TRUST V1.7.6 Developer’s Training Session

DE LA RECHERCHE À L'INDUSTRIE

cea

CS

La force de l'innovation

Table of contents

Introduction

Prerequis

For this training session:

- TRUST/TrioCFD (User’s training session)
- C++ (Intermediate)

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

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

Objectives

To get a general knowledge of the TRUST code

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

To acquire reflexes to develop while following TRUST rules of coding

Useful links

TRUST:

http://sourceforge.net/projects/trust-platform/files/

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

mailto:triou@cea.fr

C++:

http://www.tutorialspoint.com/cplusplus

Git:

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

http://www.alexgirard.com/git-book/index.html

TRUST
An object oriented CFD code

Interest of TRUST

- 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 TRUST support team

Interest of TRUST

- 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 TRUST)

What is TRUST CFD code ?

It provides :

- 3 spatial discretizations (VDF, VEF, EF)
- 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

TRUST

- What can handle TRUST
  - Runs on every Linux box (32/64 bits)
  - Runs on the CEA clusters
    - Has already run a LES on a 400.10^{e-6} cells mesh with 10000 cores (curie on CCRT)

TRUST
Specifications/Choices explained

Main specifications:

Enable developments with the following characteristics:

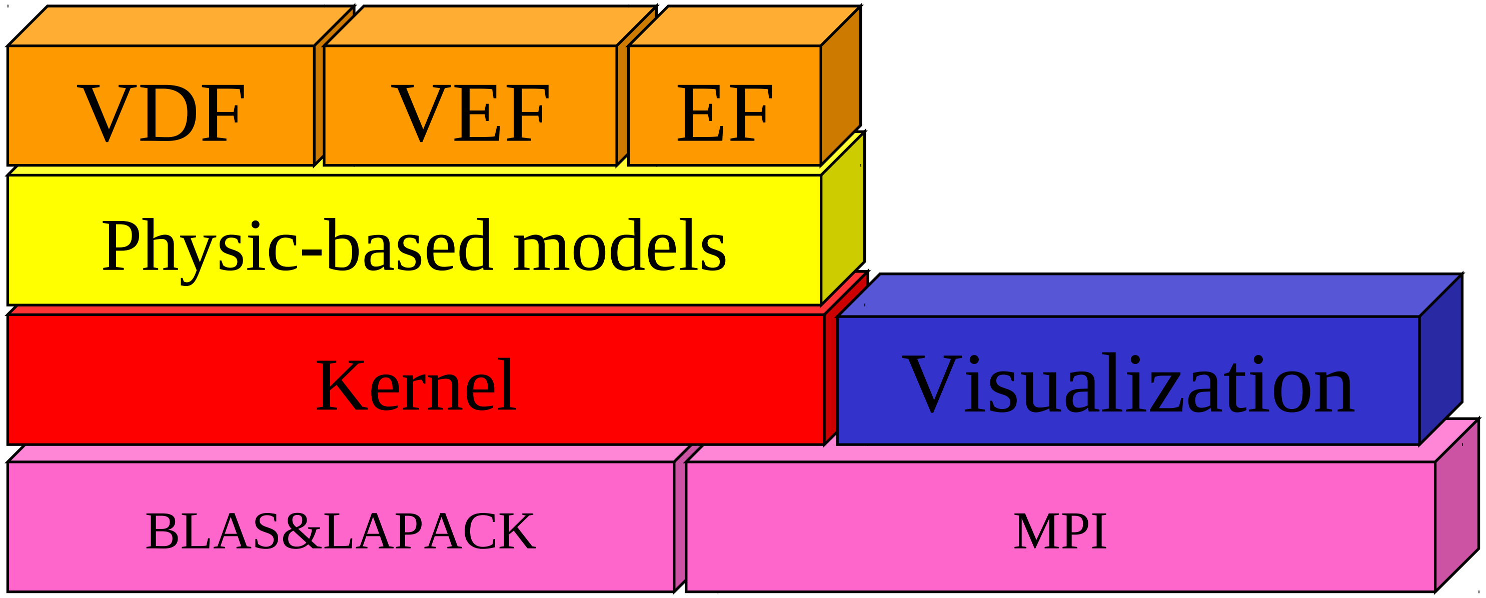
- fast
- reliable
- reusable
- effective
- documented
- enable encapsulation of Fortran modules

Main Choices:

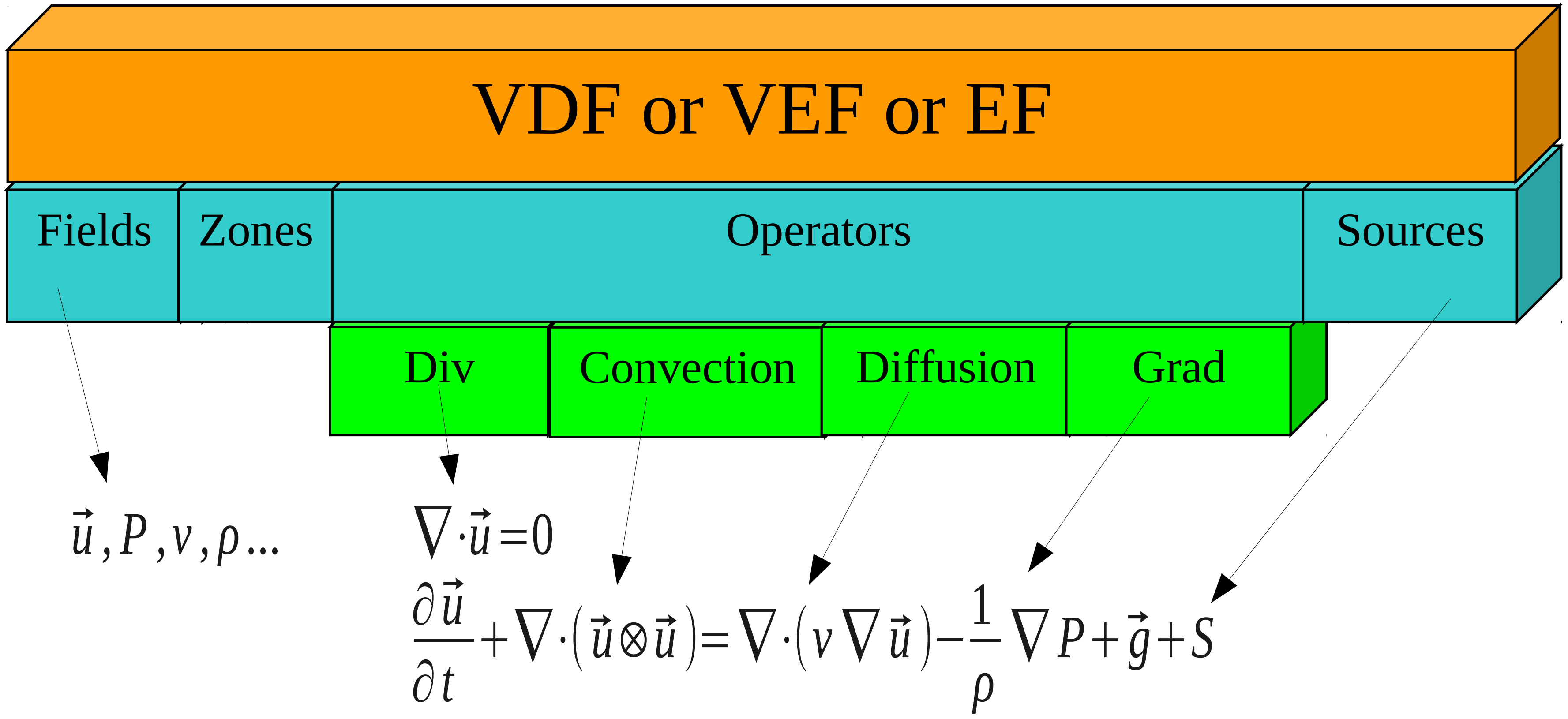
- Object Oriented Conception
  - Modularity, maintainability, library encapsulation
- C++ implementation
  - Standard, performances, C/Fortran compatibility
- Parallelism by sending/receiving messages (MPI)
  - Standard, portable
- Multi-site configuration management (Git)
  - Co-developing
- Automatic generation via Doxygen of HTML documentation from code sources
  - Documentation is up to date
- Automatic generation of the documentation of your new classes and keywords with XData tool

TRUST modules

TRUST modules



Discretization modules



VDF or VEF or EF

Fields

Zones

Operators

Sources

Div

Convection

Diffusion

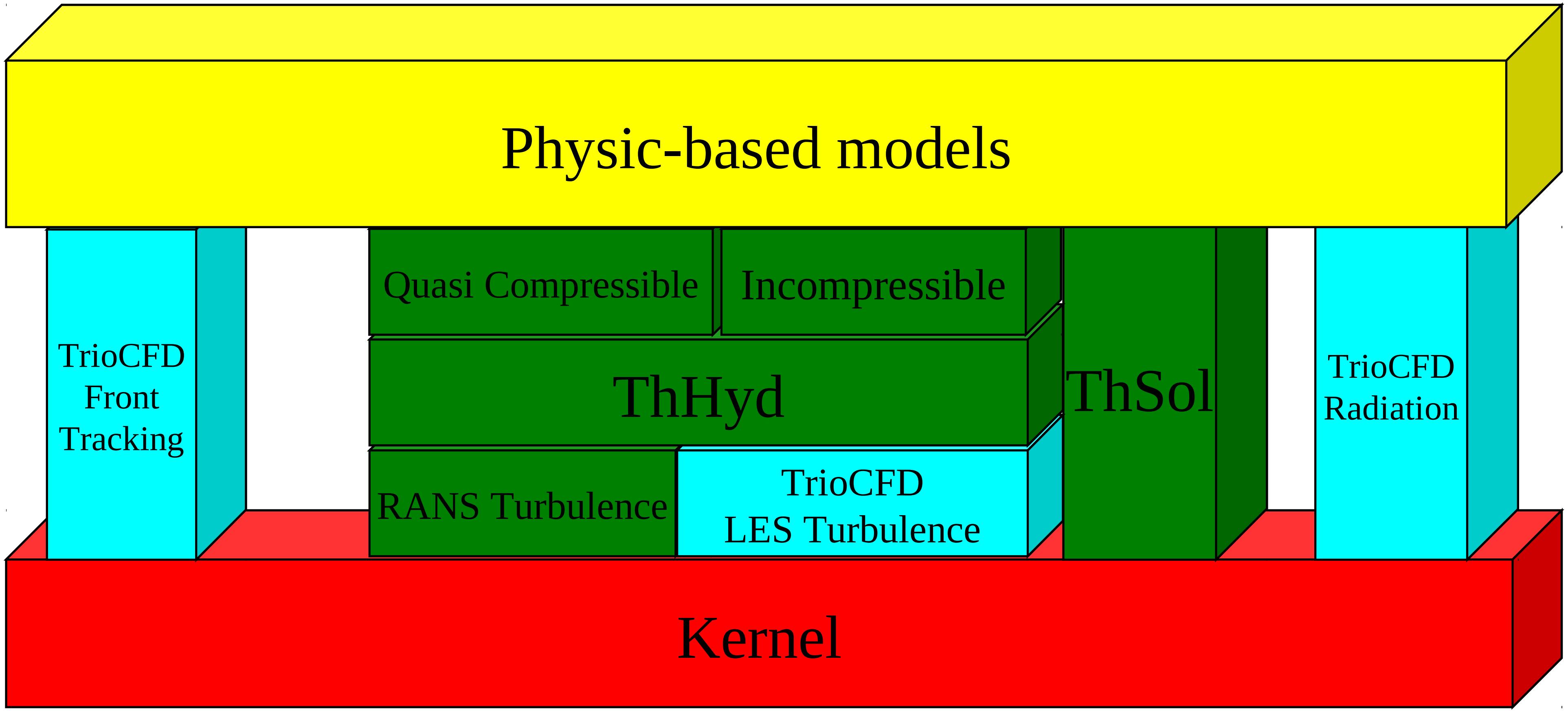
Grad

$\vec{u}, P, \nu, \rho \ldots$

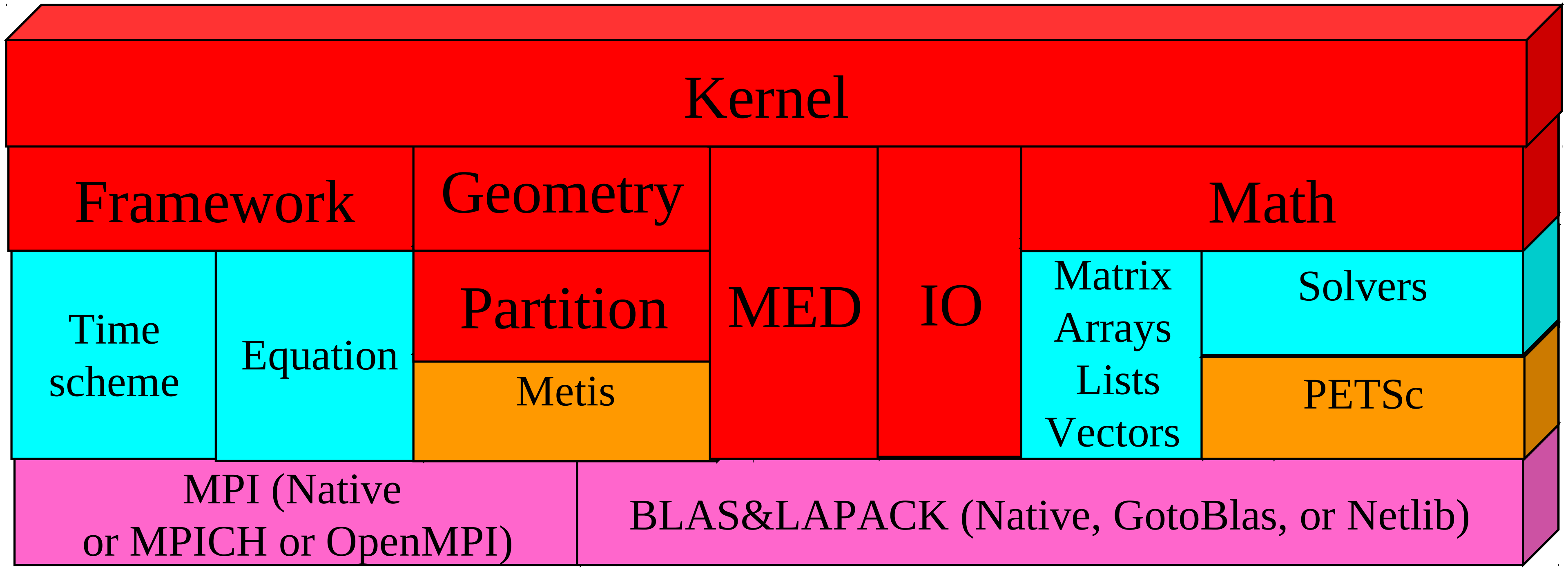
$\nabla \cdot \vec{u} = 0$

$$\frac{\partial \vec{u}}{\partial t} + \nabla \cdot (\vec{u} \otimes \vec{u}) = \nabla \cdot (\nu \nabla \vec{u}) - \frac{1}{\rho} \nabla P + \vec{g} + S$$

Physics modules



Kernel module



Kernel

Framework

Geometry

MED

IO

Math

Time scheme

Equation

Partition

Metis

Matrix
Arrays
Lists
Vectors

Solvers

PETSc

MPI (Native
or MPICH or OpenMPI)

BLAS&LAPACK (Native, GotoBlas, or Netlib)

TRUST sources

➤ TRUST code is made of:

- 1600 classes
- Declared in include files (.h)
- Implemented in sources files (.cpp)
- Within 74 directories

➤ Kernel constitutes 47% of the TRUST code.

➤ HTML documentation to browse and see the class hierarchy under:

```
$TRUST_ROOT/doc/html
```

Or

```
trust -index
```

TRUST tests

~60 **TRUST Verification forms** to check analytical results under:

$TRUST_ROOT/Validation

~150 **TrioCFD Validation forms** to compare with experimental results or with results from other codes under:

$project_directory/validation

~2050 **Non regression test cases**:

- ~750 TRUST non regression test cases under **$TRUST_ROOT**/tests
- ~ 1300 TrioCFD non regression test cases under **$project_directory**/build/tests

Using Eclipse

TRUST Baltik project Tutorial

- Load the TRUST environment:

```
source /home/triou/env_TRUST_X.Y.Z.sh
```

- Open the TRUST tutorial:

```
trust -index
```

→ « Developer Tutorial » link in the developer block

→ TRUST Initialization exercise

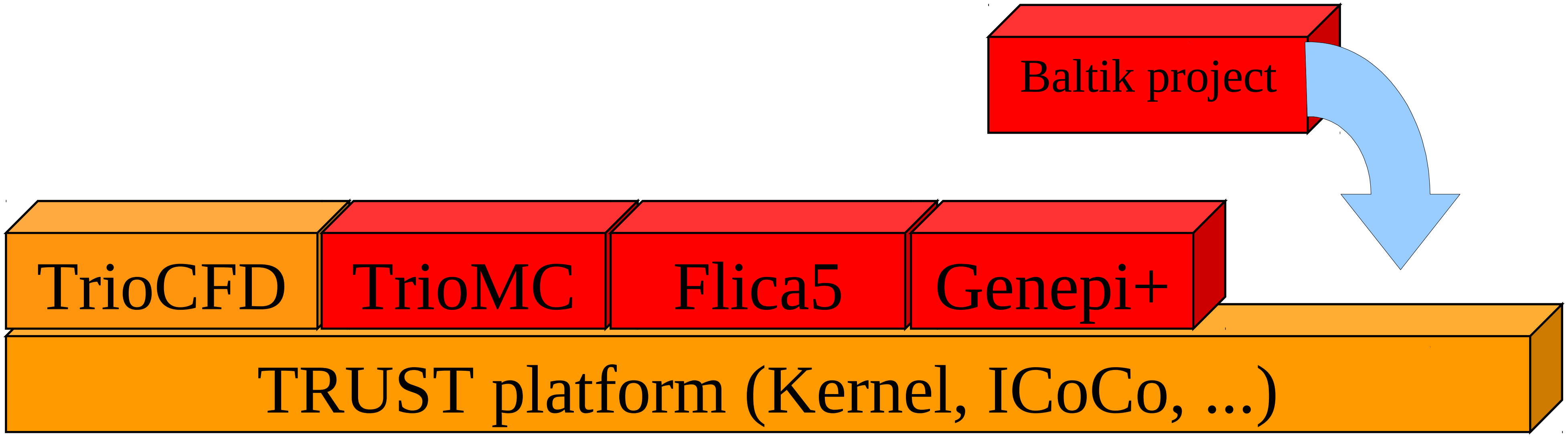
Main page: http://www.eclipse.org

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

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

Baltik
Building **A**pplication **L**inked with **T**r**i**o_U **K**ernel

Develop in a TRUST Baltik project



I) with new features

II) modifying TRUST functions

You need to first load TRUST environment.

Develop in a TRUST Baltik project

I) Develop in a Baltik project based on TRUST

- You want to develop your own project
  - more freedom about the update of TRUST version
- Baltik means **B**uilding an **A**pplication **L**inked to **T**r**i**o_U **K**ernel

II) Integrate your project in TRUST base

- You want to contribute to TRUST
- But if you want to share your work, you will need :
  - To follow the TRUST roles of coding
  - To check and respect the non regression of others parts of the code
  - To add new validation forms or test cases

TRUST Baltik project Tutorial

→ Baltik initialization exercise

- Creation of a Baltik project
- Creation of your git repository
- Builds
- Using Eclipse

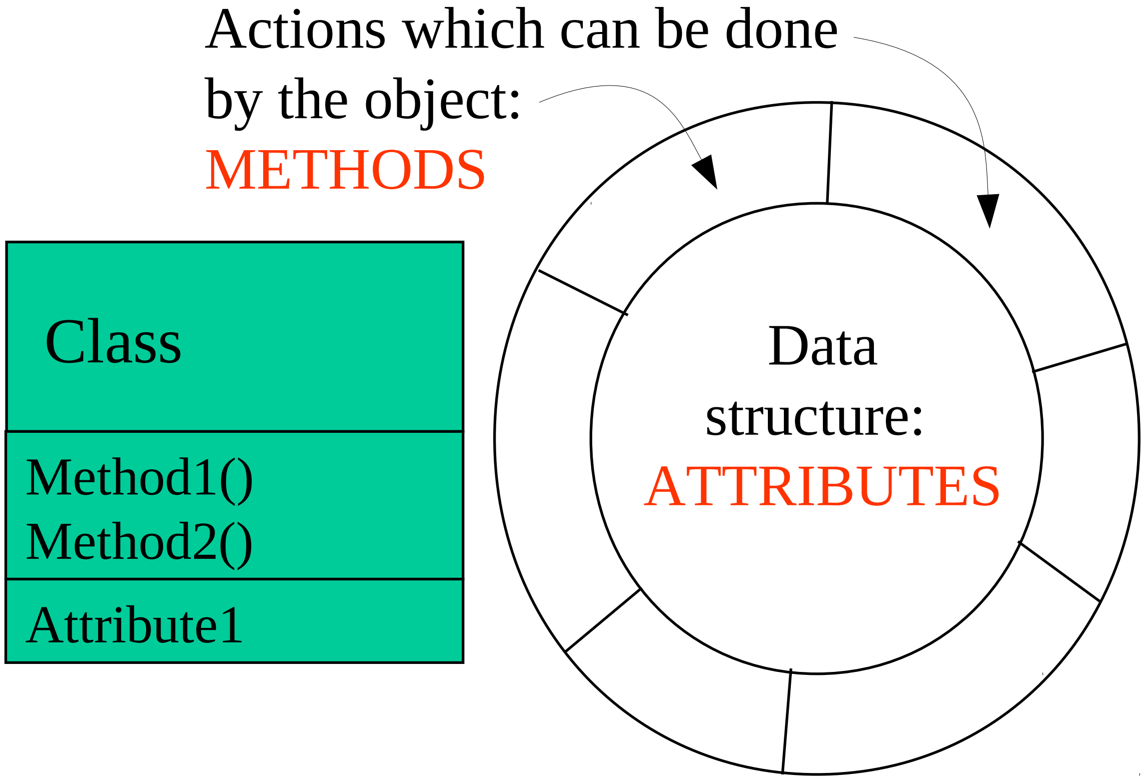
Basic Oriented Object Conception (OOC) concepts used in TRUST

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



Object attributes can only be modified by:

- the object itself,
- by other objects using the methods of this object.

➡ Data encapsulation

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 TRUST 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 (ρ, μ, λ,...)
- 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 :

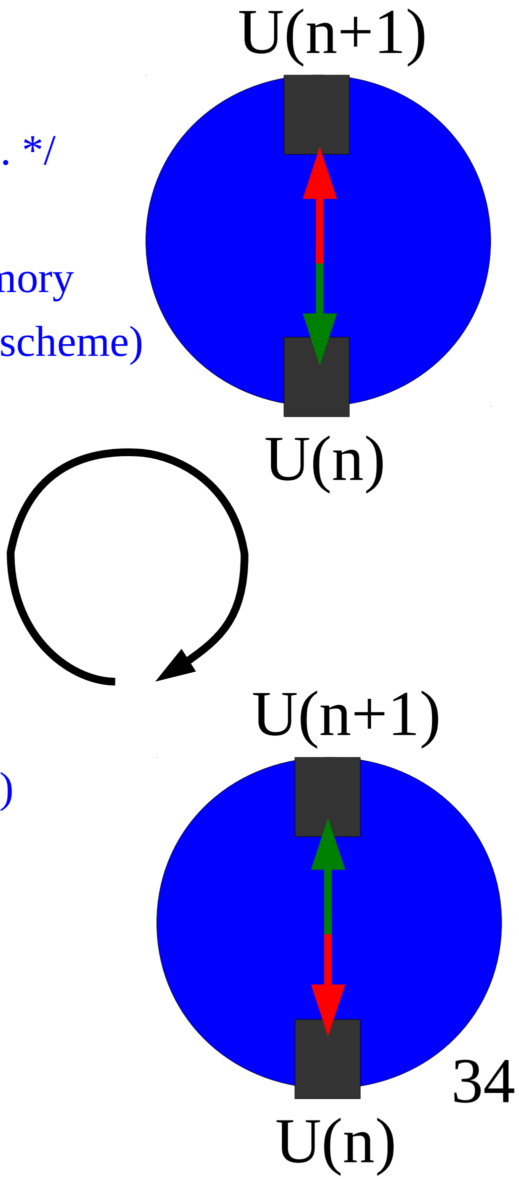
Roue_ptr les_valeurs // Pointer to a "wheel" mechanism to manage the different times for the unknown field

Code example:

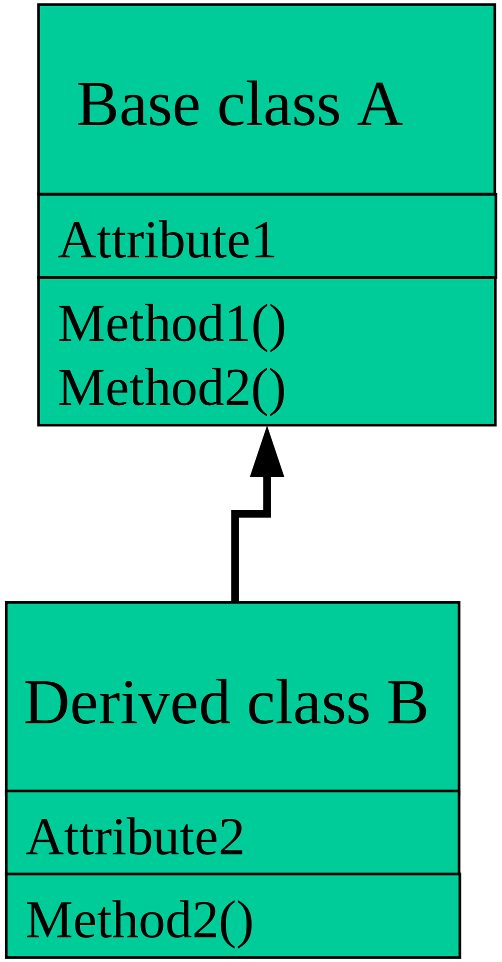
```
inconnue.fixer_nb_valeurs_temporelles(2);  // 2 memories to store the different times of the unknown inconnue
//  present (it is an alias or link) points to U(n) (first memory)
DoubleTab& present = inconnue.valeurs();
/* DoubleTab present = inconnue.valeurs();  ←  Warning! It is a copy here... */

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)  <=> U(n+1)=U(n) + dt*f(U(n))
...
// At the end of the time step, we turn the « wheel » with:
inconnue.avancer();

// 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).
```



Inheritance



Base class A with 2 methods and 1 attribute.

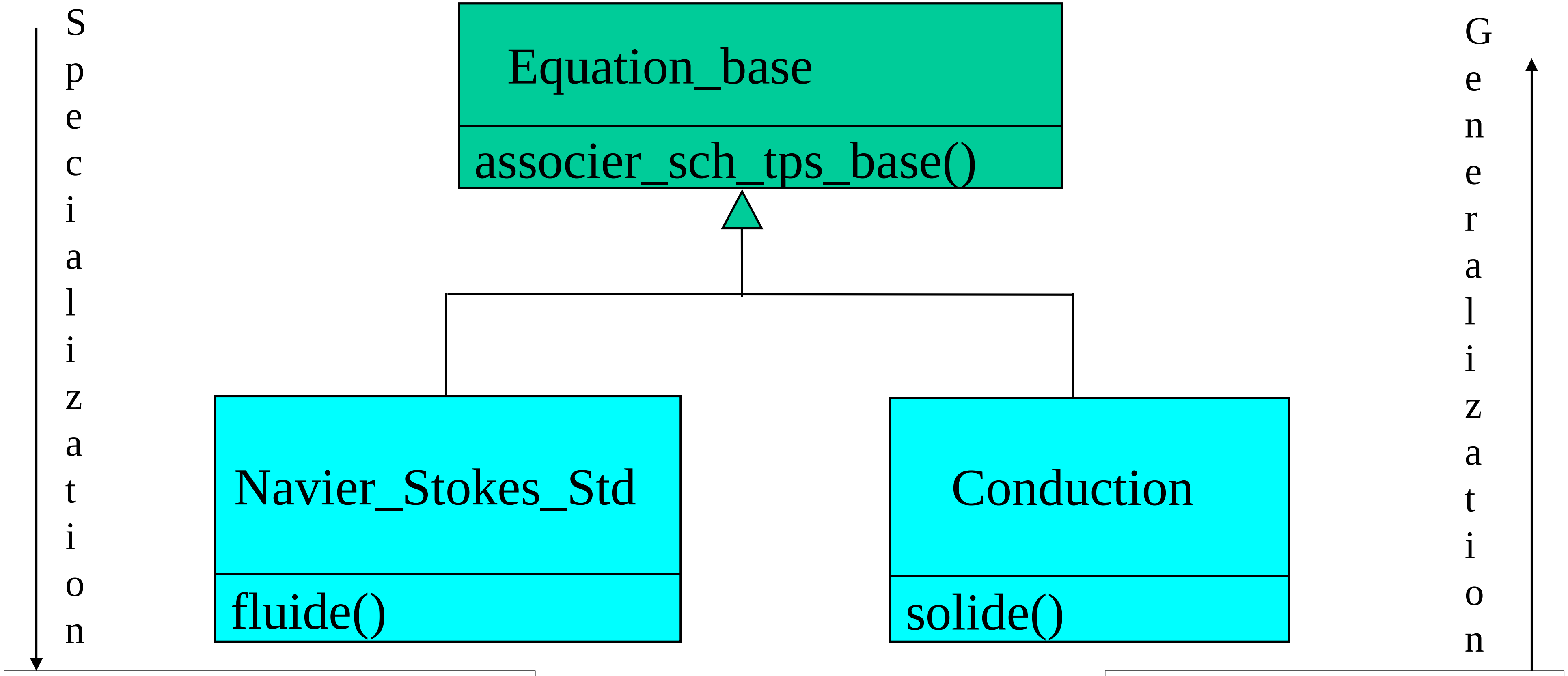
Derived class B inherits from base class A:

->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



Early process leading to a specialisation of the code

Late process leading to factorize the code

Polymorphism use in TRUST

→ Example of the ***derivee_en_temps_inco()*** method which implements the calculation of F(U) in ∂U/∂t=F(U), where U is the main unknown of the equation

_ Static polymorphism (decision is made at the compile time):

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

_ Dynamic polymorphism (decision is made at the run time):

```
Equation eqn;  // Equation is a generic class in TRUST
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 real method (default case):

- can be overloaded
- enable only **static polymorphism**

→ In the example, A()

-A virtual method:

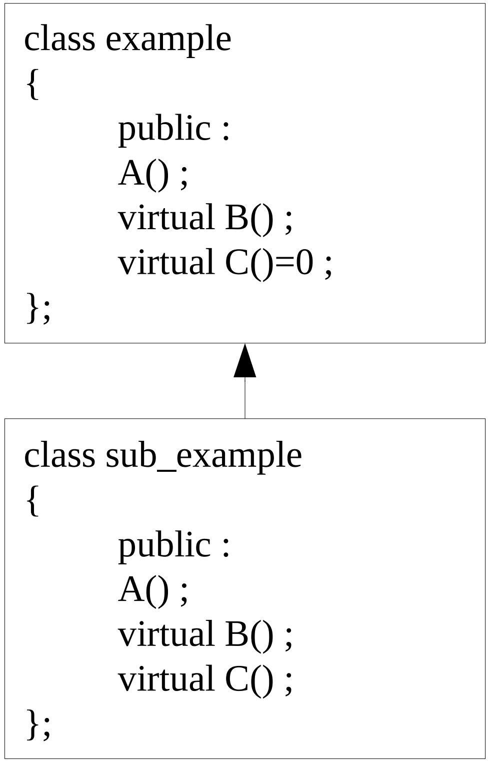
- can be overloaded
- enable **dynamic polymorphism**

→ in the example, B()

-A pure virtual method (abstract method):

- **must** be overloaded (otherwise compilation fails),
- make the class abstract (used for example in base classes),
- enable **dynamic polymorphism**

→ 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 Equation_base : public Objet_U
{
public :
        // Evaluate ∂U/∂t (returned in F array) for the equation :
        virtual DoubleTab& derivee_en_temps_inco(DoubleTab& F);
       …
};
```

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

Navier Stokes equation

TRUST 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):

$$1)\ BU=0$$

$$2)\ M\partial U/\partial t = -B^TP -CU + LU + S$$

Or by inverting 2) by M gives 2'):

$$2')\ \partial U/\partial t = -M^{-1}B^TP + M^{-1}(LU-CU+S)$$

$$= -M^{-1}B^TP + F(U)$$

Then using 1) on 2') leads to 1'):

$$1')\ BM^{-1}B^TP = BM^{-1}(LU-CU+S) \qquad \Rightarrow \mathbf{P^{n+1}}$$

Solving 2'):

$$2')\ \partial U/\partial t = -M^{-1}B^TP + F(U) \qquad \Rightarrow \mathbf{U^{n+1}}$$

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

Virtual method example

```
DoubleTab& Navier_Stokes_std::derivee_en_temps_inco (DoubleTab&  F)
{
        // for explicite case
        // ∂U/∂t=F(U)-M^-1B^TP
        Equation_base::derivee_en_temps_inco(F);   // F(U)-M^-1B^TP
        return F;                                   // ∂U/∂t = F(U)-M^-1B^TP
}
```

Navier_Stokes_std::derivee_en_temps_inco(F)

→ Equation_base::derivee_en_temps_inco(F)

→ corriger_derivee_expl(secmem) **which is overloaded in** Navier_Stokes_std class to calculate -GradP !

Virtual method example

derivee_en_temps_inco() is a virtual method of Equation_base class, who calculates $\partial U/\partial t = F(U) = M^{-1}(\Sigma Op_i(U)+\Sigma S_i)$:

```
DoubleTab& Equation_base::derivee_en_temps_inco(DoubleTab&  F)
{
    // for explicit case
    F=0;
    DoubleTrav secmem(F);                        // Initialisation by copy
    // Loop on the operators to add them to the second member of the equation
    for(int i=0; i<nombre_d_operateurs(); i++)
        operateur(i).ajouter(secmem);             // $\Sigma Op_i(U)=LU-CU$
    // Adding source terms
    les_sources.ajouter(secmem);                  // $\Sigma Op_i(U)+\Sigma S_i=LU-CU+S$
    // Call to an other virtual method
    corriger_derivee_expl(secmem);                 // do nothing except for Navier_Stokes_std (overloaded): returns  $LU-CU+S -B^TP$
    solveur_masse.appliquer(secmem);              // -> $M^{-1}(LU-CU+S)$, and for Navier_Stokes_std: $M^{-1}(LU-CU+S -B^TP)=F(U)-M^{-1}B^TP$
    F=secmem;
    F.echange_espace_virtuel();                   // parallel instruction
    corriger_derivee_impl(F);                     // for Navier_Stokes_std: calculates  $P^{n+1}$, also used by Transport_K_Eps
    return F;
}
```

Note: This method is overloaded in the Navier_Stokes_std equation class

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 &);
};
```

Pure virtual method example

```
int Schema_Euler_Explicite::faire_un_pas_de_temps_eqn_base(Equation_base& eqn)
{
    // ∂U/∂t = F(Un)       -->   $U^{n+1} = U^n + dt* F(U^n)$   for forward Euler scheme
    DoubleTab& present = eqn.inconnue().valeurs();   // Contains $U^n$
    DoubleTab& futur = eqn.inconnue().futur();          // Location to store $U^{n+1}$
    DoubleTab dudt(futur);                              // Copie of $U^{n+1}$
    // Using boundary conditions applied on Un+1:
    ...
    eqn.derivee_en_temps_inco(dudt);                   // $F(U^n)$
    ...
    // Un+1=Un+dt_*dU/dt
    futur=dudt;
    futur*=dt_;                                       // $dt* F(U^n)$
    futur+=present;                                   // $dt* F(U^n) + U^n$
    eqn.zone_Cl_dis()->imposer_cond_lim(eqn.inconnue(),temps_courant()+pas_de_temps());
    ...
    return 1;
}
```

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 : ...

-> ...

TRUST Baltik project Tutorial

→ PRM file and validation test cases exercise

The extensive use of macros in TRUST

TRUST important points

TRUST does not use, for historical reasons:

- Templates
- STL (Standard Template Library)
- Exceptions (until recently)

-Instead of templates, TRUST uses macros

-Instead of using STL, TRUST defines LIST, VECTORS,...

TRUST important points

No pointers in TRUST:

- to avoid coding error
- to differentiate the aggregation of the reference

You will never see:

```
     class A {
     A    private: B *b_;
     B};
```

But instead:

```
   class A {
       private: REF(B) b_;
   };
```

TRUST important points

Why no pointers in TRUST?

```
First case:
A::A()
{
   b_ = new B;
   // Initialize b_
   b_ = ...
}

A::~A()
   // Delete b_
   delete b_;
}
```

```
Second case:
A::A()
{
   // Just initialize b_
   b_ = ...
}

A::~A()
{
   // Nothing to do. b_ is deleted by the
   // destruction of the object REF(B)
}
```

TRUST macros

Macros are widely used to implement plumbing of several features of TRUST. 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)

TRUST 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)

-To ensure a correspondence dataset /class

Four different kinds of classes in TRUST:

Base class

Instanciate class

Associated class

Generic class

Base class

Definition:
A base class is a prototype for other classes.
It is an abstract class, which **can't be instantiated**.

TRUST examples:

Probleme_**base**	Problem base class
Equation_**base**	Equation base class

Base class

Declaration file: A_base.h

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

Implementation file: A_base.cpp

```
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 »
}
```

Four different kinds of classes in TRUST:

Base class

Instanciate class

Associated class

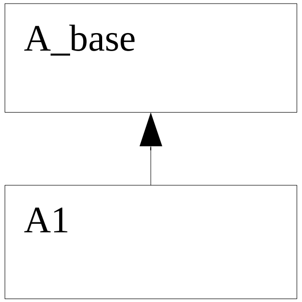
Generic class

Instanciate class

from a base class

Declaration file: A1.h

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



Implementation file: A1.cpp

```
Implemente_instanciable(A1, «A1», A_base);

Entree& A1::readOn(Entree& is)
{
...
}

Sortie& A1::printOn(Sortie& os)
{
...
}
…
```

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
_sans_constructeur :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)

Four different kinds of classes in TRUST:

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. of 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) :
  - Object pointed by c_ exists independently of any instance of A
  - Implemented by the REF macro in TRUST:

    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.

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

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

WARNING : use only REF(A) in your code.

Associated class (REF)

Declaration file: Ref_A.h

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

Implementation file: Ref_A.cpp

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

Four different kinds of classes in TRUST:

Base class

Instanciate class

Associated class

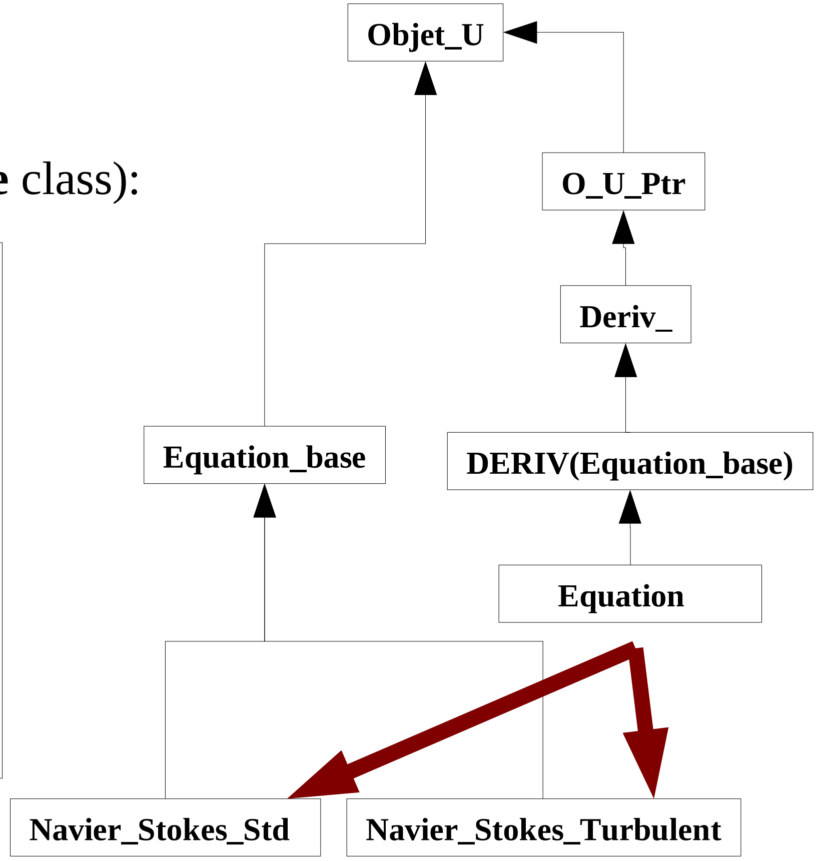
Generic class

Generic class (DERIV)

- Definition: A generic class A is useful to create objects which can be typed at every moment to any object inheriting from A_base class.

- 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();
```



Generic class (DERIV)

Declaration file: A.h

```
#include <Deriv.h>
#include <A_base.h>
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();
}
```

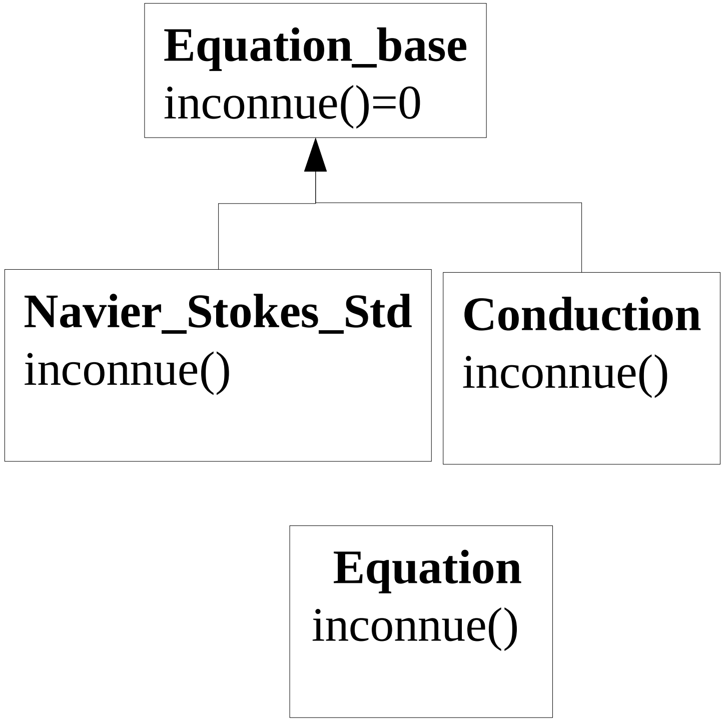
Implementation file: A.cpp

```
Implemente_deriv(A_base);
Implemente_instanciable(A, « A»,DERIV(A_base));

Entree& A::readOn(Entree& is)
{
...
}

Sortie& A::printOn(Sortie& os)
{
...
}
…
```

Generic class



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

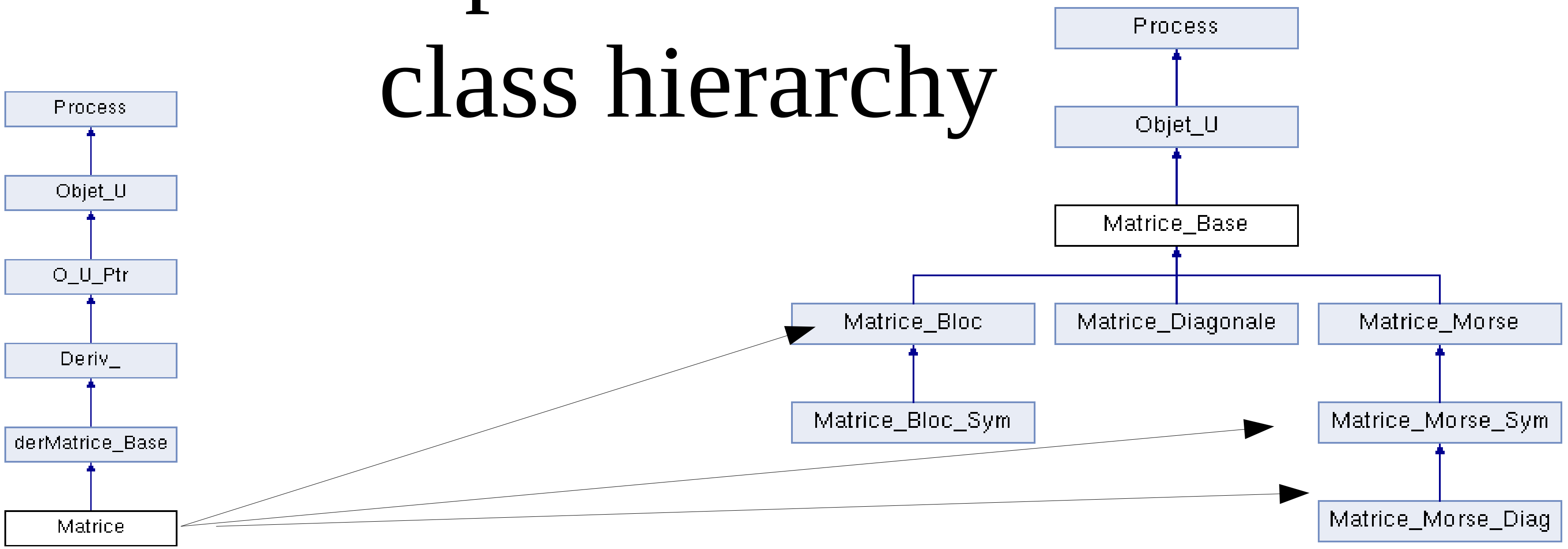
```
Conduction cond; // Instanciated class
Cerr << cond.que_suis_je() << finl ; // Prints « Conduction »

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

- 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() ;
}
```

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) ; … } ;
```

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 ?

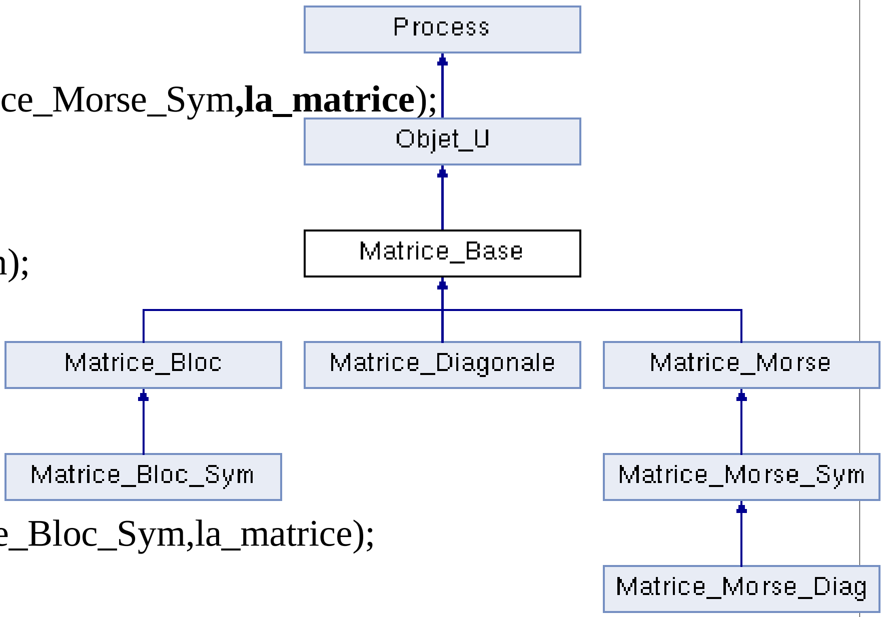
ref_cast(classA,B) : cast the object B in a classA type object or produces an error if object B is not from a derived class of classA.

Type casting

sub_type and ref_cast macros

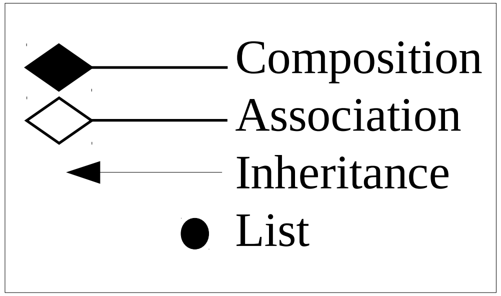
Solv_Petsc.cpp example :

```
Int  Solv_Petsc::resoudre_systeme(const Matrice_Base& la_matrice, const DoubleVect& secmem, DoubleVect&
solution)
...
        if(sub_type(Matrice_Morse_Sym,la_matrice))
        {
          const Matrice_Morse_Sym& matrice = ref_cast(Matrice_Morse_Sym,la_matrice);
          assert(matrice.get_est_definie());
          Matrice_Morse mat;
          MorseSymHybToMorse(matrice,mat,secmem,solution);
          Create_objects(mat,secmem);
        }
      else if(sub_type(Matrice_Bloc_Sym,la_matrice))
        {
          const Matrice_Bloc_Sym& matrice = ref_cast(Matrice_Bloc_Sym,la_matrice);
          Matrice_Morse_Sym mat_sym;
           ...
```



Hierarchy examples and UML notations

UML (Unified Modeling Language)



Base class

Instanciate class

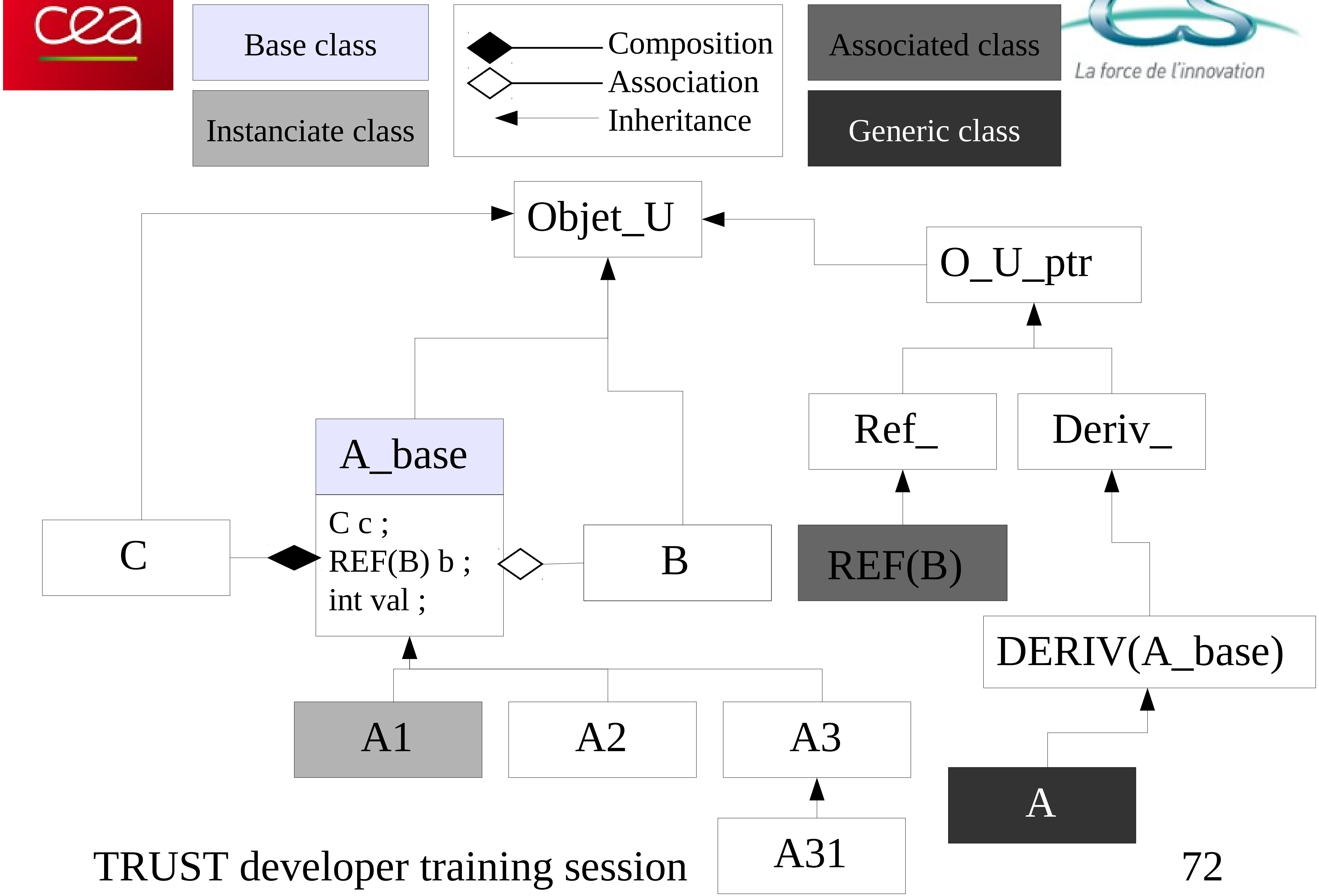
◆— Composition

◇— Association

◄— Inheritance

Associated class

Generic class



Objet_U

O_U_ptr

Ref_

Deriv_

A_base

C c ;
REF(B) b ;
int val ;

C

B

REF(B)

DERIV(A_base)

A1

A2

A3

A31

A

Exercise:
Use HTML doc

# Browse the TRUST ressources index file :

$ trust -index

# Notice when you select a class, the **localisation of his .cpp/.h files are specified at the bottom of the html page**.

# 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 ?

Interpretors: Links between data file and the code

Read: keyword to read an Object
Solve: keyword to solve a Problem

Which method is called ?

```
Dimension 3
Conduction pb
Domaine dom
...
Associate pb dom
...
Read pb { … }
```

-**Read** (as other keywords like Associate) are interpretor 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 **Interprete** is called when the data file is read :

Interprete::interpreter(Entree&) { … }

-For example : Lire.cpp

Interpretors: Links between data file and the code

Read: keyword to read an Object

Solve: keyword to solve a Problem

Where is solved a problem ?

```
Pb_hydraulique pb
...
Read pb { … }
Solve pb
```

```
Resoudre::Interpreter()
{
        Nom problem_name;
        is >> problem_name;
        Probleme_U& pb = ref_cast(Probleme_U,
                      objet(problem_name));
        pb.initialize();
        pb.run();
        pb.terminate();
}
```

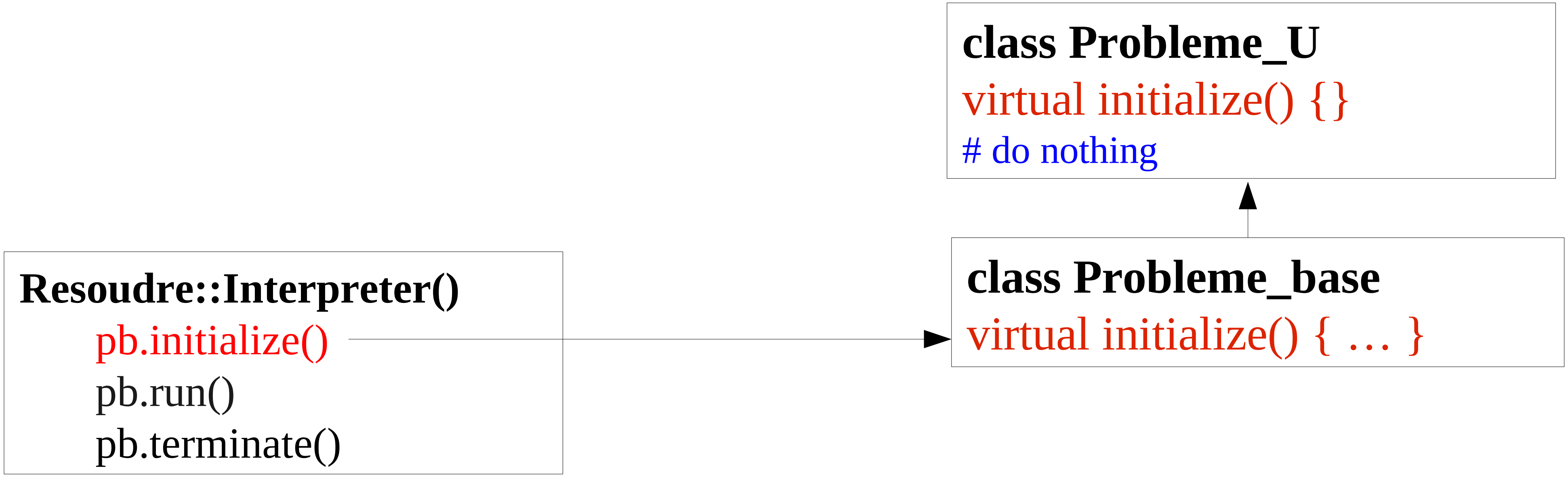
-The **Solve** interpretor solve the **problem**

-The object **problem** is described by a class which inherits from :

- **Probleme_base** (single base problem)
- **Probleme_U** (TRUST problems can be single or coupled)

Notice how an object is retrieved from its name (objet() method).

Resoudre call graph



class Probleme_U

virtual initialize() {}

# do nothing

class Probleme_base

virtual initialize() { … }

Resoudre::Interpreter()

pb.initialize()

pb.run()

pb.terminate()

Probleme_base::initialize()

→ Probleme_base::preparer_calcul()

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

→ milieu().initialiser()

→ Loop on equation(i).preparer_calcul()

→ Schema_temps_base::initialize()

```
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)
→ Loop on the time steps until stop:
        → Probleme_base::InitTimeStep()           // Initialize
            → 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:
                    →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()          // Update each unknown & BC & media
                → Schema_Temps_base::mettre_a_jour()  // t(n+1)=t(n)+dt(n)
        → computeTimeStep()                       // Prepare next: Compute next time step dt(n+1)
        → Probleme_base::postraiter()             // Post process the results
```

```
Resoudre::Interpreter()
    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()
```

Terminology/chronology of methods in TRUST

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

TRUST Baltik project Tutorial

→ **Modify the cpp sources**

- **Create a new cpp class**
- Modify your cpp class
- Add XData tags
- Adding prints

Exploring

Kernel module:

Math (Arrays, Matrix, Vect, List)

Framework (Problem, Domain, Equation, Time schemes, Fields, Operators)

ThHyd module

(Incompressible Thermalhydraulic)

Space discretization module

Math module

- Array for double :

  - ArrOfDouble A(n)

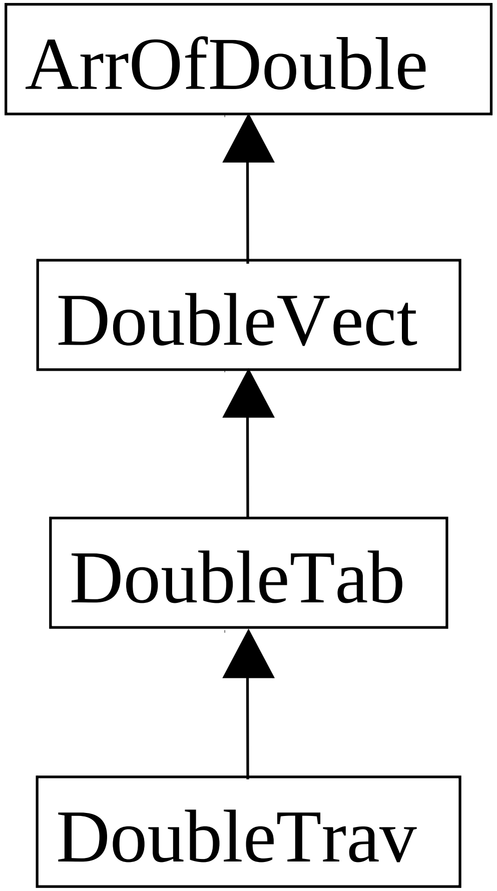
    → Basic array, no mecanism to extend data for parallelization

  - 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

Notice:

```
DoubleTab A(B); // A has the same dimensions as B, B is copied in A
DoubleTrav A(B); // A has the same dimensions as B, A is initialized to 0 !!!
```

Use TRUST 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
```

Array examples

```
// 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) ;
```

Array examples

```
// Initialize an array:
DoubleTab B(A) ;  // Dimension B and B=A
B+=A ;   // B(i)=A(i)+A(i)

// not recommanded:
DoubleTab C(n) ;
C=1 ; // C(i)=1.0
```

Array examples

```
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)
```

Array examples

```
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
```

VECT and LIST macros

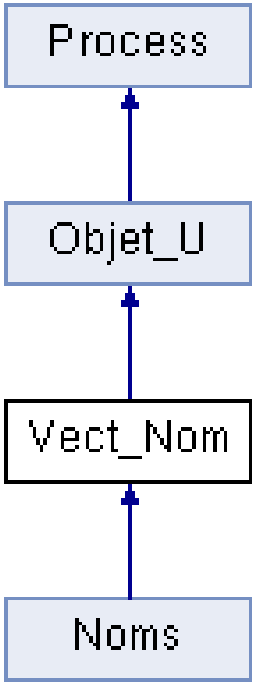
One can regroup a set of objects of the same kind by using:

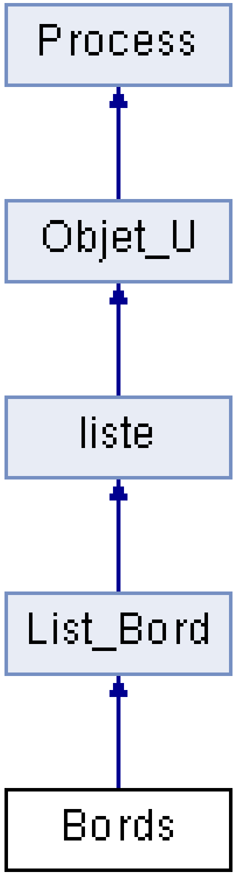
- either VECT, vector of objects
- or LIST, list of objects

Similar interface (search(), add(),...) and performances.

Examples of VECT and LIST

Noms	VECT(Nom)
Bords	LIST(Bord)
…	





VECT(class) LIST(class)

Declaration (As.h file)

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

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

Implementation (As.cpp file)

```
Implemente_vect(As);
Implemente_instanciable(As, «As»,VECT(A));

Entree& As::readOn(Entree& is)
{ … }
Sortie& As::printOn(Sortie& os)
{ … }
```

```
Implemente_liste(As);
Implemente_instanciable(As, «As»,LIST(A));

Entree& As::readOn(Entree& is)
{ … }
Sortie& As::printOn(Sortie& os)
{ … }
```

Exercise
Use HTML doc

Use the **HTML documentation** or **Eclipse** to see **Noms class**

→ 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) ;
Cerr << « The number of students is » << StudentNames.??? << finl ;
```

Exploring

Kernel module:

Math (Arrays, Matrix, Vect, List)

Framework (Problem, Domain, Equation, Time schemes, Fields, Operators)

ThHyd module

(Incompressible Thermalhydraulic)

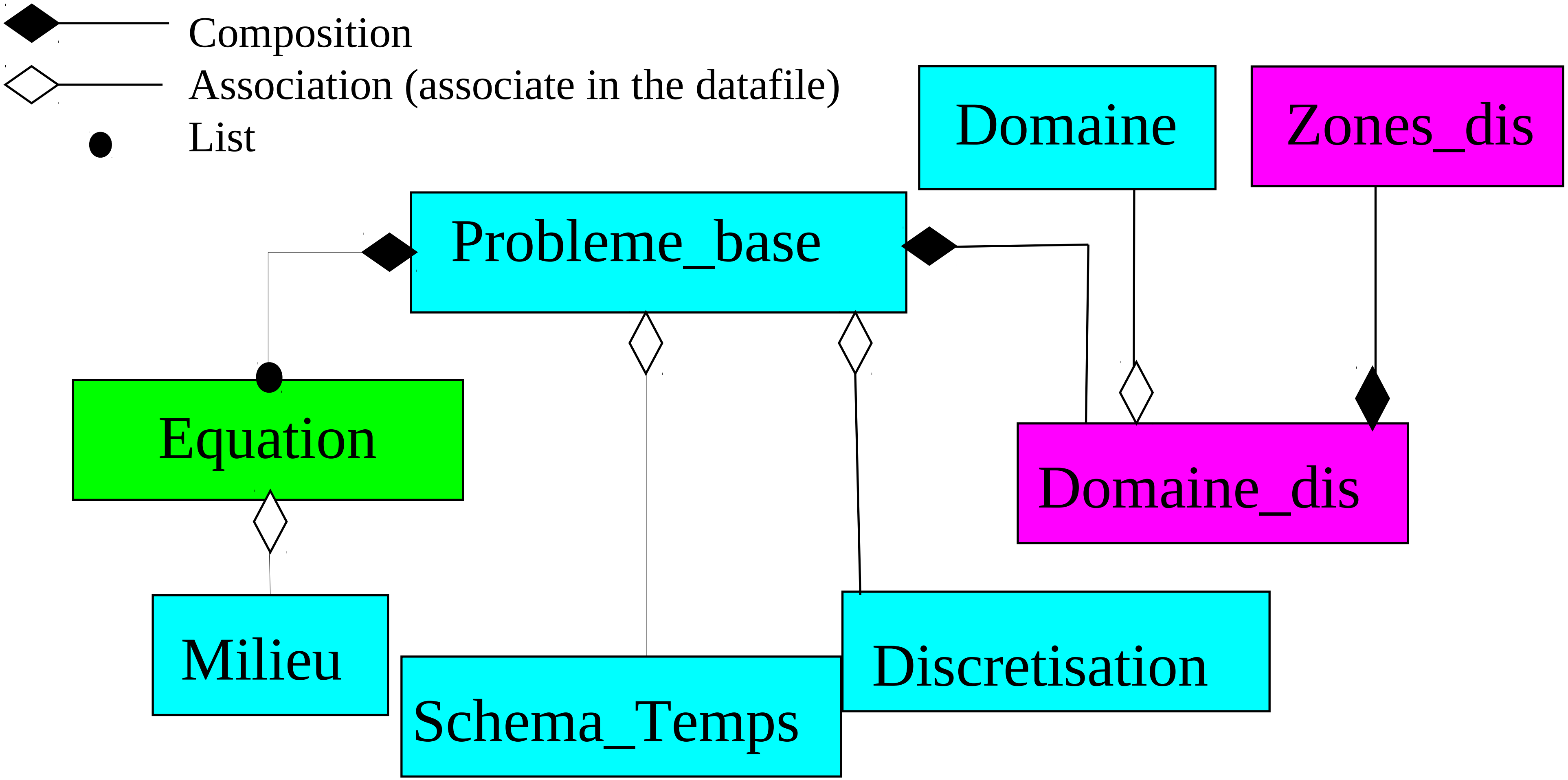
Space discretization module

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 :	**5 classes :**
Domain	Domaine
Media	Milieu
Scheme	Schema_Temps
Discretization	Discretisation
Problem	Probleme_base

Problem (Kernel framework)



Objects creation

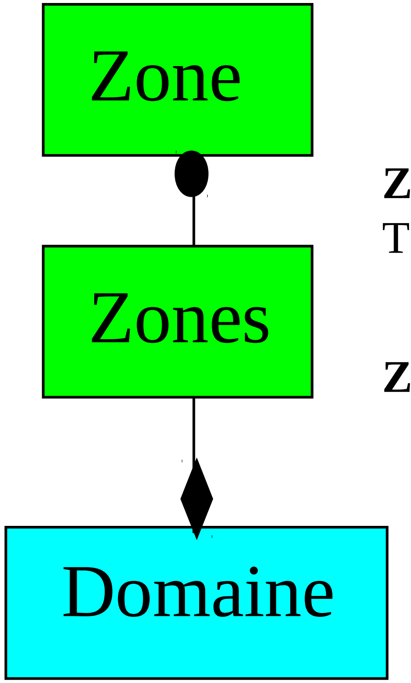
-Associated objects should be created before being associated

- – 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 TRUST, so everywhere in the code a **Zones** list has a size of 1).

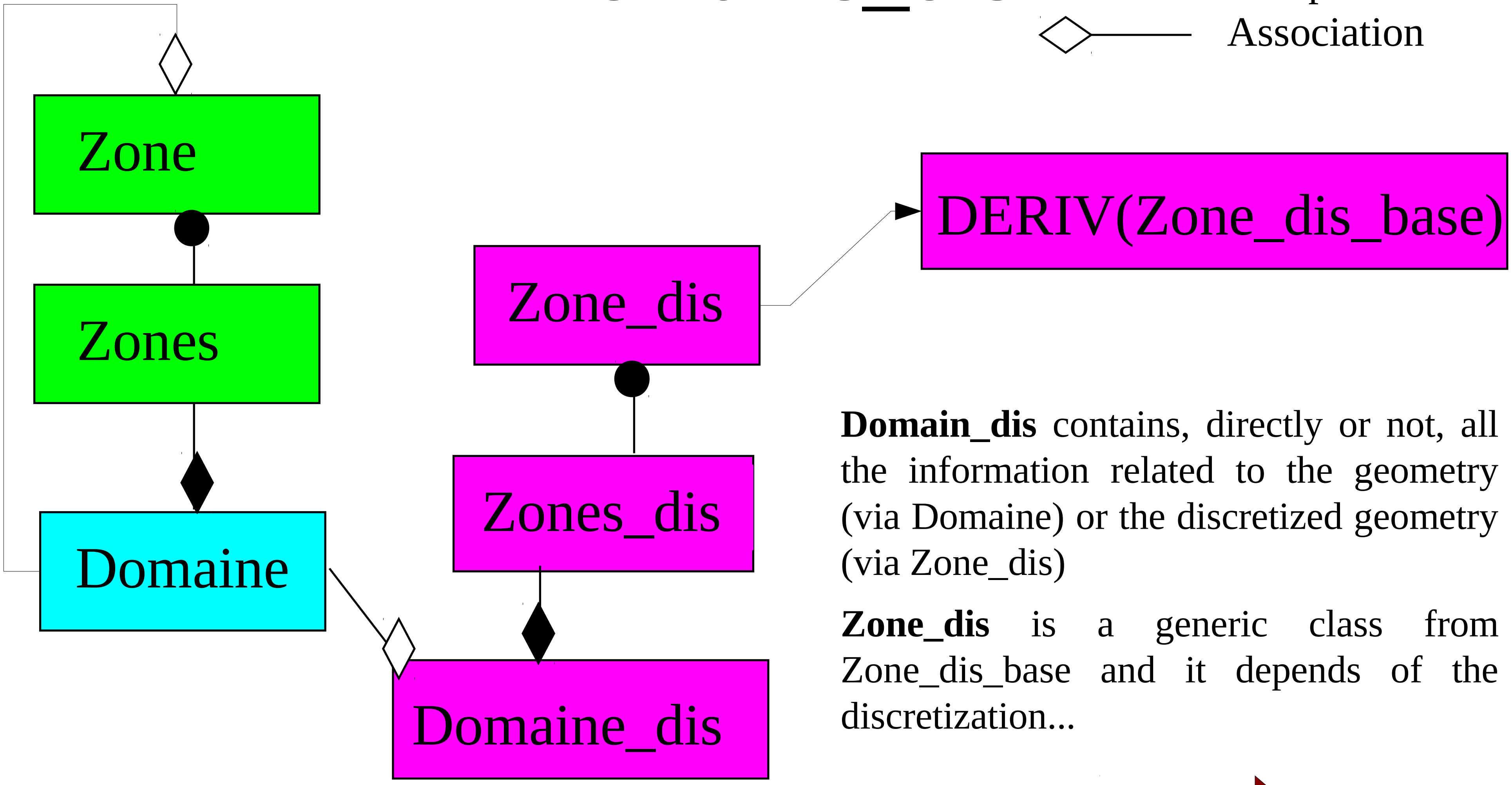
Zone : Is a mesh with cells of same type (eg : tetraedras). It contains :

- 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** »)

Domaine_dis

◆—— Composition

◇—— Association



Zone

Zones

Domaine

Zone_dis

Zones_dis

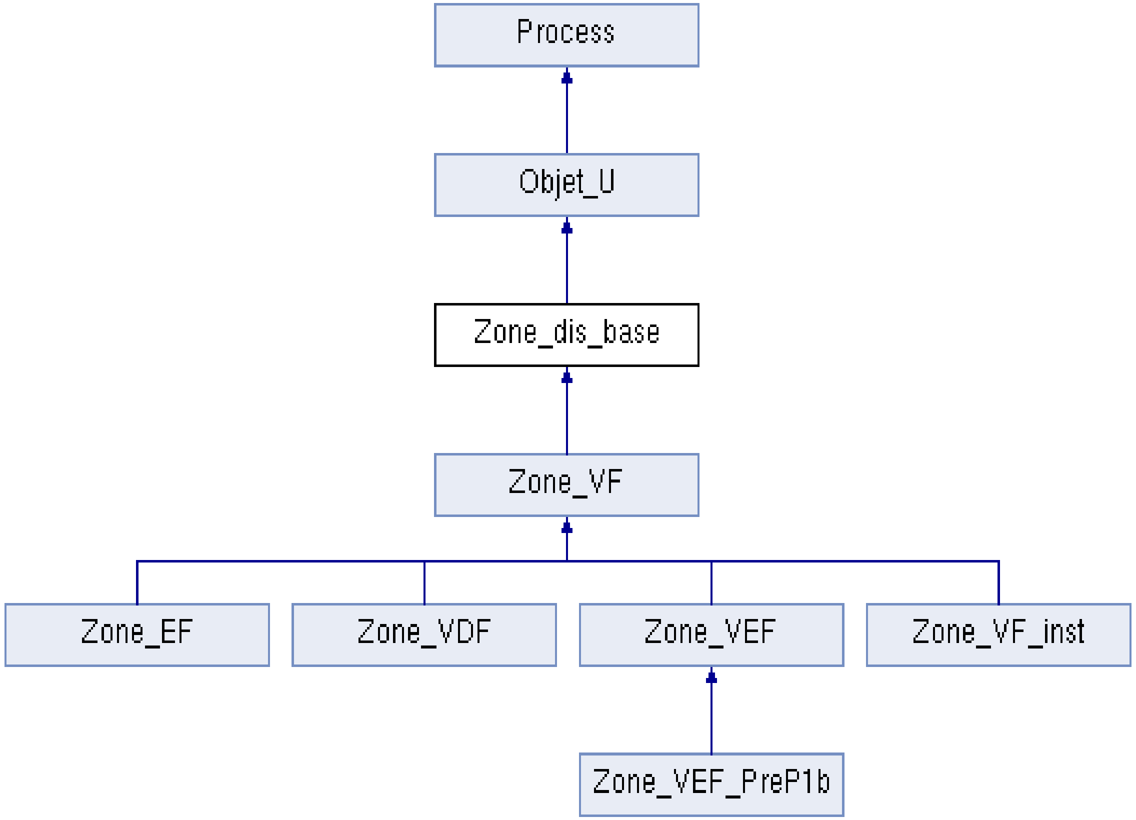
Domaine_dis

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...

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)

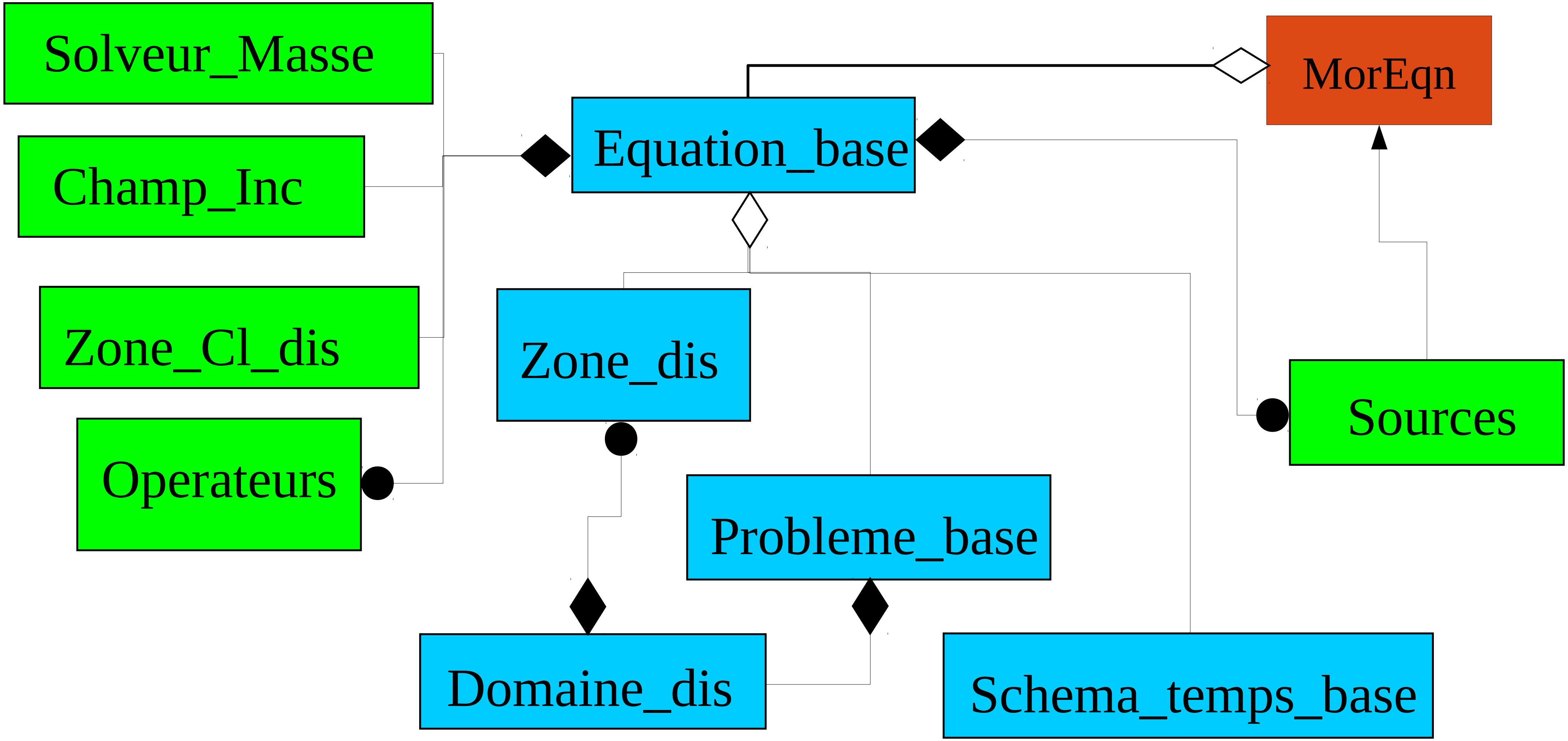
TRUST Baltik project Tutorial

→ **Modify the cpp sources**

- Create a new cpp class
- **Modify your cpp class (Part 1)**
- Add XData tags
- Adding prints

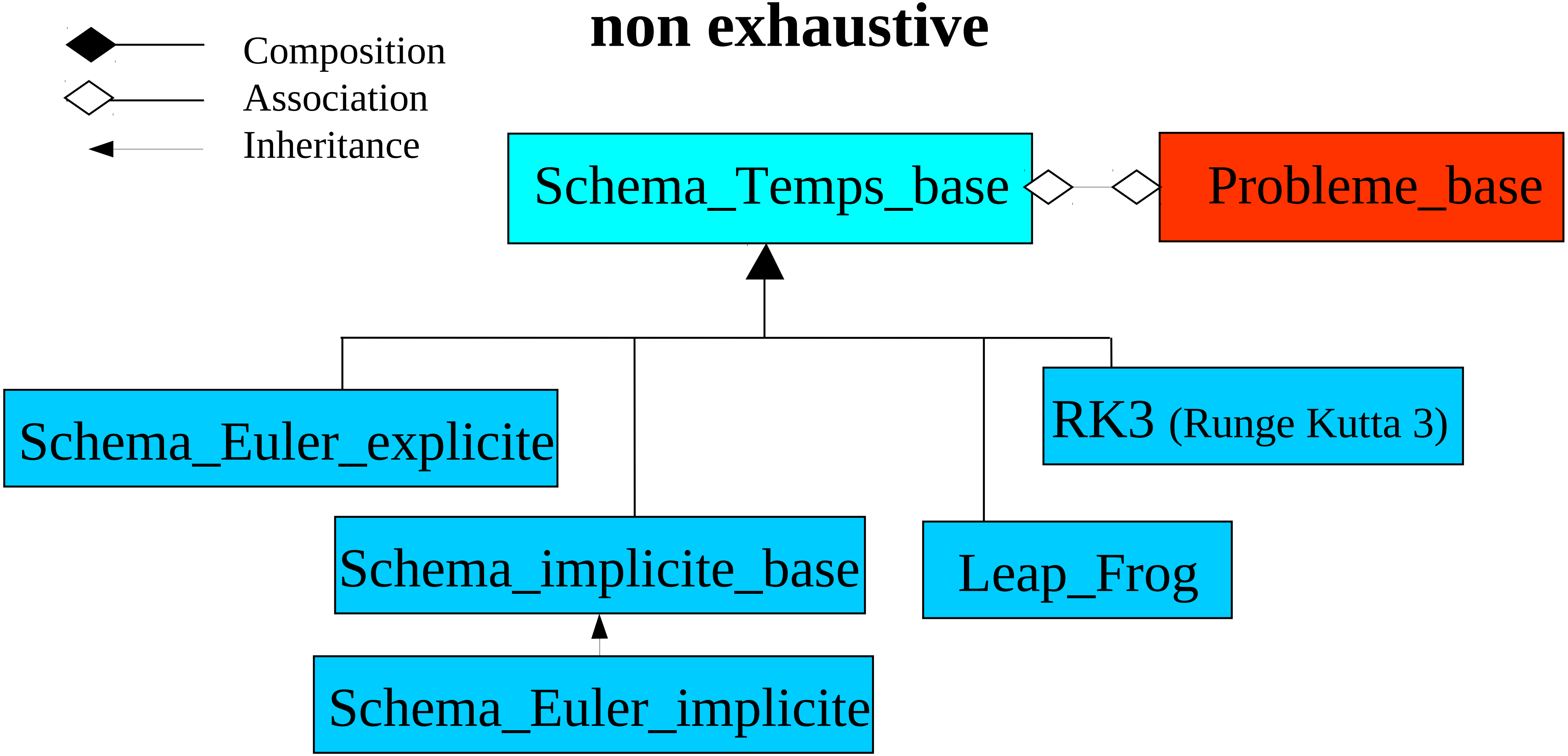
Equation (Kernel framework)

non exhaustive



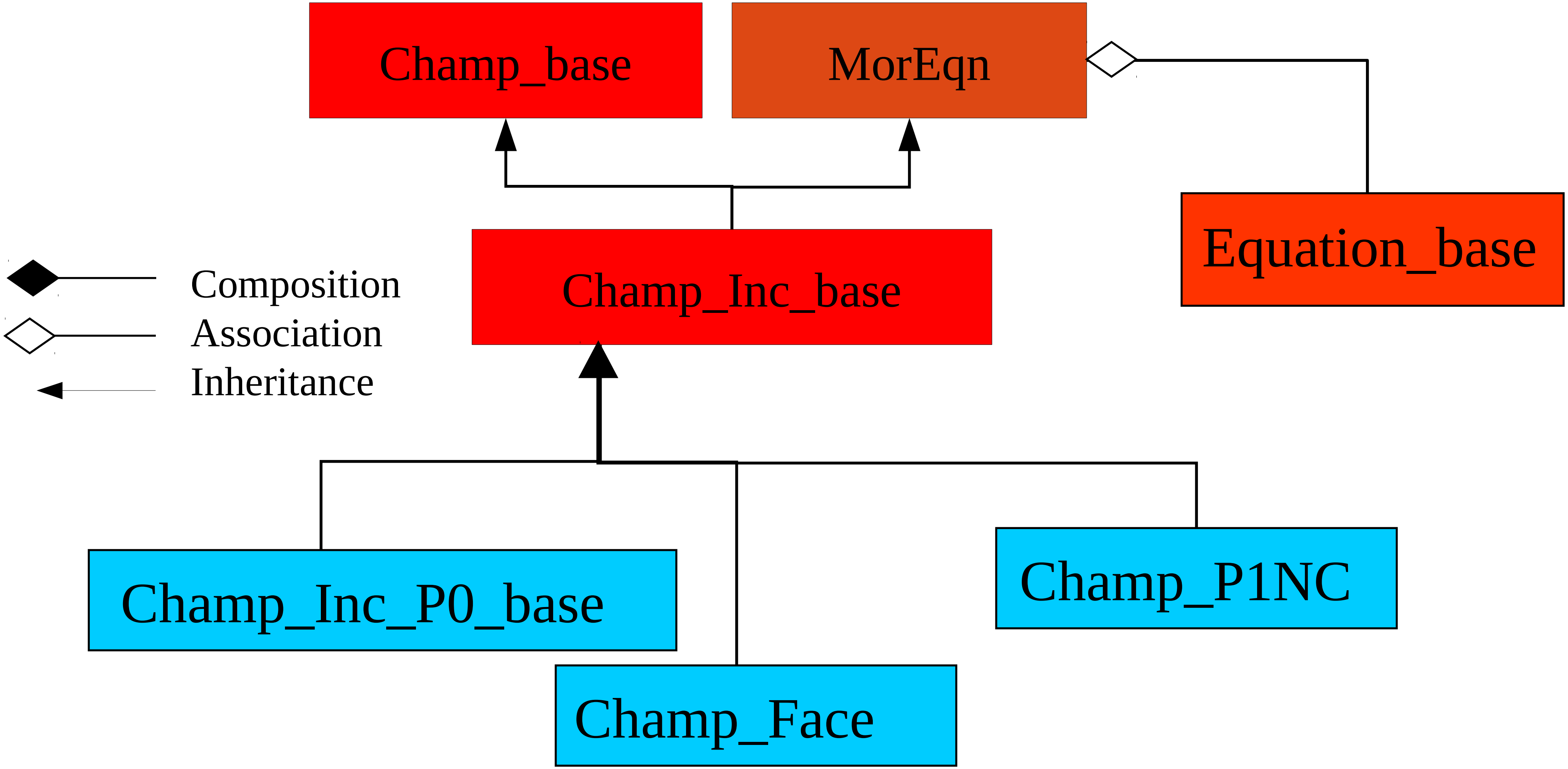
Time Schemes

non exhaustive



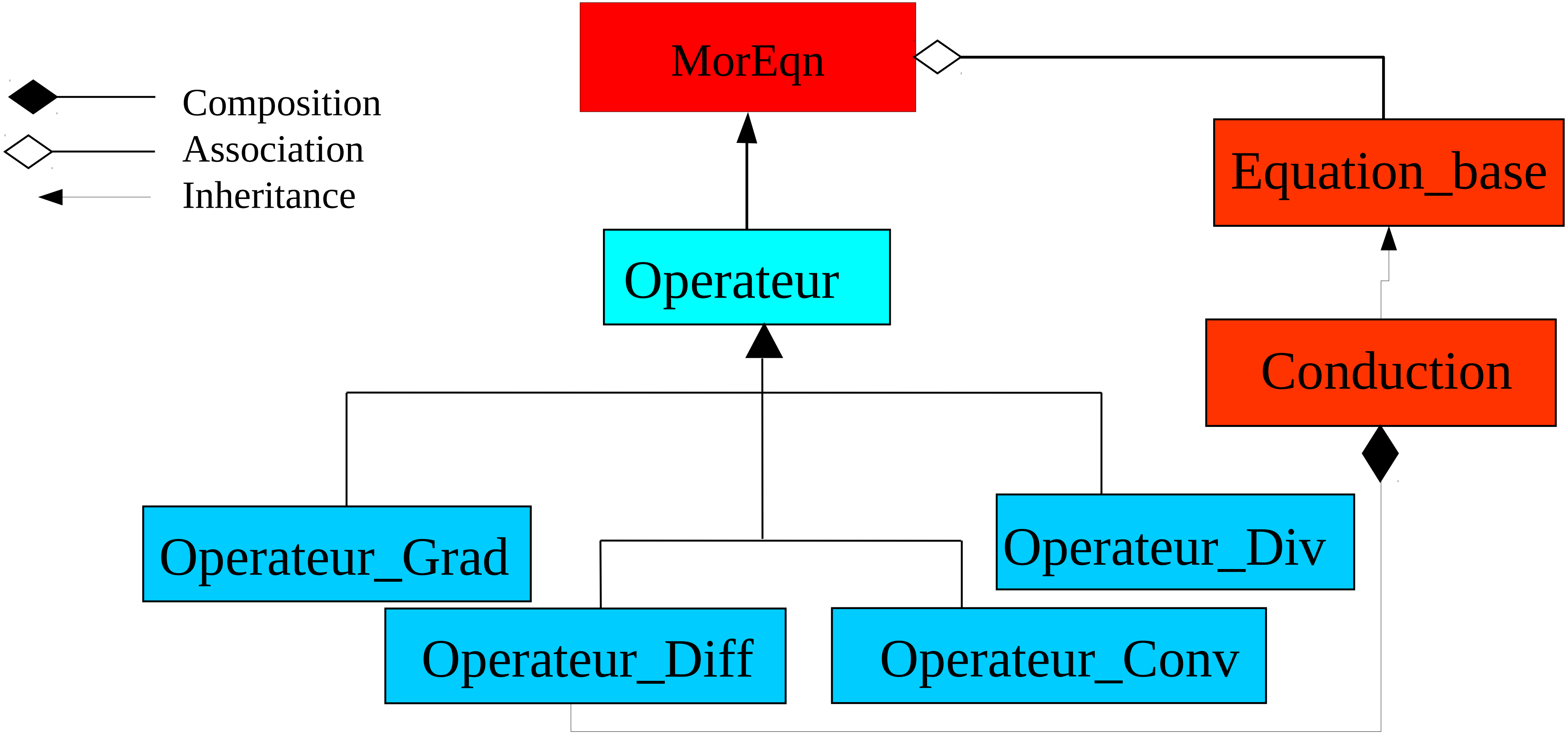
Fields

non exhaustive



Operators

non exhaustive



Exploring

Kernel module:

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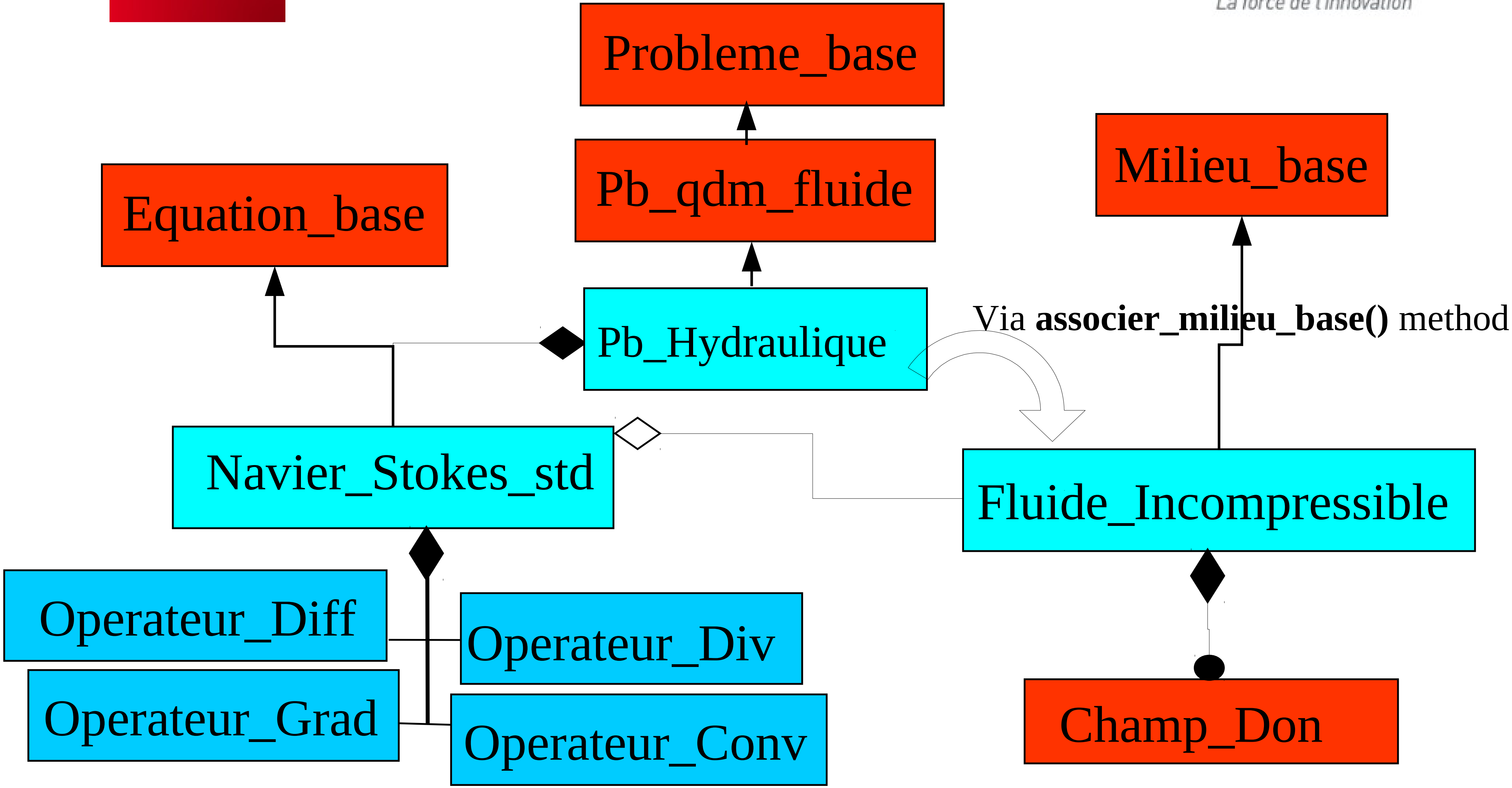
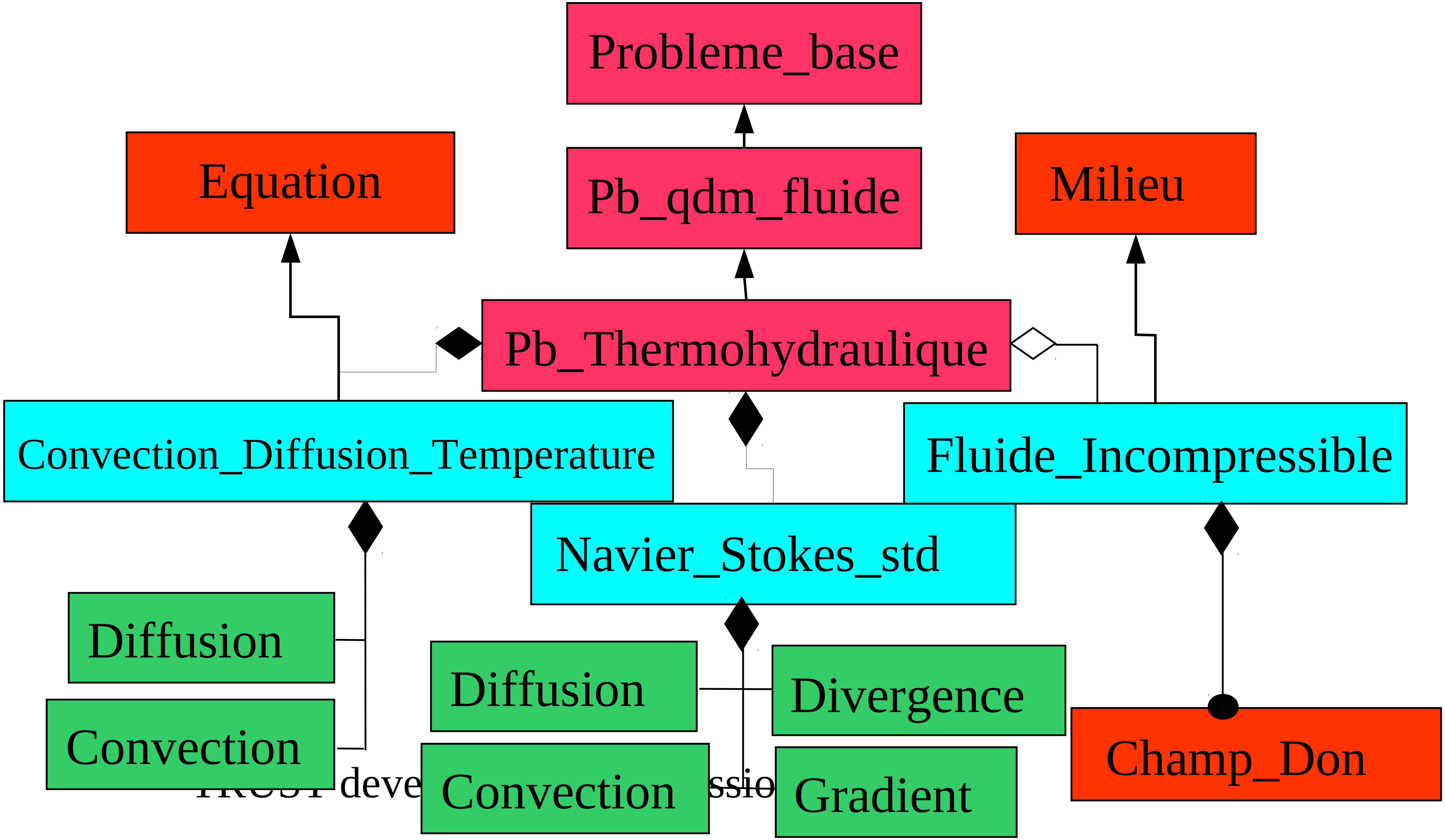
(Incompressible Thermalhydraulic)

Space discretization module

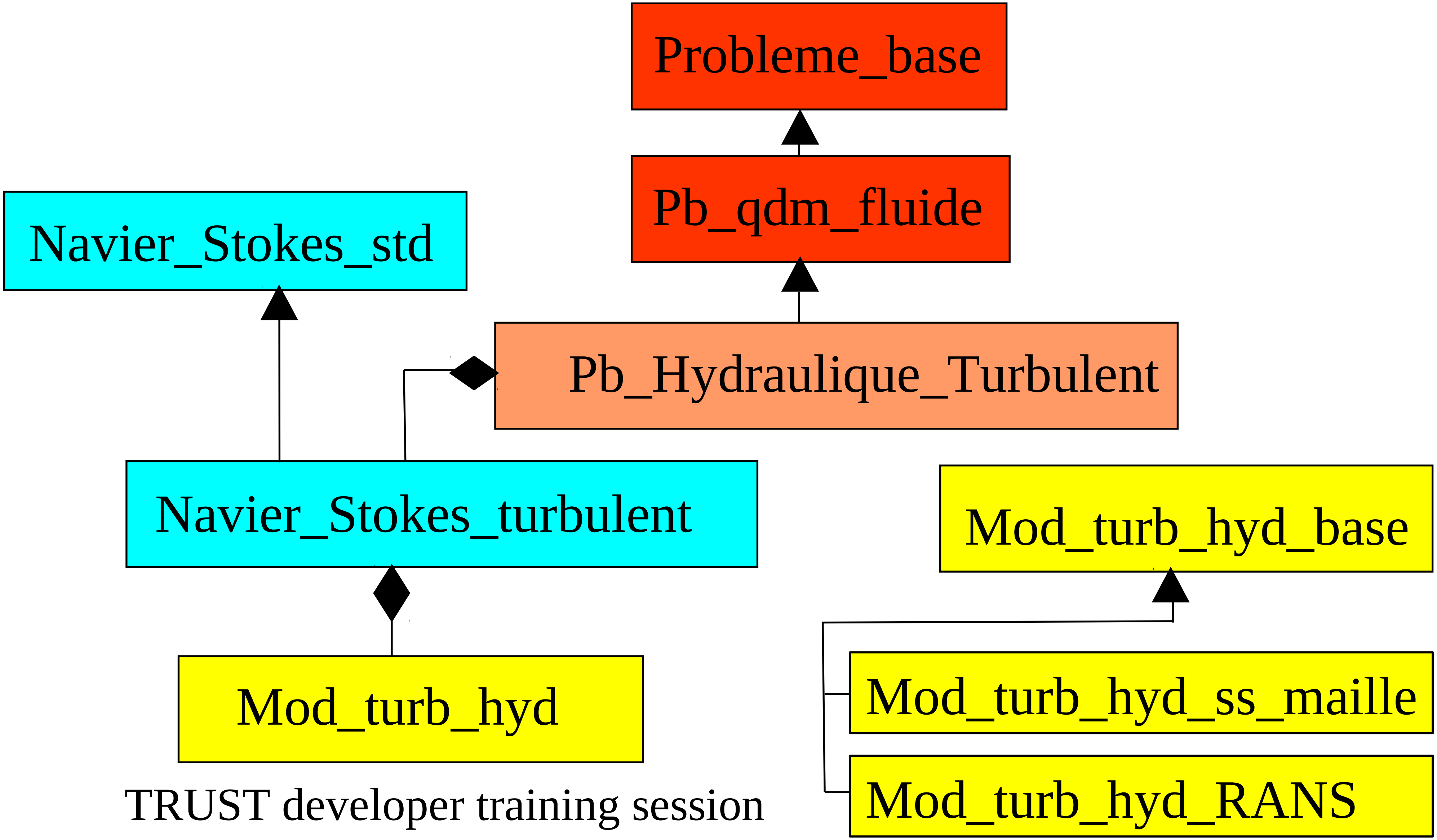
Hydraulic


Probleme_base
Pb_qdm_fluide
Milieu_base
Equation_base
Pb_Hydraulique
Via **associer_milieu_base()** method
Navier_Stokes_std
Fluide_Incompressible
Operateur_Diff
Operateur_Div
Operateur_Grad
Operateur_Conv
Champ_Don

Thermalhydraulic



Turbulent thermohydraulic



Exploring

Kernel module:

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Framework (Problem, Domain, Equation, Time schemes, Fields, Operators)

ThHyd module

(Incompressible Thermalhydraulic)

Space discretization module

Reference's Documentation

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

TrioCFD website with other PhD Thesis and articles:

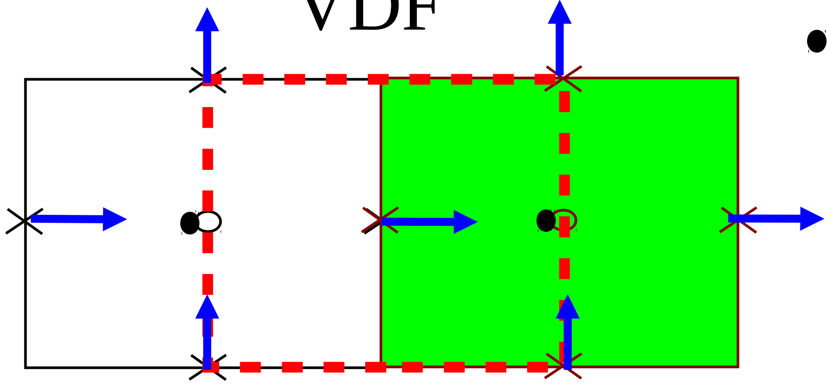
http://www-trio-u.cea.fr → More information on numerical methods

Available discretizations

↑ Velocity

● Pressure

VDF



Field localisation:

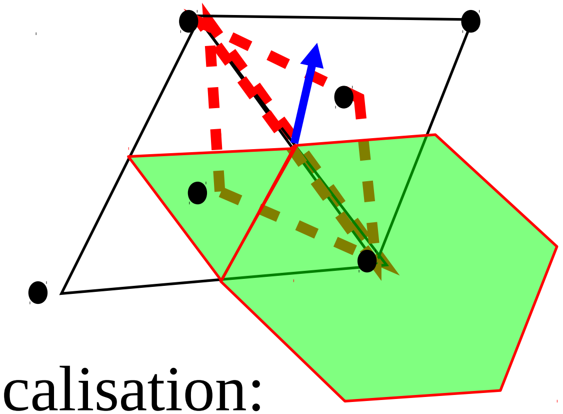
- Vector field (P1NC) at the center of the faces

control volume: ⬚

- Scalar field (P0) at the center of elements

mass control volume: 🟩

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

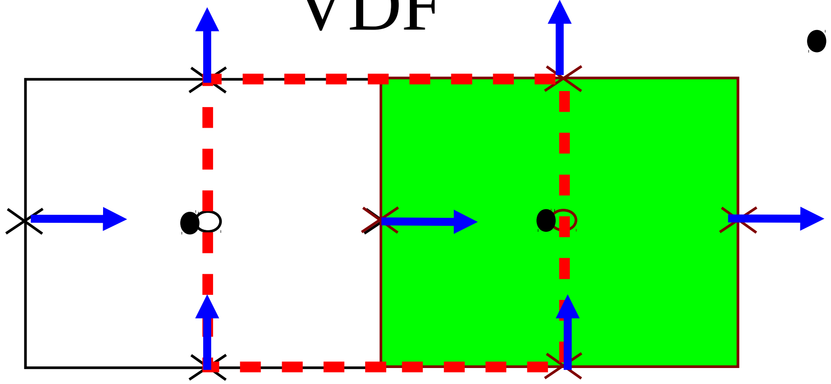
mass control volumes: ▼ ⬢

Available discretizations

↑ Velocity

● Pressure

VDF



Algorithms:

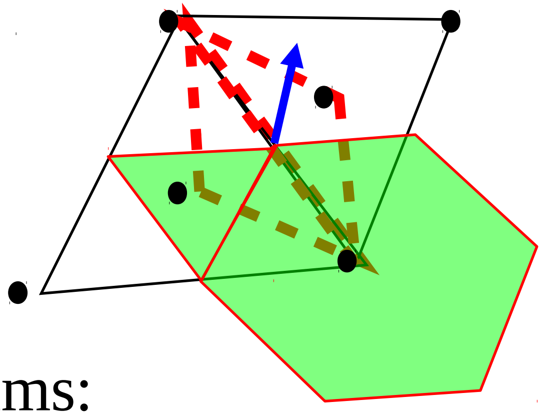
-Iterators to loop on elements or faces

-Evaluators to calculate fluxes on faces or facets

VDF/Operateurs/Iterateurs

VDF/Operateurs/Evaluateurs

VEF



Algorithms:

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

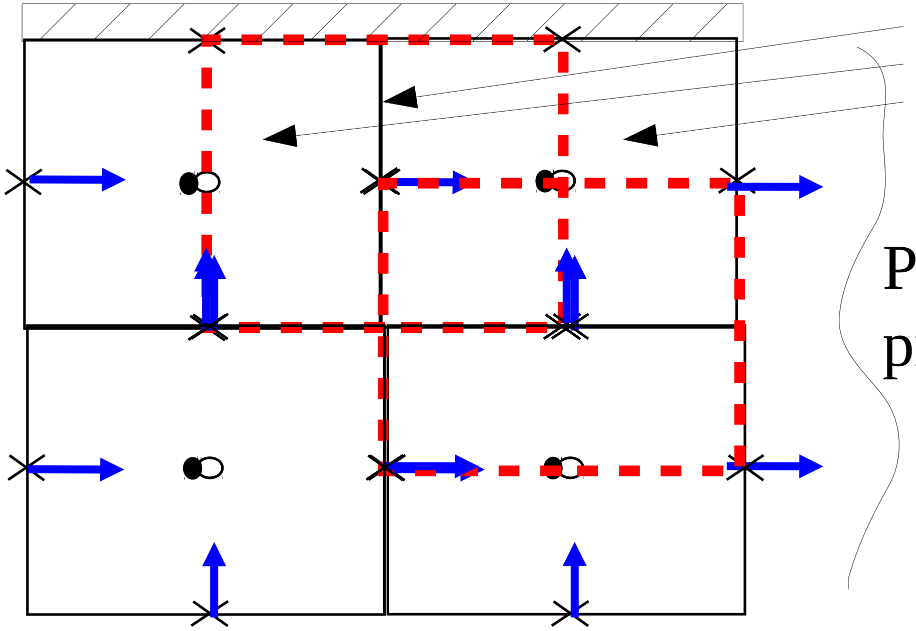
⬚ Momentum control volume

🟩 Mass control volume

Gradient operator example in VDF

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

$$On\ X\ axis,\ \iiint \nabla P\, dV = \iint P.ndS = (P(elem1) - P(elem0)) * area(num_{face})$$



Face num_face

Cell elem0=face_voisins(num_face,0)

Cell elem1=face_voisins(num_face,1)

Pimp (outlet pressure imposed)

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

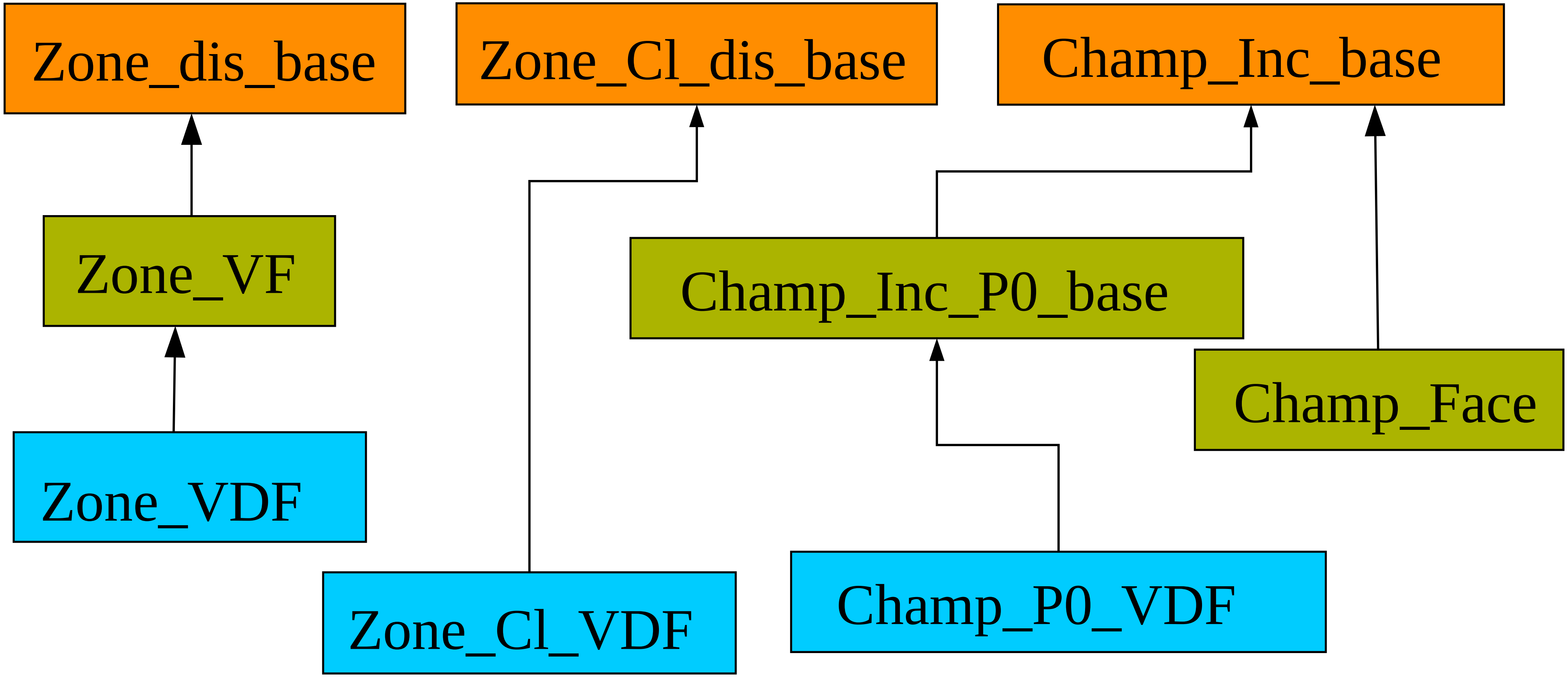
2) Loop on the internal faces :

premiere_face_int() returns the first internal face of the zone

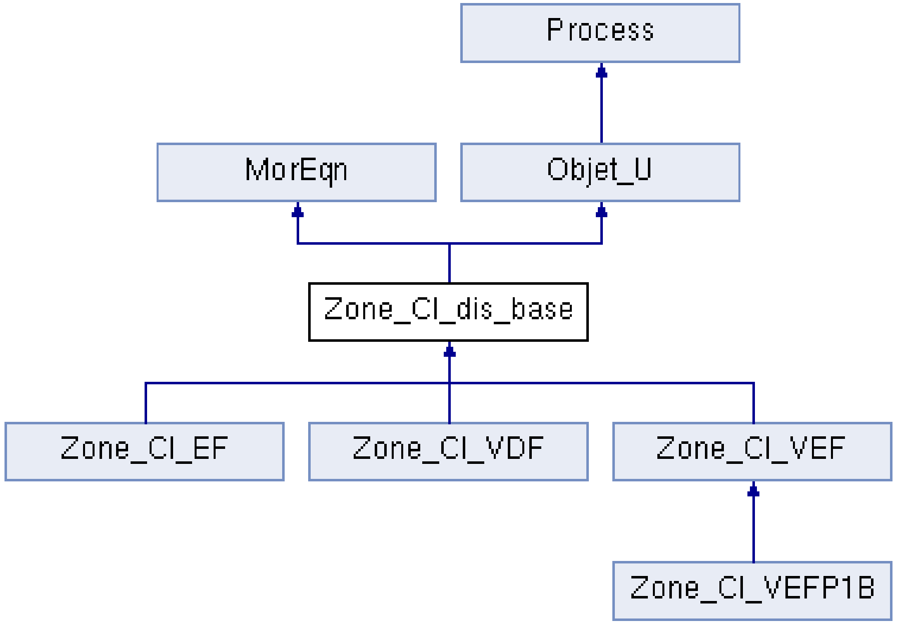
nb_faces() returns the number of faces of the zone

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

VDF Zones and Fields



Zone_Cl_dis_base

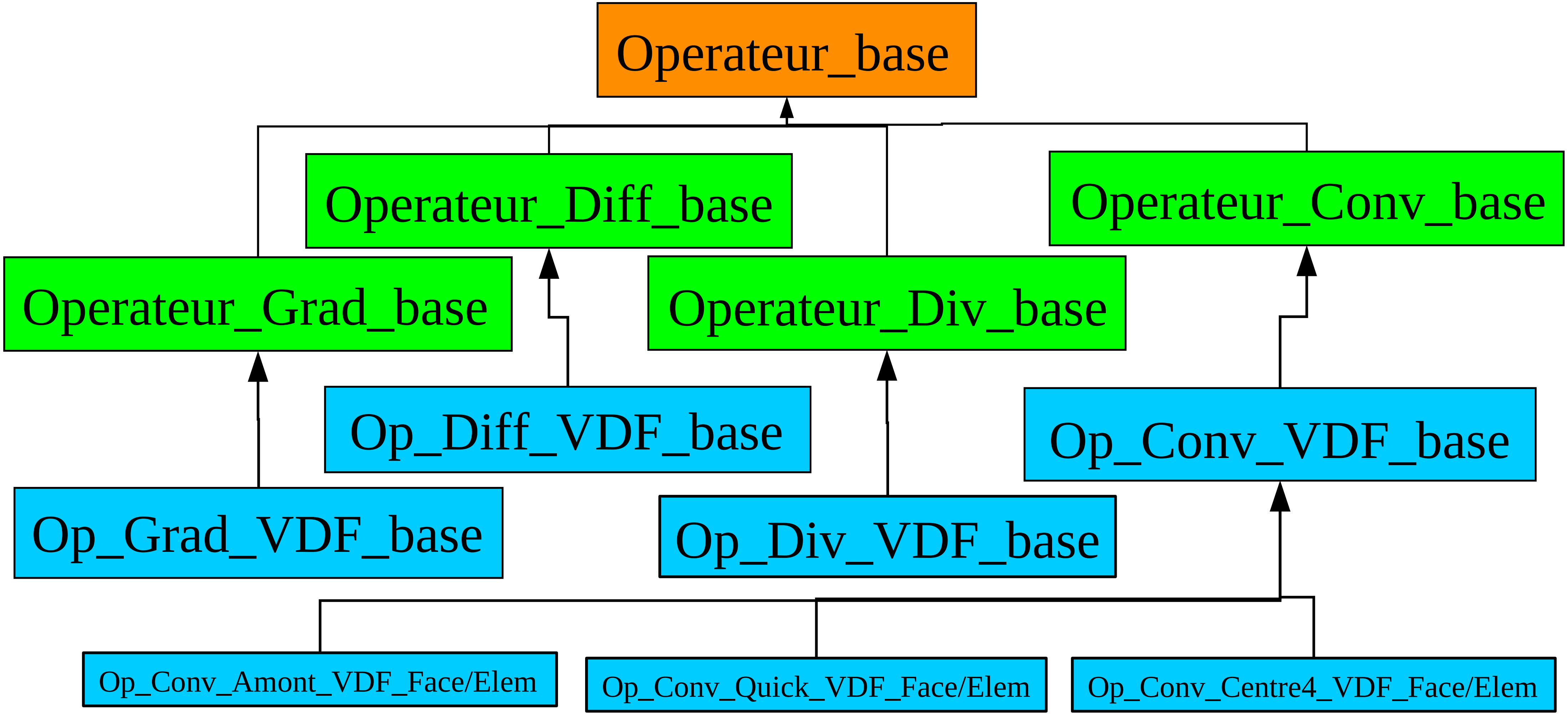


The Zone_Cl_dis_base classe describes discretized boundary conditions :

Protected :

Conds_lim les_conditions_limites_ ;

Operators VDF implementation



TRUST Baltik project Tutorial

→ **Modify the cpp sources**

- Create a new cpp class
- **Modify your cpp class (Part 2)**
- Add XData tags
- Adding prints

How to parallelize in TRUST

Managing input/output files

Parallelism

Parallelism

-SPMD (Single Program, Multiple Data)

-Definitions of the TRUST parallelism :

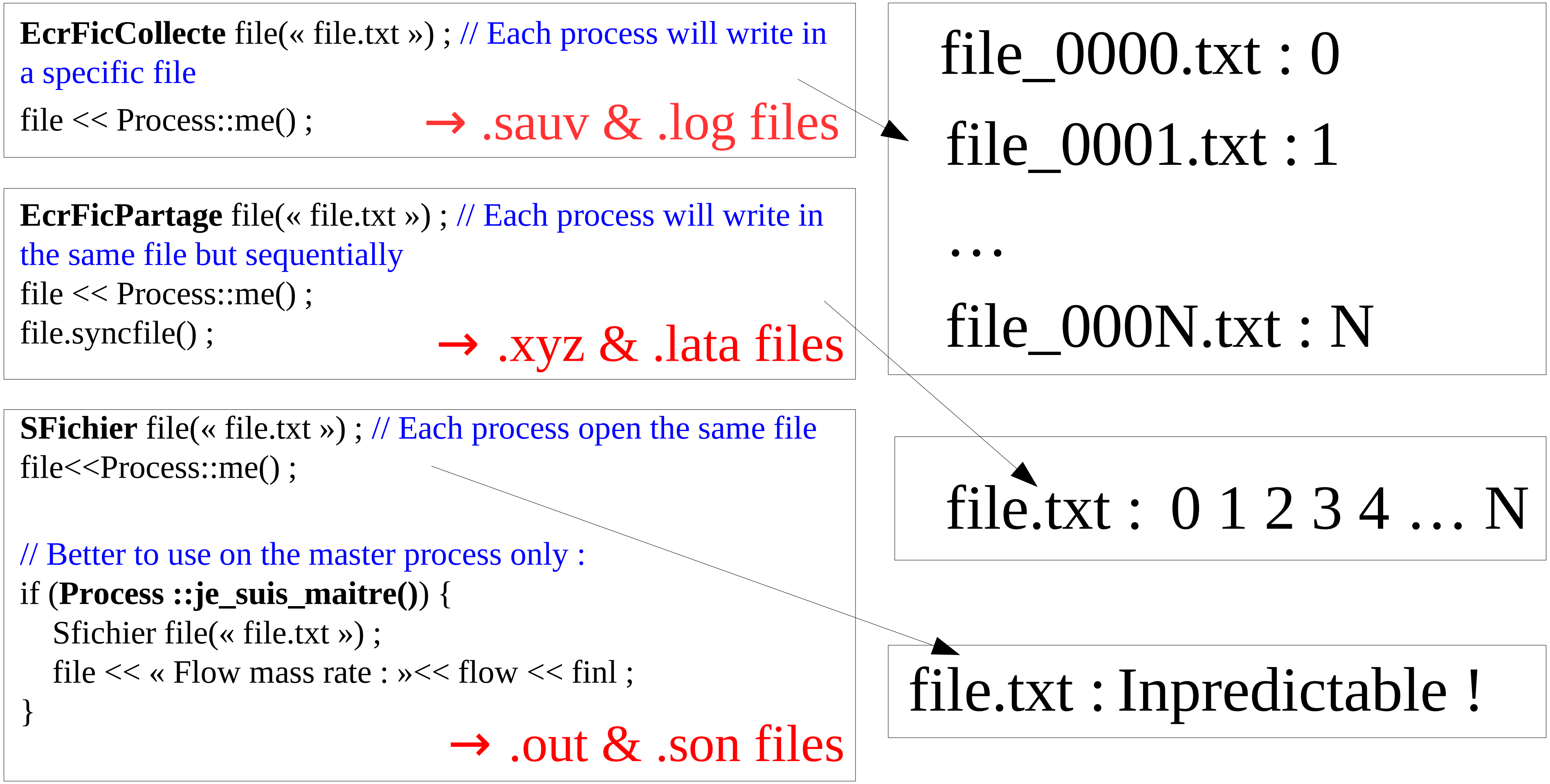
- Domain partition create several Zones
- Each process works on one Zone
- Joint (faces that connect different Zones)
- Items (which constitute a Zone)
  - cell, vertex, face, edge (3D)
  - may be real (physically located on the Zone) or virtual (located on the remote Zone, but known by the local process)

How to parallelize in TRUST

Managing input/output files

Parallelism

Dedicated classes to **Output**



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

→ .sauv & .log files

```
EcrFicPartage file(« file.txt ») ; // Each process will write in the same file but sequentially
file << Process::me() ;
file.syncfile() ;
```

→ .xyz & .lata files

```
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 ;
}
```

→ .out & .son files

file_0000.txt : 0

file_0001.txt : 1

…

file_000N.txt : N

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 ;
```

```
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;
```

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 »); // TRUST class to read a file
is >> a ; // Read the 2 attributes from a file
          // '>>': call the readOn method
Cerr << a << finl ; // Print the 2 attributes of a
                    // '<<': call the printOn method
SFichier os(« newfile.txt ») ;
os << a ; // Write the 2 attributes of a in a new file
```

readOn - printOn

* “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.

TRUST Baltik project Tutorial

→ **Modify the cpp sources**

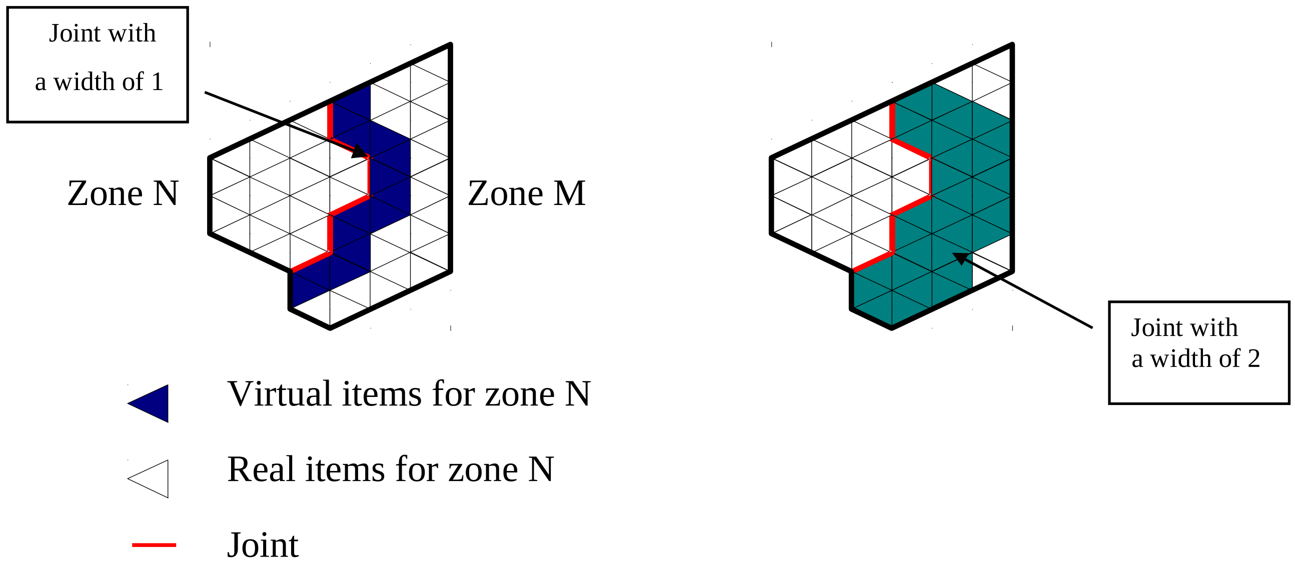
- Create a new cpp class
- Modify your cpp class
- **Add XData tags**
- **Adding prints**

How to parallelize in TRUST

Managing input/output files

Parallelism

Parallelism



Joint with a width of 1

Zone N

Zone M

Joint with a width of 2

◀ Virtual items for zone N

◁ Real items for zone N

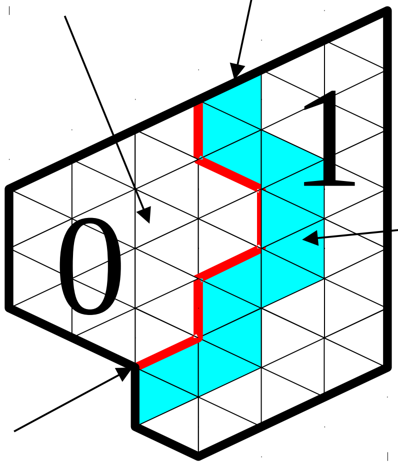
— Joint

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

Parallelism

Virtual boundary face
for the process 0

Real cells for process
0



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.

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

Parallelism

- Number of real items:

  Zone_VF::nb_faces()

  Domaine::nb_som()

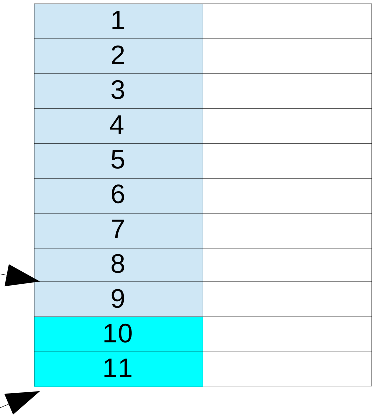
  Zone::nb_elem()

- Number of real+virtual items:

  Zone_VF::nb_faces_tot()

  Domaine::nb_som_tot()

  Zone::nb_elem_tot()

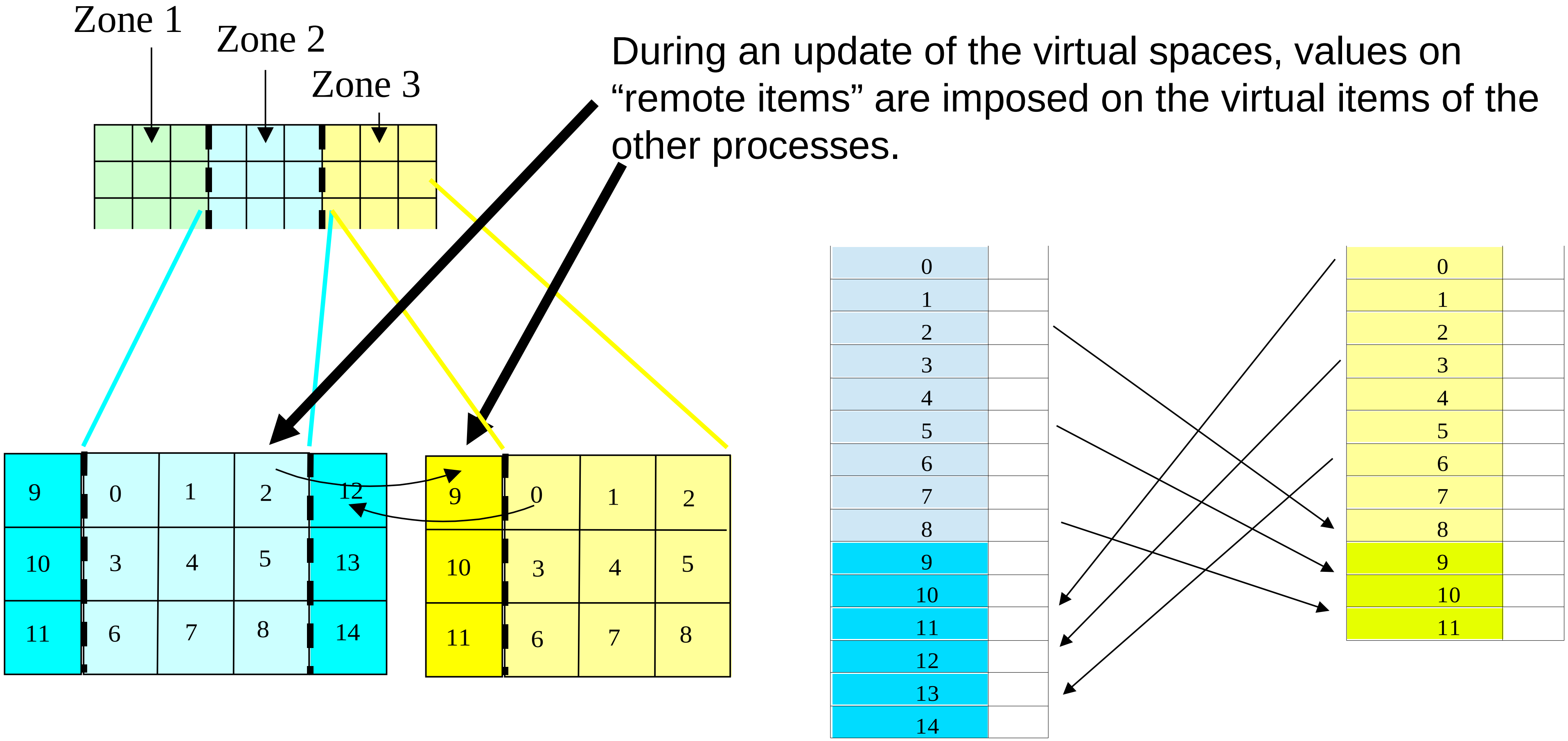


1	
2	
3	
4	
5	
6	
7	
8	
9	
10	
11	

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

Parallelism

Example of a distributed array on cells



During an update of the virtual spaces, values on “remote items” are imposed on the virtual items of the other processes.

Parallelism

- 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();

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 : */
```

Parallelism

```
DoubleVect A2(la_zone_vef.nb_faces());
const MD_Vector& md2 = la_zone_vef.md_vector_faces();
MD_Vector_tools::creer_tableau_distribue(md2, A2);

DoubleVect A3(la_zone_vef.zone().nb_aretes());
const MD_Vector& md3 = la_zone_vef.md_vector_aretes();
MD_Vector_tools::creer_tableau_distribue(md3, A3);

DoubleVect A4(la_zone_vef.zone().nb_faces_frontiere());
const MD_Vector& md4 = la_zone_vef.md_vector_faces_front();
MD_Vector_tools::creer_tableau_distribue(md4, A4);

DoubleVect A5(la_zone_vef.nb_som());
const MD_Vector& md5 = la_zone_vef.zone().domaine().md_vector_sommets();
MD_Vector_tools::creer_tableau_distribue(md5, A5);
```

Parallelism

– 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
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
Cerr << A.size_reelle() << finl ;   // nb_elem
Cerr << A.size_totale() << finl ;   // nb_elem_tot
```

Parallelism

- 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));
```

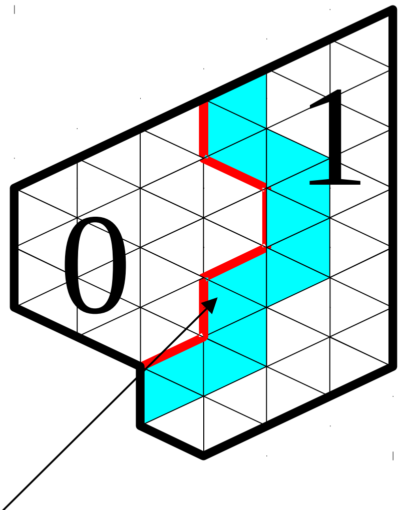
Parallelism

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 :

Parallelism

```
// 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
…
```



Parallelism

- Some useful TRUST 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 the scalar x on the whole processes
  - **Process::mp_min(**x**)** returns the smallest value of the scalar x on the whole processes
  - **Process::mp_max(**x**)** returns the biggest value of the scalar x on the whole processes
  - **Process::barrier()** waits that all processes reach this point

Parallelism

- 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(**DoubleVect& x**)** 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
  - Journal() : all the processes write to the .log files

Parallelism

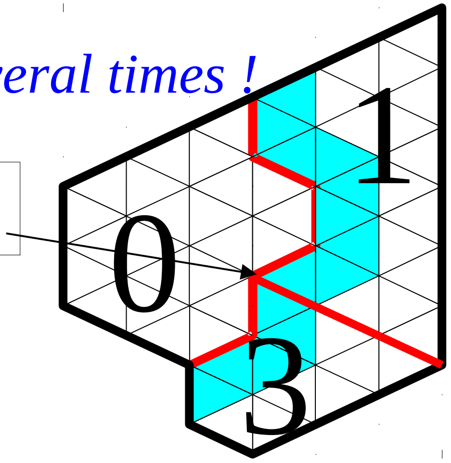
- Send/receive methods (envoyer/recevoir). Well described in the file :
  - $TRUST_ROOT/Kernel/Utilitaire/communications.cpp
  - Example of use in the Sous_Zone.cpp file. An array is sent by the master processor (0) and received by all the other ones.

Parallelism

– 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

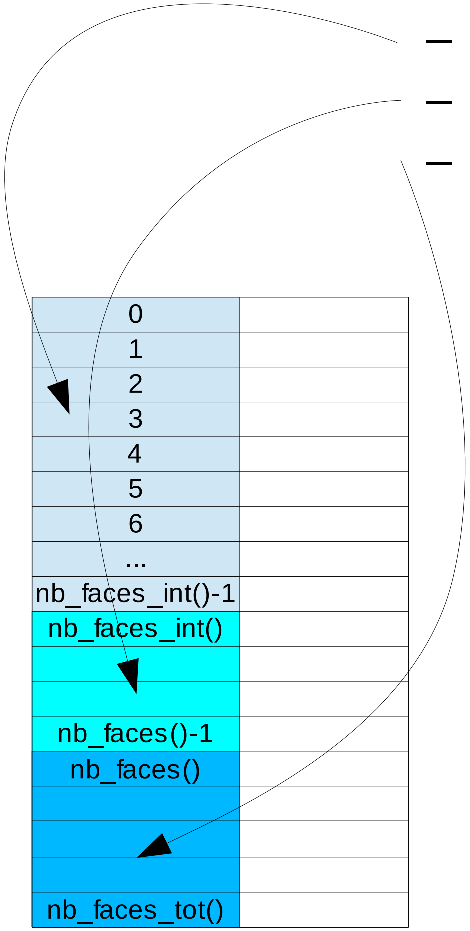


NB: In this case, you would use :
double sum = **mp_somme_vect(tab) ;**

Parallelism

-Pitfall with how the faces are ranked in TRUST (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())



0
1
2
3
4
5
6
...
nb_faces_int()-1
nb_faces_int()
nb_faces()-1
nb_faces()
nb_faces_tot()

```
// So, to loop on the internal faces, you will write :
const int nint=zone_VF::premiere_face_int();
const int nb_faces_tot=zone_VF::nb_faces_tot();
 for (int face=nint;face<nb_faces_tot;face++)
  if (!zone_VF.est_une_face_virt_bord(face))
      …. // Internal face (real or virtual)
```

Parallelism

```
// 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++)
    {
       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

TRUST Baltik project Tutorial

→ **Parallel exercise :**

- **Part 1**
- **Part 2 Optional**
- Part 3
- Part 4 Debog

Parallelism

– How to validate parallelization in TRUST

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):

  trust datafile

- Run you parallel calculation on N cpus and compare the LATA results :

  trust parallel_datafile 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

Parallelism

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              0.805794 70% (1 appel/pas de temps)
Dont operateurs convection        0.157865 13% (2 appels/pas de temps)
Dont operateurs diffusion         0.053469 4% (2 appels/pas de temps)
Dont operateurs gradient          0.02917 2% (2 appels/pas de temps)
Dont operateurs divergence        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          17.7 % of total time
Communications max          21.4 % of total time
Communications min          14 % of total time
Network latency benchmark 7.10487e-07 s
Network bandwidth max      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
```

Parallelism

– How to debug parallelization in TRUST

- 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 :

    exec=$exec_debug trust datafile N

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

    exec=$exec_debug trust -gdb **datafile N**

Parallelism

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

-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.

TRUST Baltik project Tutorial

→ **Parallel exercise :**

- Part 1
- Part 2 Optional
- **Part 3**
- **Part 4 Debog**

TRUST test coverage

Code coverage

→ Created by gcov tool, as a nightly task on ~2000 test cases.

→ 70% of TRUST & his Baltiks 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.

→ TRUST/TrioCFD code coverage and tools exploiting it are available for the developer

→ TRUST keywords coverage verified nightly in order to have more keywords covered at each new version

Useful code coverage tools

- TRUST tool to know and run the test cases covering a method:

trust -check class::method

***Example* :**

```
$ trust -check Navier_Stokes_std::mettre_a_jour
$ nedit liste_cas
```

- To check the non-regression on one or several test cases

trust -check all|testcase|list

Some examples for Baltik developer:

```
$ make check_optim|check_debug  # Check the project non-regression on Baltik test cases
$ make check_last_pb_debug      # Running last pb test suite (see test in liste_pb.all file)
$ make check_deps_debug         # Check the project non-regression on dependencies test cases
$ make check_all_debug          #  Check the project non-regression on all test of project = baltik test + dependencies test
$ make check_trust_optim        # Check the project non-regression on TRUST test cases
$ make check_full_debug         #  Check the project non-regression on full test suite (all test of project + all test of TRUST
platform)
```

How to debug TRUST

gdb
valgrind

Use gdb tool to debug or understand the code

GDB web site and documentation:

https://www.gnu.org/software/gdb/

https://doc.ubuntu-fr.org/gdb

Online tutorials:

http://www.linux-france.org/article/memo/node119.html
http://perso.ens-lyon.fr/daniel.hirschkoff/C_Caml/docs/doc_gdb.pdf

With TRUST, run with **Eclipse** or in a **terminal**:

```
# To describe all the commands:
$ man gdb

# To debug the TRUST binary program compiled with -g:
$ exec=$exec_debug trust -gdb datafile
```

Use gdb tool to debug or understand the code

```
# 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)
   up              # To move up in the stack
   down            # To move down in the stack
   list            # List the source code
   cont or c       # To continue the calculation after a stop
   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 TRUST error message is printed (before the stack is left)
   next or n       # Execute next line
   step or s       # Execute next line and enter in a method/function if any
   print var       # Print a variable
```

Use gdb tool to debug or understand the code

# Specific gdb commands for TRUST (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:

$ make_PAR.data datafile N

$ exec=$exec_debug trust **-gdb** PAR_datafile N

Use valgrind to find memory bugs

- Valgrind is a memory checker tool: http://www.valgrind.org

- You can check a binary with:

$ **VALGRIND=1 trust** datafile

- It detects uninitialized variables, memory leaks, outbound array values,...

- TRUST has 0 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,...)

TRUST 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 all modules
- All news (classes, keywords, ...) in english

Rules to contribute

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

If you develop in a Baltik project based on TRUST:

- 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 (no errors) on the debug binary and possible differences should be explained :
  - make check_full_debug # Check the project non-regression on full test suite (all test of project + dependances + TRUST)
  - VALGRIND=1 make check_optim # Same in optimized mode with Valgrind check

After the training session...

Read the commented solution of the exercise:

$TRUST_ROOT/doc/TRUST/exercices/my_first_class

Practice on a tutorial:

$TRUST_ROOT/doc/TRUST/exercices/equation_convection_diffusion/rapport.pdf

Or

trust -index → « Other baltik tutorial »

TRUST Baltik project Tutorial

→ **Code coverage exercise**

→ **Tools**

- **GDB exercise**
- **Use Valgrind to find memory bugs**

The End

Good luck!

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