TRUST/TrioCFD 1.7.4
developer's training session

Table of contents

Introduction

Prerequisites

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

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

$TRUST_ROOT/src

We are only in an evaluation phase...

Exercise: eclipse install

 # If you are on a CEA Saclay PC:
$ cd /export/home/yourlogin

 # Initialize TRUST environment
$ source /home/triou/env_TRUST_1.7.4.sh

 # Create your eclipse project:
$ vi $TRUST_ROOT/src/README_ECLIPSE

$TRUST_ROOT/src/README_ECLIPSE

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 :

- 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

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:

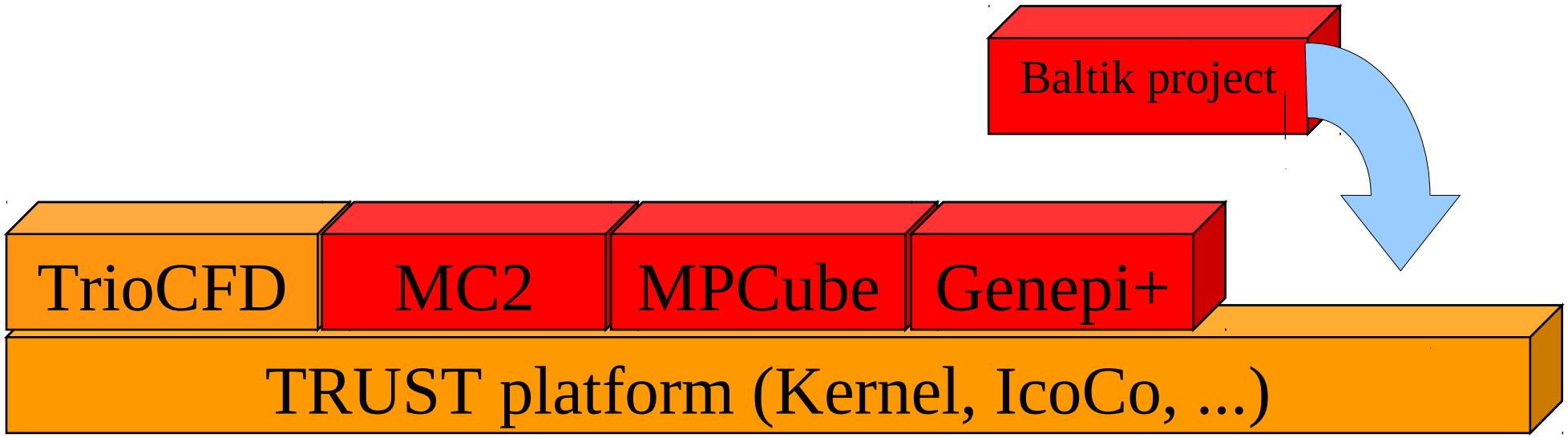
Enable developments with the following characteristics:

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

Main Choices:

- Object Oriented Conception 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 (Git)
  - Co-developing
- Automatic generation via Doxygen of HTML documentation from code sources
  - Documentation is up to date

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 or TrioCFD

- 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 **Tri**o_U **K**ernel

II) Integrate your project in TRUST base

- You want to contribute to TRUST/TrioCFD
- 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

Baltik
Building Application Linked with Trio_U Kernel

Exercise
Create a Baltik project

 # Create your project from a basic project template:
$ mkdir –p /export/home/yourlogin/my_project
$ cd /export/home/yourlogin/my_project
$ cp -r $TRUST_ROOT/bin/baltik/templates/basic/* .

 # Prepare of exercises:
$ cp $TRUST_ROOT/src/MAIN/mon_main.cpp src/.
$ mkdir -p /export/home/tourlogin/my_project/tests/Reference/NonRegression
$ cd /export/home/tourlogin/my_project/tests/Reference/NonRegression
$ trust -copy Cx
$ mv Cx myCx
$ cd /export/home/yourlogin/my_project

Exercise
Setting configuration

 # Initialize git base:
$ git init
$ git status
Git add --all
$ git commit --all -m "Initial commit"
$ git status

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

 # Track changes via gitk (GUI interface of Git)
$ git status
$ git status --u=no
$ gitk

Exercise: BALTIK build

 # Basic build

$ cd /export/home/yourlogin/my_project

 # Configure:

$ ./configure

 # Compilation:

$ make *optim # Build an optimized (-03 option) version*

$ make debug *# Build a debug (-g -O0 option with asserts) version*

$ source env_basic.sh

$ ls $exec_opt

$ ls $exec_debug

Other possible builds

 # List other options available for the make command:

$ make

 # 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 # NB : TRUST exe matching must exist

$ ls $exec_gcov

 # Build an semi optimized binary (option -O3 with asserts)

$ make semi_opt # NB : only for TRUST exe

$ ls $exec_semi_opt

Other basic commands

 # To run the non regression tests with a binary

$ make check_all_optim

$ make check_all_debug

 # To share your work

$ make distrib

 # Clean the install

$ git status

$ make clean

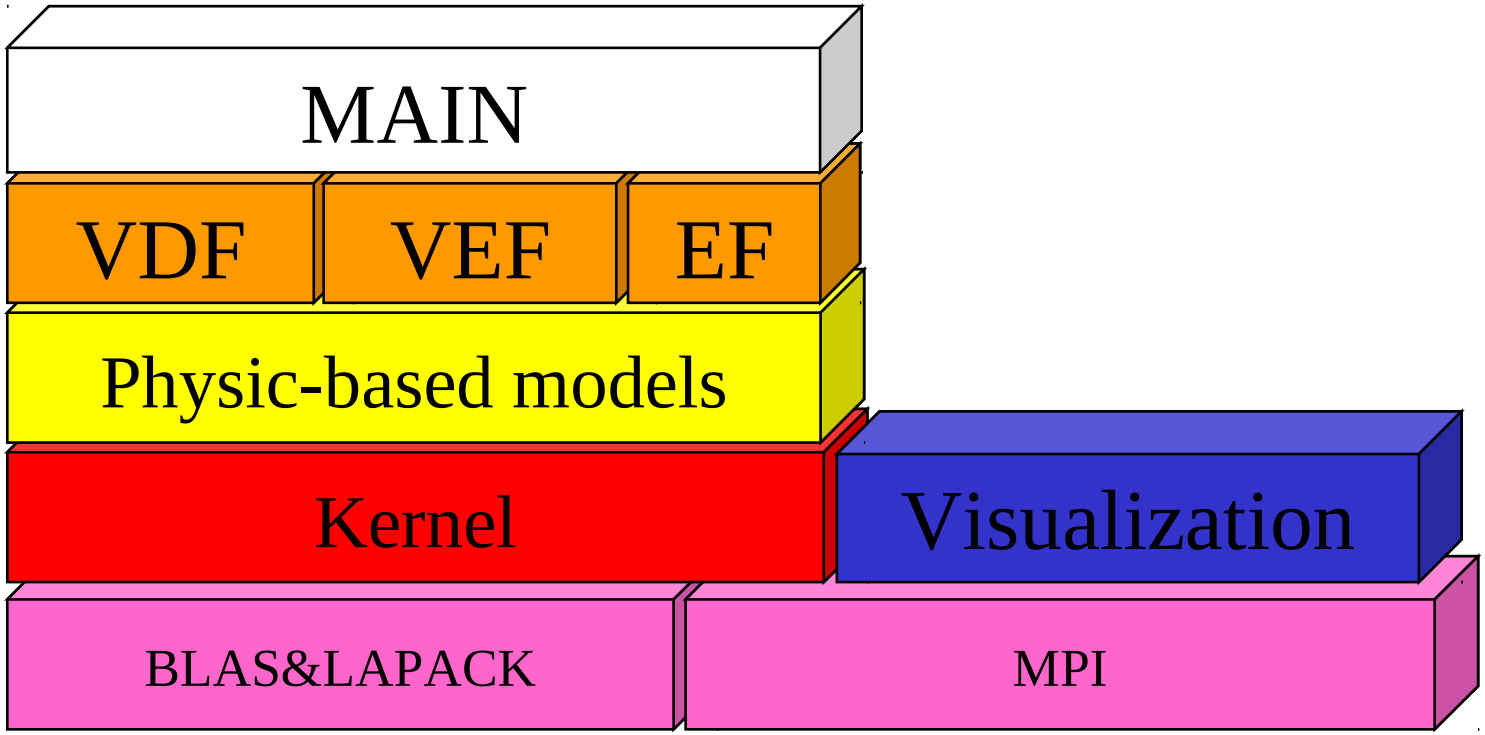
$ git status

$ ./configure

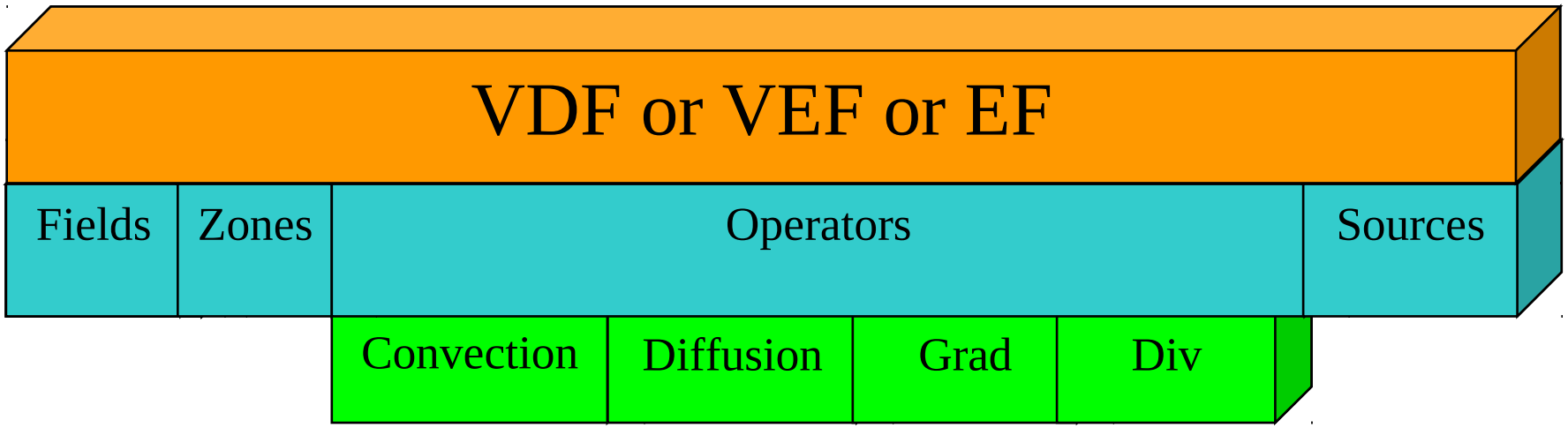
$ make optim debug

TRUST/TrioCFD modules

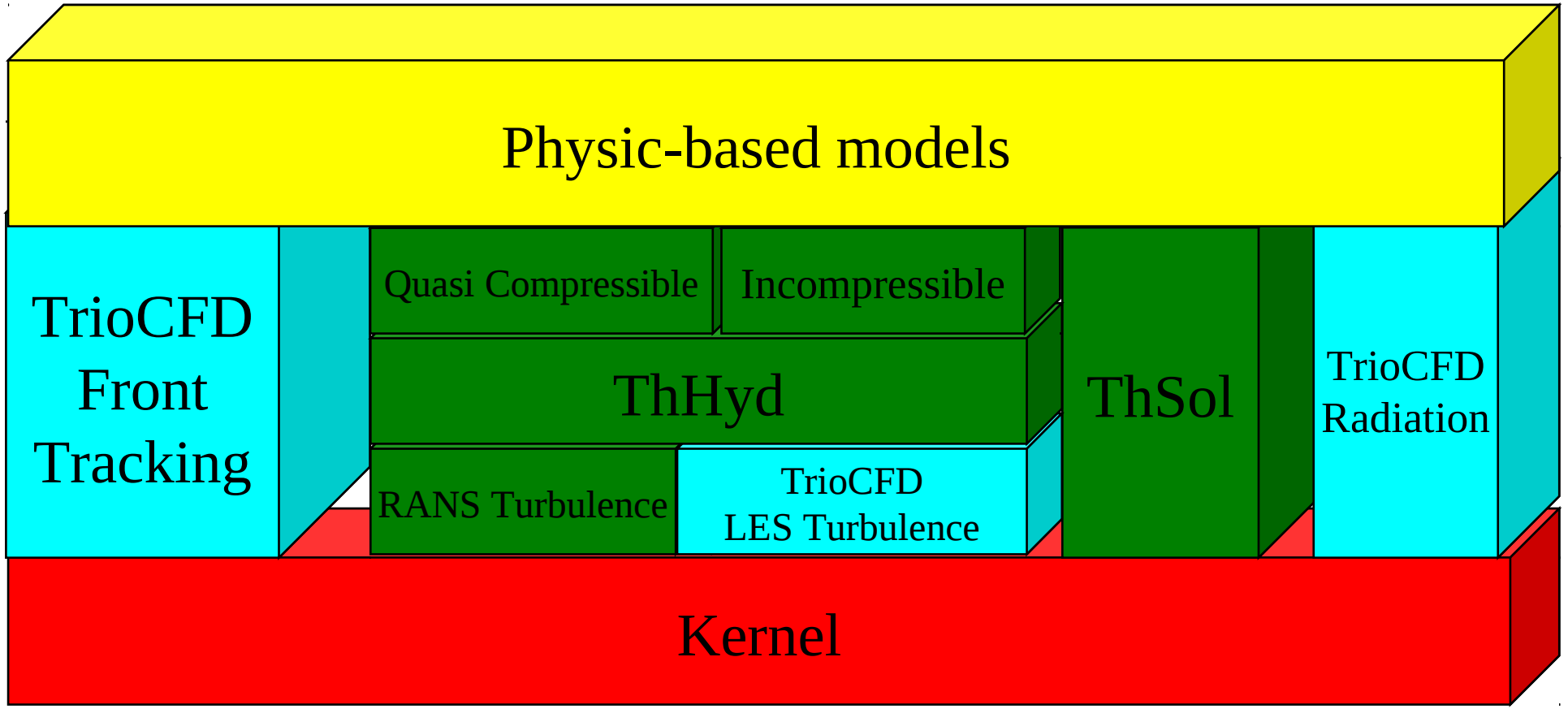
TRUST/TrioCFD modules



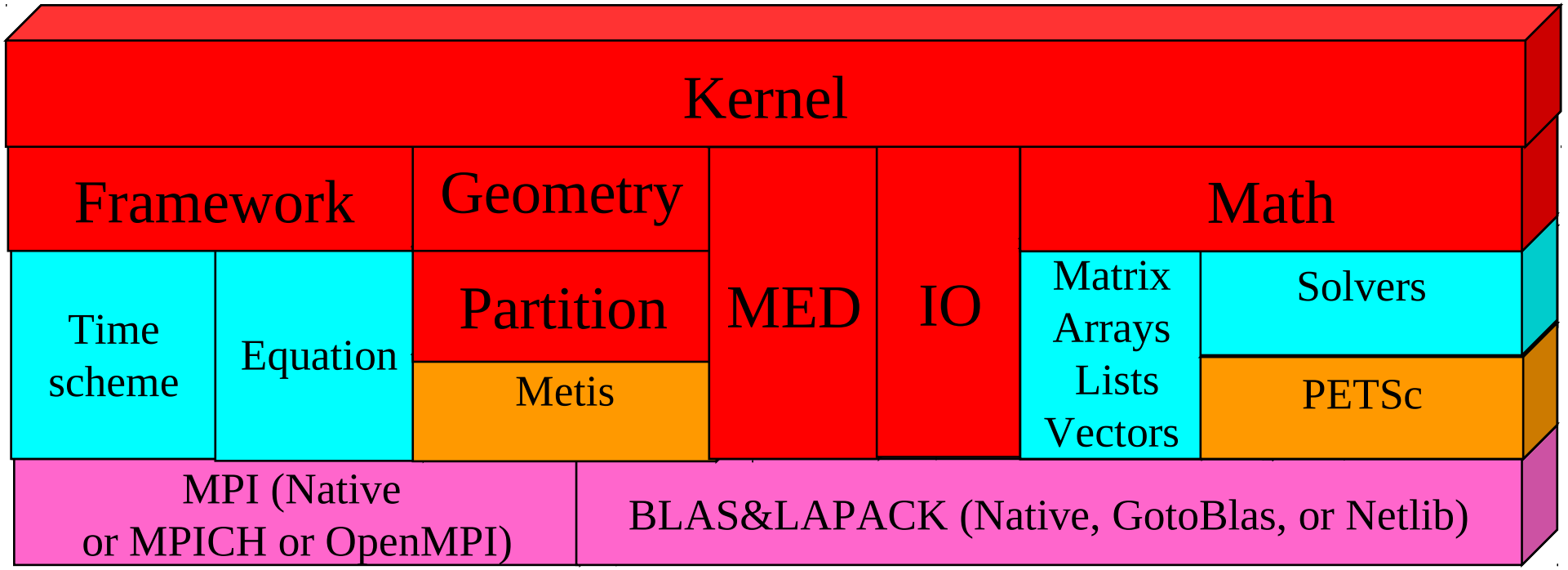
Discretization modules



Physics modules



Kernel module



TRUST/TrioCFD

➤ TRUST/TrioCFD 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 TRUST/TrioCFD code.

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

$TRUST_ROOT/doc/html

TRUST/TrioCFD tests

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

$TRUST_ROOT/Validation/Rapports_automatiques/Verification

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

$TrioCFD_ROOT/validation/share/Validation/Rapports_automatiques/Validant

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

$TRUST_ROOT/tests

$TrioCFD_ROOT/validation/tests

Kernel source directories

Under $TRUST_ROOT/src/Kernel

./Champs	Generic fields
./Champs_dis	Discretized generic fields
./Cond_Lim	Generic boundary conditions
./Framework	Generic problem, equation, time scheme
./Geometrie	Domain, cell geometry, mesh utilities
./Geometrie/Decoupeur	Partition utilities
./ICoCo	IcoCo coupling interface
./MEDimpl	MED utilities
./Math	Math utilities (arrays...)
./Math/Matrices	Matrix
./Math/SolvSys	Linear system solvers
./Operateurs	Generic operators (gradient,...)
./Schemas_Temps	Time schemes
./Solveurs	Solvers
./Statistiques_temps	Statistical utilities
./Utilitaires	IO, memory, MPI
./VF/Champs	Finite volume fields
./VF/Zones	Finite volume geometry description

TRUST source directories

./MAIN	Directory with main.cpp
./VDF	VDF discretization
./VDF/Axi/Operateurs	Operators in VDF with axis symmetry
./VDF/Axi/Operateurs/Evaluateurs	Flux evaluators in VDF with axis symmetry
./VDF/Axi/Sources	VDF source terms for axis symmetry
./VDF/Axi/Turbulence	VDF turbulence model for axis symmetry
./VDF/Champs	VDF fields
./VDF/Cond_Lim	VDF boundary conditions
./VDF/Elements	VDF cells description
./VDF/Operateurs	VDF operators
./VDF/Operateurs/Evaluateurs	Flux evaluators in VDF
./VDF/Operateurs/Iterateurs	Flux iterators in VDF
./VDF/Solveurs	VDF solvers
./VDF/Sources	VDF source terms
./VDF/Sources/Evaluateurs	Source term evaluators in VDF
./VDF/Sources/Iterateurs	Source term iterators in VDF
./VDF/Turbulence	Turbulence models VDF implementation
./VDF/Zones	VDF geometry description

TRUST source directories

./VEF	VEF discretization
./VEF/Champs	VEF fields
./VEF/Cond_Lim	VEF boundary
./VEF/Operateurs	VEF operator
./VEF/Solveurs	VEF source terms
./VEF/Sources	Source evaluators in VEF
./VEF/Sources/Evaluateurs	Source iterarators in VEF
./VEF/Sources/Iterateurs	Turbulence model implemented in VEF
./VEF/Turbulence	VEF geometry description
./VEF/Zones	
./P1NCP1B	VEF discretization
./P1NCP1B/Champs	VEF fields
./P1NCP1B/Cond_Lim	VEF boundary conditions
./P1NCP1B/Operateurs	VEF operators
./P1NCP1B/Solveurs	VEF solvers
./P1NCP1B/Turbulence	VEF turbulence
./P1NCP1B/Zones	VEF geometry description

TRUST source directories

./EF	EF discretization
./EF/Champs	EF fields
./EF/Operateurs	EF operators
./EF/Sources	EF source terms
./EF/Zones	EF geometry description
./EF/fortran	EF fortran functions
./ThHyd	Thermalhydraulic models
./ThHyd/Chimie	Chemical species model
./ThHyd/Quasi_Compressible	Quasi compressible model
./ThHyd/Quasi_Compressible/Turbulence	Turbulence models
./ThHyd/Quasi_Compressible/VDF	VDF implementation
./ThHyd/Quasi_Compressible/VEF	VEF implementation
./ThHyd/Schemas_Temps	Time schemes
./ThHyd/Turbulence	Turbulence models
./ThHyd/Turbulence/Spectres	Turbulence utilities
./ThSol	Conduction model

Basic Oriented Object Conception (OOC) concepts used in TRUST

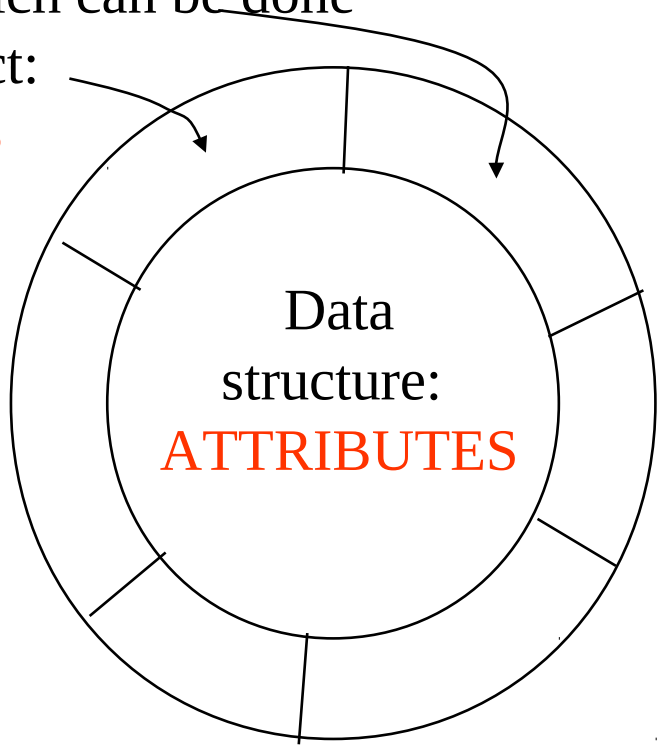
What are C++ class/object?

-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

Actions which can be done by the object: METHODS



Class
Method1() Method2()
Attribute1

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 :

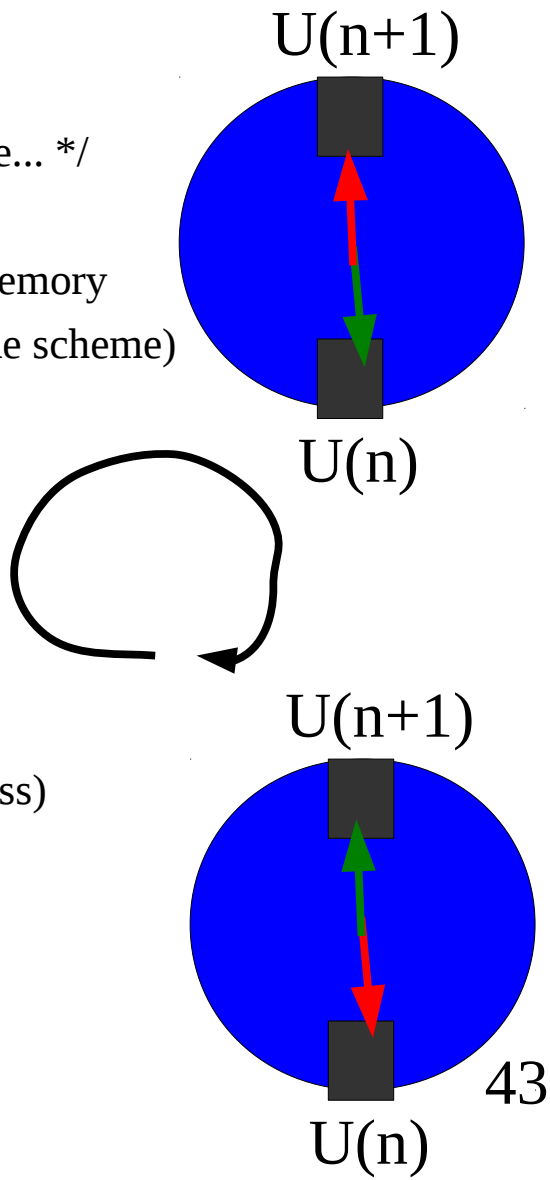
Roue_ptr les_valeurs // Pointer to a “wheel” mechanism to manage the different times for the unknown field

Code example:

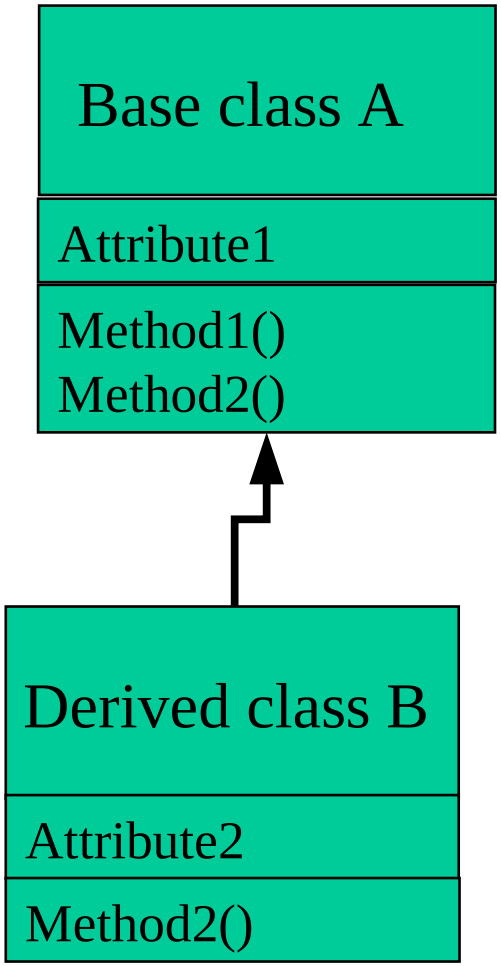
```
inconnue.fixer_nb_valeurs_temporelles(2);  // 2 memories to store the different times of the unknown inconnue
//  present (it is an alias or link) points to U(n) (first memory)
DoubleTab& present = inconnue.valeurs();
/* DoubleTab present = inconnue.valeurs();  ←  Warning! It is a copy here... */

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.

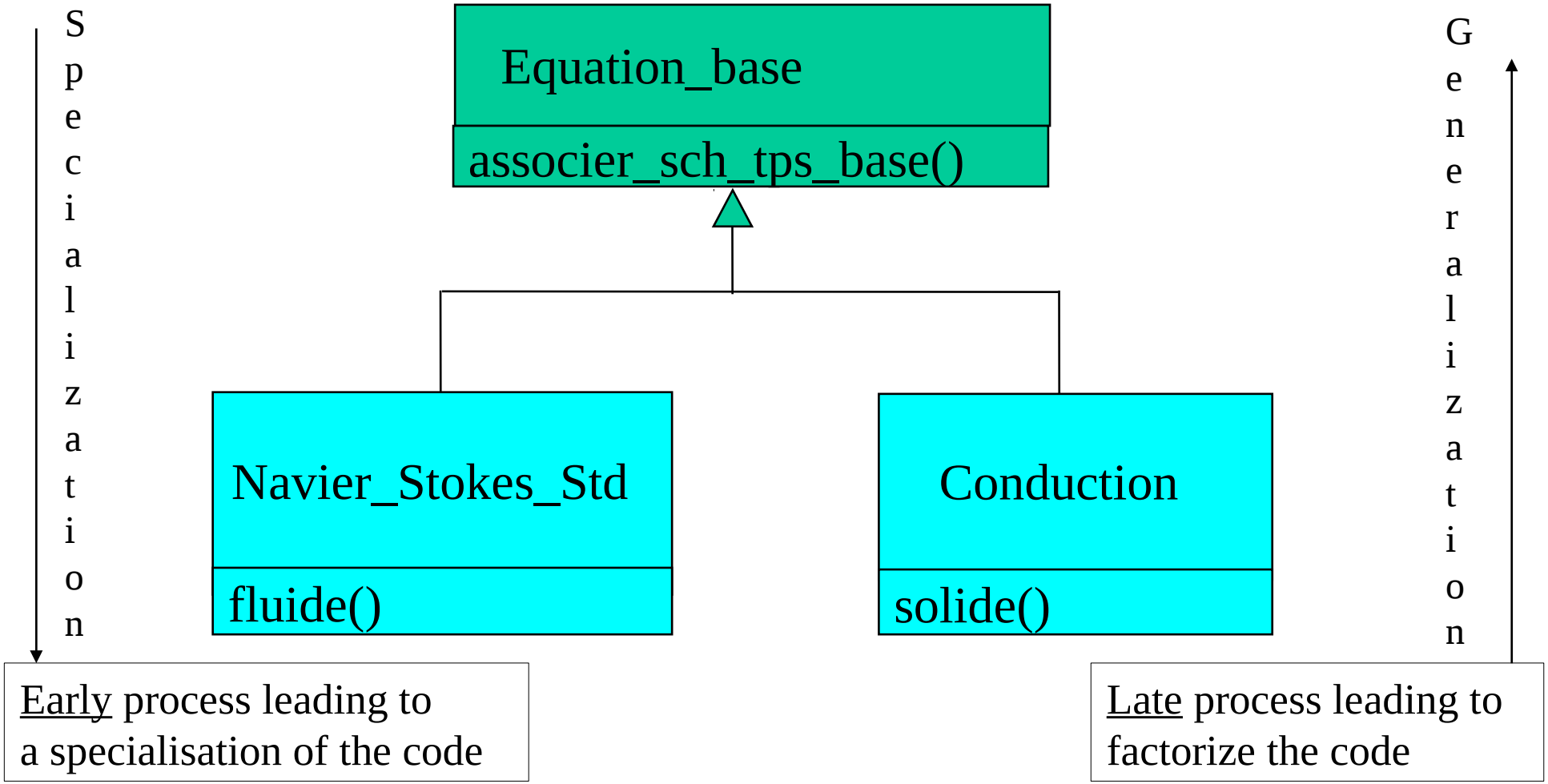
Derived class B inherits from base class A:

->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



Exercise: Use HTML doc

Browse the TRUST ressources index file :

$ konqueror|firefox $TRUST_ROOT/index.html

Or :

$ trust -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 ?

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()

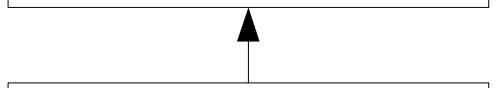
-A virtual method:
- can be overloaded
- enable dynamic polymorphism

→ 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):

$$1)\ BU=0$$

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

Or by inverting 2) by M gives II):

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

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

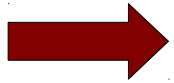
$$I)\ BM^{-1}B^TP = BM^{-1}(LU-CU+S)$$

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

Virtual method example

```
DoubleTab& Equation_base::derivee_en_temps_inco(DoubleTab&  F)
{
    // ∂U/∂t = F(U) =M-1( ΣOpi(U)+ΣSi)
    F = 0;
    for(int i=0; i<nombre_d_operateurs(); i++)
          operateur(i).ajouter(F);              // ΣOpi(U)
    les_sources.ajouter(F);                     // ΣOpi(U)+ΣSi
    return solveur_masse.appliquer(F);          // M-1(ΣOpi(U)+ΣSi)
}
```

Note: This method is overloaded in the Navier_Stokes equation class



Virtual method example

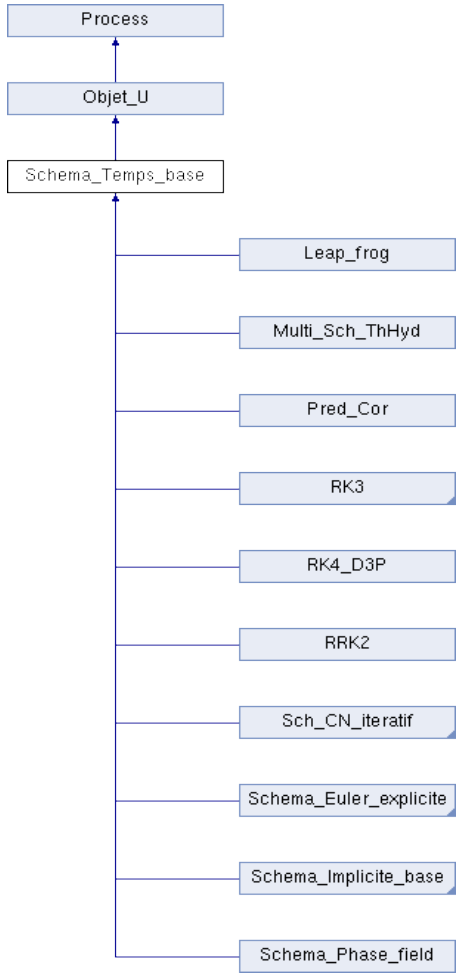
```
DoubleTab& Navier_Stokes_std::derivee_en_temps_inco (DoubleTab&  F)
{     // MdU/dt + grad P = MF(U) = ΣOp_i(U)+ΣS_j
      // div U = 0  -> div M^-1grad P = div F(U)
      DoubleTab& pression = la_pression.valeurs();  // Storage for P
      DoubleTab& vitesse = la_vitesse.valeurs();  // U^n
      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^-1B^TP=div(F(U))
      gradient.calculer(pression, gradP);        // gradP
      solveur_masse.appliquer(gradP);         //  M^-1gradP
      F -= gradP;                             // F(U)-M^-1gradP
      return F;                     // dU/dt = F(U)–M^-1gradP
}
```

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
     Champ_Inc& inconnue = eqn.inconnue();            // Equation unknown
      DoubleTab& present = inconnue.valeurs();        // Contains U^n
      DoubleTab& futur = inconnue.futur();            // Location to store U^(n+1)
   futur = eqn.derivee_en_temps_inco();               // F(U^n)
     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

- $TRUST_ROOT/src/MAIN/mon_main.cpp
- Edit the src/mon_main.cpp in your baltik project 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 /export/home/yourlogin/my_project

  ./configure

  make optim

- Run the code sequentially

  cd $TRUST_TMP

  touch hello.data

  trust hello

- Run the code in parallel and see the differences

  trust 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:
  - trust -clean
  - trust hello 4 -journal=0

Baltik exercise

 # Create a first class and have a look at the 2 files my_first_class.h|cpp
$ cd /export/home/yourlogin/my_project/src
$ baltik_gen_class my_first_class
$ git status .

 # Build your project:
$ cd ..
$ ./configure # Necessary each time a source file is added to the project
$ make optim debug

 # Look for more infos here:
vi README.BALTIK

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 inTRUST?

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 kind 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 (.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)

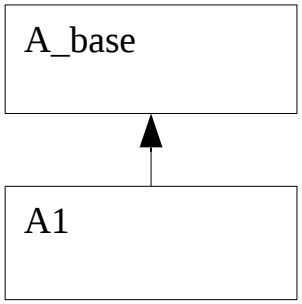
```
Implemente_base(A_base, «A_base», Objet_U);

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 »); // TRUST 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
_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)

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 ?

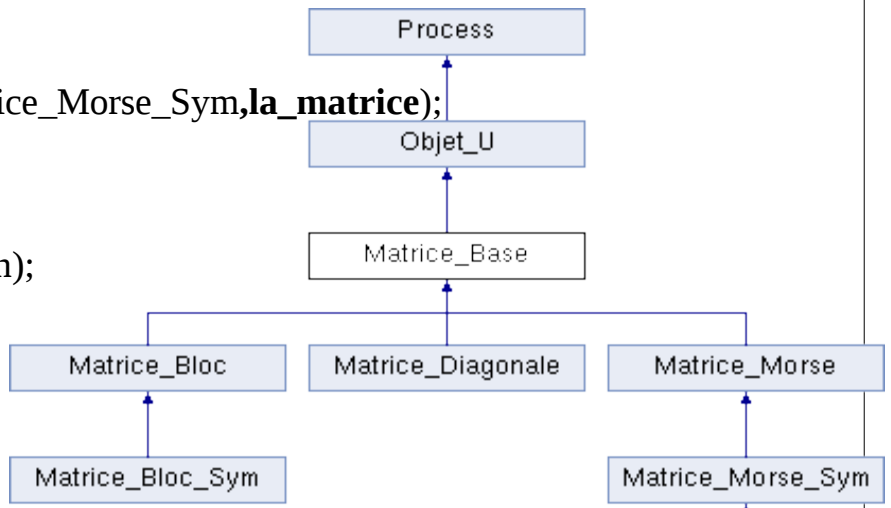
ref_cast(classA,B) : cast the object B in a classA type object or produces an error if object B is not from a derived class of classA.

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;
         ...
```



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 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 **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

...

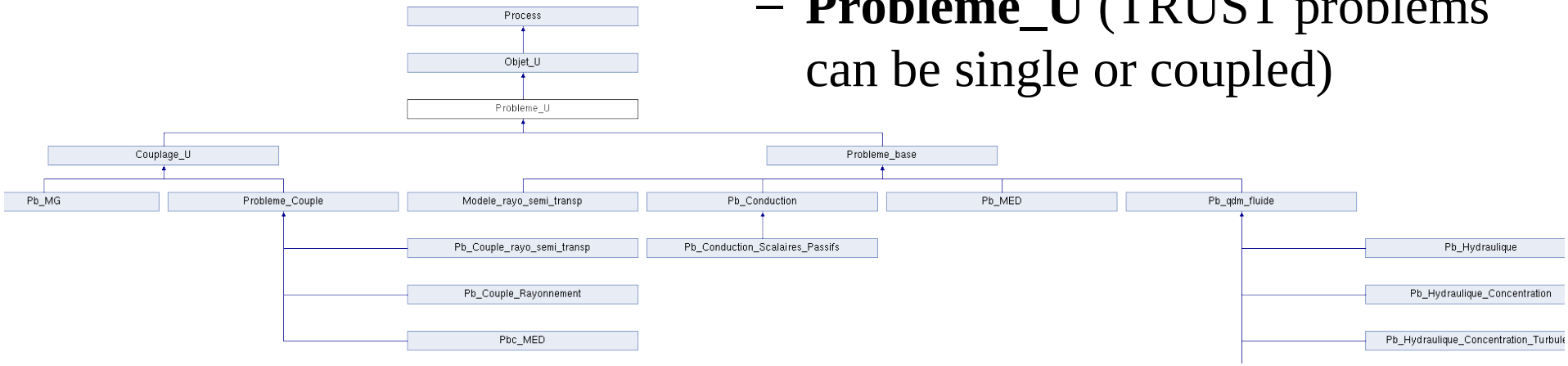
Read pb { … }

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** (TRUST problems can be single or coupled)



Resoudre call graph

Dimension 3

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();
}
```

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

class Probleme_U

virtual initialize() {}

class Probleme_base

virtual initialize() { … }

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)

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()

→ Loop on equation(i).mettre_a_jour() *// Update each unknown & BC*

→ milieu().mettre_a_jour() *// Update the media*

→ Schema_Temps_base::mettre_a_jour() *// t(n+1)=t(n)+dt(n)*

→ computeTimeStep() // **Prepare next**

→ schema_temps().computeTimeStep() *// 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()

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

# Edit the 2 files:
$ cd /export/home/yourlogin/my_project
$ nedit|xemacs|gedit src/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:
$ make debug # An error will occur

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 $TRUST_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,...)

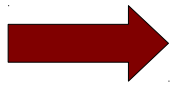
Define the public method **interpreter_(Entree&)** in the include file and implement it (just print a message with Cerr like “My first keyword!”) into the cpp file. **Entree** is a TRUST class to read an input stream (from a file for example):

```
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 /export/home/yourlogin/my_project

$ make debug



Baltik exercise

# Modify 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):
$ cd /export/home/yourlogin/my_project/tests/Reference/NonRegression

# 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
$ cd myCx
$ nedit|gedit|xemacs Cx.data

Baltik exercise

# And run your binary to check that this new keyword is recognized:
$ cd /export/home/yourlogin/my_project/build/tests
$ trust -copy myCx
$ cd myCx
$exec=$exec_debug trust 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 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_;
}
```

```
C c;
{
   A a;
   a.c_=&c;
}
```

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

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

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
```

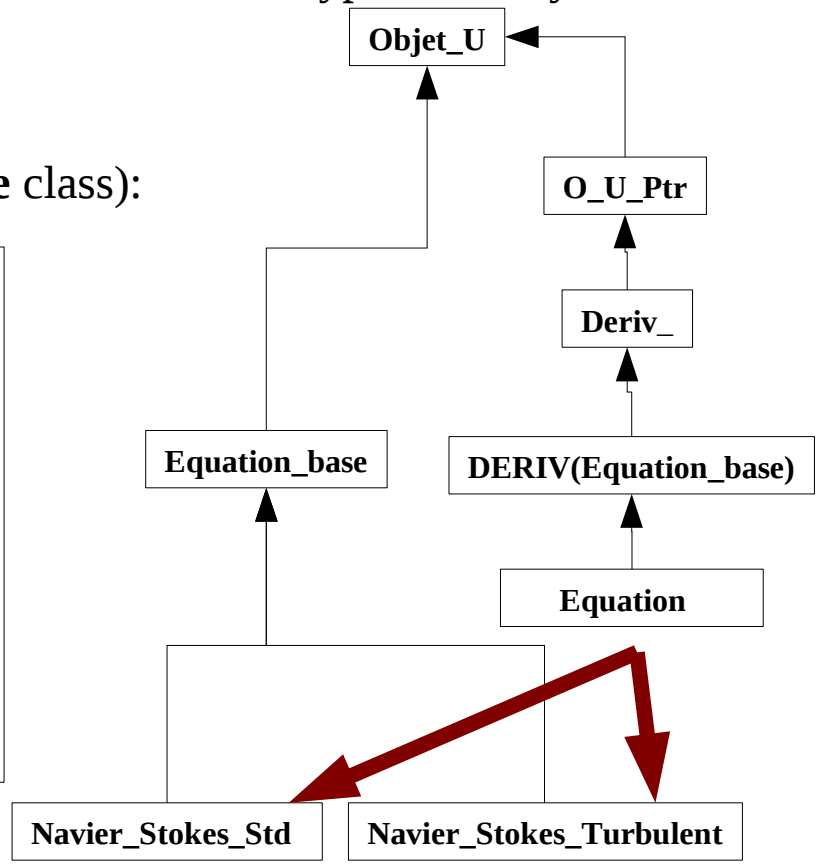
```
#include <Ref_A.h>
#include <A.h>
Implemente_ref(A);
```

Generic class (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 (.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();
}
```

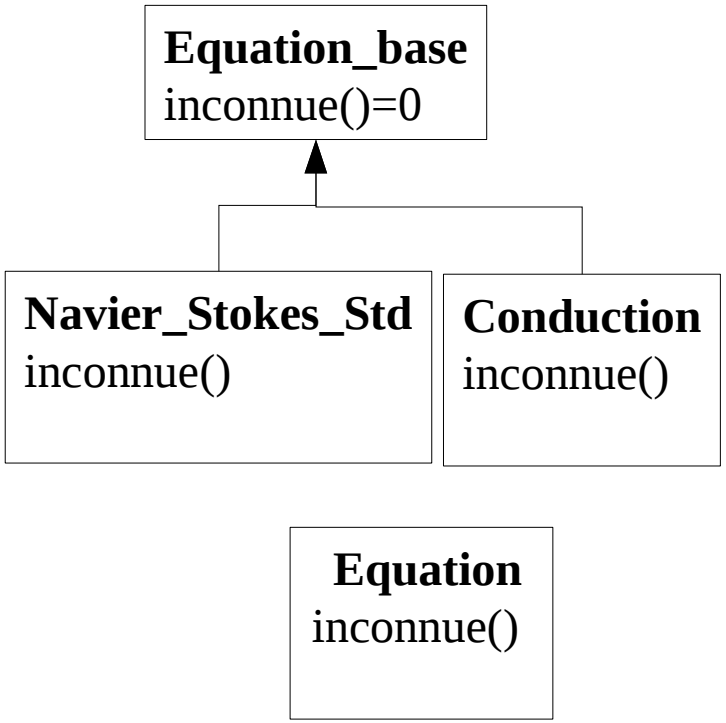
Implementation (.cpp file)

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

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

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

Generic class



- 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 »

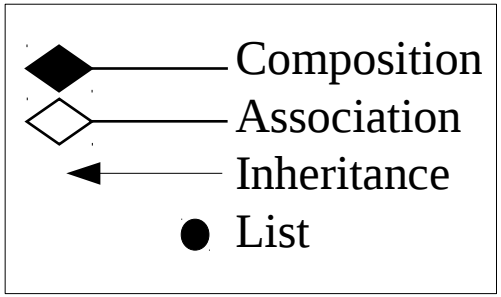
Equation eqn; // Generic class
eqn.typer(Conduction) ;
Cerr << eqn.que_suis_je() << finl ;// Prints « Equation »
Cerr << eqn.valeur().que_suis_je() << finl; // Prints « Conduction »

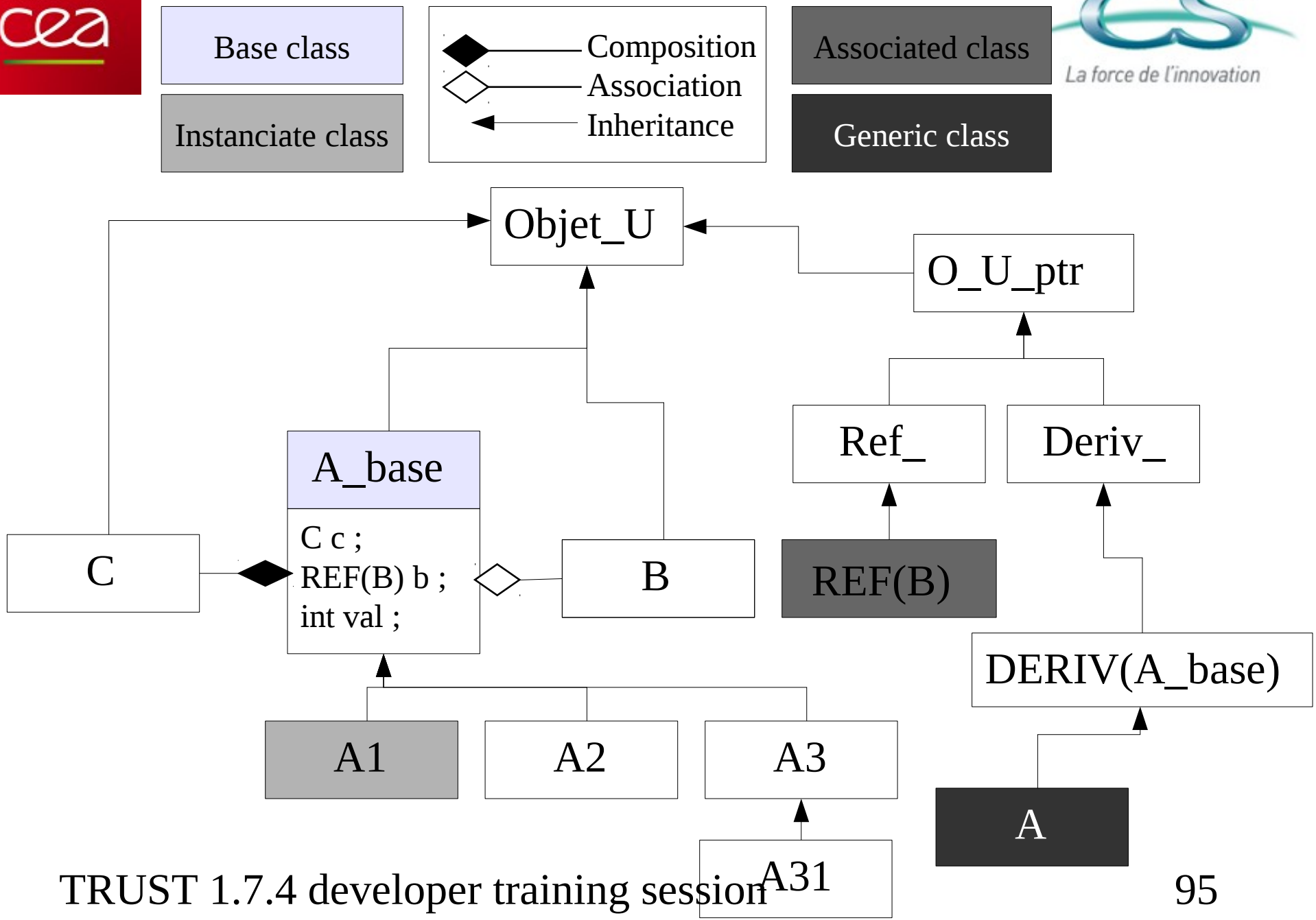
- Often (but not always), hierarchy methods are also coded in generic classes to avoid the use of .valeur(). Example :

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

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
A_base
C c ;
REF(B) b ;
int val ;
C
B
Ref_
Deriv_
REF(B)
DERIV(A_base)
A1
A2
A3
A31
A

Exploring the Kernel modules

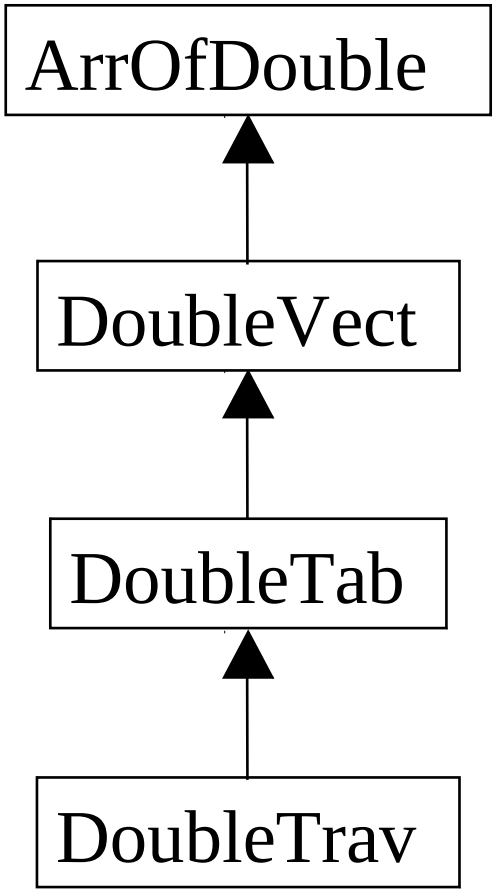
Math (Kernel)
Part I: Arrays

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 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 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
```

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
```

How to debug TRUST

gdb

valgrind

Use gdb tool to debug or understand the code

To describe all the commands:
$ man gdb
To debug the TRUST binary program compiled with -g:
$ exec=$exec_debug trust -gdb datafile

```
# 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]

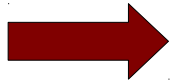
To debug a parallel calculation with N processes:

make_PAR.data datafile N

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

Exercise with gdb

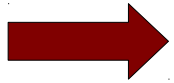
```
# Build a debug version of TRUST if necessary:
$ cd /export/home/yourlogin/my_project
$ make debug
# Access to all tests cases: your baltik + TRUST
$ source full_env_basic.sh
# Copy example case
$ cd /export/home/yourlogin/my_project/tests/Reference/NonRegression
$ trust -copy upwind
$ mv upwind myupwind
$ cd /export/home/yourlogin/my_project/
$ ./configure   # update baltik
$ cd /export/home/yourlogin/my_project/build/tests
$ trust -copy myupwind
```



Exercise with gdb

```
$ cd /export/home/yourlogin/my_project/build/tests/myupwind
$ exec=$exec_debug trust -gdb upwind

(gdb) break SSOR::ssor    # Stop into the SSOR preconditionner
(gdb) run upwind
(gdb) where  # Have a look at the stack
(gdb) n
(gdb) print tab1      # Or print matrice.tab1_ if “optimized out” message printed
(gdb) print tab1[10]          # Print only a value of an array
(gdb) dumpint tab1      # Dump the array
(gdb) print tab1.size_array()  # Array size
```



Exercise with gdb

(gdb) up
(gdb) list 100 # Print lines after the 100th 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:

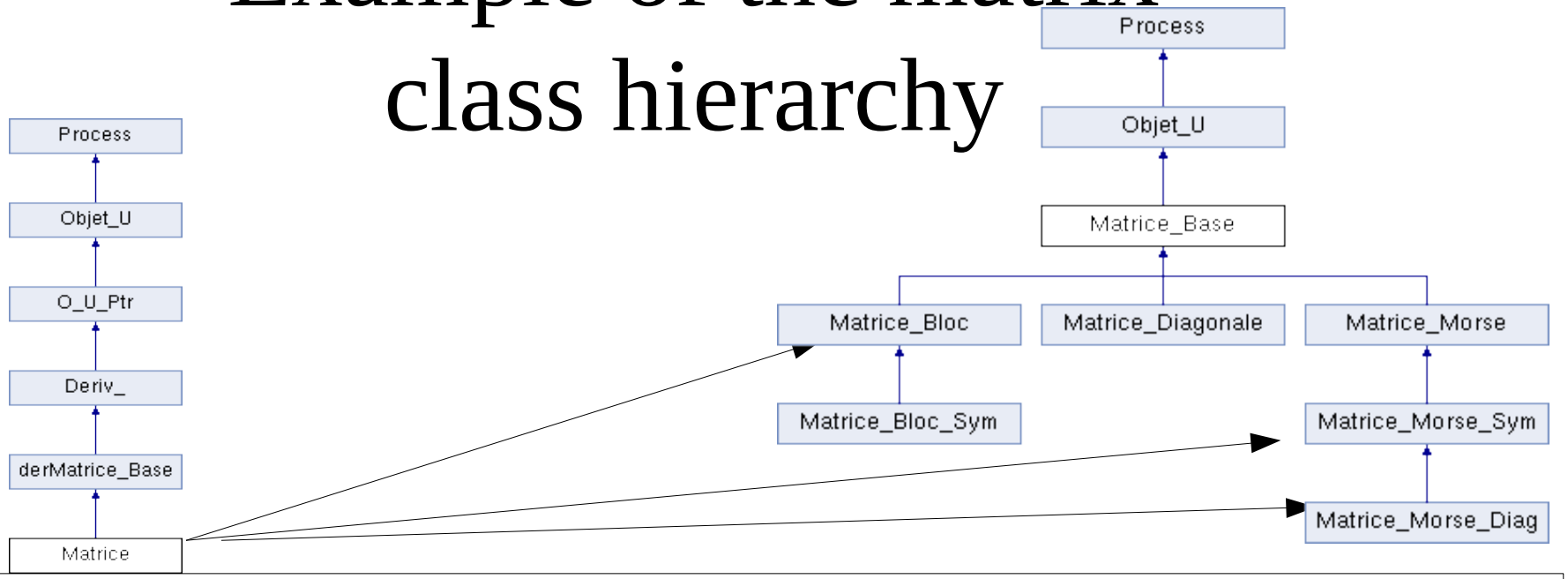
$ gdb -valgrind $exec_debug

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

-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,...)

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) ; … } ;

VECT and LIST macros

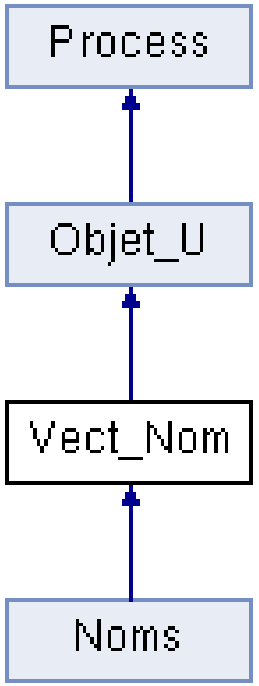
One can regroup a set of objects of the same kind
by using:

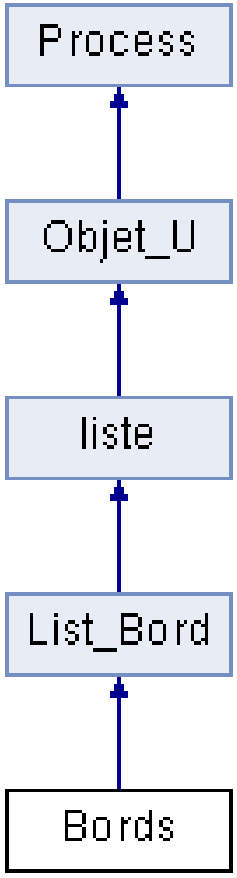
- either VECT, vector of objects
- or LIST, list of objects

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)
{ … }
```

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)
{
      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;
}
```

```
A a
Read a { dimension 3 option fast }
```

Baltik exercise

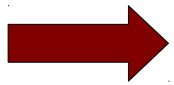
Add into the interpreter_(Entree&) method the read of a domain and some parameters into brackets. In the data file, the syntax will be:

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



Baltik exercise

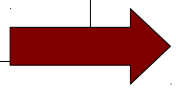
Then use the **Param** object to read the keyword parameter option in the data file. **Param** use is the recommended choice in this case (even if a lot of current TRUST classes still use the old fashion to read parameters), cause it simplifies greatly the coding.

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;



Baltik exercise

```
# Build/fix/re-build/run the test case:
$ cd /export/home/yourlogin/my_project
$ make debug
$ cd build/tests/myCx
$ export exec=$exec_debug
$ trust Cx    # in this case trust runs with exec_debug
```

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

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

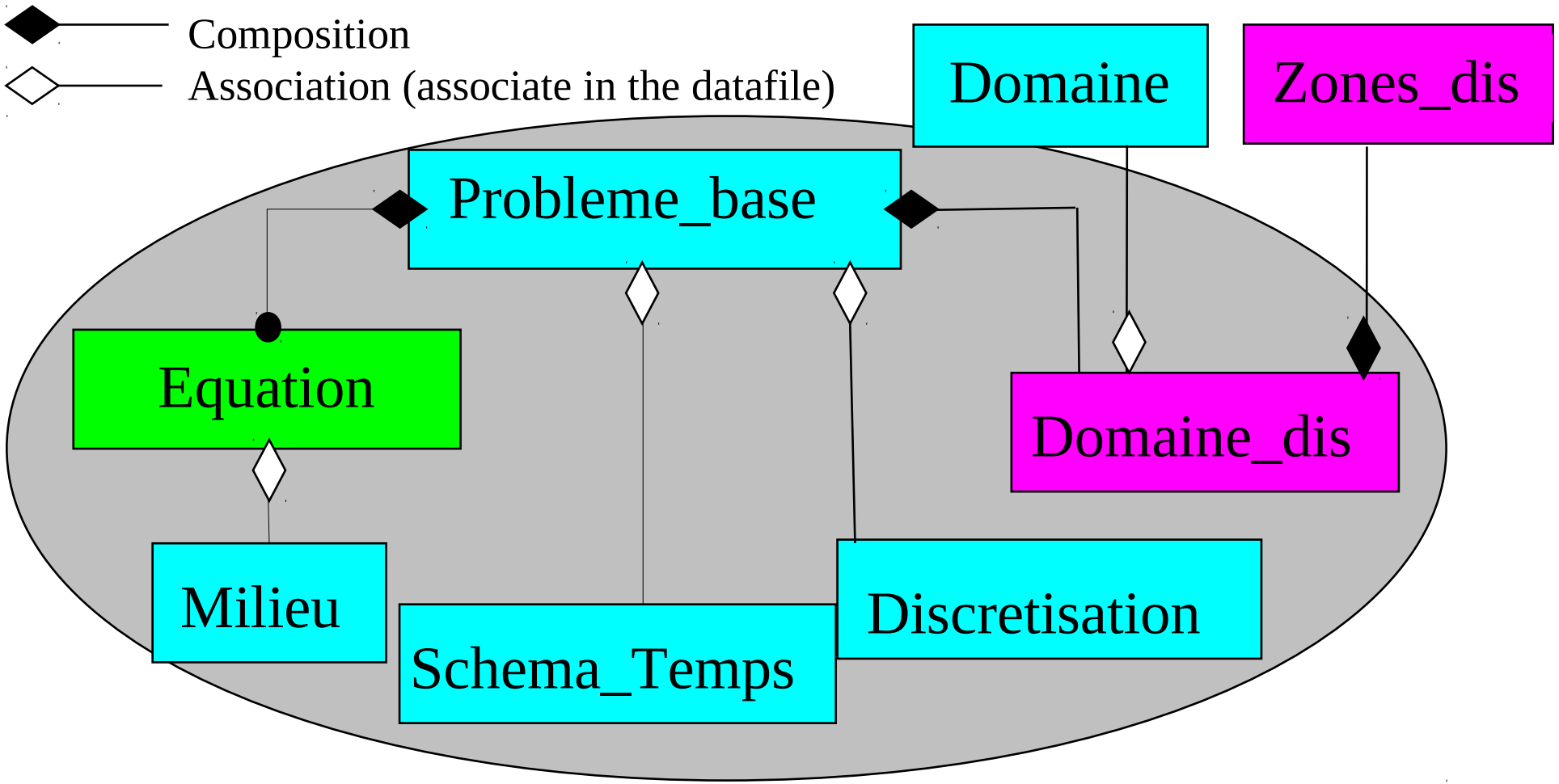
Discretize problem discretization

Read problem { … }

Solve problem

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

Problem (Kernel framework)



Objects creation

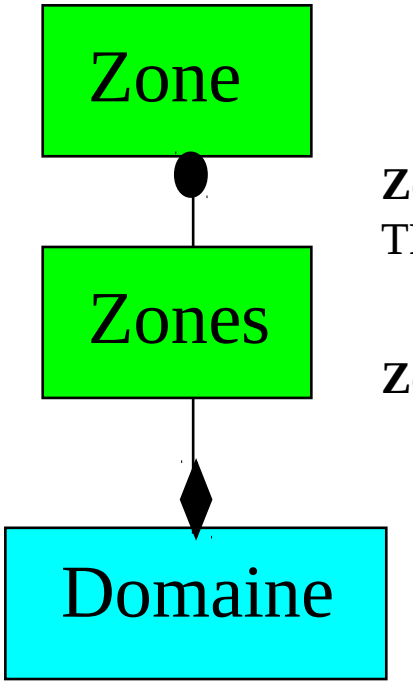
-Associated objects should be created before being associated

- 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

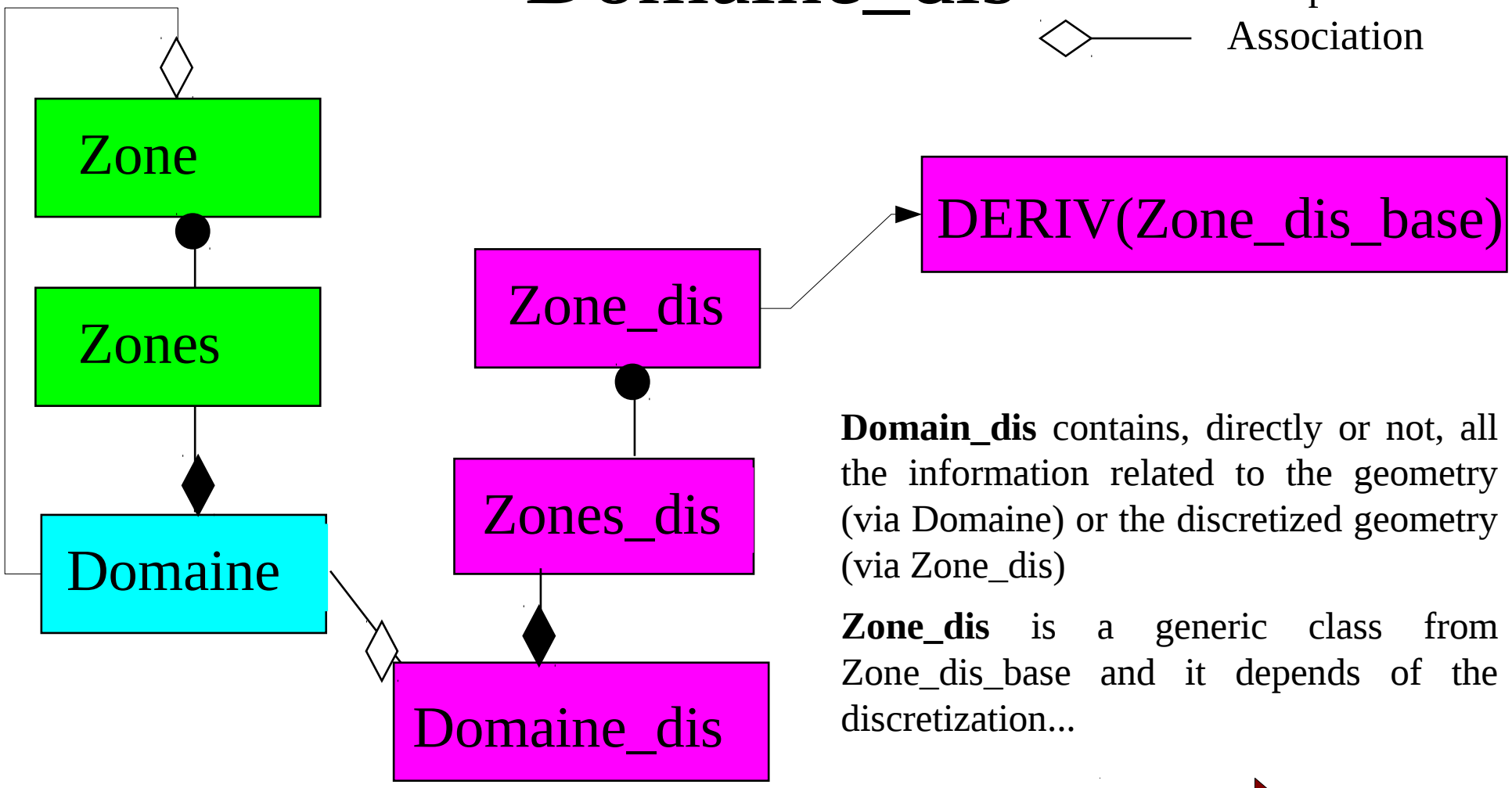
- Contains the **Zones** and the vertexes (**DoubleTab** sommets) used by the **Zones**

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** »)

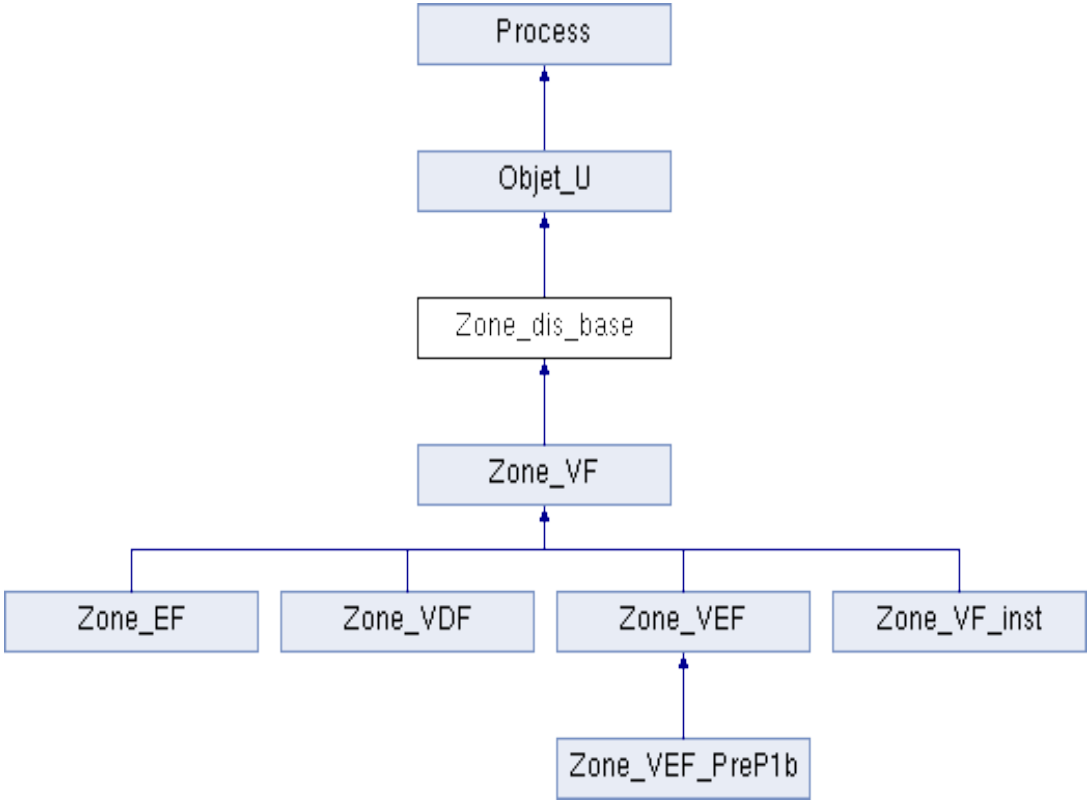
Domaine_dis



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)

Baltik exercise

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.

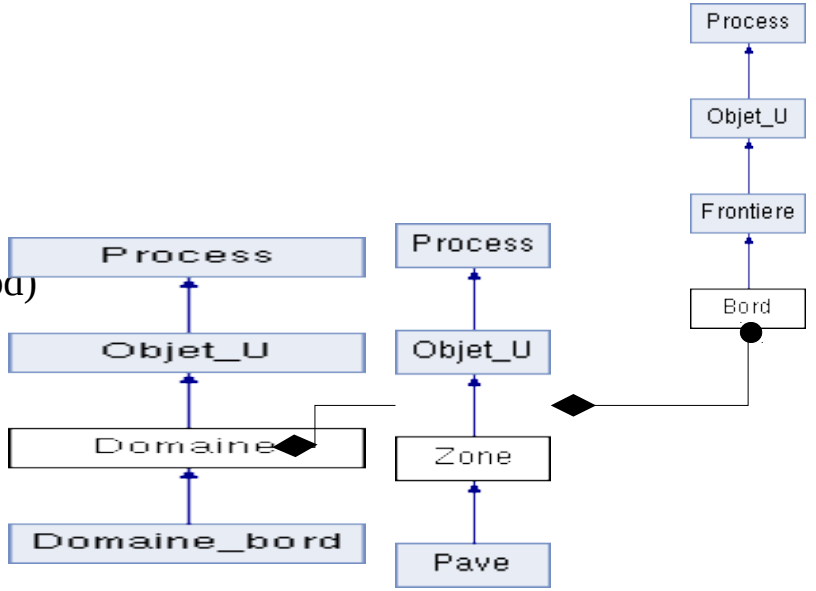
Look for help inside the Domaine, Zone, Bord, Frontiere classes into the HTML documentation to access to the:

-Number of boundaries (**nb_bords()** method)

-Boundaries (**bord(int)** method)

-Name of the boundaries (**le_nom()** method)

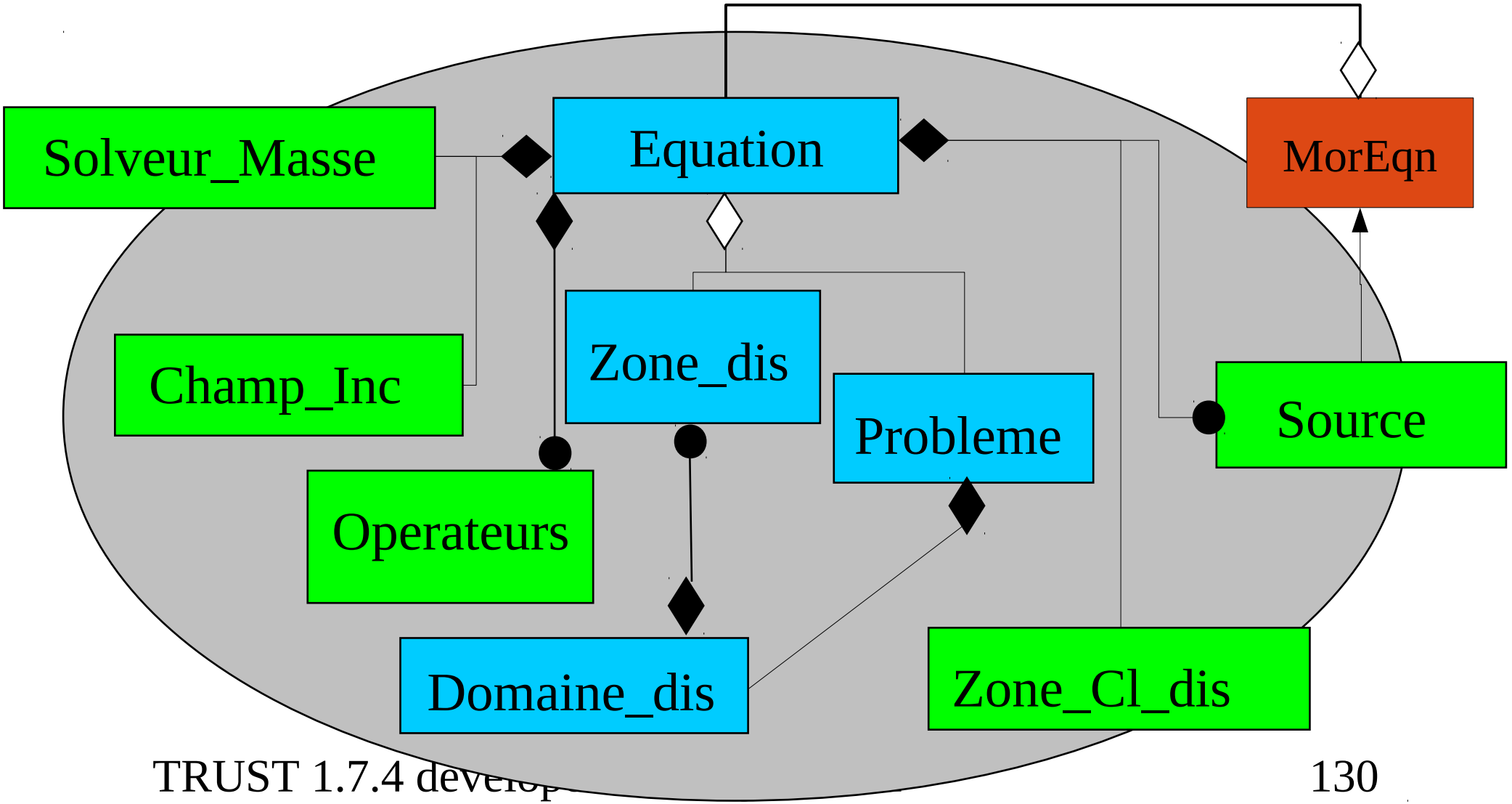
-Number of faces of each boundary (**nb_faces()** method)



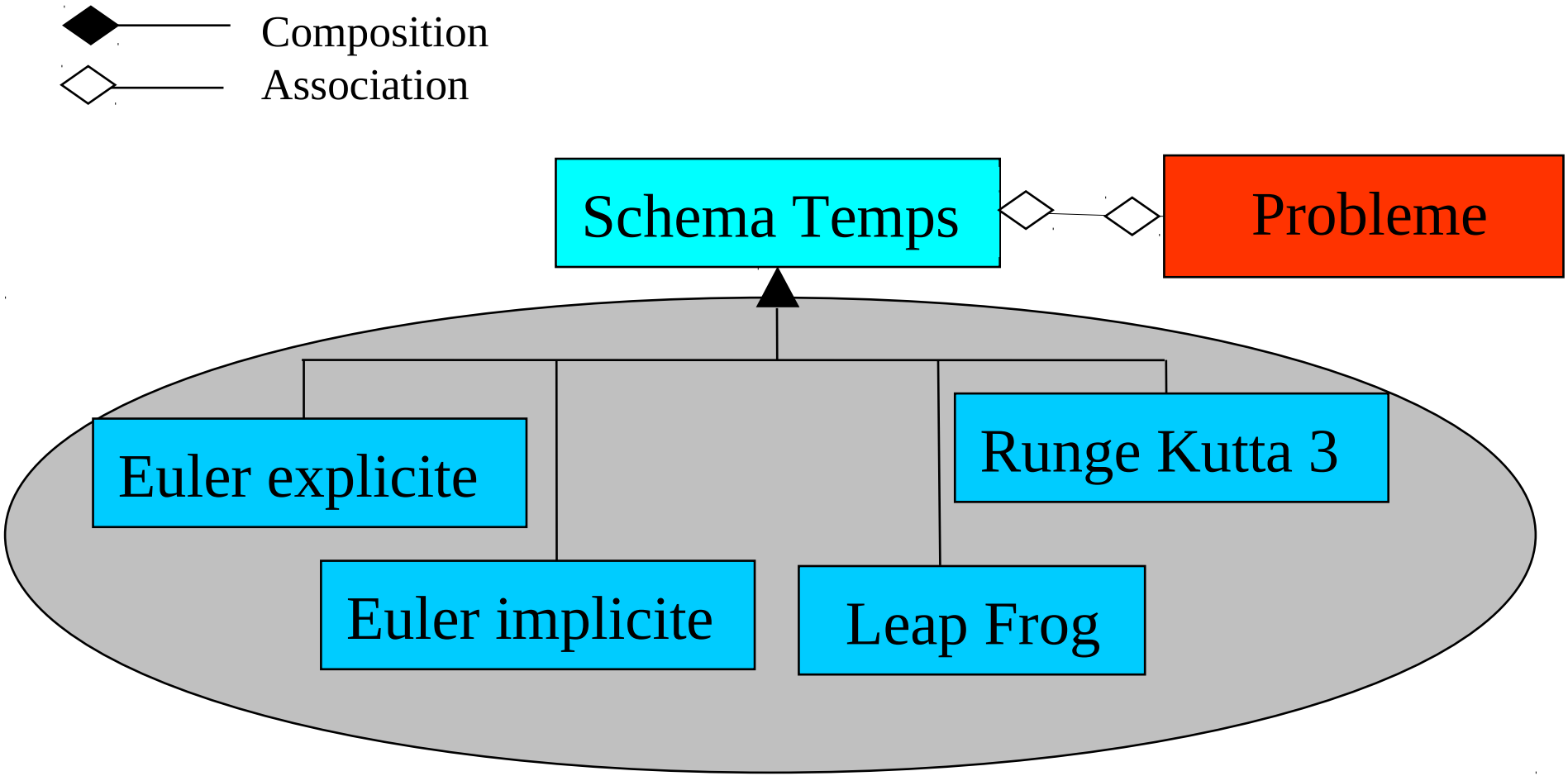
You will print the infos with something like:

Cerr << “The boundary named “ << ??? << “ has “ << ??? << “ faces.” << finl;

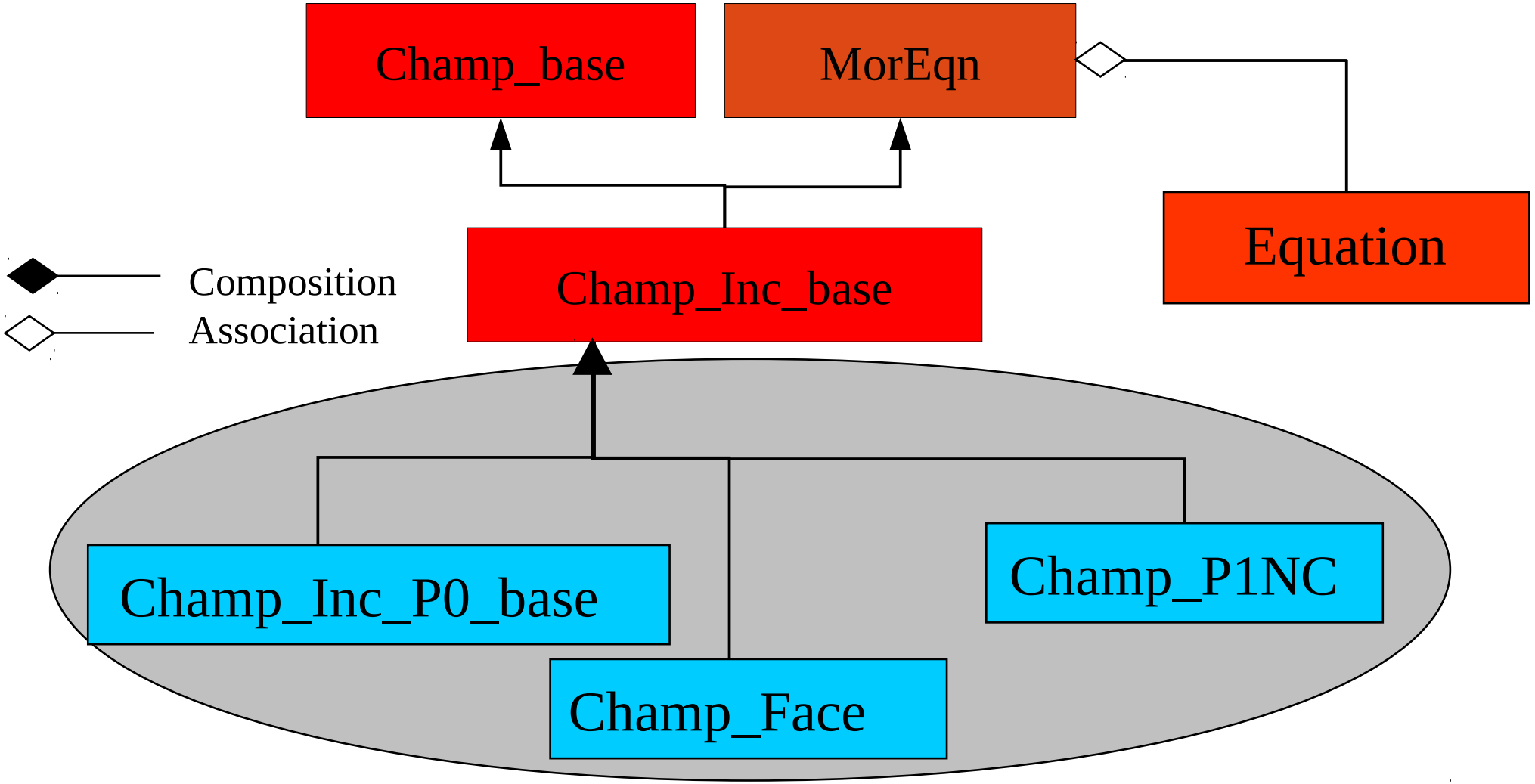
Equation (Kernel framework)



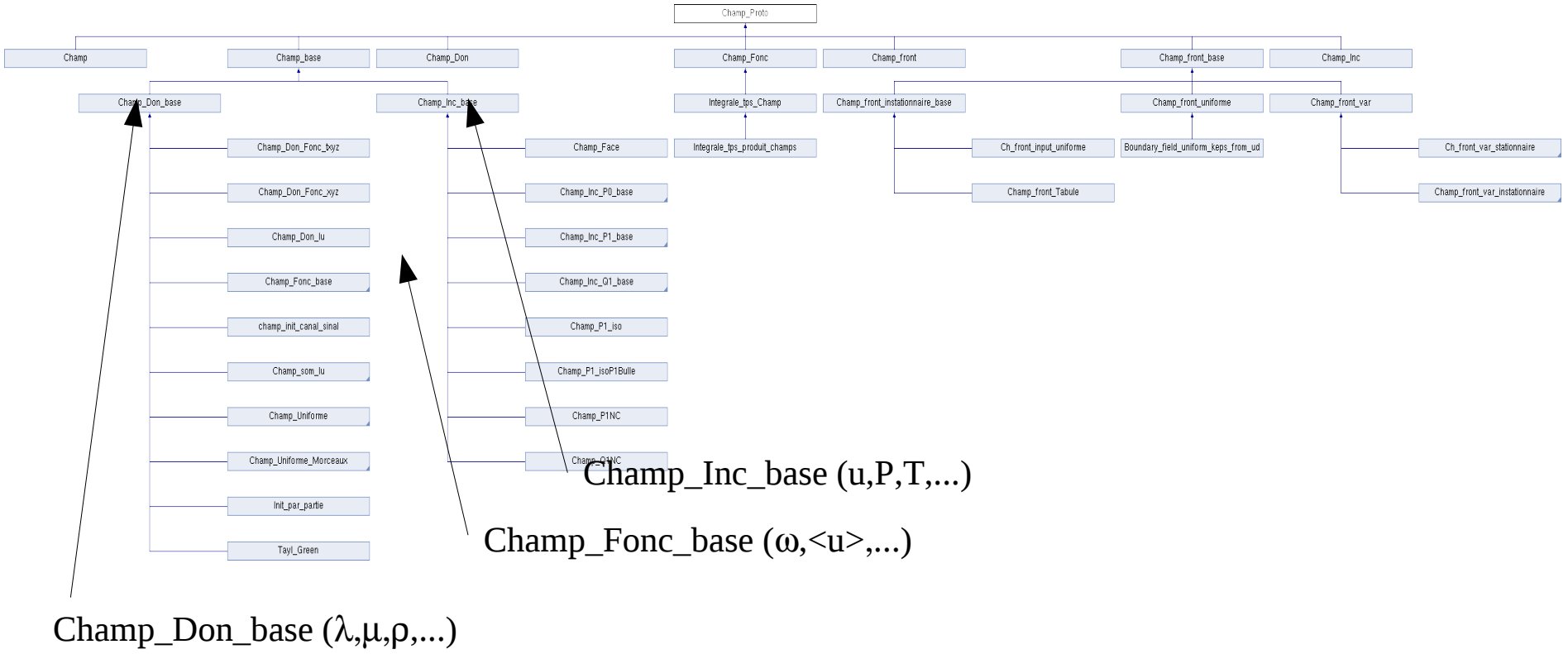
Time Schemes



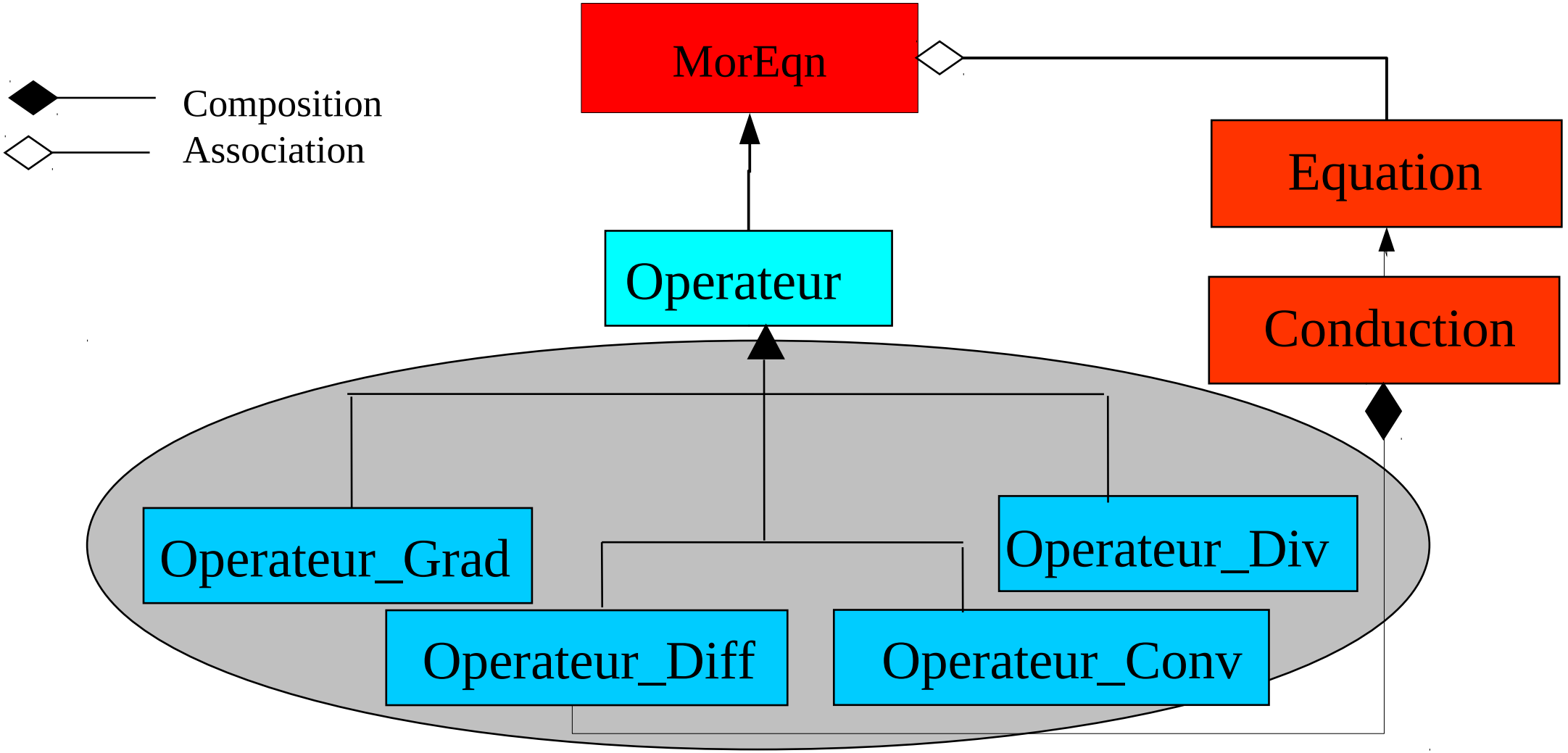
Fields


Champ_base
MorEqn
Equation
Champ_Inc_base
Composition
Association
Champ_Inc_P0_base
Champ_P1NC
Champ_Face

Field hierarchy



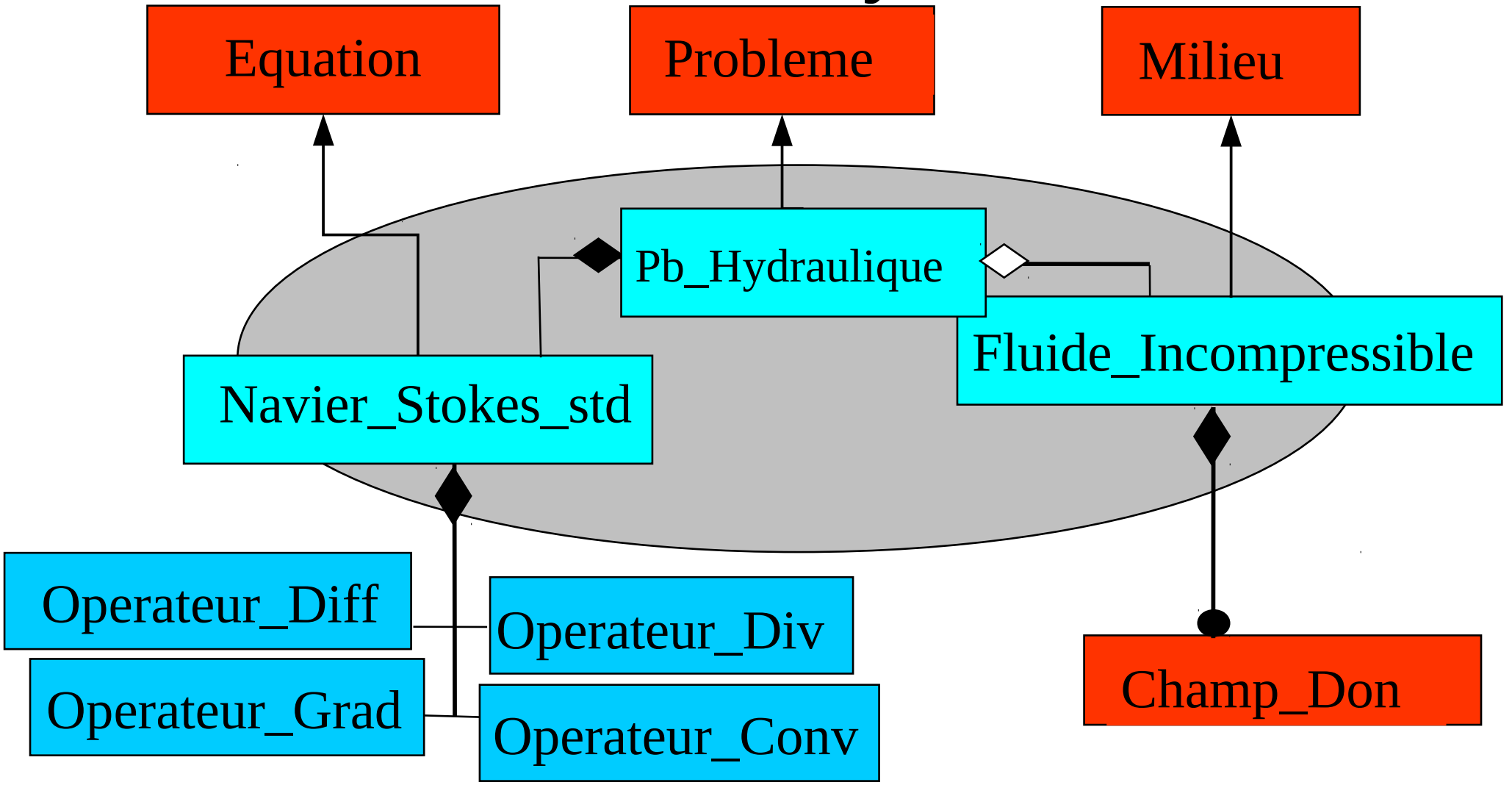
Operators


Composition
Association
MorEqn
Equation
Operateur
Conduction
Operateur_Grad
Operateur_Div
Operateur_Diff
Operateur_Conv

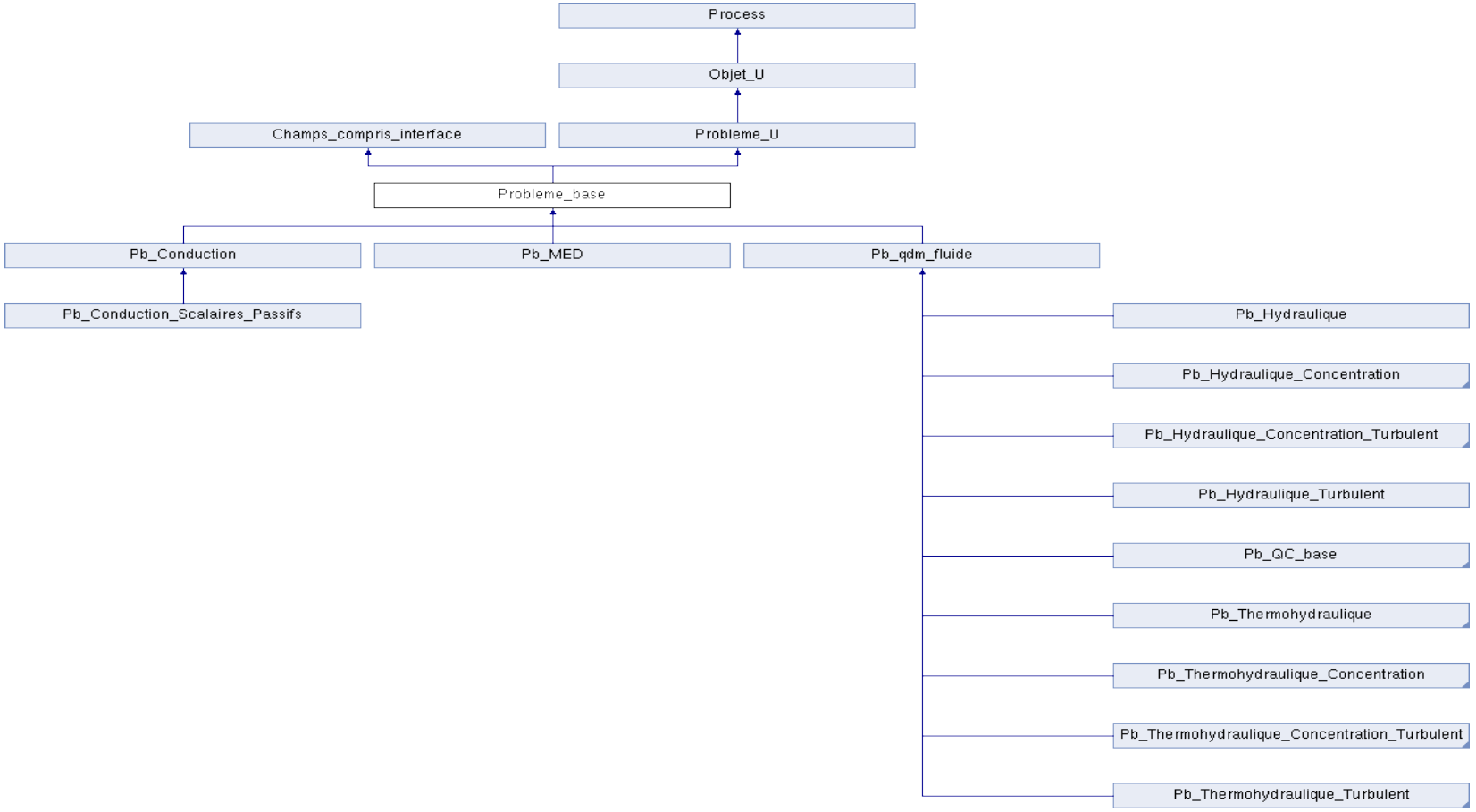
TRUST ThHyd module

Incompressible Thermalhydraulic

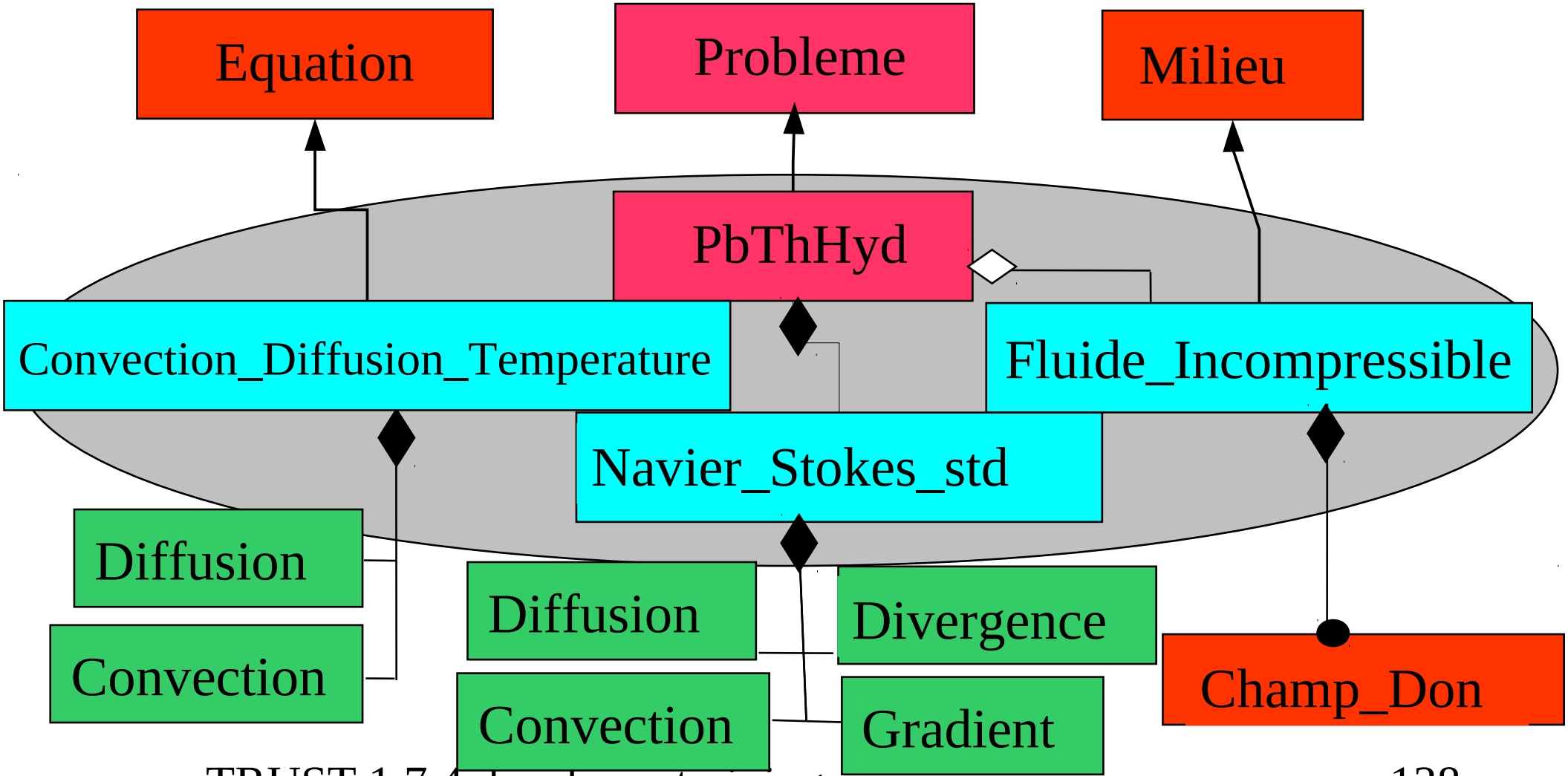
Thermalhydraulic



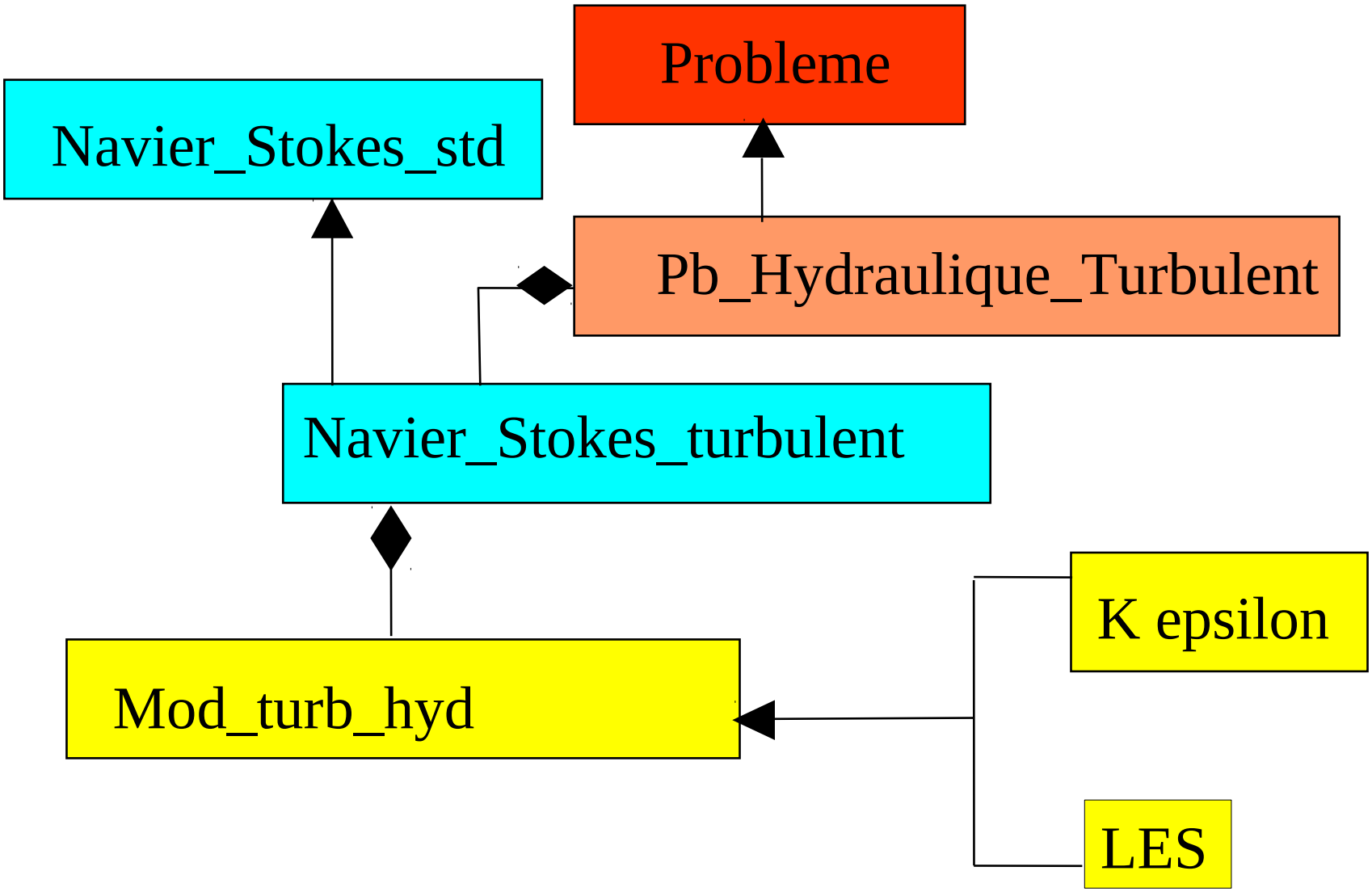
Problem hierarchy



Thermalhydraulic



Thermohydraulic



TRUST spatial discretization modules

VDF: Finite-volume differences method

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

VEF: Finite-volume elements method

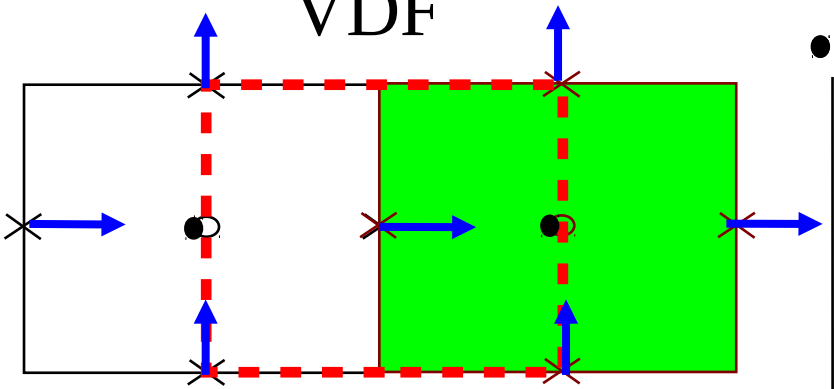
More details in FORTIN T. thesis: http://www.theses.fr/2006PA066526

Available discretizations

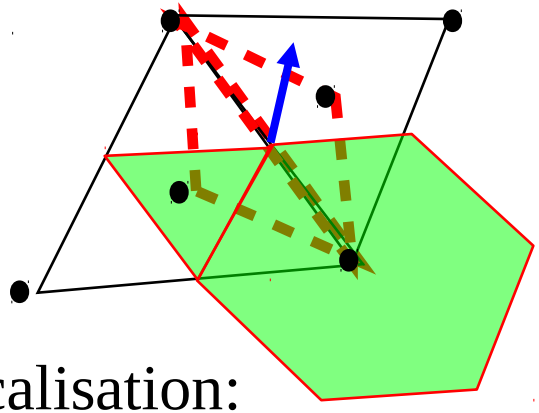
Velocity

Pressure

VDF



VEF



Field localisation:

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

Field localisation:

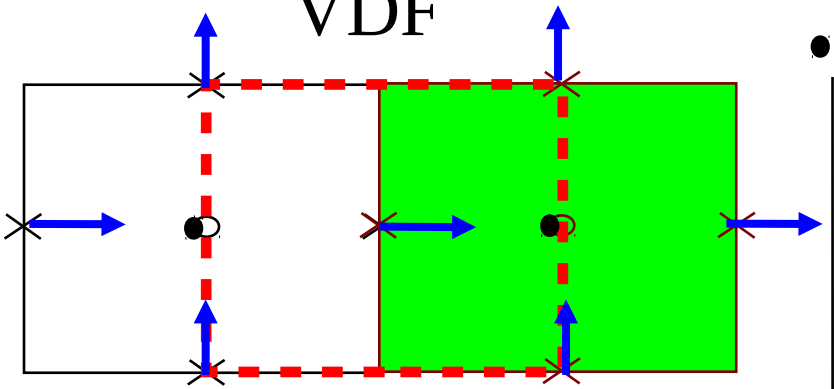
- Vector and scalar fields (P1NC) at the center of the faces control volume:
- Pressure (P0P1Bulle) at the nodes and the center of elements mass control volumes:

Available discretizations

Velocity

Pressure

VDF



Algorithms:

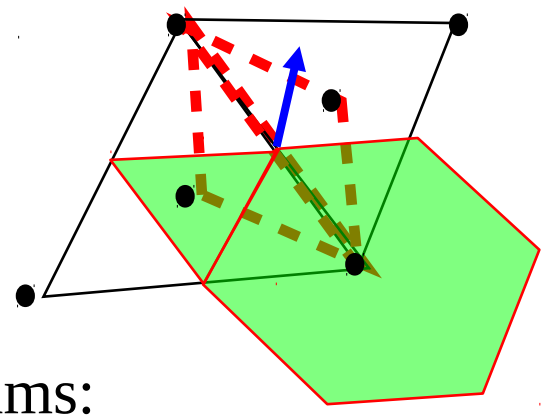
-Iterators to loop on elements or faces

-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

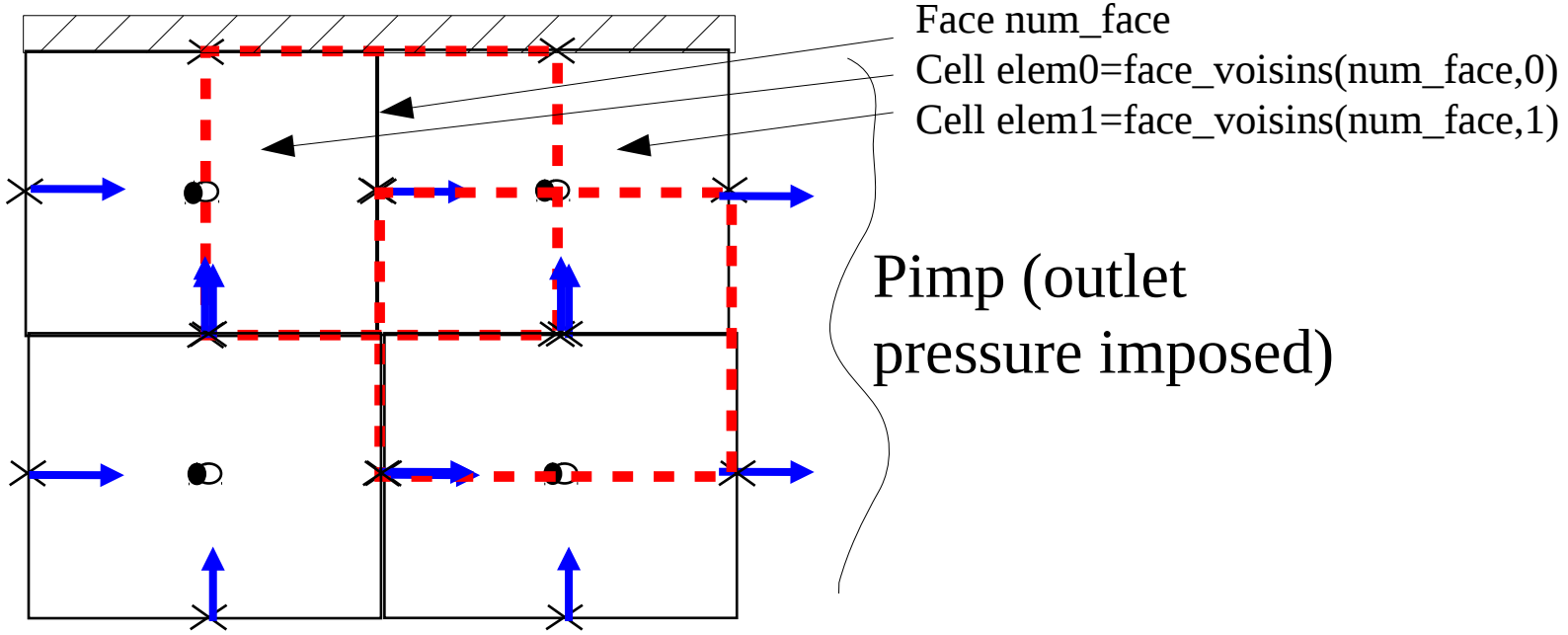
Momentum control volume

Mass control volume

Gradient operator example in VDF

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

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



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

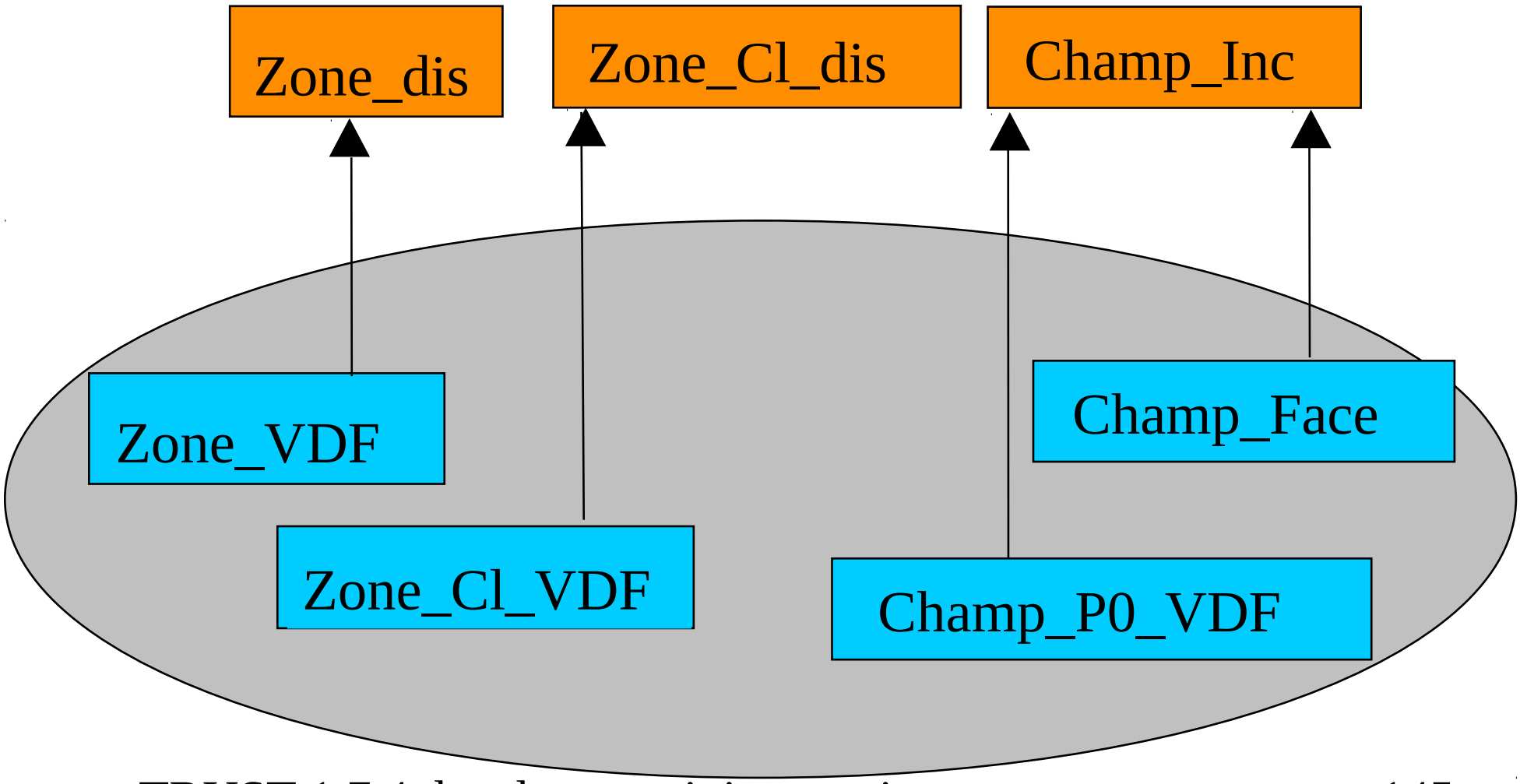
2) Loop on the internal faces :

premiere_face_int() returns the first internal face of the zone

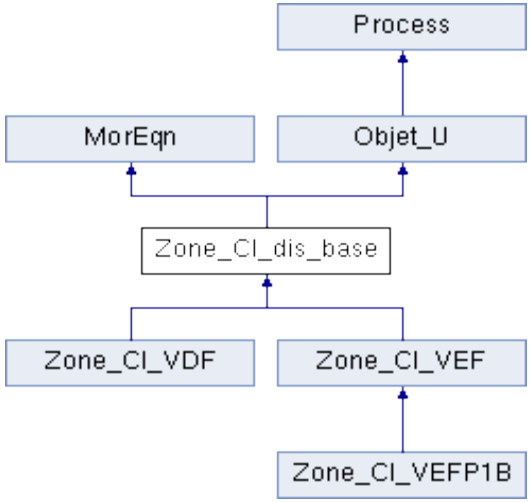
nb_faces() returns the number of faces of the zone

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

VDF Zones and Fields



Zone_Cl_dis_base

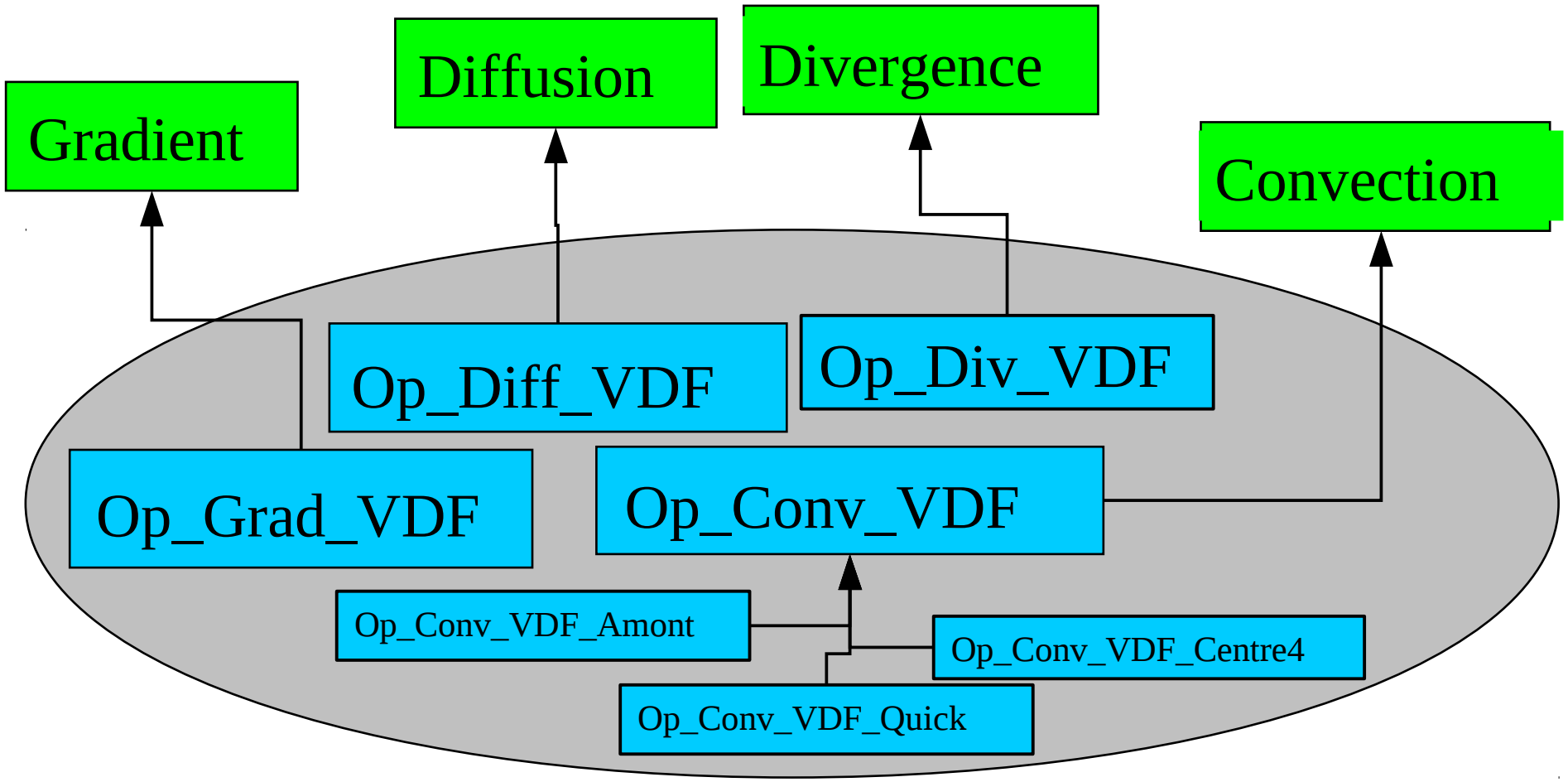


The Zone_Cl_dis_base classe describes discretized boundary conditions :

Protected :

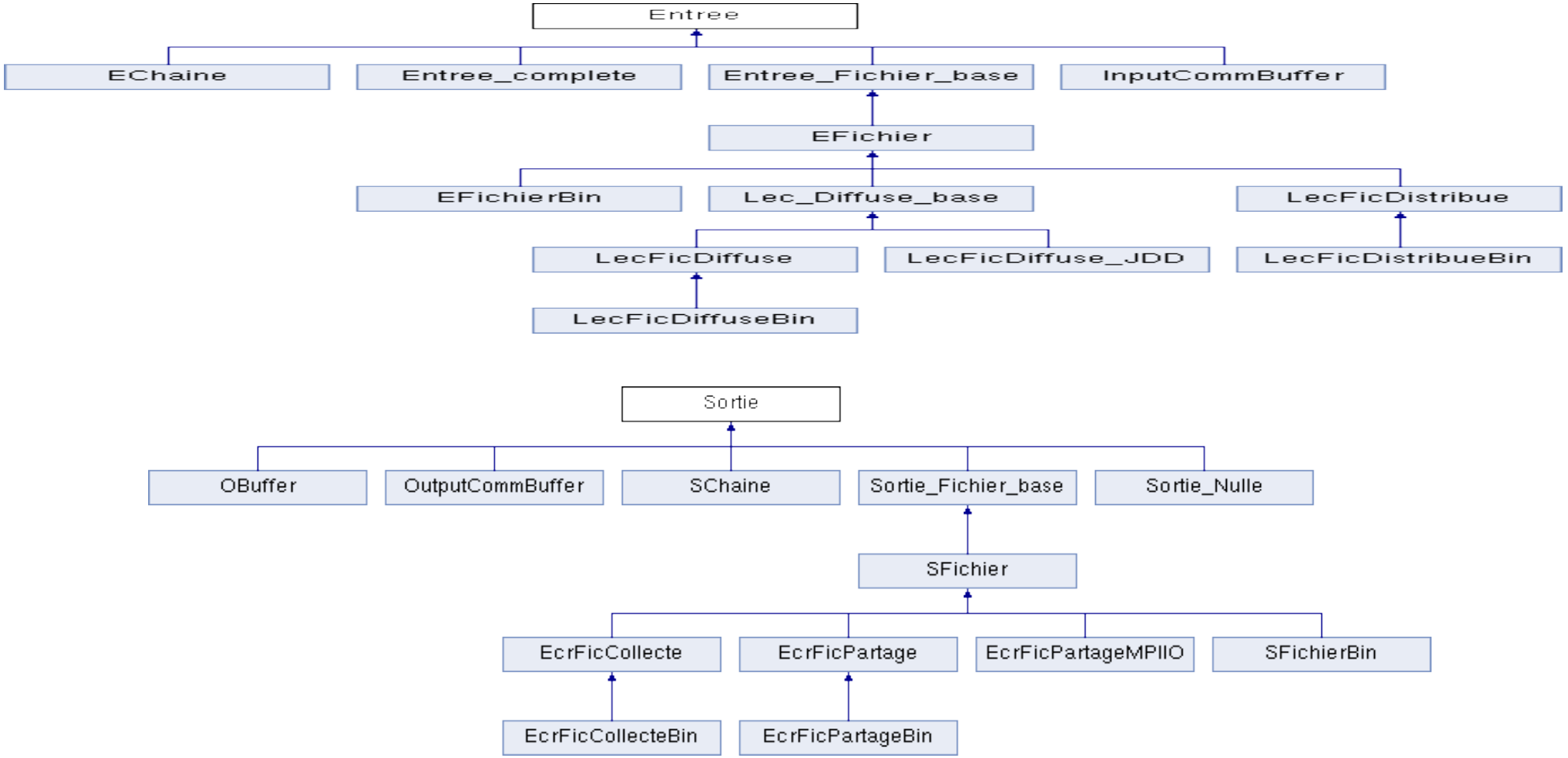
Conds_lim les_conditions_limites_ ;

Operators VDF implementation



Managing input/output files with TRUST classes

Dedicated classes to input/output



Dedicated classes to output

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

```
file << Process::me() ;
```

file_0000.txt : 0

file_0001.txt : 1

…

file_000N.txt : N

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

```
file << Process::me() ;
file.syncfile() ;
```

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 ;
}
```

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;

Baltik exercise

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.

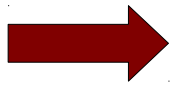
Then, remember the equation UML diagram page 123.

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)



Baltik exercise

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;

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 ?

Baltik exercise

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 /export/home/yourlogin/my_project/build/tests/myCx

$ exec=$exec_debug trust Cx

How to parallelize in TRUST

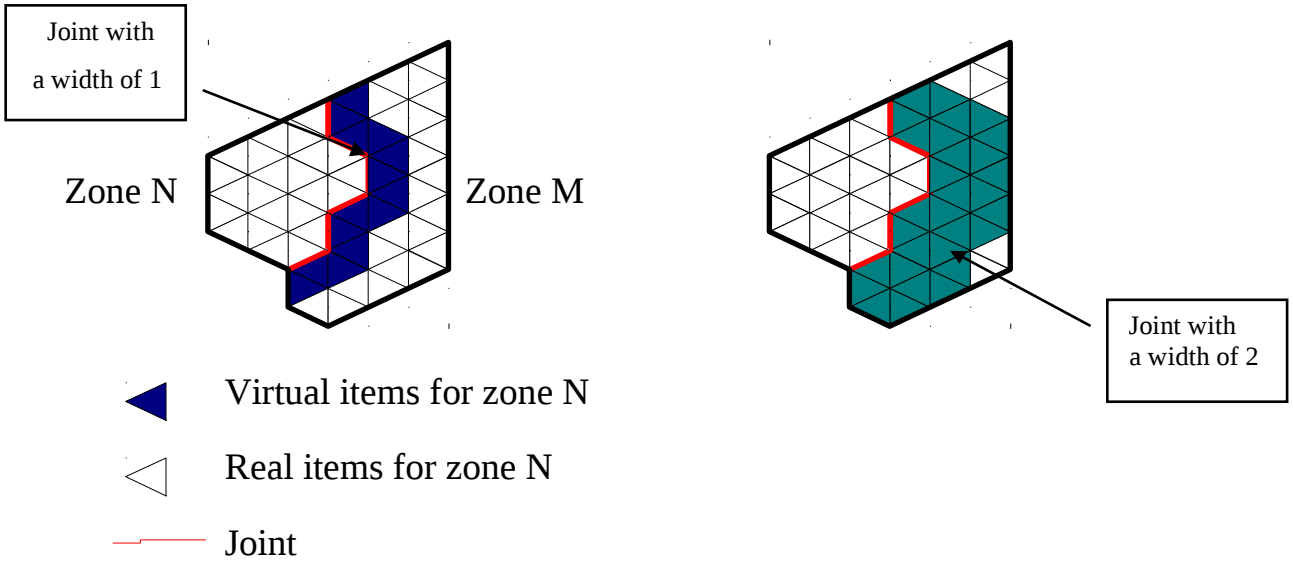
Parallelism

-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)

Parallelism

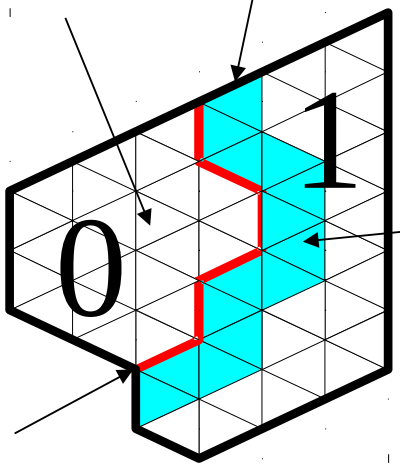


The virtual items of the local Zone are the remote items constituted of vertexes located up to n vertexes of the n-width joint.

Parallelism

Virtual boundary face for the process 0

Real cells for process 0



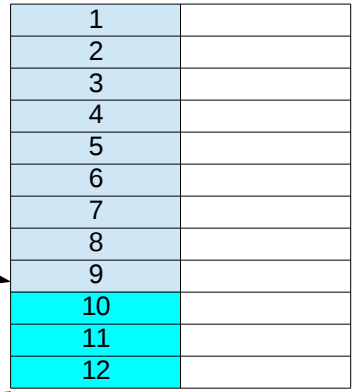
Virtual items in blue (faces, cells, vertexes) constitute the « virtual space » of the process 0.

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

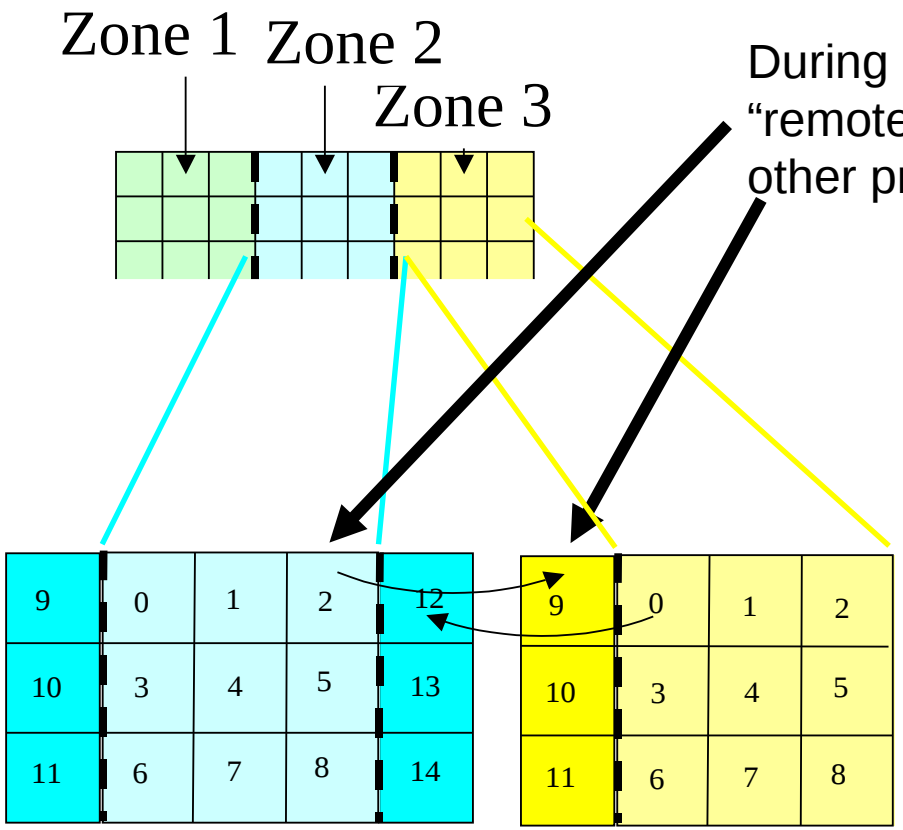
- Number of real items:
  - Zone_VF::nb_faces()
  - Domaine::nb_som()
  - Zone::nb_elem()
- Number of real+virtual items:
  - Zone_VF::nb_faces_tot()
  - Domaine::nb_som_tot()
  - Zone::nb_elem_tot()



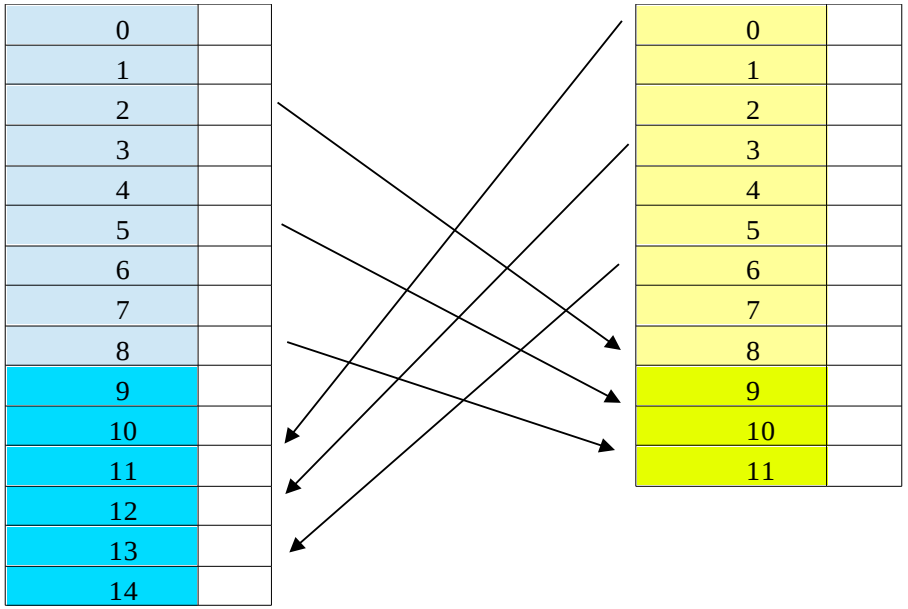
Example of distributed array with additionnal data stucture (**MD_Vector** in TRUST)

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();
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 : */
```

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();
```

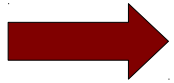
- Notes:
  - echange_espace_virtuel() does **nothing** on real arrays
  - It is possible to check if an update of the virtual space is useful or not with :

```
#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

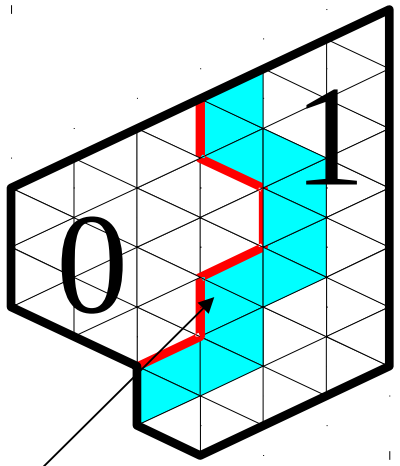
When do I need to create a distributed array ?

- 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 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

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()** 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

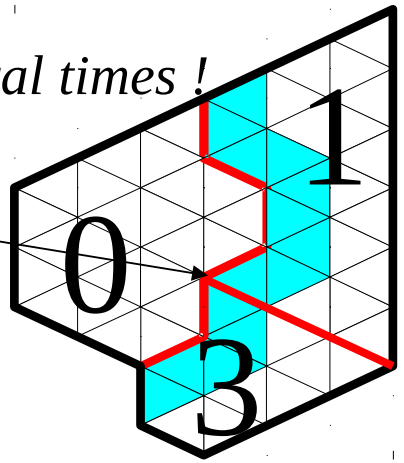
- Send/receive methods (envoyer/recevoir). Well described in the file :
  - $TRUST_ROOT/Kernel/Utilitaire/communications.cpp
  - Example of use in the Sous_Zone.cpp file. An array is sent by the master processor (0) and received by all the other ones.

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) ;**

Baltik exercise

 # Run your test case Cx in parallel mode:

$ cd /export/home/yourlogin/my_project/build/tests/myCx

$ make_PAR.data Cx 2 # Partition in 2 subdomains

$ export exec=$exec_debug

$ trust 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.*

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 no particular order (from nb_faces() to 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

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 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.data

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

  trust 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

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.

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
```

TRUST test coverage

Code coverage

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

→ 66% of TRUST/TrioCFD 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

Useful code coverage tools

trust -check class::method

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

-For Baltik developer : Not available yet ?

***Example* :**

$ trust -check Navier_Stokes_std::mettre_a_jour

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

Example :

$ trust -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 TRUST test cases

Code coverage exercice

Browse the TRUST ressources index file :

trust -index

Select the Test coverage link :

Q: Which is the less covered matrix class ?

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

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 Kernel module
- …

Rules to contribute

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

I) If you develop directly in TRUST/TrioCFD :

- 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 (no errors) on the debug binary and possible differences should be explained. Run :

exec=$exec_debug trust -check all

Rules to contribute

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

II) If you develop in a Baltik project based on TRUST/TrioCFD :

- 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_all_debug # Check non regression of the Baltik and TRUST
  - VALGRIND=1 make check_all_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

The End

Good luck!

triou@cea.fr