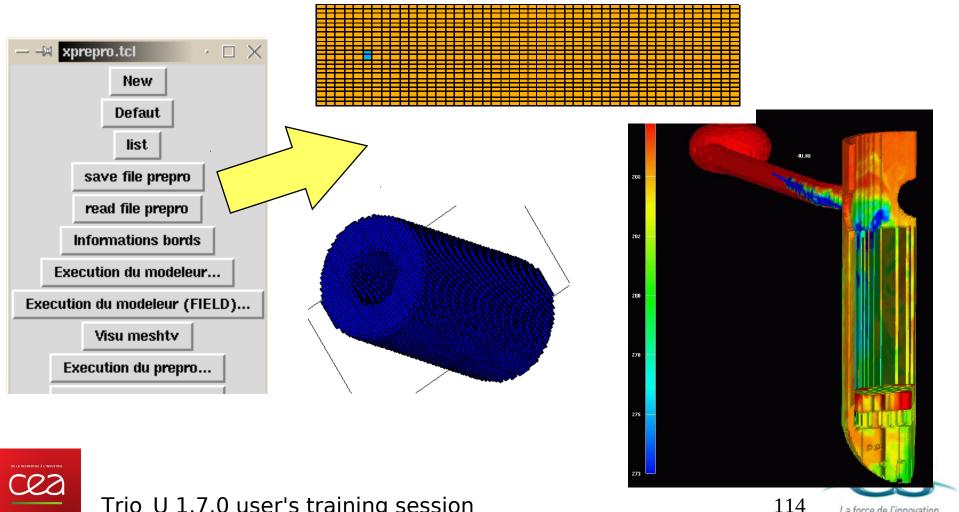


Xprepro -> Salomé

- 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 Trio_U data file (Lire_MED keyword)



Modeling/mesh tool created by the Trio_U team



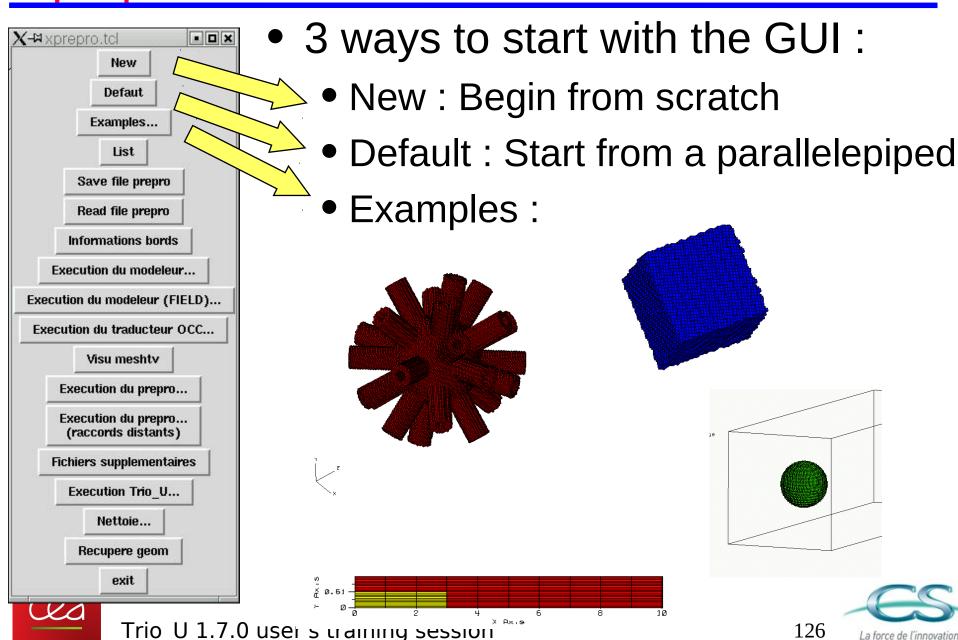
Main features:

- 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



- 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





La force de l'innovation

```
real xomin, xomax, yomin, yomax, zomin, zomax, eps
C Cotes extremes de la geometrie maillee
     xomin=?
     xomax=?
     vomin=?
     yomax=?
     zomin=?
     zomax=?
 eps sert a l'epaisseur des paves bords
     eps=0.01
    XM(1)=xomin-eps
    XM(nx)=xomax+eps
    YM(1)=yomin-eps
    YM(ny)=yomax+eps
    ZM(1)=zomin-eps
    ZM(nz)=zomax+eps
```

Button Default

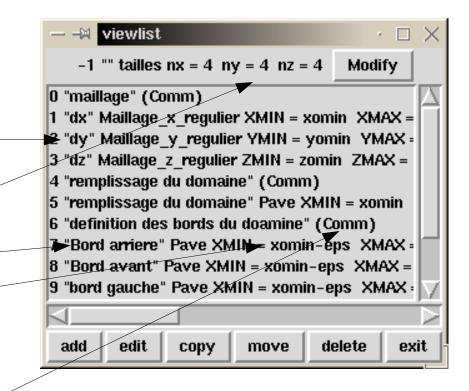
- A parallelepiped domain
- 6 boundaries already defined

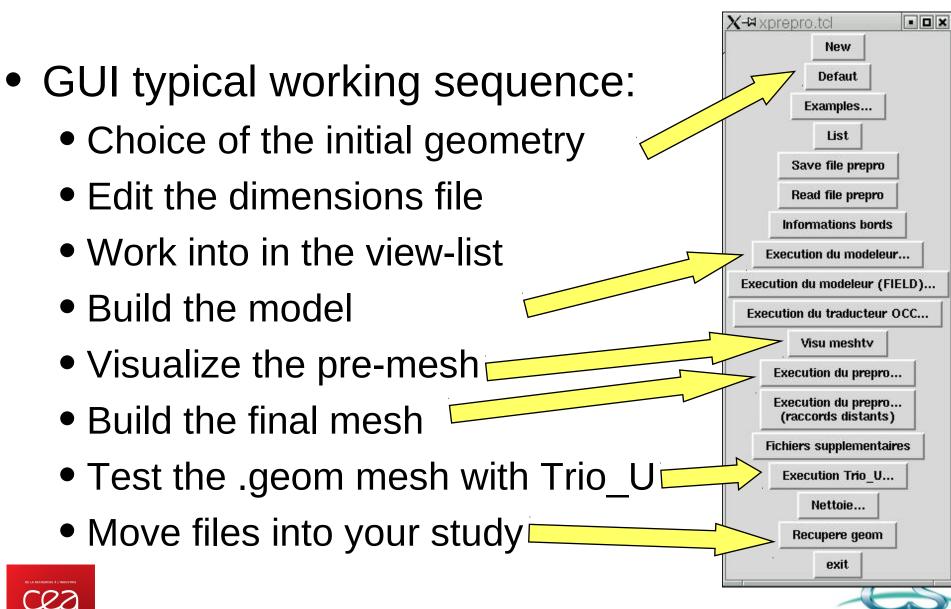
Edit a dimensions file

- Define the parallelepiped coordinates
- Define a tolerance eps
- It is possible to add new variables
- Take care: it is fortran language!



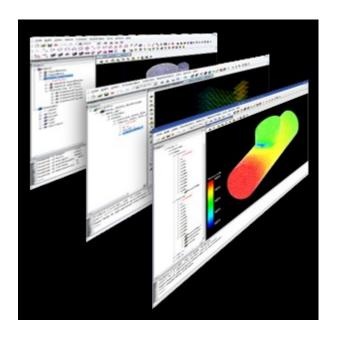
- The GUI Viewlist contains:
 - The pre-mesh
 - The grids according X,Y,Z
 - The number of pts Nx, Ny, Nz
 - Shapes definition
 - The name
 - The coordinates
 - Take care of the definition order (read from top to bottom)
 - Some comments (COMM)





La force de l'innovation

Salomé



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

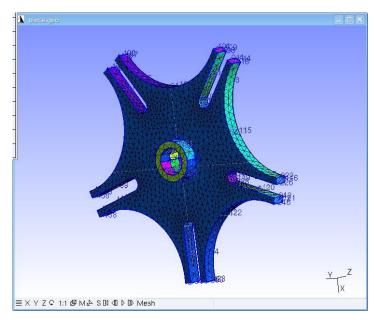
- -> **Salomé** is not provided in the Trio_U package
- -> To have a full training session, or receive support for install or use, see:

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

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



Gmsh



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 Trio_U install. There are tutorials and examples under:

\$TRIO_U_ROOT/exec/gmsh/share/doc/gmsh/tutorial

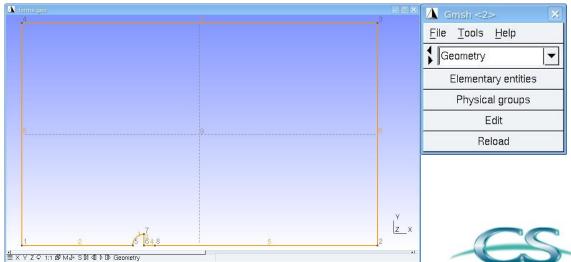
\$TRIO_U_ROOT/exec/gmsh/share/doc/gmsh/demos

-> 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

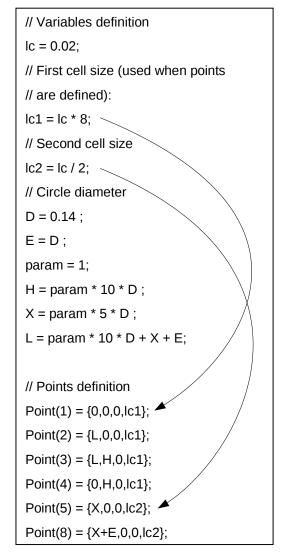
Edit and change your .geo file and use the **Reload** button to update the geometry visualization.



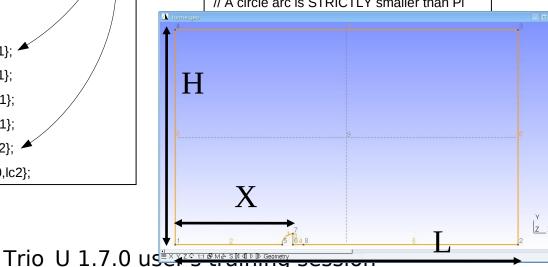


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Gmsh (Example of .geo file)



```
// 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
```

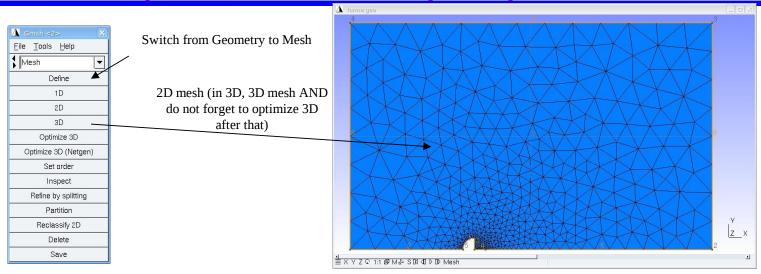


// Naming the boundaries is MANDATORY // and it is thanks to the // Physical Line (use Lines or Circle to define it) // DO NOT USE LINE LOOPS !!!! Physical Line("Shape") = {1,3}; Physical Line("Axis") = $\{2,4,5\}$; Physical Line("Outlet") = {6}; Physical Line("Top") = {7}; Physical Line("Inlet") = {8}; // 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 (Mesh and import)



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 Trio_U datafile:

Dimension 2

Domaine dom

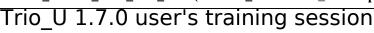
Lire_MED family_names_from_group_names dom mesh_name file.med # By default, the mesh name is the name of the file, so there mesh_name=file #

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 a mesh tool (2nd day morning)

VEF calculation with Trio_U

- 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 Trio_U



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Examples of Data files

- If one is interested by Quasi compressible model:
 - The Low mach flow data file should be presented



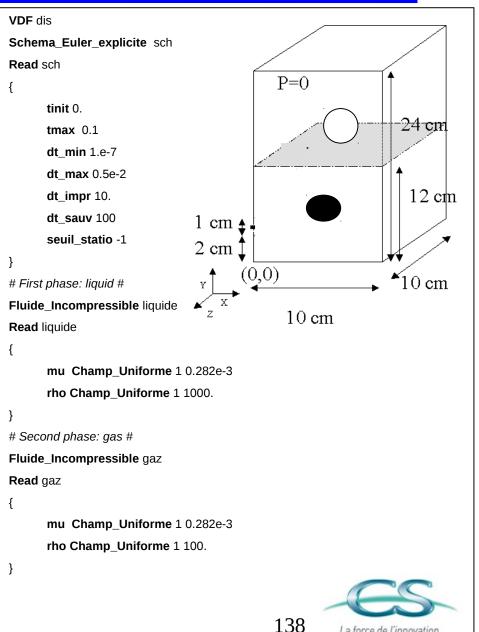
- Exercise 5 (Low mach number flow)
- If one is interested by Front Tracking model:
 - The Front Tracking data file should be presented



- Exercise 11 (3D Tank filling exercise)
- If one is interested by Genepi+ data file (old) :
 - See p146



```
# 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. \leq Y \leq 0.04 0. \leq Z \leq 0.06
                         bord paroi X = 0.04 \ 0. \le Y \le 0.04 \ 0. \le Z \le 0.06
                         bord paroi Y = 0. 0. \langle = X \langle = 0.04 \ 0. \langle = Z \langle = 0.06 \ 
                         bord paroi Y = 0.04 \ 0. \le X \le 0.04 \ 0. \le Z \le 0.06
                         bord bas Z = 0. 0 <= X <= 0.04 0 <= Y <= 0.04
                         bord haut Z = 0.06 \, 0. \le X \le 0.04 \, 0. \le Y \le 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 #
```



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```
# 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
```

```
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))^2+((y-0.02)/0.6)^2+((z-0.02))^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+((y-0.02)/0.6)^2+(
                           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
```

```
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 }
```

Practice

Exercise 11 on Front tracking:

Tank Filling 3D

```
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, \le Y \le 0.4
      },
Pave Sortie1
      Origine 0. 5.4
      Nombre de Noeuds 43
      Longueurs 0.6 0.4
      Bord outlet1 Y = 5.8 0. <= X <= 0.6
      Bord wall X = 0. 5.4 \le Y \le 5.6
      Bord wall X = 0.6 5.4 <= Y <= 5.8
      Bord P imp X = 0. 5.6 \le Y \le 5.8
      },
Pave Entree2
      Origine 1.0.
      Nombre de Noeuds 43
      Longueurs 0.6 0.4
```

```
Bord inlet2 Y = 0.
                        1. <= X <= 1.6
      Bord wall X = 1.
                          0. \le Y \le 0.4
      Bord wall X = 1.6 0. <= Y <= 0.4
Pave Sortie2
      Origine 1, 5,4
      Nombre de Noeuds 43
      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 \le Y \le 5.8
Pave Enceinte
      Origine 0. 0.4
      Nombre_de_Noeuds 9 26
      Longueurs 1.6 5.
      Bord wall Y = 0.4  0.6 \le X \le 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 #
```

```
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
```



```
# 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)
```





```
Convection Diffusion chaleur OC
             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*(v]1.4)*(v<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
```



```
Postraitements
                    # List of postprocessing blocks #
entree1 {
       # Restrict postprocessing on surface meshes previouslyy 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
```

```
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
```

```
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 }
```

```
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

```
# File plagues.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.
```





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Trio_U automated validation test case

- What is an automated test case?
- How to generate an automated test case?
- How to run an automated test case?

Trio_U automated validation test case

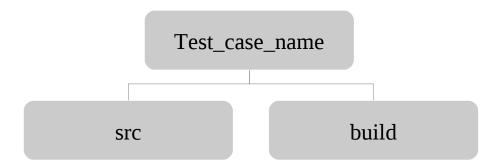
What is an automated test case?

- Tool to compare Trio_U 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 Trio_U version or to compare different versions of the code



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





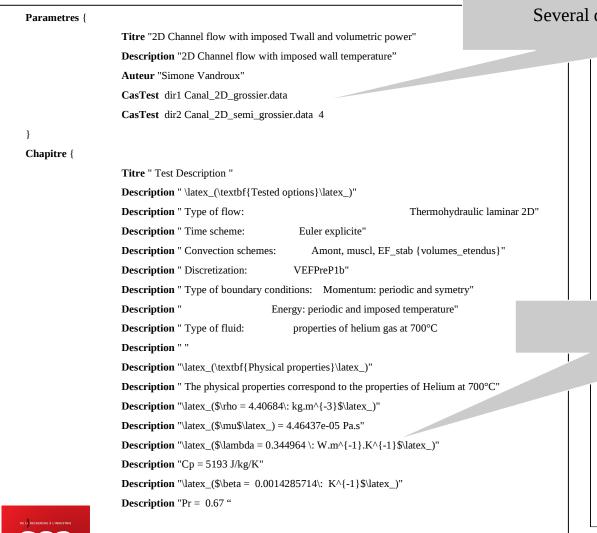


How to generate an automated test case?

- 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,...



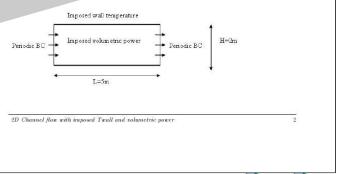
• Example of a **prm** file (and final PDF result):

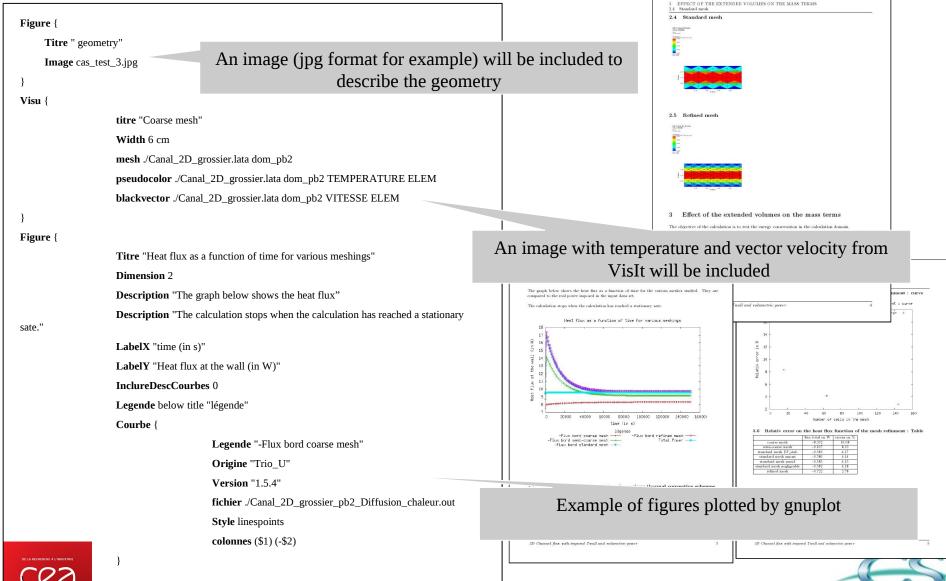


Several data files will be run by Trio_U

Test Description Tested options Type of flow: Thermohydraulic laminar 2D Time scheme: Euler explicite Convection schemes: Amont, muscl, EF_stab {volumes_etendus} Discretization: VEEPreP1b Type of boundary conditions: Momentum: periodic and symetry Energy: periodic and imposed temperatur Type of fluid: properties of helium gas at 700°C Physical properties The physical properties correspond to the properties of Helium at 700°C $\rho = 4.40684 \; kg.m^{-3}$ a = 4.46437e-05 Pa.s $\lambda = 0.344964 \ W.m^{-1}.K^{-}$ Cp = 5193 J/kg/K $\beta = 0.0014285714 K$ Pr = 0.67Boundary limits Hydraulic: symetry at walls Energy: imposed temperature T=0 at walls, imposed volumetric power=1 in the calculation domain 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

Latex format can be integrated





• Example of a **prepare** script:

```
#!/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 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 ..
```

• 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
```



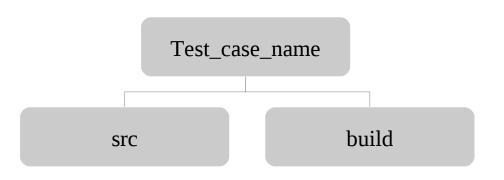
• Example of **post_run** script:

```
#!/bin/bash
# The first parameter is the name of the data file:
datafile=$1
file=${datafile%.data}
# Read the pressure drag on the 5<sup>th</sup> 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
```



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:
 - -runs the **pre_run** script
 - -runs the calculation
 - -runs the **post_run** script
- » Then builds the PDF report file



User guide:

-\$TRIO U ROOT/doc/Trio U/HowTo Validation.pdf

.prm syntax documented in:

-\$TRIO_U_ROOT/Validation/Outils/Genere_courbe/doc/manuel.xhtml

Examples of automated validation test case:

-\$TRIO_U_ROOT/Validation/Rapports_automatiques/Validant/Fini

Examples of automated verification test case:

-\$TRIO U ROOT/Validation/Rapports automatiques/Verification/Fini

• Demo:

cd \$TRIO_U_ROOT/Validation/Rapports_automatiques/Validant/pas_fini/Drag Run_fiche -xpdf Run_fiche -help # Give all the options #



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Trio_U Support (1/2)

Subscribe to the Trio_U 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

Ftp site: ftp://ftp.cea.fr/pub/Trio_U/a87pour/index.html

- Download new versions
- Release Notes

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

Hot line

- triou@cea.fr
- Céline CAPITAINE
- Marthe ROUX

01 69 08 42 68 (Saclay bât 451 pièce 43)

01 69 08 00 02 (Saclay bât 451 pièce 43)





Trio_U Support (2/2)

- A release every 3 months:
 - Linux version only
 - Installed on several CEA clusters and TGCC/CCRT (HPC CEA institute)
 - Installation by users or Trio_U support
- Documentation available here ftp://ftp.cea.fr/incoming/y2k01/Trio_U/doc/ or under \$TRIO_U_ROOT/doc/Trio_U directory:

Trio_U_and_Xprepro_presentation.pdf (these slides)

Models_Equations_Trio_U.pdf "Methodology for incompressible single phase

flow" (~Trio_U equations & models)

• Best_Practice_Trio_U.pdf "Validation of Trio_U code" (~Trio_U User Guide)

User_Manual_Trio_U.pdf
 Manuel_Xprepro.pdf
 "User Manual Trio_U"
 "User Manual Xprepro"

Developer_Trio_U_presentation.pdf
 Trio_U development Presentation

Tutorial_Trio_U.pdf
 Trio_U & Xprepro tutorial

