



Introduction





Prerequisites

For this training session:

- Trio_U (User's training session)
- C++ (Intermediate)

Later, if you want to develop/contribute to Trio_U:

- Git (Basic)
- MPI (Basic)
- French skills (Mandatory)





Objectives

To get a general knowledge of the Trio_U code

To be able to look for useful information in the code for a specific development

To acquire reflexes to develop while following Trio_U rules of coding





Useful links

Trio_U:

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

mailto:triou@cea.fr

C++:

http://www.tutorialspoint.com/cplusplus

Git:

http://www-cs-students.stanford.edu/~blynn/gitmagic/index.html





Exercise: Trio_U download

```
# If you are on a CEA Saclay PC:
$ cd /export/home/yourlogin
# From everywhere on the CEA network, download (~5mn) with:
$ git clone git://is223196/official/trio_u
# Go into your workspace :
$ cd trio_u
$ ls
# Create a new work branch :
$ git checkout -b YourNewBranch
```





Trio_U An object oriented CFD code





Interest of Trio_U

- Implement and test your numerical or physical models
- Reuse existing validated data structures
- Run your models on very large meshes thanks to parallelism
- Consolidate your work
 - Developments are integrated, documented, ported, tested, maintained by Trio_U support team





Interest of Trio_U

- Need an investment:
 - to acquire the knowledge of the data structure
 - because of lack of documentation or obsolete one
 - to avoid several pitfalls (from C++ or Trio_U)





What is Trio_U CFD code?

It provides:

- 2 spatial discretizations (VDF, VEF)
- Several time schemes
 - Explicit forward Euler, backward Euler, Runge Kutta 2-3-4,...
- Several schemes according the discretization
 - Quick, Upwind, EF_stab, Muscl,...
- Templates to create new Equation, Problem, Field,...
- Several efficient tools to solve linear systems through the PETSc library :
 - Solvers : CG, BiCGstab, GMRES, Cholesky
 - Preconditioners : SSOR, ILU, Jacobi, Boomeramg,
- Data structures and functions to quickly parallelize your developments





Trio_U

- What can Trio_U can handle
 - Runs on every Linux box (32/64 bits)
 - Runs on all the CEA clusters
 - Has already run a LES on a 300.10⁶ cells mesh with 4600 cores (curie on CCRT)





Trio_U Specifications/Choices explained





Main specifications:

Enable developments with the following characteristics:

- fast
- reliable
- reusable
- effective
- documented
- enable encapsulation of Fortran modules





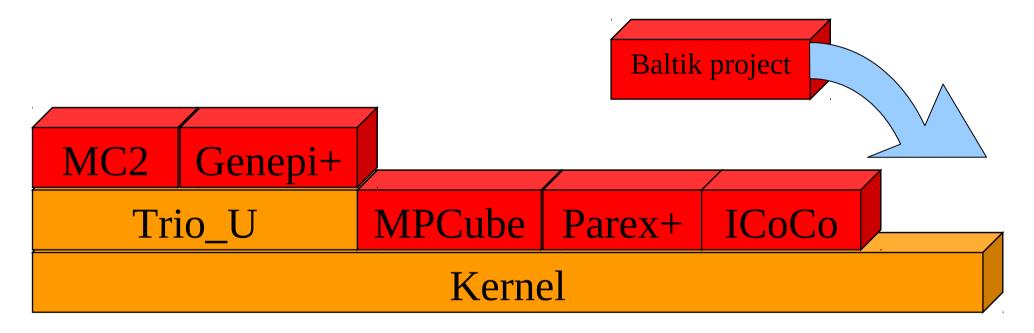
Main Choices:

- Object Oriented Conception using UML method
 - Modularity, maintainability, library encapsulation
- C++ implementation
 - Standard, performances, C/Fortran compatibility
- Parallelism by sending/receiving messages (MPI)
 - Standard, portable
- Multi-site configuration management (previously Clearcase, now Git)
 - Co-developing
- Automatic generation via Doxygen of HTML documentation from code sources
 - Documentation is up to date





2 ways to develop in Trio_U



I) In Trio_U/Kernel

II) In a Baltik project on top of Trio_U/Kernel

In the 2 cases, you need to first install and build Trio_U/Kernel. Trio_U 1.7.0 developer training session





2 ways to develop in Trio_U

- I) Develop directly in Trio_U/Kernel
 - You want to contribute to Trio_U/Kernel
 - But if you want to share your work, you will need:
 - to follow the Trio_U rules of coding
 - to check and respect the non regression of other parts of the code
- II) Develop in a Baltik project based on Trio_U/Kernel
 - You want to develop your own project
 - more freedom about rules of coding/non regression of the Trio U/Kernel
 - Baltik means Building an Application Linked to Trio_U Kernel





Exercise: Trio_U build

```
# Basic build
$ cd Trio_U
# Configure (~5mn):
$ ./configure -without-visit # Configure Trio_U without the VisIt install
# Initialize Trio_U environment :
$ source bin/Init_Trio_U
$ make optim # Build an optimized (-03 option) version (~15mn)
$ ls $exec_opt
$ make debug # Build a debug (-g -O0 option) version (~5mn)
$ ls $exec_debug
```





Other possible builds

```
# Build a semi optimized binary (option -O3 with asserts)
$ make
$ ls $exec
# Build an optimized binary for profiling (option -pg -O3)
$ make prof
$ ls $exec_pg
# Build an optimized binary for test coverage (option -gcov -O3)
$ make gcov
$ ls $exec_gcov
```





Other basic commands

```
# Clean the install
$ cd $TRIO_U_ROOT
$ make clean
# To run the non regression tests with a binary (by default: $exec)
$ triou -check all
# To share your work on the Trio_U shared Git repository
$ cd $TRIO_U_ROOT
$ git commit --all -m"My wonderful work »
$ git remote add shared git://is223196/shared/trio_u
$ git push shared
```



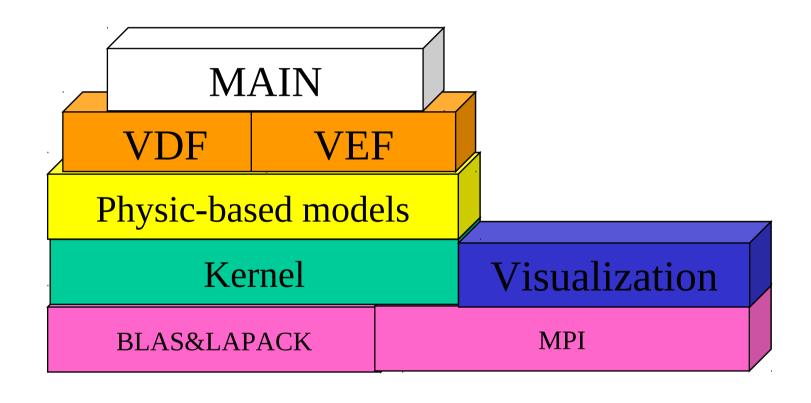


Trio_U modules





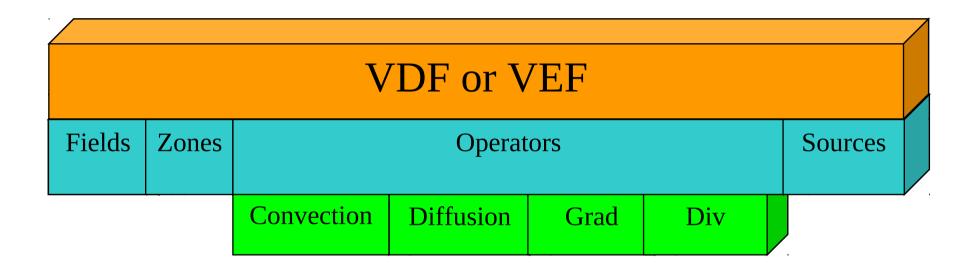
Trio_U modules







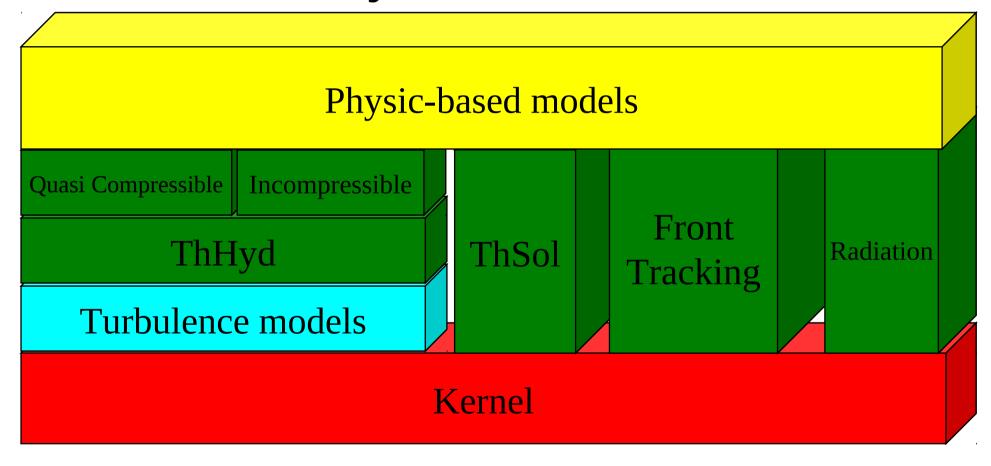
Discretization modules







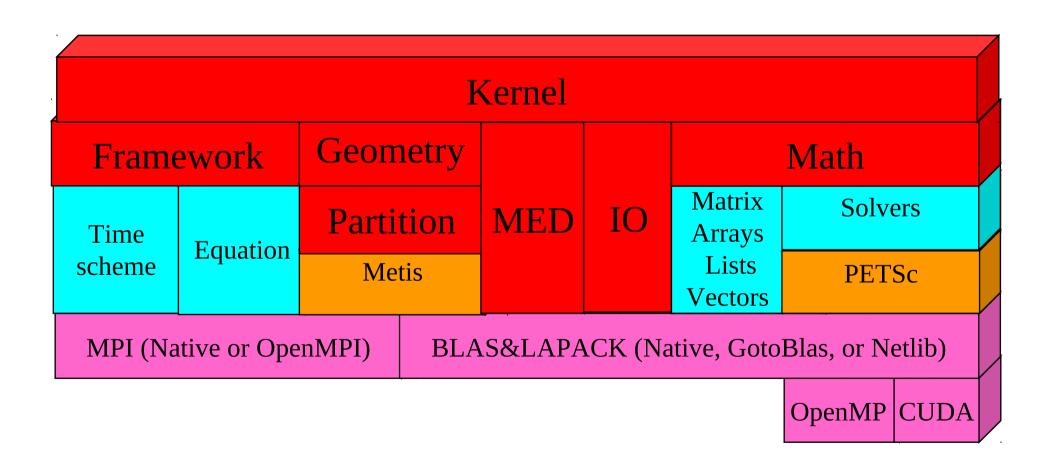
Physics modules







Kernel module







Trio_U/Kernel

- ➤ Trio_U code is made of :
 - -1500 classes
 - -Declared in 1500 include files (.h)
 - -Implemented in 1500 sources files (.cpp)
 - -Within 84 directories
- ➤ Kernel constitutes 40% of the Trio_U/Kernel code.
- ➤ There is a HTML documentation to browse and see the class hierarchy under :

\$TRIO_U_ROOT/doc/Trio_U/html





Trio_U/Kernel tests

~40 **Verification forms** to check analytical results under :

\$TRIO_U_ROOT/Validation/Rapports_automatiques/Verification

~100 **Validation forms** to compare Trio_U with experimental results or with results from other codes under :

\$TRIO_U_ROOT/Validation/Rapports_automatiques/Validant

~1900 **Non regression test cases** under :

\$TRIO_U_ROOT/tests



Kernel source directories



Under \$TRIO_U_ROOT/src/Kernel

./Champs

./Champs_dis

./Cond_Lim

./Framework

./Geometrie

./Geometrie/Decoupeur

./ICoCo

./MEDimpl

./Math

./Math/Matrices

./Math/SolvSys

./Operateurs

./Schemas_Temps

./Solveurs

./Statistiques_temps

./Utilitaires

./VF/Champs

./VF/Zones

Generic fields

Discretized generic fields

Generic boundary conditions

Generic problem, equation, time scheme

Domain, cell geometry, mesh utilities

Partition utilities

IcoCo coupling interface

MED utilities

Math utilities (arrays...)

Matrix

Linear system solvers

Generic operators (gradient,...)

Time schemes

Solvers

Statistical utilities

IO, memory, MPI

Finite volume fields

Finite volume geometry description



Trio_U source directories



Under \$TRIO_U_ROOT/src

./ALE ALE method

./Front_tracking_discontinu Discontinous front tracking method

./Front_tracking_discontinu/VDF VDF implementation

./Front_tracking_discontinu/VEF VEF implementation

./P1NCP1B

VEF discretization

VEF fields

./P1NCP1B/Champs VEF fields
./P1NCP1B/Cond Lim VEF boundary conditions

./P1NCP1B/Operateurs VEF operators VEF operators

./P1NCP1B/Solveurs VEF solvers

./P1NCP1B/Turbulence VEF turbulence

./P1NCP1B/Zones VEF geometry description

./Phase_field Phase_field method

./Phase_field/VDF VDF implmentation

./Rayonnement Transparent media radiation model

./Rayonnement/VDF VDF implementation

./Rayonnement/VEF VEF implementation

./Rayonnement_semi_transp Semi transparent media radiation model

./Rayonnement_semi_transp/VEF VEF implementation



Trio_U source directories



./7	Γh	Н	v	d
•/ -			- у	u

./ThHyd/Chimie

./ThHyd/Quasi_Compressible

./ThHyd/Quasi_Compressible/Turbulence

./ThHyd/Quasi Compressible/VDF

 $./ThHyd/Quasi_Compressible/VEF$

./ThHyd/Schemas_Temps

./ThHyd/Turbulence

./ThHyd/Turbulence/Spectres

./ThSol

./UtilitairesAssemblages

./VDF

./VDF/Axi/Operateurs

./VDF/Axi/Operateurs/Evaluateurs

./VDF/Axi/Sources

./VDF/Axi/Turbulence

./VDF/Champs

 $./VDF/Cond_Lim$

./VDF/Elements

./VDF/Operateurs

./VDF/Operateurs/Evaluateurs

./VDF/Operateurs/Iterateurs

./VDF/Solveurs

./VDF/Sources

./VDF/Sources/Evaluateurs

./VDF/Sources/Iterateurs

./VDF/Turbulence

./VDF/Zones

Thermalhydraulic models

Chemical species model

Quasi compressible model

Turbulence models

VDF implementation

VEF implementation

Time schemes

Turbulence models

Turbulence utilities

Conduction model

Assembly utilities

VDF discretization

Operators in VDF with axis symmetry

Flux evaluators in VDF with axis symmetry

VDF sources term for axis symmetry

VDF turbulence model for axis symmetry

VDF fields

VDF boundary conditions

VDF cells description

VDF operators

Flux evaluators in VDF

Flux iterators in VDF

VDF solvers

VDF source terms

Source term evaluators in VDF Source term iterators in VDF

Turbulence models VDF implementation

VDF geometry description



Trio_U source directories



./VEF

./VEF/Champs

./VEF/Cond_Lim

./VEF/Operateurs

./VEF/Solveurs

./VEF/Sources

./VEF/Sources/Evaluateurs

./VEF/Sources/Iterateurs

./VEF/Turbulence

./VEF/Zones

./Zoom/Algos

./Zoom/Geometrie

./Zoom/Kernel

./Zoom/Noyau

./Zoom/Operateurs

./Zoom/VDF

./Zoom/VDF/Cond_Lim

./Zoom/VDF/Turbulence

./MAIN

VEF discretization

VEF fields

VEF boundary

VEF operator

VEF source terms

Source evaluators in VEF

Source iterarators in VEF

Turbulence model implemented in VEF

VEF geometry description

Zoom (multi scale simulation)

Algorithms

Geometry

Kernel

Operator

VDF implementation

VDF boundary condition

VDF turbulence model

Directory with main.cpp

Note:

Some directories need to be merged

(e.g : VEF and P1NCP1B)!





Basic Oriented Object Conception (OOC) concepts used in Trio_U



Class

What are C++ class/object?



-A class is an association of a set of methods and a data structure -The class defines the plan to create the object -The object is an instance of the class

Actions which can be done by the object: Object attributes can only be **METHODS** modified by: - the object itself, Data - by other objects using the structure: methods of this object. Method1() **ATTRIBUTES** Method2() Attribute1 Data encapsulation

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Data encapsulation



- The aim of data encapsulation is to:
- hide the attributes
- hide the implementation of the methods

- Respecting encapsulation enables a good maintainability. At any time, one can easily :
- Add/change the implementation of the methods
- Add/change attributes

with no (or limited) changes to the rest of the code.





Example of Trio-U objects:

Problem (Conduction, Hydraulic,...)

• Equation (PDE as $\partial U/\partial t + \Sigma Op(U) = \Sigma F$)

• Operator (grad, div, laplacian,...)

Unknown field (solution of an equation)

• Physical fields $(\rho, \mu, \lambda,...)$

• Boundary condition (Dirichlet, Neumann, symmetry, ...)

• Time scheme (Euler, Runge Kutta, Implicit, ...)

• Space discretization (VEF, VDF, ...)

• ... and many others at lower level ... Examples:

• Arrays (class DoubleTab for A(i,j), class DoubleVect for A(i), IntTab,)

String (class Nom)...



First example: Equation class



See Equation_base class

attributes:

- **Nom** nom // A name
- Ref_Probleme_base mon_probleme // A reference (link) to a problem
- Ref_Schema_Temps_base le_schema_en_temps // A reference to a time scheme

– ...

methods:

- to access to the attributes:
 - **probleme()** method returns the problem
 - **schema_temps()** method returns the time scheme
- to evaluate the time derivative of the unknown I(x,y,z,t):
 - derivee_en_temps_inco(DoubleTab& I) method returns $\partial I/\partial t = f(I)$

– ...



Second example: Unknown field class



See Champ_Inc_base class

methods:

```
fixer_nb_valeurs_temporelles(int nb) // To store fields in memory at nb different times
valeurs() // Return the values at the current time t(n)
futur(int i=1) // Return the values at the time t(n+i)
passe(int i=1) // Return the values at the time t(n-i)
avancer(int i=1) // Go to the future (by turning forward the "wheel")
reculer(int i=1) // Go to the past (by turning backward the "wheel")
...
```

attributes:

Roue_ptr les_valeurs // Pointer to a "wheel" mechanism to manage the different times for the unknown field



Code example:



```
inconnue.fixer nb valeurs temporelles(2); // 2 memories to store the different times of the unknown inconnue
// present (it is an alias or link) points to U(n) (first memory)
                                                                                       U(n+1)
DoubleTab& present = inconnue.valeurs();
/* DoubleTab present = inconnue.valeurs(); ← Warning! It is a copy here... */
DoubleTab& futur = inconnue.futur();
                                          // futur points to the second memory
// Computation of U(n+1) with an algorithm using U(n) only (one step time scheme)
// like: futur=present + dt* f(present) \leq U(n+1)=U(n) + dt*f(U(n))
                                                                                         U(n)
// At the end of the time step, we turn the « wheel » with:
inconnue.avancer();
                                                                                        U(n+1)
// Now valeurs() will return U(n+1) and futur() will return U(n)
// So during, the next time step, the memory used to store U(n) (now useless)
// will be overwritten by the storage of U(n+2).
                                                                                                   36
```

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Base class A

Attribute1

Method1()

Method2()

Inheritance

Base class A with 2 methods and 1 attribute.

Derived class B

Attribute2

Method2()

Derived class B inherits from base class A:

->Attribute1 and Method1() are **inherited** from the class A

-> B::Method2 method **overloads** A::Method2





Interest of inheritance

Factorization

 Identical attributes and methods in different derived classes will be declared and/or implemented once in the base class.

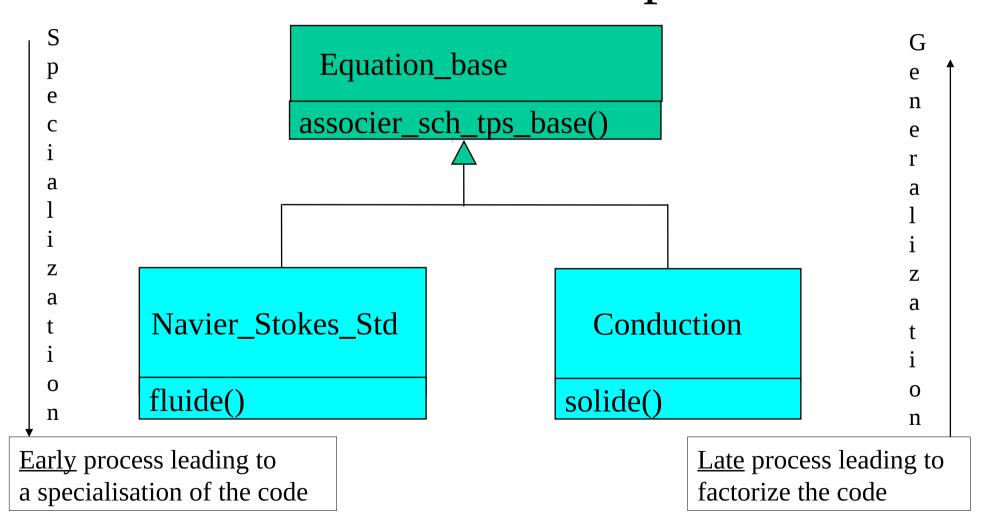
Consistency

 All the derived classes have, at least, the same interface (methods) than the base class.





Inheritance example



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Exercise: Use HTML doc



- # Browse the Trio_U ressources index file :
- \$ konqueror|firefox \$TRIO_U_ROOT/index.html
- # Or:
- \$ triou -index
- # Select the C++ classes link and look for:
 - Inheritance graph of the Navier_Stokes_Std class
 - Q: How many classes inherits from this class?
 - Code file Nom.cpp and the class Nom constructors
 - Q: What is the default value of an object Nom when created?
 - Non const **method** Intab& Zone_VF::face_voisins()
 - Q: How many methods in the code use this method?
 - List all the members of the Zone_VEF class
 - Q: In which class is implemented its nb_elem() method?

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- La force de l'innovation
- \rightarrow Example of the *derivee_en_temps_inco()* method which implements the calculation of F(U) in $\partial U/\partial t = F(U)$, where U is the main unknown of the equation
 - <u>Static</u> polymorphism (decision is made at the <u>compile</u> time):

```
Navier_Stokes_std eqn;
eqn.derivee_en_temps_inco();
```

– <u>Dynamic</u> polymorphism (decision is made at the <u>run</u> time):

```
Equation eqn; // Equation is a generic class in Trio_U

if (...)

eqn->typer(Navier_Stokes_std);

else

eqn->typer(Navier_Stokes_Turbulent);

....

eqn->derivee_en_temps_inco();
```



Polymorphism implementation with real and virtual methods



- -A <u>real</u> method (default case):
 - can be overloaded
 - enable only static polymorphism
 - \rightarrow In the example, A()
- -A <u>virtual</u> method:
 - can be overloaded
 - enable dynamic polymorphism
 - \rightarrow in the example, B()
- -A <u>pure virtual</u> method (abstract method):
 - must be overloaded (otherwise compilation fails),
 - make the class abstract (used for example in base classes),
 - enable dynamic polymorphism
 - \rightarrow In the example, C()

```
class example
{
    public :
    A();
    virtual B();
    virtual C()=0;
};

class sub_example
{
    public :
    A();
    virtual B();
```

virtual C():

};



Virtual method example



```
class Navier_Stokes_std : public Equation_base
{
  public :
    virtual DoubleTab& derivee_en_temps_inco(DoubleTab& F);
};
```



Navier Stokes equation



Trio_U equations are basically set under the form:

$$\partial U/\partial t = F(U) = M^{-1}(\Sigma Op_i(U) + \Sigma S_i)$$

But for instance, Navier Stokes equations for an incompressible fluid (U velocity, P pressure, M mass, C convection, L diffusion, B divergence, B^T gradient, S sources):

1) BU=0
2)
$$M_{\partial}U/_{\partial}t + CU = -B^{T}P + LU + S$$

Or by inverting 2) by M gives II):

II)
$$\partial U/\partial t = -M^{-1}B^{T}P + M^{-1}(LU-CU+S) <=> \partial U/\partial t = -M^{-1}B^{T}P + F(U)$$

Then applying BU=0 on II) leads to I):

I)
$$BM^{-1}B^{T}P = BM^{-1}(LU-CU+S)$$

-> One more equation (Poisson) to compute the pressure P and one additional term $-M^{-1}B^{T}P$ compared to the equation basic form $\partial U/\partial t = F(U)$ to compute velocity



Virtual method example



Note: This method is overloaded in the Navier_Stokes equation class





Virtual method example



```
DoubleTab& Navier_Stokes_std::derivee_en_temps_inco (DoubleTab& F)
    // M\partial U/\partial t + grad P = MF(U) = \Sigma Op_i(U) + \Sigma S_i
    // \operatorname{div} U = 0 -> div M<sup>-1</sup>grad P = div F(U)
    DoubleTab& pression = la_pression.valeurs(); // Storage for P
    DoubleTab& vitesse = la_vitesse.valeurs(); // U<sup>n</sup>
    DoubleTrav secmem(pression); // Second member
    DoubleTrav gradP(vitesse); // Pressure gradient
    Equation_base::derivee_en_temps_inco(F); // F(U)
    divergence.calculer(F, secmem); // secmem=div(F(U))
    solveur_pression.resoudre(secmem, pression); // Solve BM<sup>-1</sup>B<sup>T</sup>P=div(F(U))
    gradient.calculer(pression, gradP);
                                                // gradP
    solveur_masse.appliquer(gradP); // M<sup>-1</sup>gradP
                                               // F(U)-M^{-1}gradP
    F = gradP;
                               // \partial U/\partial t = F(U) - M^{-1} grad P
    return F;
```

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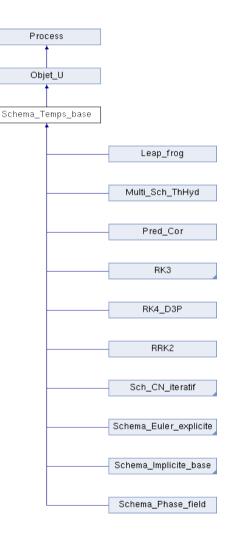
Pure virtual method example



faire_un_pas_de_temps_eqn_base(Equation_base& equation) method implements the time scheme to calculate U^{n+1} for $\partial U/\partial t = F(U)$ where U is the main equation unknown

```
class Schema_temps_base : public Objet_U
{
    Public :
        virtual int faire_un_pas_de_temps_eqn_base(Equation_base&) =0;
        ...
};

class Schema_Euler_Explicite : public Schema_temps_base
{
    public :
        virtual int faire_un_pas_de_temps_eqn_base(Equation_base &);
};
```



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```
int Schema_Euler_Explicite::faire_un_pas_de_temps_eqn_base(Equation_base& eqn)
   // \partial U/\partial t = F(Un) --> U^{n+1} = U^n + dt * F(U^n) for forward Euler scheme
   Champ_Inc& inconnue = eqn.inconnue();
                                                          // Equation unknown
                                                          // Contains U<sup>n</sup>
    DoubleTab& present = inconnue.valeurs();
    DoubleTab& futur = inconnue.futur();
                                                          // Location to store U<sup>n+1</sup>
  futur = eqn.derivee_en_temps_inco();
                                                          // F(U<sup>n</sup>)
   futur *= dt:
                                                          // dt^* F(U^n)
   futur += present;
                                                          // dt^* F(U^n) + U^n
   return 1;
Note: These (simplified) example may differ from the current version of the code
```





Hello world exercise

• Edit the \$TRIO_U_ROOT/src/MAIN/mon_main.cpp file and add this lines after "Process::imprimer_ram_totale(1);":

```
std::cout << "Hello World to cout." << std::endl;
std::cerr << "Hello World to cerr." << std::endl;
Cout << "Hello World to Cout." << finl;
Cerr << "Hello World to Cerr." << finl;
Process::Journal() << "Hello World to Journal." << finl;
```





Hello world exercise

• Rebuild the code:

cd \$TRIO_U_ROOT make optim

 Run the code sequentially cd \$TRIO_U_TMP touch hello.data triou hello

• Run the code in parallel and see the differences triou hello 4





Hello world exercise

- Cout <=> std::cout on the master process only
 Use this output for infos about the physics (convergence, fluxes,...)
- Cerr <=> std::cerr on the master process only
 Use this output for warning/errors only
- finl <=> std::endl + flush() on the master process
- Journal() prints to datafile_000n.log files

Use this output during parallel development to print plumbing infos which would be hidden during later production runs

During run, this output can be deactivated with: triou hello -journal=0





Baltik Building Application Linked with Trio_U Kernel





Exercise Create a Baltik project

```
# Initialize Trio_U/Kernel environment
$ source $TRIO_U_ROOT/bin/Init_Trio_U

# Create your project from a basic project template:
$ mkdir -p ~/test/my_project
$ cd ~/test/my_project
$ cp -r $TRIO_U_ROOT/bin/baltik/templates/basic/*.

# Edit your project file project.cfg to specify name, author and executable
# Then configure your project:
$ baltik_build_configure
$ ./configure
```





Baltik exercise

```
# Create a first class and have a look at the 2 files my_first_class.h|cpp
$ cd src
$ baltik_gen_class my_first_class
# Build your project:
$ cd ..
$ ./configure # Necessary each time a source file is added to the project
$ make optim
# List other options available for the make command:
$ make
# Look for more infos here:
# $TRIO_U_ROOT/bin/baltik/doc/README.BALTIK
```





The extensive use of macros in Trio_U





Trio_U important points

Trio_U does not use, for historical reasons:

- Templates
- STL (Standard Template Library)
- Exceptions (until recently)
- -Instead of templates, Trio_U uses macros
- -Instead of using STL, Trio_U defines LIST, VECTORS,...





Trio_U important points

Trio_U hides pointers as much as possible.

```
You will never see:

class A {

private:

B *b_;

};

But instead:

class A {

private:

REF(B) b_;

};
```





Trio_U important points

Why Trio_U hides pointers as much as possible?

```
Second case:
First case:
A::A()
                                            A::A()
  b = new B;
                                              // Just initialize b_
 // Initialize b_
                                              b = \dots
  b = \dots
                                            A::~A()
A::~A()
 // Delete b
  delete b_;
                                              // Nothing to do. b_ is deleted by the
                                              // destruction of the object REF(B)
```





Trio_U macros

Macros are widely used to implement plumbing of several features of Trio_U. For instance:

- To declare and define the class type:
 - -base class (base macros)
 - -instanciated class (instanciable macros)
 - -generic class (deriv macros)
 - -associated class (ref macros)





Trio_U macros

- -To define default class constructor/destructors
- -To define default class methods like printOn(), readOn() to print/read objects on output/input streams
- -To define easily vector (VECT) or list (LIST) of objects
- -For type casting (sub_type & ref_cast macros)





Four different kind of classes in Trio_U:

Base class
Instanciate class
Associated class
Generic class





Base class

Definition:

A base class is a <u>prototype</u> for other classes. It is an <u>abstract</u> class, which can't be instantiated.

Trio_U examples:

Probleme_base Problem base class

Equation_base Equation base class





Base class

Declaration (.h file)

```
class A_base : public Objet_U
{
    Declare_base (A_base);
    public : ...
    virtual DoubleTab& calculer();
    protected : ...
    private :
        int attribute1;
        B attribute2;
}
```

Implementation (.cpp file)

```
Implemente_base(A_base, «A_base», Objet_U);
Entree& A_base::readOn(Entree& is)
     is >> attribute1;
     is >> attribute2;
Sortie& A_base::printOn(Sortie& os)
     os << attribute1;
     os << attribute2;
DoubleTab& A_base::calculer()
... // que_suis_je() methods returns string « A_base »
```

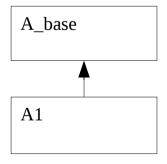




Instanciate class from a base class

Declaration (.h file)

```
class A1 : public A_base
{
         Declare_instanciable (A1);
         public : ...
         protected : ...
         private : ...
}
```



Implementation (.cpp file)

```
Implemente_instanciable(A1, «A1», A_base);
Entree& A1::readOn(Entree& is)
{
...
}
Sortie& A1::printOn(Sortie& os)
{
...
}
...
```





readOn - printOn

printOn and **readOn** methods are useful to print and read an instanciated object (example, here from A1 class):

```
A1 a;
```

EFichier is(« file.txt »); // Trio_U class to read a file is >> a ; // Read the 2 attributes from a file

Cerr << a << finl; // Print the 2 attributes of a SFichier os(« newfile.txt »); os << a; // Write the 2 attributes of a in a new file





But other macros!

Declare_TYPEOPTION(ClassName);

Implemente_TYPEOPTION(ClassName, »Name »,ParentClassName);

TYPE:

base :For an abstract class

instanciable :For an instanciate class

OPTION:

:Class with a constructor/destructor by default

<u>_sans_constructeur</u> :Class without a constructor by default (*you* define the

constructor)

__sans__destructeur :Class without a destructor by default (*you* define the

destructor

_sans_constructeur_ni_destructeur : Class without a constructor or a destructor by default (*you* define the constructor/destructor)



Type casting



sub_type and ref_cast macros

sub_type(classA,B) : useful to check that a
cast is possible <=> is the class of the object B
a derived class of classA ?

ref_cast(classA,B): cast the object B in a classA type object or produces an error if object B is not from a derived class of classA.



Type casting



sub_type and ref_cast macros

Solv_Petsc.cpp example:

```
Int Solv Petsc::resoudre systeme(const Matrice Base& la matrice, const DoubleVect& secmem, DoubleVect&
solution)
    if(sub_type(Matrice Morse Sym,la_matrice))
                                                                                 Process
      const Matrice Morse Sym& matrice = ref cast(Matrice Morse Sym,la matrice);
                                                                                 Objet_U
      assert(matrice.get est definie());
      Matrice Morse mat;
                                                                               Matrice_Base
     MorseSymHybToMorse(matrice,mat,secmem,solution);
      Create objects(mat,secmem);
                                                            Matrice_Bloc
                                                                             Matrice_Diagonale
                                                                                                 Matrice_Morse
   else if(sub_type(Matrice_Bloc_Sym,la_matrice))
                                                          Matrice_Bloc_Sym
                                                                                               Matrice_Morse_Sym
      const Matrice Bloc Sym& matrice = ref cast(Matrice Bloc Sym,la matrice);
      Matrice Morse Sym mat sym;
                                                                                               Matrice_Morse_Diag
```





Interpretors keywords in the data file Eg: **Read** keyword to read an Object





Which method is called?

Dimension 3

Conduction pb

Domaine dom

•••

Associate pb dom

• • •

Read pb { ... }

-Read (as other keywords like Associate) are <u>interpretor</u> keywords. They do several tasks on objects specified by their name (e.g. « pb » name of the problem)

-For each Interpretor, the method of the class **Interpretor** is called when the data file is read:

Interpretor::interpreter(Entree&) { ... }

-For example : Lire.cpp





Link between data file and the code Eg: **Solve** keyword to solve a Problem



Where is solved a problem?



Dimension 3

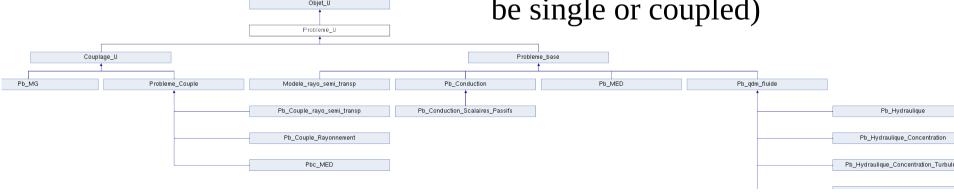
Pb_hydraulique pb

...

Read pb { ... }

Solve pb

- -The **Solve** interpretor solve the problem
- -The object problem is described by a class which inherits from :
 - **Probleme_base** (single base problem)
 - Probleme_U (Trio_U problems can be single or coupled)



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Resoudre call graph



```
Dimension 3
Pb hydraulique pb
Read pb { ... }
Solve pb
```

```
class Probleme_U
virtual initialize() {}
```

class Probleme_base

```
virtual initialize() { ... }
```

```
Resoudre::Interpreter()
    Nom problem_name;
    is >> problem_name;
    Probleme_U& pb = ref_cast(Probleme_U,
        objet(problem_name));
    pb.initialize();
    pb.run();
                      Notice how an object is retrieved
    pb.terminate();
                       from its name (objet() method).
```

Probleme_base::initialize()



- → Probleme_base::preparer_calcul()
 - → milieu().initialiser()
 - → Loop on equation(i).preparer_calcul()
- Schema_temps_base::initialize()

preparer_calcul() methods make further initializations (eg : set time to 0 in fields)

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Resoudre::Interpreter()

pb.initialize()

pb.run()

pb.terminate()



```
Probleme_U::run()
     → computeTimeStep()
                                                     // Call to Probleme_base::computeTimeStep()
          → schema_temps().computeTimeStep()
                                                     // Calculate first time step dt(0)
     \rightarrow Loop on the time steps until stop:
               → Probleme_base::InitTimeStep()
                                                         // Initialize
                    \rightarrow schema_temps().initTimeStep(); // Set dt=dt(n), initialize flags & residuals
                    → Loop on equation().initTimeStep(); // Set new time on each unknown & BC
               → Probleme_U::solveTimeStep()
                                                          // Solve
                    → Probleme_base::iterateTimeStep(); // Loop on each problem for this call
                        → schema_temps().iterateTimeStep(); // Inside, loop on each equation to compute:
                             \rightarrow faire_un_pas_de_temps_eqn_base(equation(i)) //U(n+1)=U(n)+dt*f(U(n))
               → Probleme_base::validateTimeStep()
                                                          // Update
                    → Schema_Temps_base::validateTimeStep()
                        → Probleme_base::mettre_a_jour()
                             → Loop on equation(i).mettre_a_jour() // Update each unknown & BC
                             → milieu().mettre_a_jour()
                                                                   // Update the media
                        \rightarrow Schema_Temps_base::mettre_a_jour() // t(n+1)=t(n)+dt(n)
               → computeTimeStep()
                                                          // Prepare next
                                                                   // Compute next time step dt(n+1)
                    → schema_temps().computeTimeStep()
             → Probleme_base::postraiter() // Post process the results Trio_U 1.7.0 developer training session
                                                                                                 74
```



Resoudre::Interpreter()

La force de l'innovation

pb.initialize()
pb.run()

pb.terminate()

Problem_U::terminate()

- → Probleme_base::terminate()
 - → Probleme_base::finir()



- → Loop on postraitement(i).finir()
- → Probleme_base::sauver()
 - → Probleme_base::sauvegarder()
 - → Loop on equation(i).sauvegarder() // Write unknown in backup file
 - → Loop on postraitement(i).sauvegarder()
- → schema_temps().terminate()





Know some typical C++ compiler message errors before exercise...

Error: Forward declaration « struct example ...

Error: Invalid use of incomplet type « example ...

-> Missing #include <example.h> where example.h declares the example class.

Error: Cannot declare variable 'a' to be of abstract type 'A' because the following virtual functions are pure within 'A':

-> You need to implement a virtual method declared pure virtual method in the base class

Error : ...





Baltik exercise

Process

Cities Lu

The process

Interprofe Comment repro-come

Edit the 2 files:

\$ cd ~/test/my_project/src

\$ nedit|xemacs|gedit my_first_class.* &

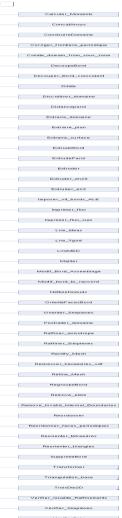
Change the inheritance of the class in order that it inherits not from **Objet_U** but Interprete_geometrique_base class instead. It is the base class of all the keywords doing tasks on domains (eg: **Mailler**, **Lire_fichier**,...).

You will:

- a) add an #include <Interprete_geometrique_base.h> in my_first_class.h
- b) switch **Objet_U** to **Interprete_geometrique_base** in the .h and .cpp files
- c) rebuild your app with:
- \$ cd ~/test/my_project
- \$ make debug # An error will occur



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Baltik exercise

You will have an error indicating a pure virtual function (interpreter_) should be implemented. Look at the **Interprete_geometrique_base** class thanks to HTML documentation from \$TRIO_U_ROOT/index.html and notice the **interpreter()** method.

This method is called each time a keyword is read in the datafile (eg: **Read_file** dom dom.geom, **Solve** pb,...)

Define the public method **interpreter_(Entree&)** in the include file and implement it (just print a message with Cerr like "My first keyword!") into the cpp file. **Entree** is a Trio_U class to read an input stream (from a file for example):

virtual Entree& interpreter_(Entree&);

Rebuild your project and fix your files until the binary of your project is built (named basic if you have not changed the name in the project.cfg file):

\$ cd ~/test/my_project

\$ make debug







Baltik exercise

Create a test case into the tests/Reference directory of your Baltik project (it should be the directory location of all your test cases for the project):

\$ mkdir -p ~/test/my_project/tests/Reference/NonRegression

\$ cd ~/test/my_project/tests/Reference/NonRegression

\$ triou -copy Cx

\$ cd Cx

\$ nedit|gedit|xemacs Cx.data

Add into the data file *Cx.data* the keyword **my_first_class** just after the line where the problem is discretized, reduce the number of time step to only 1 and run your binary to check that this new keyword is recognized:

\$ ~/test/my_project/basic Cx

Understand that **Interprete_geometrique_base::interpreter()** method is called first, which calls then the **my_first_class::interpreter_()** method.





Four different kind of classes in Trio_U:

Base class
Instanciate class
Associated class
Generic class





Associations between objects

An object A can have other objects as attributes:

- Either by composition (e.g. <u>of</u> an object from class B) :
 - Object b_ is created (or destroyed) when an instance from A is created (or destroyed)
- Or by association (e.g. with an object from class C):

```
Class A: public Objet_U
{
    public:
        B b_;
        REF(C) c_;
}
```

- Object pointed by c_ exists independently of any instance of A
- Implemented by the REF macro in Trio_U:
 REF(C) c_; <=> C *c_;
- When an instance of A is destroyed, the pointer c_
 is deleted but the pointed object is still in memory:





Real life example

```
-Class Car-Class Tires-Class Plate_number
```

```
Class Car
{
    Tires set_of_tires_;
    Plate_number* number_;
    ...
};
```

In blue, object attributes by composition In red, object attributes by association Trio_U 1.7.0 developer training session





Equation_base class example

```
protected:
  Nom nom;
  Solveur_Masse solveur_masse;
  Sources les_sources;
  REF(Schema_Temps_base) le_schema_en_temps;
  REF(Zone_dis) la_zone_dis;
  Zone_Cl_dis la_zone_Cl_dis;
  REF(Probleme_base) mon_probleme;
 In blue, object attributes by composition
 In red, object attributes by association
 NOTE : REF(A) is noted Ref_A in the HTML documentation
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                                                           83
```





Associated class (REF)

```
Class A : public Object_U
{ }
Class REF(A) : public Ref_
{ }
```

Generally declared/implemented in a Ref_A.h/Ref_A.cpp files with the 2 macros Declare_Ref/Implemente_Ref:

```
#ifndef RefA_inclus
#define RefA_inclus
#include <Ref.h>
class A;
Declare_ref(A);
#endif
```

```
#include <Ref_A.h>
#include <A.h>
Implemente_ref(A);
```





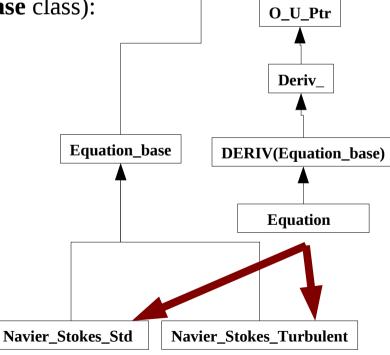
Generic class

– <u>Definition</u>: A generic class A is useful to create objects which can be typed at every moment to any object inheriting from A_base class.

Objet_U

- Example: The Equation class (vs the Equation_base class):

```
Equation eqn;
if (...)
    eqn->typer(Navier_Stokes_std);
else
    eqn->typer(Navier_Stokes_Turbulent);
....
eqn->derivee_en_temps_inco();
```



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Generic class (DERIV)

Declaration (.h file)

```
Declare_deriv(A_base);
class A : public DERIV(A_base)
{
    Declare_instanciable (A);
    public : ...
    // Generally inline all the methods
    DoubleTab& method()
    protected : ...
    private : ...
}
inline DoubleTab& A::method()
{
    return valeur().method();
}
```

Implementation (.cpp file)

```
Implemente_deriv(A_base);
Implemente_instanciable(A, « A»,DERIV(A_base));
Entree& A::readOn(Entree& is)
{
...
}
Sortie& A::printOn(Sortie& os)
{
...
}
...
```



Generic class



Equation_base inconnue()=0

Navier_Stokes_Std inconnue()

Conduction inconnue()

- All generic classes have a valeur() method to return the the pointed type of the object, which is different of the object type given by the que_suis_je() method. Example :

```
Conduction cond; // Instanciated class
Cerr << cond.que_suis_je() << finl ; // Prints « Conduction »</pre>
```

```
Equation eqn; // Generic class
eqn.typer(Conduction);
Cerr << eqn.que_suis_je() << finl ;// Prints « Equation »
Cerr << eqn.valeur().que_suis_je() << finl; // Prints « Conduction »</pre>
```

- Often (but not always), hierarchy methods are also coded in generic classes to avoid the use of .valeur(). Example :

```
Champ_Inc& Equation::inconnue() {
   return valeur().inconnue();
}
```

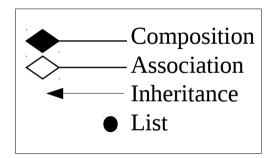
Equation inconnue()

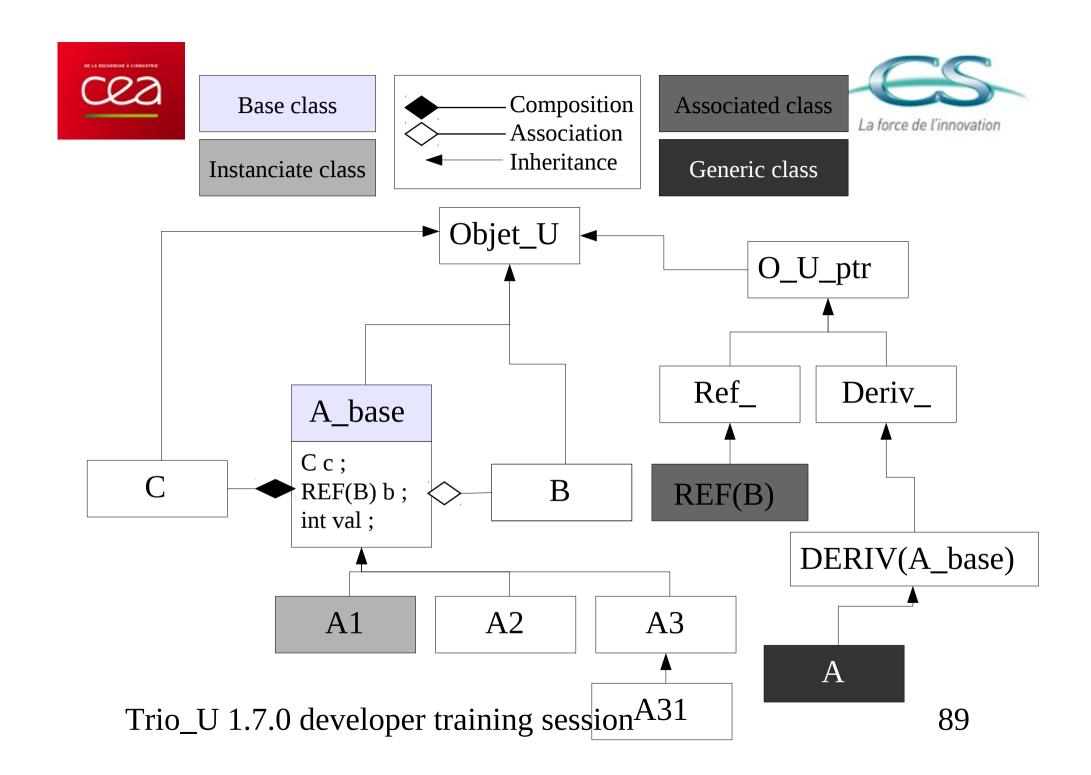


Hierarchy examples and UML notations



UML (Unified Modeling Language)









Exploring the Kernel modules





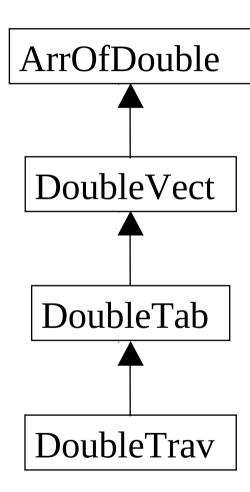
Math (Kernel)
Part I: Arrays





Math module

- Array for double :
 - ArrOfDouble A(n)
 - → Basic array, no mecanism to extend data for parallelization
 - DoubleVect A(n)
 - DoubleTab A(n) or A(n,m) or..
 - DoubleTrav A(n)
 - → same than DoubleTab except memory managment
- -Array for Integer (same but Int instead of Double), example:
 - ArrOfInt, IntVect,...







Math module

Difference between DoubleTab and DoubleTrav

- -DoubleTab does a memory allocation/deallocation
- -DoubleTrav does a memory allocation but don't deallocate for a future reuse

Use Trio_U arrays cause manage memory for you and detect out of bounds during debug mode runtime.

Example:

DoubleTab A(n);

Cerr << A(n) << finl; // Error detected

Cerr << A(0,0) << fin; // Error detected





```
// Create and size :
DoubleTab A(n);
// Create (A.size_array()=0) then resize :
DoubleTab A;
if (nb\_comp==1)
 A.resize(n);
else
 A.resize(n,2);
```





```
// Initialize an array :
DoubleTab A(n); // A(i)=0.0
DoubleTab A(n,1.0); // A(i)=1.0
DoubleTab A(n,1); // A(i,0)=0.0
DoubleTab C(n);
C=1; // C(i)=1.0
DoubleTab B(A); // Dimension B and B=A
B+=C; // B(i)=A(i)+1
```





```
DoubleTab C;
  C=B; // Dimension C according to B and copy values
  C.copy(B, Array_base::COPY_INIT); // Same than previous
  DoubleTab C;
  C.copy(B, Array_base::NOCOPY_NOINIT);
  // Dimension C according to B. C(i)=? (uninitialized)
  C.resize_array(n+10, Array_base::COPY_NOINIT);
  // C(i<n) is kept. C(n<=i<n+10)=? (uninitialized)
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```





```
DoubleTab A(n,m);
Cerr << A.nb_dim() << finl;  // 2
Cerr << A.size() << finl;  // n*m
Cerr << A.size_array() << finl;  // n*m
Cerr << A.dimension(0) << finl;  // n
Cerr << A.dimension(1) << finl;  // m</pre>
```





How to debug Trio_U gdb valgrind





Use gdb tool to debug or understand the code

```
# To describe all the commands:
$ man gdb
# To debug the Trio_U binary program compiled with -g:
$ gdb $exec_debug
  # List of the gdb commands:
  run datafile # Run the calculation on the datafile
  where or bt # Todisplay the program stack (useful to understand who called what)
               # To move up in the stack
  up
               # To move down in the stack
  down
  list
               # List the source code
               # To continue the calculation after a stop
  cont or c
  break class::method # To add a breakpoint on a method of a class
  break line# To add a breakpoint on a line of the file once inside a method
  break exit # Useful to set a breakpoint just after a Trio_U error message is printed (before the stack is left)
               # Execute next line
  next or n
               # Execute next line and enter in a method/function if any
  step or s
               # Print a variable
  print var
```





Use gdb tool to debug or understand the code

- # Specific gdb commands for Trio_U (macros in a gdb wrapper)
 # to dump an array or print array values:
 - -To dump a DoubleVect : dump array
 - -To dump a DoubleTab: dumptab array
 - -To dump a IntVect : dumpint array
 - -To dump a IntTab: dumpinttab array
 - -To print tab(i)of a DoubleVect array: print tab.operator()(i) or tab[i]
 - -To print tab(i,j)of a DoubleTab array : print tab.operator()(i,j) or tab[i,j]

To debug a parallel calculation with N processes: mpirun **-gdb** -np N \$exec_debug datafile N

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Exercise with gdb

```
Build a debug version of Trio U if necessary:
cd $TRIO U ROOT
(OPT="";monodir)
cd tests/Reference/upwind
gdb $exec_debug
(gdb) break SSOR::ssor # Stop into the SSOR preconditionner
(gdb) run
(gdb) where # Have a look at the stack
(gdb) n
                # Or print matrice.tab1_ if "optimized out" message printed
(gdb) print tab1
                        # Print only a value of an array
(gdb) print tab1[10]
(gdb) dumpint tab1
                     # Dump the array
(gdb) print tab1.size_array() # Array size
```

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Exercise with gdb

```
(gdb) up
(gdb) list 100 # Print lines after the 100<sup>th</sup> line
(gdb) print matrice
(gdb) print matrice.que_suis_je() # Kind of matrix ?
(gdb) print matrice.que_suis_je().nom_ # Kind of matrix ?
(gdb) up 5 # Move up 5 levels
(gdb) list 900
(gdb) print la_pression.que_suis_je().nom_ # Pressure field
(gdb) print la_pression.valeurs() # Pressure values (DoubleTab)
(gdb) print la_pression.valeurs().nb_dim() # DoubleTab dimension
(gdb) dumptab la_pression.valeurs() # Dump the field values
```





Use valgrind to find memory bugs

- -Valgrind is a memory checker tool: http://www.valgrind.org
- -You can check a binary with:
- **\$ valgrind** \$exec_debug datafile

Or within the gdb debugger:

- \$ gdb -valgrind \$exec_debug
- It detects uninitialized variables, memory leaks, outbound array values,...
- -Trio_U has <u>0</u> errors/warnings/memory leaks according to valgrind on the 2000 non-regression test cases (checked every night). Some errors in third party code (OpenMPI, MUMPS, OpenBlas,...)

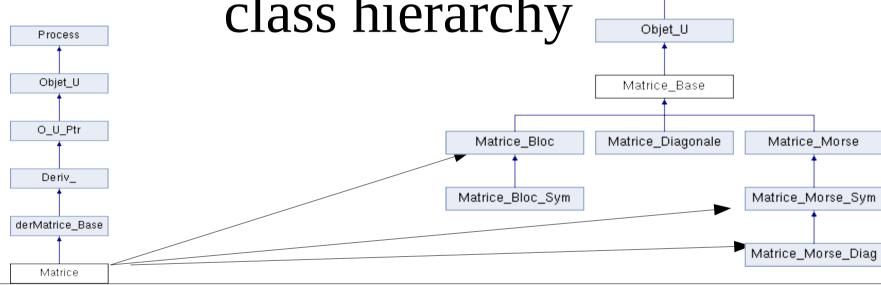




Math (Kernel) Part II: Matrix, Vect, List



Example of the matrix class hierarchy



```
class Matrice_Base : public Objet_U // Base class (and also abstract cause pure virtual method defined)
{ Declare_base(Matrice_Base);
public :
    virtual int ordre() =0 ; ... } ;
class Matrice_Morse : public Matrice_Base // Instanciate class :
{ Declare_instanciable_sans_constructeur(Matrice_Morse); ... } ;
class Matrice : public DERIV(Matrice_Base) // Generic class
{ Declare_instanciable_sans_constructeur(Matrice) ; ... } ;
```

La force de l'innovation





VECT and LIST macros

One can regroup a set of objects of the same kind by using:

- either VECT, vector of objects
- or LIST, list of objects

Similar interface (search(), add(),...) and performance except for an access to one specific element (LIST slower than VECT in this case)

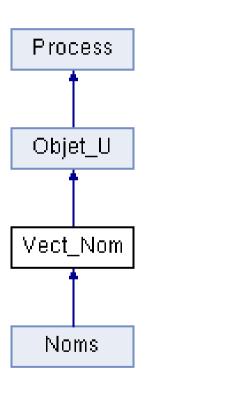


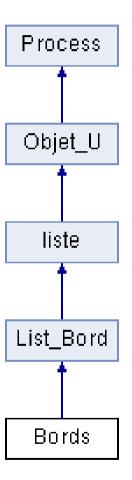


Examples of VECT and LIST

Noms VECT(Nom)
Bords LIST(Bord)

• • •







VECT(class) LIST(class)



Declaration (.h file)

```
Declare_vect(As);
class As : public VECT(A)
{
     Declare_instanciable (As);
     public : ...
     protected : ...
     private : ...
}
```

Implementation (.cpp file)

```
Implemente_vect(As);
Implemente_instanciable(As, «As», VECT(A));
Entree& As::readOn(Entree& is)
{ ... }
Sortie& As::printOn(Sortie& os)
{ ... }
```

```
Declare_liste(As);
class As : public LIST(A)
{
          Declare_instanciable (As);
          public : ...
          protected : ...
          private : ...
}
```

```
Implemente_liste(As);
Implemente_instanciable(As, «As»,LIST(A));
Entree& As::readOn(Entree& is)
{ ... }
Sortie& As::printOn(Sortie& os)
{ ... }
```

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Practice exercise

Use the HTML documentation to see MacVect.h and have a look at the VECT methods.

→ Find the method names for ??? in the code :

```
Noms StudentNames;
StudentNames.???(3);
StudentNames[0]=...;StudentNames[1]=...;StudentNames[2]=...;
int number = StudentNames.???(« Betty » );
Nom NewStudent(« Bart »);
StudentNames.???(NewStudent);
```



Read the data file



The class **Param** use is the recommended choice to read parameters in the data file:

```
#include <Param.h>
Entree& A::readOn(Entree& is)
                                       A a
                                       Read a { dimension 3 option fast }
    Nom opt;
    int dim;
    Cerr << « Reading parameters of A from a stream (cin or file) » << finl;
    Param param(que_suis_je());
    // Register parameters to be read:
    param.ajouter("option",&opt);
    param.ajouter("dimension",&dim,Param::REQUIRED); // Mandatory parameter
    // Read now the parameters from the stream is and produces an error if unknown
    // keyword is read or if brackets are not found at the beginning and the end:
    param.lire_avec_accolades_depuis(is);
    return is;
```





Add into the interpreter_(Entree&) method the read of a domain and some parameters into brackets. In the data file, the syntax will be:

my_first_class dom { option 0 } # dom is the domain name #

Use the following method to read the name of the domain Interprete_geometrique_base::associer_domaine(Entree&). Look the HTML documentation. What is the task of this method?

To help you, have a look at a Interprete_geometrique_base sub-classe, for instance Raffiner_anisotrope to see how the domain is read. The datafile syntax is:

Raffiner_anisotrope DomainName







Then use the **Param** object to read the keyword parameter option in the data file. **Param** use is the recommended choice in this case (even if a lot of current Trio_U classes still use the old fashion to read parameters), cause it simplifies greatly the coding.

Add #include <Param.h> into the cpp file and if help needed, have a look at the Interprete_geometrique_base sub-classe Extruder. The datafile syntax is:

Extruder { domaine DomainName nb_tranches N direction X YZ }

Once implementation is finished, add a check at the end of the method *interpreter_(Entree&)* and find how to print the domain name:

Cerr << "Option number " << option_number << " has been read on the domain named " << ??? << finl;







- # Build/fix/re-build/run the test case:
- \$ cd ~/test/my_project
- \$ make debug
- \$ cd tests/Reference/NonRegression/Cx
- \$ ~/test/my_project/basic Cx





Terminology/chronology of methods in Trio_U

interpreter()/readOn()

→ The parameters of the keyword are read

associer()

→ Called by a **Associate** keyword, generally to fill the references (pointer) to other objects (eg: link to an Equation)

discretiser()

→ Called by **Discretize** keyword, complete tasks related to the selected discretization (eg : discretize a field)

completer()

→ All the data file is read, and some initializations are completed now

Loop in the Probleme_base class on each equation -> Probleme_base.cpp

Loop in Equation_base class on each operator, discretized boundary condition, sources and time sheme -> Equation_base.cpp

preparer_calcul()

→ Before the first time step (eg : initialize arrays, set time to 0)

Loop in the Probleme_base class on each equation -> Probleme_base.cpp

calculer()

→ During the time step, perform the main task of the class

mettre_a_jour()

→ At the end of the time step (eg : update time field)

Loop in the Probleme_base class on each equation -> Probleme_base.cpp

postraiter()

→ At the end of the time step, post process the fields into the result files

Example : LES Turbulence model in Mod_turb_hyd_ss_maille.cpp





Framework (Kernel)

Problem, Domain, Equation, Time steps





Simple datafile

Dimension 2

Domaine domain **Read_file** domain file.geom

Fluide_Incompressible media **Read** media **{ ... }**

Schema_Euler_explicite scheme **Read** scheme { ... }

VDF discretization **Read** discretization { ... }

Pb_hydraulique problem

Associate problem domain

Associate problem media

Associate problem scheme

Discretize problem discretization

Read problem { ... }

Solve problem

5 objects:

Domain

Media

Scheme

Discretization

Problem

5 classes:

Domaine

Milieu

Schema_Temps

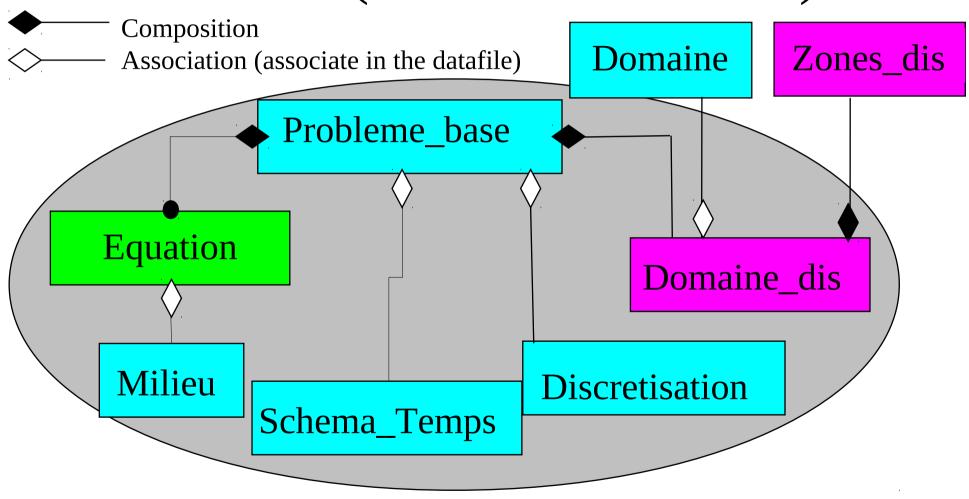
Discretisation

Probleme_base





Problem (Kernel framework)



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Objects creation

- -Associated objects should be created before being associated
 - e.g. : Milieu, Schema_Temps,...
- -Objects by composition are automatically created
 - e.g.: Equation and Domaine_dis by the problem
 - What is a **Domaine_dis** vs a **Domaine**?





First, Domain and Zone

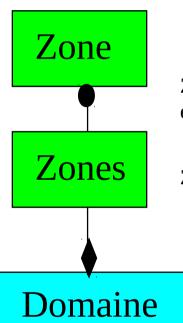
Domaine : Spatial domain of resolution of a problem

Contains the **Zones** and the vertexes (**DoubleTab** sommets) used by the **Zones**

Zones: List of meshes to support multi meshes domain (not fully implemented in Trio_U, so everywhere in the code a **Zones** list has a size of 1).

Zone: Is a mesh with cells of same type (eg: tetraedras). It contains:

- The cells (IntTab mes_elems)
- The type cell (**elem**)
- The boundaries (« **Bord** » and « **Raccord** ». **Bord** is a boundary, **Raccord** is a boundary where coupling is possible to another domain)
- The boundaries between sub domains for parallelism (« **Joint** »)

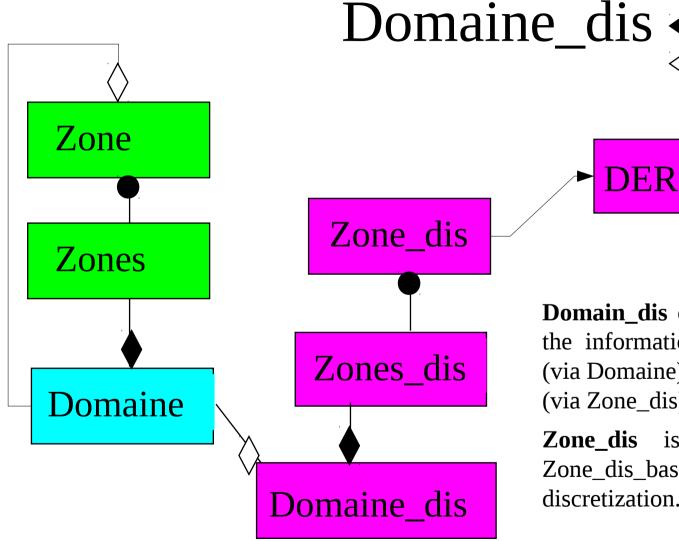






Composition

Association



DERIV(Zone_dis_base)

Domain_dis contains, directly or not, all the information related to the geometry (via Domaine) or the discretized geometry (via Zone_dis)

Zone_dis is a generic class from Zone_dis_base and it depends of the discretization...

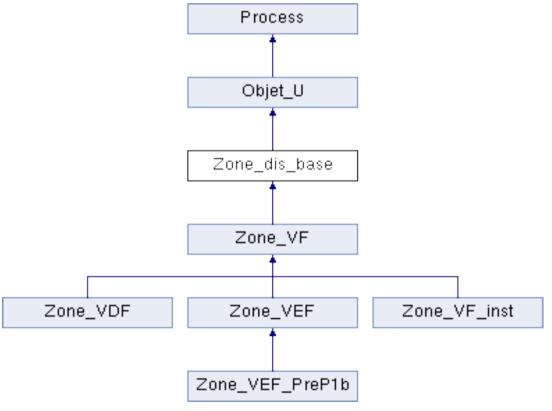
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Zone_dis_base



Zone_VF: Finite volume description class. Describes control volumes, with xp (center of cells), xv (center of faces)

Zone_VDF: VDF class description with face surfaces, face orientation, ...

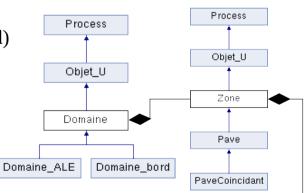
Zone_VEF: VEF class description with face normals, face surfaces, ...

Zone_VEF_PreP1B: Addition to the VEF class (possible edge discretization)





- # We are going to try to print informations of the domain boundaries in our current project:
- # Edit the *my_first_class.cpp* file and add into the interpreter_() method a loop on the boundaries.
- # Look for help inside the Domaine, Zone, Bord, Frontiere classes into the HTML documentation to access to the:
- -Number of boundaries (**nb_bords()** method)
- -Boundaries (**bord(int)** method)
- -Name of the boundaries (**le_nom()** method)
- -Number of faces of each boundary (**nb_faces()** method)



You will print the infos with something like:

Cerr << "The boundary named " << ??? << " has " << ??? << " faces." << finl;

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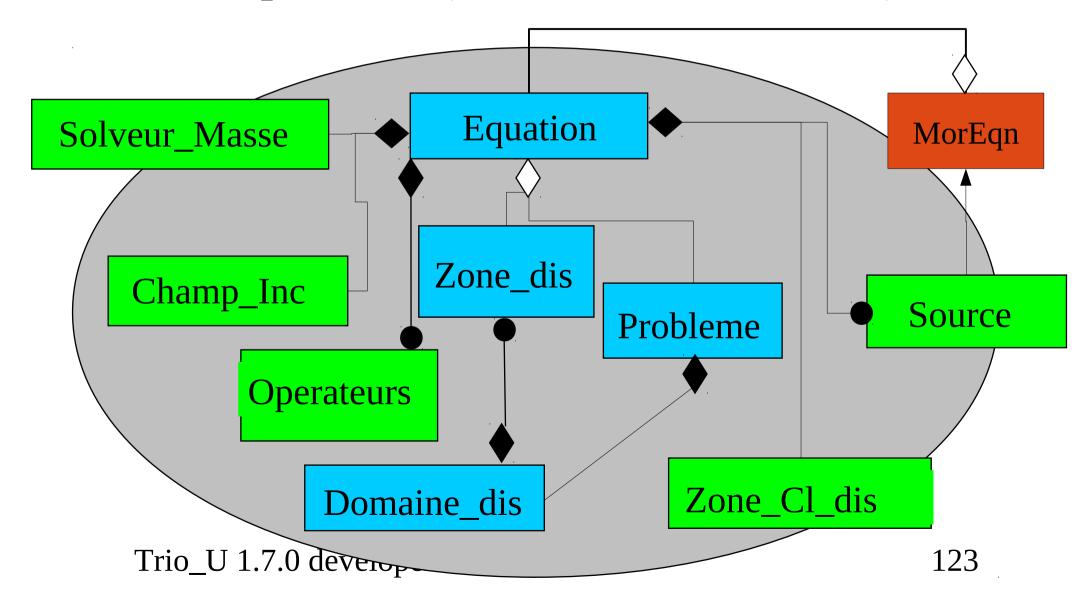
Objet U

Frontiere

Bord



Equation (Kernel framework) ce de l'innovation

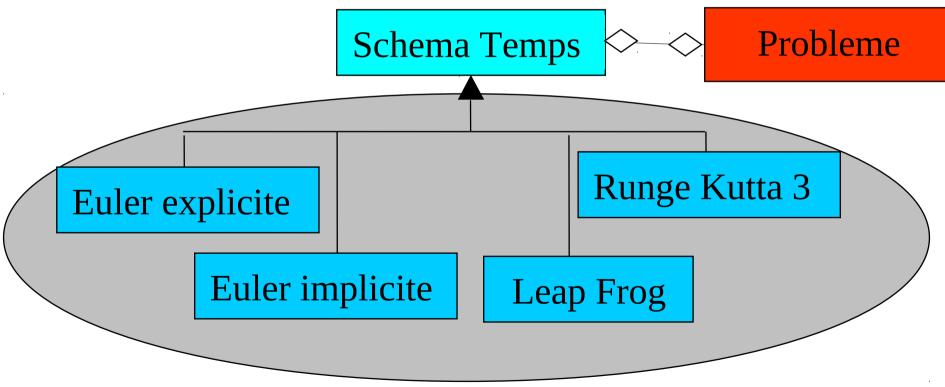






Time Schemes



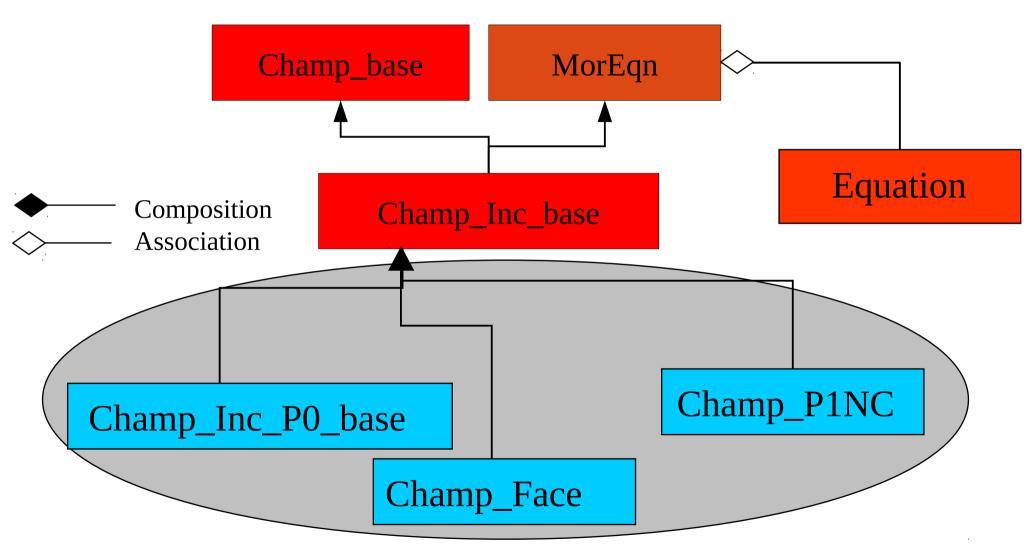


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Fields



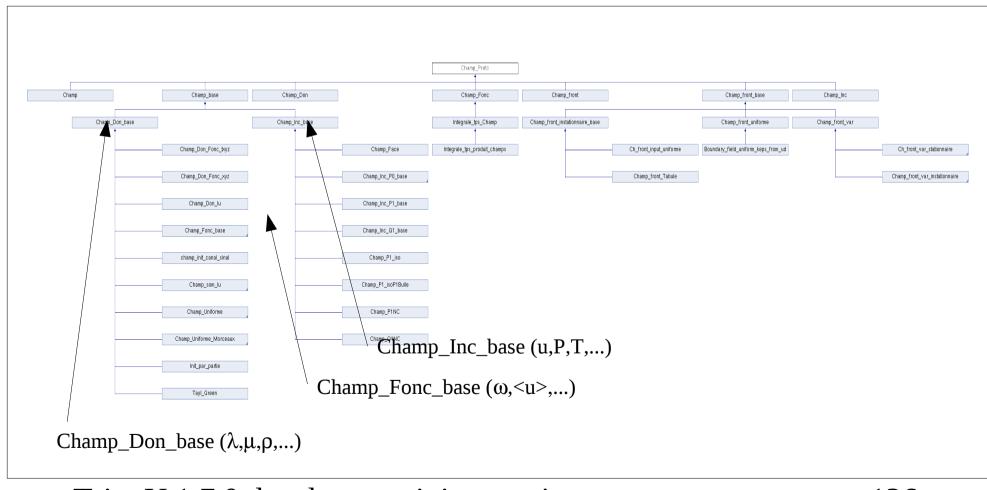


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Field hierarchy

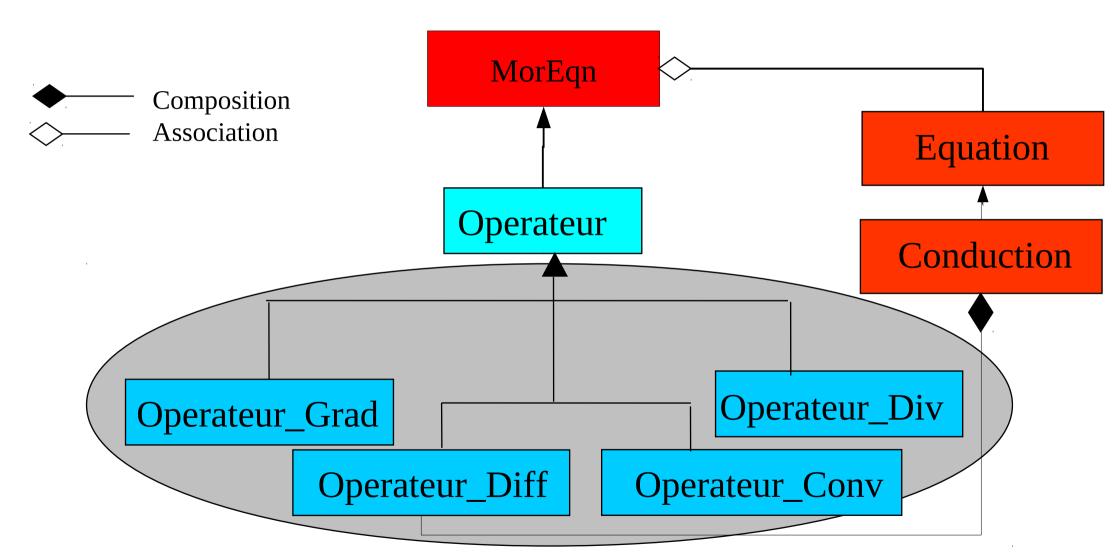


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Operators





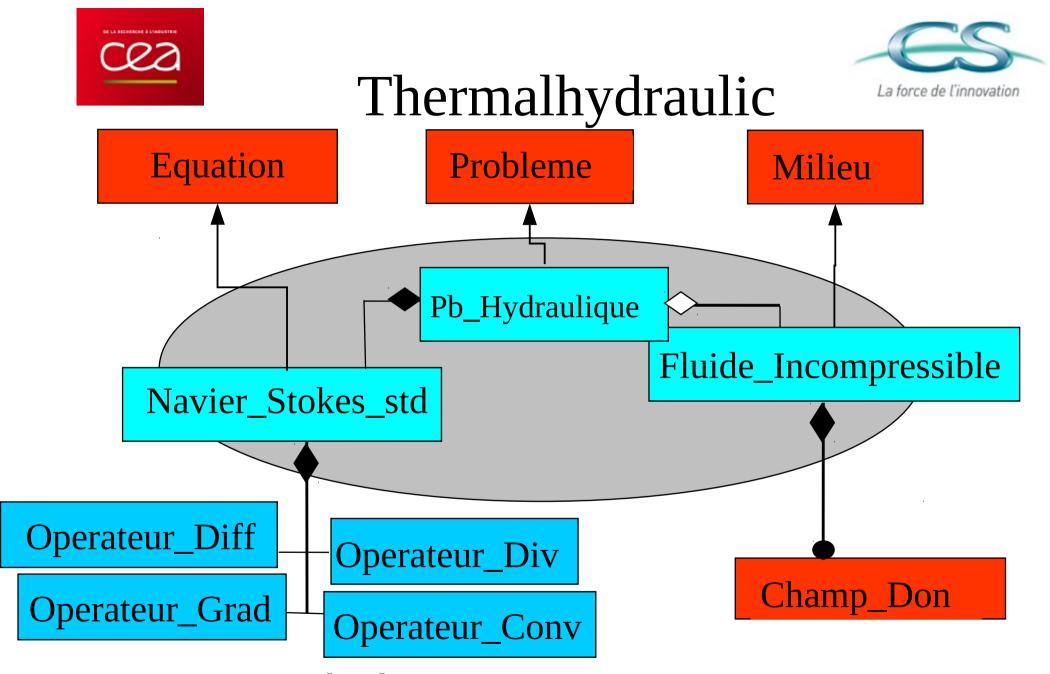
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Trio_U ThHyd module

Incompressible Thermalhydraulic

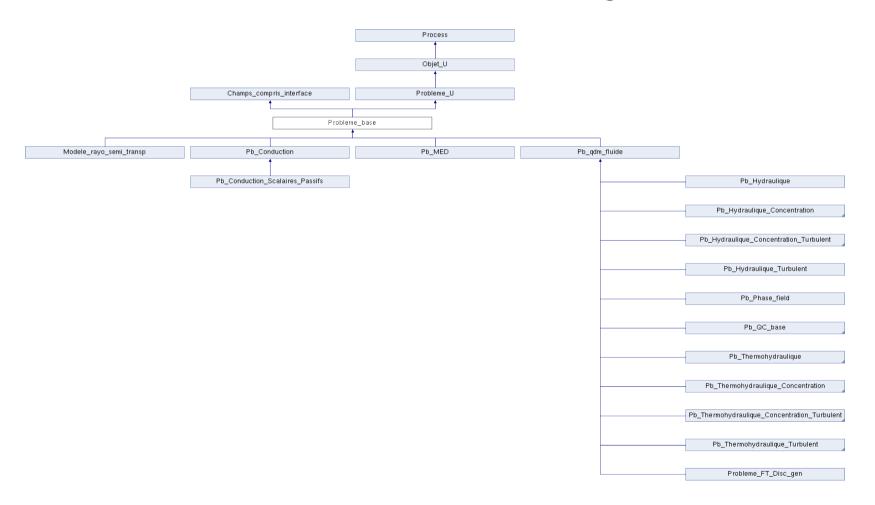


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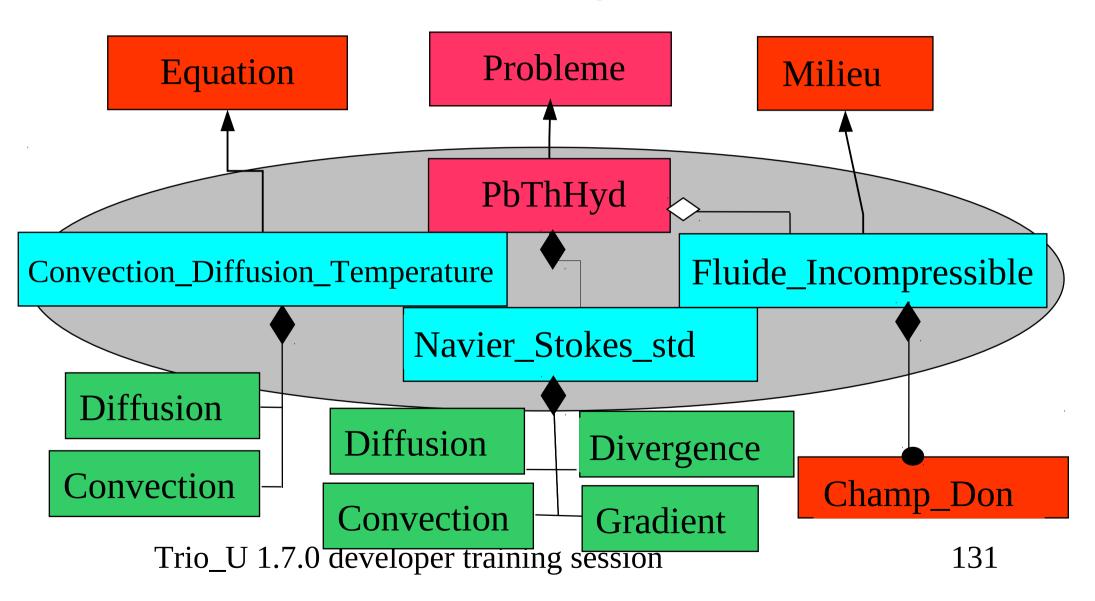
Problem hierarchy







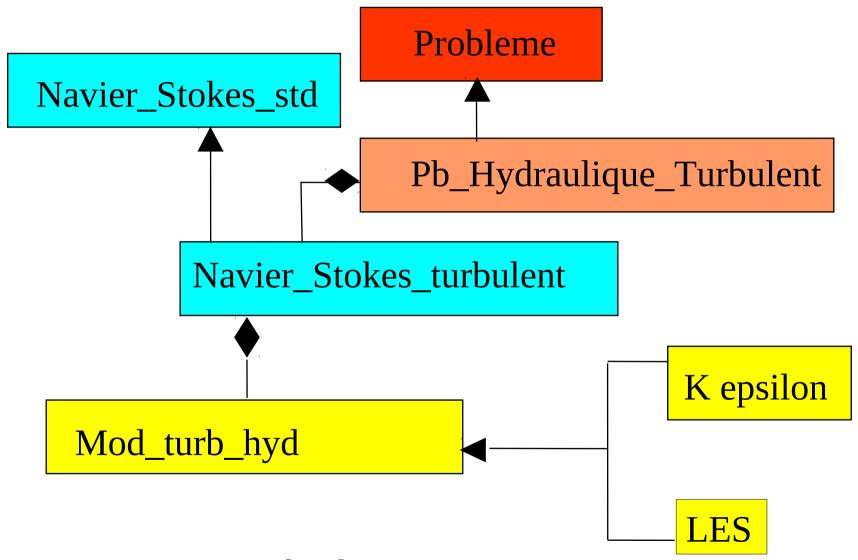
Thermalhydraulic





Thermohydraulic





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Trio_U spatial discretization modules

VDF: Finite-volume differences method

More details in CHATELAIN A. thesis: http://www.theses.fr/2004INPG0065

VEF: Finite-volume elements method

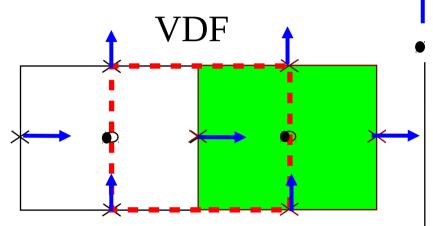
More details in FORTIN T. thesis: http://www.theses.fr/2006PA066526





La force de l'innovation

Available discretizations

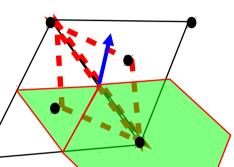


Field localisation:

- Vector field (P1NC) at the center of the faces control volume:
- Scalar field (P0) at the center of elements mass control volume:



Pressure



 \mathbf{VEF}

Field localisation:

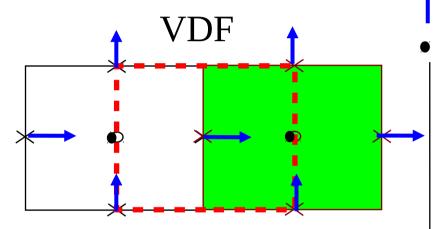
- Vector and scalar fields (P1NC) at the center of the faces control volume:
- Pressure (P0P1Bulle) at the nodes and the center of elements mass control volumes:





Available discretizations

La force de l'innovation

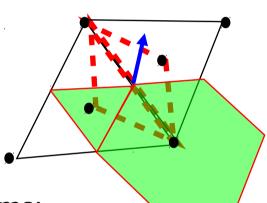


Algorithms:

- -Iterators to loop on elements or faces
- -Evaluators to calculate fluxes on faces or facets VDF/Operateurs/Iterateurs VDF/Operateurs/Evaluateurs

Velocity

Pressure



 VEF

Algorithms:

-Repeated loops on elements, faces or facets to calculate fluxes on the control volumes for <u>each</u> scheme



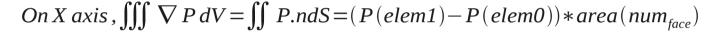
Momentum control volume
Mass control volume

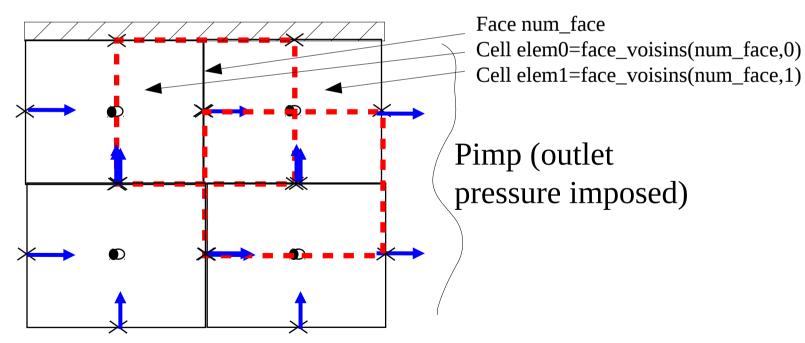




Gradient operator example in VDF

To evaluate the volume control integration of the gradient (eg : pressure) :





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Gradient operator example in VDF

See Op_Grad_VDF_Face::ajouter(const DoubleTab& inco, DoubleTab& resu)

1) Loop on the boundaries :

nb_front_cl() returns the number of boundaries
les_conditions_limites(i) returns the boundary condition on the ith boundary
face_voisins(face,0:1) returns the two elements surrounding the face
face_surfaces(face) returns the area of the face
bord.num_premiere_face() returns the first face of the boundary bord
bord.nb_faces() returns the number of faces of the boundary bord

2) Loop on the internal faces:

premiere_face_int() returns the first internal face of the zone
nb_faces() returns the number of faces of the zone

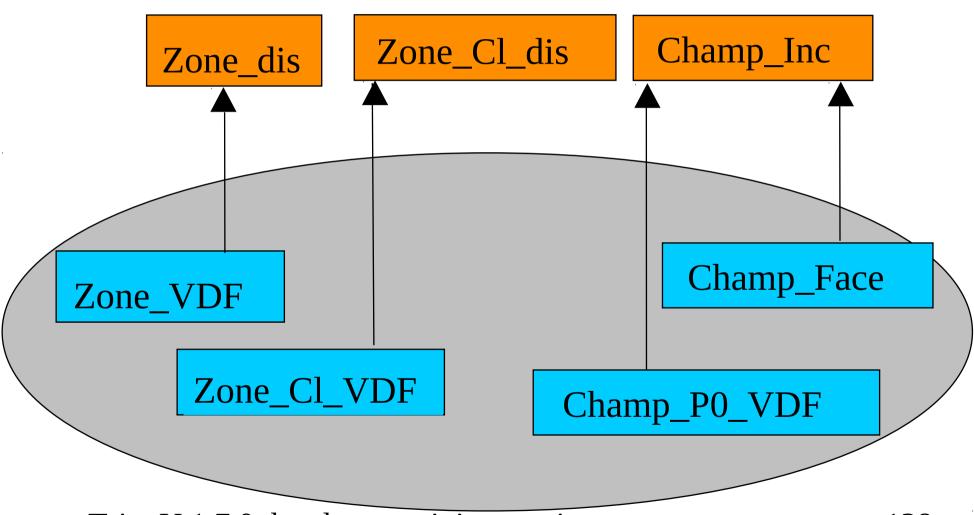
Remember: Boundary faces are ranked first then internal faces in the zone.

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VDF Zones and Fields

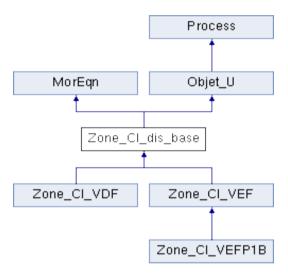


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Zone_Cl_dis_base



The Zone_Cl_dis_base classe describes discretized boundary conditions :

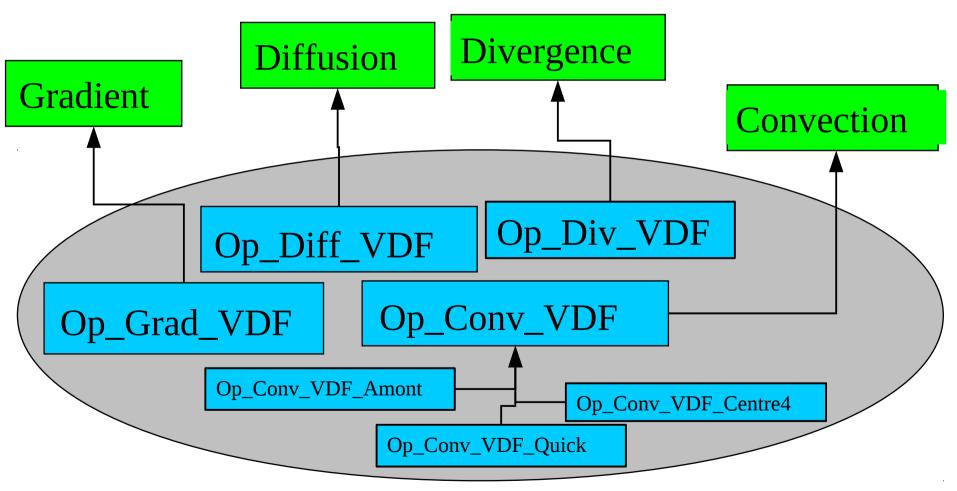
Protected:

Conds_lim les_conditions_limites_;





Operators VDF implementation



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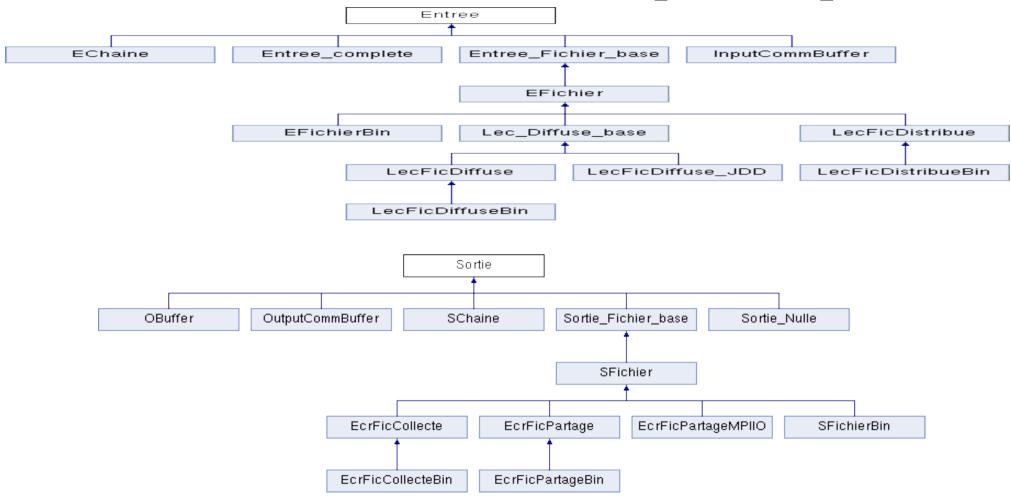


Managing input/output files with Trio_U classes





Dedicated classes to input/output



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Dedicated classes to output

```
EcrFicCollecte file(« file.txt »); // Each process will write in a specific file

file << Process::me();

EcrFicPartage file(« file.txt »); // Each process will write in the same file but sequentially

file << Process::me();

file_0000.txt:0

file_0001.txt:1

...

file_0001.txt:1
```

```
SFichier file(« file.txt »); // Each process open the same file
  file<<Process::me();
  // Better to use on the master process only:
  if (Process ::je_suis_maitre()) {
        Sfichier file(« file.txt »);
        file << « Flow mass rate : »<< flow << finl;
  }</pre>
```

file.txt: 0 1 2 3 4 ... N

file.txt : Inpredictable !





Dedicated classes to input

```
LecFicDistribue file(« file.txt »); // Each process will read in a specific file_000i.txt file >> value;
```

```
LecFicPartage file(« file.txt »); // Each process will read in the same file but sequentially file >> value;
```

```
EFichier file(« file.txt ») ; // Each process will read the same file
file>>value;
// In this case, better to use (cause opening the same file by a lot of process is not efficient) :
```

LecFicDiffuse file(« file.txt »); // Only the master process read the file and send to other processes : file>>value;





Now, we are going to try to calculate the sum of the VEF control volumes on the domain in our project.

The information is in the Zone_VF class (a Zone_dis discretized zone) which can't be accessed from the domain, only from the problem. So we need to read another parameter in our data file:

my_first_class dom { option 0 problem pb }

Add the read of a new parameter problem (see Extraire_plan::interpreter_(Entree&) method for instance) into the *my_first_class.cpp* file.

Then, remember the equation UML diagram page 123.

Look for help inside the Zone_VF, Probleme_base and Equation_base into the HTML documentation to access to the:

- -equation (equation(int) method)
- -discretized zone (zone_dis(int) method)
- -control volumes (volumes_entrelaces() method)







You will need to cast the discretized zone returned by the **zone_dis()** method into a Zone_VF object.

You will print the size of the control volumes array with something like:

Cerr << control_volumes.size() << finl;</pre>

Where control_volumes is a **DoubleVect** returned by the **Zone_VF::volumes_intrelaces()** method.

If you look at the previous Problem UML diagram, you will notice a better path to access to the discretized zone: _____. What is this path ?





Now, compute and print the sum of the control volumes into a file whose name is something like:

DataFileName_result.txt where DataFileName is the name of the data file (eg: Cx).

For that, you will create the previous filename with the class **Nom** by adding to the name of the data file (given by **Objet_U::nom_du_cas()** method) the string "_result.txt" thanks to the operator+= method of the class **Nom**.

Then you will create the file with the **SFichier** class and print the sum into this file.

Once everything is implemented, run the test case (but, first add the keyword **FIN** just after the line where **my_first_class** is used in order to not run the whole calculation...)

\$ cd ~/test/my_project/tests/Reference/NonRegression/Cx

\$ ~/test/my_project/basic Cx





How to parallelize in Trio_U

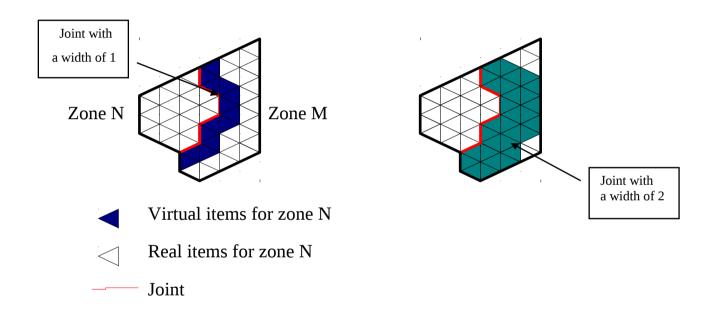




- -SPMD (Single Program, Multiple Data)
- -Definitions of the Trio_U parallelism :
 - Domain partition create several Zones
 - Each process works on one Zone
 - Joint (faces that connect different Zones)
 - Items (which constitute a Zone)
 - cell, vertex, face, edge (3D)
 - may be real (physically located on the Zone) or virtual (located on the remote Zone, but known by the local process)





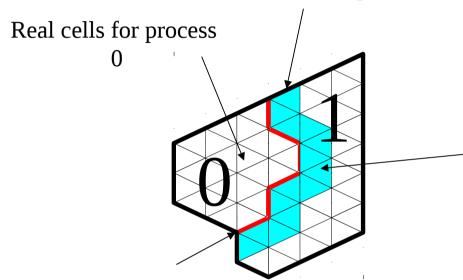


The virtual items of the local Zone are the remote items constituted of vertexes located up to n vertexes of the n-width joint.





Virtual boundary face for the process 0



Joint with <u>common</u> faces and <u>common</u> vertexes for the processes 0 et 1. These <u>common</u> items are <u>real</u> items for the 2 processes.

Virtual items in blue (faces, cells, vertexes) constitute the « virtual space » of the process 0.

For the process 1, the same items are real and constitute the « remote space » of process 0.







• Number of real items:

Zone_VF::nb_faces()

Domaine::nb_som()

Zone::nb_elem()

• Number of real+virtual items:

Zone_VF::nb_faces_tot()

Domaine::nb_som_tot()

Zone::nb_elem_tot()

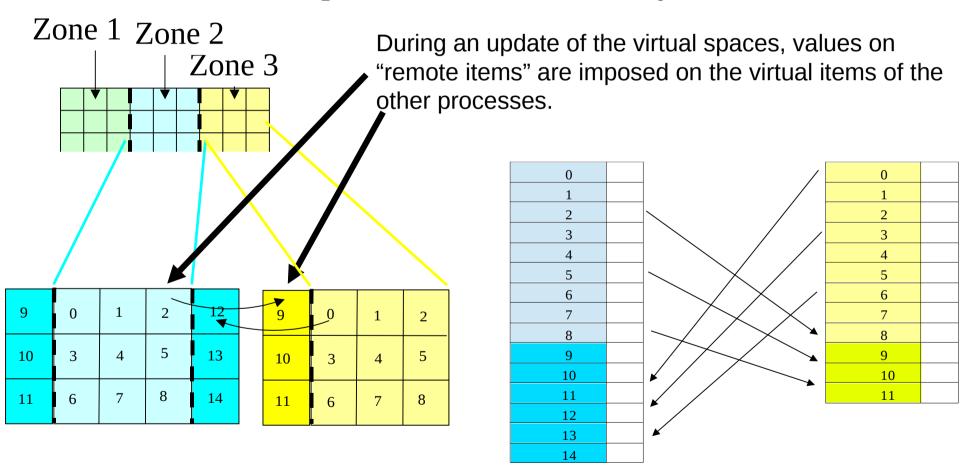
	1	
	2	
	3	
	4	
	5	
	6	
	7	
	8	
	9	
	10	
	11 12	
	12	-

Example of distributed array with additionnal data stucture (**MD_Vector** in Trio_U)





Example of a distributed array on cells



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 Example to create a distributed array : #include <MD_Vector_tools.h> int nb_elem=la_zone_vef.nb_elem(); int nb_elem_tot=la_zone_vef.nb_elem_tot(); const Domaine& dom=la_zone_vef.domaine(); DoubleVect A(nb_elem); const MD_Vector& md = la_zone_vef.zone().md_vector_elements(); **MD_Vector_tools::creer_tableau_distribue(md, A);** /* A has now nb_elem_tot values */ DoubleVect A(B); /* Or use an existing distributed array, here B */ DoubleVect C(nb_elem_tot); /* Warning, C is NOT a distributed array: */





Sizes before and after the creation of a distributed array :

```
DoubleVect A(nb_elem);
// Before:
Cerr << A.size() << finl; // nb_elem
Cerr << A.size_array() << finl; // nb_elem</pre>
Cerr << A.size_reelle() << finl; // nb_elem
Cerr << A.size_totale() << finl; // nb_elem
const MD_Vector& md = domaine().zone().md_vector_elements();
MD_Vector_tools::creer_tableau_distribue(md,A);
// After:
Cerr << A.size() << finl; // nb elem
Cerr << A.size_array() << finl ; // nb_elem_tot</pre>
Cerr << A.size_reelle() << finl; // nb_elem</pre>
Cerr << A.size_totale() << finl; // nb_elem_tot
```





 Update of the virtual space of a distributed array is done by: tableau.echange_espace_virtuel();

- Notes:

- echange_espace_virtuel() does **nothing** on real arrays
- It is possible to check if an update of the virtual space is useful or not with : #include <Check_espace_virtuel.h>

. . . .

/* Exit in error if the virtual spaces of the distributed array A are not up to date */ assert(check_espace_virtuel_vect(A));





When do I need to create a distributed array?

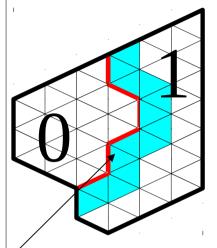
- It depends of your algorithm and the items you are using
- Use carefully distributed arrays. It will slow down the parallel execution during each virtual spaces update
- Example where you need it: You want to calculate the interpolation of a cell centered field to the faces of the mesh:







```
// Non distributed array of a cell centered field :
const entier nb elem=zone VEF.nb elem();
DoubleVect Field(nb_elem);
// Loop on cells to fill the array Field :
// Now to calculate the faces interpolation of this field
const entier nb faces=zone VEF.nb faces();
DoubleVect A(nb_faces);
// Loop on the real faces and use Zone VF :: face voisins() distributed array
// Problem: values on joint common faces are not well evaluated
// cause there is no virtual space on Field array to access virtual cells, so the
// good solution would be to create a distributed version for Field :
MD_Vector_tools::creer_tableau_distribue(md, Field);
// Loop on real cells to fill the array Field
Field.echange_espace_virtuel(); // To update the virtual spaces of Field array
// Loop on real faces to fill A
```







- Some useful Trio_U methods to know from the **Process** class:
 - **Process::je_suis_maitre()** returns 1 if the current process is the master process 0
 - **Process::me()** returns the current number process
 - **Process::nproc()** returns the process numbers
 - **Process::mp_sum(**x**)** returns the sum of x on the whole processes
 - **Process::mp_min(**x**)** returns the smallest value of x
 - **Process::mp_max(**x**)** returns the biggest value of x
 - **Process::barrier()** waits that all processes reach this point





- On the arrays:
 - **mp_somme_vect(**DoubleVect& x) returns the sum of all the elements from the distributed vector x
 - **mp_norme_vect(**DoubleVect& x**)** returns the L2 norm of the distributed array vector x
 - **mp_norme_tab(**const DoubleTab& x, ArrOfDouble& y**)** returns in the array y the L2 norm of each component of the distributed array x
 - **DoubleVect::mp_moyenne_vect()** returns the mean of the distributed vector **x**
- Standard/error output:
 - Cout : only the master process writes to standard output
 - Cerr: only the master process writes to error output, but other processes write to .log files
 - Cout_Global/Cerr_Global : all the processes write to standard/error output
 - Journal(): all the processes write to the .log files





- Send/receive methods (envoyer/recevoir). Well described in the file :
 - \$TRIO_U_ROOT/Kernel/Utilitaire/communications.cpp
 - Example of use in the Sous_Zone.cpp file. An array is sent by the master processor (0) and received by all the other ones.





– Pitfall with the common items :

```
/* During the sum of the values of a vertex located array tab, the following loop is incomplete: */
double sum=0;
for (int i=0;i<nb_som;i++)
    sum+=tab(i);
sum=Process::mp_sum(sum);
// Cause the common vertexes are counted several times!

Common vertex counted 3 times in the sum
```

```
NB: In this case, you would use : double sum = mp_somme_vect(tab);
```





- # Run your test case Cx in parallel mode:
- \$ cd ~/test/my_project/tests/Reference/NonRegression/Cx
- \$ make_PAR.data Cx 2 # Partition in 2 subdomains
- \$ export exec=~/test/my_project/basic
- \$ triou PAR_Cx 2 # 2 processes used

Compare the files: Cx_result.txt, PAR_Cx_result.txt and explain the discrepancies between the values.

To parallelize the algorithm, rewrite it, according to the previous slide with the help of the **mp_somme_vect(DoubleVect&)** method and change the way the result is written in the .txt file. You should find the same value for the sequential and parallel calculation.





-Pitfall with how the faces are ranked in Trio_U (Zone_VF class):

- First, the real boundary faces (from 0 to nb_faces_int()-1)
- Second, the real internal faces (from nb_faces_int() to nb_faces()-1)
- Last, the virtual faces, internal or boundary with <u>no particular order</u> (from nb_faces() to nb_faces_tot())





```
// Loop on the boundary faces
for (int i=0;i<les_cl.size();i++)
  const Cond_lim& la_cl = les_cl[i];
  const Front_VF& le_bord=ref_cast(Front_VF,la_cl.frontiere_dis());
  int nb_faces_bord_tot = le_bord.nb_faces_tot();
  // Loop on real and virtual faces of a boundary :
  for (j=0 ;j< nb_faces_bord_tot;j++)</pre>
    int face=le_bord.num_face(j);
```

Warning: Some obsolete code is still using the old way to access virtual faces on boundaries: Zone_VF::ind_faces_virt_bord





- How to debug parallelization in Trio_U
 - build your code in debug mode to take advantage of all the implemented checks (asserts) in the code
 - test your parallelization :
 - on several test cases with different meshes
 - vary the partition number N of the different meshes
 - the explicit parallel run command is :

mpirun –np N \$exec_debug datafile N

- What if the parallel calculation crashes/hangs?
 - Give a try with the debugger to know exactly where the issue is :

mpirun –gdb –np N \$exec_debug datafile N





How to validate parallelization in Trio_U

Check the results <u>are the same</u> on N=1 and N>1 cpus:

 Create a reference with a sequential calculation (post process some fields at LATA format):

triou datafile.data

Run you parallel calculation on N cpus and compare the LATA results :triou parallel_datafile.data N

compare_lata datafile.lata parallel_datafile.lata

- The **compare_lata** tool will compare all the post-processed fields in the two files and will warn if the relative differences are bigger than 1.e-5, which may indicate an incorrect parallelization





How to find the source(s) of parallelism differences in Trio_U ?

-Use the **Debog** keyword by inserting in the sequential and parallel data files after the **Discretize** keyword:

Debog problem_name seq faces 1.e-6 0 # In the sequential datafile **Debog** problem_name seq faces 1.e-6 1 # In the parallel datafile

-Run the sequential then the parallel calculation. The **Debog** keyword will compare arrays each time this line is found in the code :

Debog::verifier(« I am checking array », array);

-Look at the log files to detect when the parallel difference appears.





169

How to validate performance improvements

- Run sequential and parallel calculations on clusters with an optimized version of the code
- Look the CPU measures into the files :
 - datafile.TU # Contains the global performances
 - datafile_detail.TU # Contains the per process performances

Statistiques d'initialisation du calcul

Temps total 2.99584

Statistiques de resolution du probleme

Temps total 3.46542

Timesteps 3

Secondes / pas de temps 1.14932

Dont solveurs Ax=B

Dont operateurs convection

Dont operateurs diffusion

Dont operateurs gradient

Dont operateurs divergence

0.805794 70% (1 appel/pas de temps)

0.157865 13% (2 appels/pas de temps)

0.053469 4% (2 appels/pas de temps)

0.02917 2% (2 appels/pas de temps)

0.00428367 0% (2 appels/pas de temps)

Dont operateurs source 0.01545 1% (1 appel/pas de temps)

Dont operations postraitement 0.0103403 0% (1 appel/pas de temps)

Dont calcul dt 0.00864567 0% (4 appels/pas de temps)

Dont modele turbulence 0.0473803 4% (1 appel/pas de temps)

Dont calcul divers 0.0169207 1%

Nb echange_espace_virtuel / pas de temps 404.333

Nb solveur / pas de temps 1

Secondes / solveur 0.805794 Iterations / solveur 126.667

Communications avg
Communications max
Communications min
Network latency benchmark 7.10487e-07 s
Network bandwidth max
Total network traffic

17.7 % of total time
21.4 % of total time
14 % of total time
236.697 MB/s
Total network traffic
66.9368 MB / timestep

Average message size 41.0824 kB
Min waiting time 1.7 % of total time
Max waiting time 9.1 % of total time
Avg waiting time 5.4 % of total time





Trio_U test coverage





Code coverage

- → Created by gcov tool, as a nightly task on ~2000 test cases.
- → 65% of Trio_U total lines are covered (Cerr & exit lines excluded)
- → Knowing the coverage of methods/functions of the code gives confidence (or not) when re-using it for your development.
- → Trio_U code coverage and tools exploiting it are available for the developer





Useful code coverage tools

triou -check class::method

-Trio_U tool to know and run the test cases covering a method.

-For Baltik developer : Not available yet ?

Example:

\$ triou -check Navier_Stokes_std::mettre_a_jour

triou -check all|testcase: Option to check the non-regression on one or several test cases

Example:

\$ triou -check VAHL_DAVIS

For Baltik developer (version=optim|debug):

\$ make check_version # Check the project non-regression on Baltik test cases

\$ make check_trio_version # Check the project non-regression on Trio_U test cases





Code coverage exercice

Browse the Trio_U ressources index file:

triou -index

Select the <u>Test coverage</u> link:

Q: Which is the less covered matrix class?

Q: Run the test cases using the RRK2 time scheme.





Trio_U coding rules





Coding rules

- -Class name = File name
- -One class per file
- -Respect modularity :
 - Kernel should be built without VDF or VEF module
 - VDF application should be built without VEF module

— ...

- -Use assert() for pre and post conditions when coding a method
- -Use Param object to read keyword parameters

-...





Coding rules

- Do not use pointers but instead the classes:
 - REF for association
 - DERIV for generic class
 - VECT/LIST
- Use Kernel arrays (Double|IntVect...)
- No french accents
- Cerr/Cout in english in Kernel module

- ...



Rules to contribute



You want your work to be merged in the next release of the Trio_U/Kernel, then provide to the Trio_U support team :

I) If you develop directly in Trio_U/Kernel:

- English description/syntax of the new keywords
- The name of the branch under Git you have pushed to the shared repository containing:
 - New/modified sources
 - New validation forms or test cases
- Non regression should have been checked (<u>no errors</u>) on the debug binary and possible differences <u>should</u> be explained. Run :

exec=\$exec_debug triou -check all



Rules to contribute



You want your work to be merged in the next release of the Trio_U/Kernel, then provide to the Trio_U support team :

II) If you develop in a Baltik project based on Trio_U/Kernel:

- English description/syntax of the new keywords
- If not using Git, provide a tar.gz package containing your work (new/modified sources, validation forms/test cases,...) with :
 - make distrib
- Non regression should have been checked (<u>no errors</u>) on the debug binary and possible differences <u>should</u> be explained :
 - make check_all_debug # Check non regression of the Baltik and Trio_U/Kernel
 - VALGRIND=1 make check_all_optim # Same in optimized mode with Valgrind check





Using Eclipse





IDE Eclipse

Download: http://www.eclipse.org

Check you have also:

Egit (Git support): http://www.eclipse.org/egit

Cdt (C++ support): http://www.eclipse.org/cdt

-> Create a new C/C++ project (Makefile Project with Existing Code) under \$TRIO_U_ROOT/src

We are only in an evaluation phase...





After the training session...

Read the commented solution of the exercise:

\$TRIO_U_ROOT/doc/Trio_U/exercices/my_first_class

Practice on a tutorial:

\$TRIO_U_ROOT/doc/Trio_U/exercices/equation_convection_diffusion





The End

Good luck! triou@cea.fr