CFD code Notus (0.2.0) : environment, architecture, verification and validation, performances

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Contents

What is (not) Notus

Open-source project started from scratch in 2015 (CeCILL Licence)

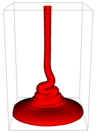
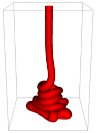
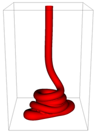
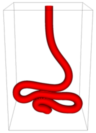
- Modelisation and simulation of **incompressible fluid flows**
- **Massively parallel**
- 2D/3D Finite Volume methods on staggered grids
- Multiphysics

Intended users

- **Mechanical community**: easy to use and adapt, proven state-of-the-art numerical methods
- **Mathematical community**: develop new numerical schemes, fast and efficient framework for comparative and qualitative tests
- Industrials, students

What is not Notus

- A concurrent of, a commercial tool, a click button code

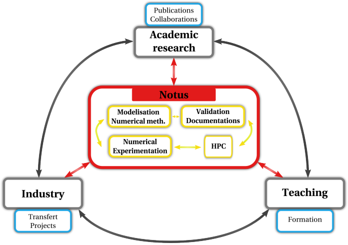
Notus - some objectives

Objectives

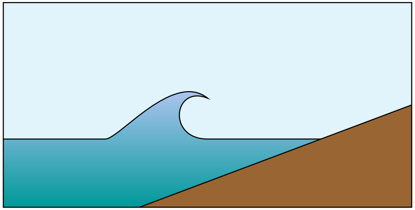
- **Rationalize research efforts**
- Benchmark methods on identified physical test cases
- Numerical toolbox
- Towards numerical experiments

Means

- Take advantage of synergies between Research / Teaching / Industry / HPC
- A clear development environment
- **Mask parallelism** complexities for easy programming
- **Porting** on GENCI, PRACE, mesocentres
- A thoroughly **validated and documented code**
- **Non-regression** approach



Research guidelines for next years



Interfaces

- Fluid / fluid interfaces (advection, surface tension)
- Fluid / solid boundaries (with or wihtout wetting)
- Fluid / porous media interface
- Fluid / solid phase change

2nd order “everywhere” ? Efficiency ?

- 2nd order advection scheme, one-fluid model ?
- 2nd order immersed boundaries, but scalable ?
- 2nd order interface reconstruction, even if immersed boundaries ?
- 2nd order interface reconstruction, and curvature ?
- ...

Notus: models

Domain

- 2D/3D Cartesian, axisymmetric
- 2nd order immersed boundary

Incompressible Navier-Stokes equations

- Buoyancy force (Boussinesq approximation)
- Surface tension force (CSF model)

Energy equation

- liquid/solid phase change

Multiphase immiscible flows

- N advected phases

Species transport equations

- N passive scalars

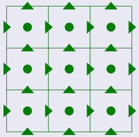
Turbulence

- Large Eddy Simulation model (mixed scale)

Notus: numerical methods

Discretisation

- 2D/3D Cartesian Finite Volume on staggered grids, automatic partitioning
- Time discretisation: implicit, up to 2nd order
- Spatial discretisation: up to 2nd order implicit schemes (advection and diffusion)
- Spatial discretisation: 3rd / 5th order WENO schemes (advection)
- 2nd order immersed boundary method



Navier-Stokes

- Velocity/pressure coupling: time splitting methods (Goda, Timmermans)
- 2nd order open and traction boundary condition
- Surface tension: Closest-Point method to compute curvature ($\rightarrow$ Level-set only)
- Wetting: macroscopic/microscopic approach

Fluid / fluid interface representation and transport

- Volume-of-Fluid method / PLIC
- Moment-of-Fluid method 2D / 3D
- Level-set / WENO
- MOF + Level-set

User Interface

Concept

- ASCII *.nts* files
- Self-explanatory keywords, precise grammar
- Efficient parser that supports:
  - variable declaration
  - formula
  - 'include'
  - if condition and loop

Organisation

- Physical fluid properties data base
- One *.nts* file per test case
  - domain{}
  - mesh{}
  - modelisation{}
  - numerical_methods{}
  - post_processing{}

User Interface

```
include std "physical_properties.nts";
system {measure_cpu_time;}
domain {
   spatial_dimension 2;
   corner_1_coordinates (0.0, 0.0);
   corner_2_coordinates (1.0, 2.0);
}
grid {
   grid_type regular;
   number_of_cells (32, 32);
}
modeling {
   fluids {fluid "one";}
   equations {
     energy {
       boundary_condition {
         left dirichlet 0.0;
         right dirichlet 1.0;
         top neumann 0.0;
         bottom neumann 0.0;
       }
       source_term {constant -2.0;}
       disable_advection_term;
       disable_temporal_term;
     }
   }
}
numerical_parameters {
   time_iterations 1;
   energy {
     solver mumps_metis;
   }
}
post_processing {
   output_library adios;
   output_frequency 1;
   output_fields temperature;
}
```

Contents

Development environment

Development framework

- Fortran 2008
  - Allocatable arrays, structured and derived type
  - Module-oriented programming (private or public internal subprograms)
  - Optional arguments & intent attribute
  - Generic subroutine
  - Preprocessor
  - Interoperability with C (binding)
- MPI parallel coding library
- Git distributed version control system
- CMake cross-platform build system
- Doxygen documentation generator from source code
- Linux

Compilers and MPI libraries

- GNU compilers ($>$ 5.2) and Open MPI (2.10)
- Intel compilers ($>$ 14) and SGI MPT (2.11) and BullxMPI (1.2.8.3)
- IBM XL compilers (14.1) and MPI libraries (2.21.1)

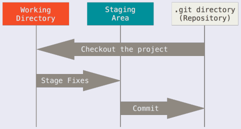
Supercomputers

- Curie at TGCC
- Occigen at CINES
- Turing at IDRIS
- Condor at I2M

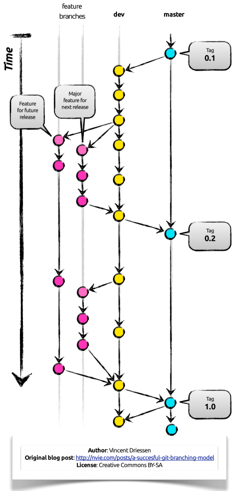
Development environment - Git

About Git VCS

- Records changes to a file(s) over time
- Allows to revert files back to a previous state
- Reverts the entire project back to a previous state



- Compares changes over time
- See who last modified something
- Recovers lost files
- Fully mirrors the repository


feature branches
dev
master
Time
Tag 0.1
Feature for future release
Major feature for next release
Tag 0.2
Tag 1.0
Author: Vincent Driessen
Original blog post: http://nvie.com/posts/a-succesful-git-branching-model
License: Creative Commons BY-SA

Notus Git repository server

```
https://git.notus-cfd.org
git clone https://git.notus-cfd.org/notus/notus.git notus
```

Installation: third party librairies

Third party libraries

- → ADIOS (MXML), HYPRE, MUMPS (METIS, Scalapack), LIS
- BLAS & LAPACK → system
- Simplify the installations of these libraries
- Be sure of the version installed
- Git repository with tarballs

```
git clone https://git.notus-cfd.orgnotus/notus_third_party.git notus_third_part
```

- Installation script (default in $HOME/usr)

```
./build_notus_third_party_lib.sh -a

Options:

Compiler name: --cc --fc ...

MPI wrapper name: --mpicc --mpifc ...

Install librarie separatly: --adios --hypre ...

Download a new version and install it: --hypre-version 2.12.0 ...

Change installation directory: --install-dir
```

Development environment - CMake - Build Notus

Open-source software for managing build process

- Compiler independant
- Supports directory hierarchies
- Automatically generates file dependencies
- Supports library dependencies
- Builds a directory tree outside the source tree

CMake and Notus

- CMakeLists.txt done for several development environnement: *GNU, Intel, etc.*
- Find third party libraries
- Build scripts available for specific computers: *linux workstation, condor, occigen, avakas, curie, etc.*
- MPI (only) release or debug (default) builds

```
$ ./build_notus_curie.sh -h
Usage: buildcmakecondor.sh [OPTIONS]
-c clean the build directory
-s sequential build (default: MPI)
-r release build (default: debug)
-m use MUMPS solver (default: false)
-l use LIS solvers (default: false)
-j NUMBER number of compilation jobs (default: 1)
-h print usage
```

- Easily adaptable

Development environment - Architecture

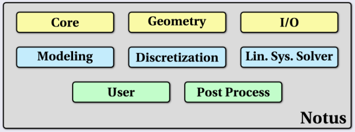
Project tree

```
src
std
test_cases
tools
```

Source tree

- `src/lib`

  `1st level:`



  `2 or 3 sub-levels`

- `src/notus`

  ```
  notus.f90
  ui/
  ```

- `src/doc`

Some development keys

Naming

- Hundreds of variables
  - self explanatory variable names (*velocity, pressure, temperature, ...*)
  - as few abbreviations as possible
- Prefix
  - module begins with *mod_*
  - scalar variable module with *variables_*
  - field array module with *fields_*
  - new derived types with *type_* ex: *struct_face_field velocity%u %v*
  - scalar names associated to an equation suffixed (*navier_time_step*, etc.)
- Explicit routine name

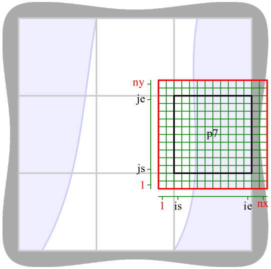
```
solve_navier
compute_mean_velocity
add_div_diffusive_flux_to_matrix
```

- → nearly “guessable” variables → Auto-documentation → Use “git grep” to locate variables, routines, etc.

Some development keys - Masking parallelism

Numerical domain and process ghost cells

- The global domain is partitioned subdomain
- Addition of a few layers of cells surrounding the local domain: *nx*.*ny*.*nz* cells



MPI generic routines to exchange data

- 2D/3D, whatever overlapping zone size
- Integer, double
- Cell array, or vector defined on staggered grid

```
call mpi_exchange(pressure)
call mpi_exchange(velocity)
```

Global reduction routines

- encapsulate MPI ones
- generic routines for min, max of local arrays, sum of scalars

Some development keys - A set of user routines

Concept

- Void routine by default
- Uncomment, modify, compile
- Specific initial condition
- Variable boundary conditions
- Source terms
- Computation of physical properties
- Schemes
- $\rightarrow$ User directory
- $\rightarrow$ Avoid a user to known very well the code

Example

```
do k=1,nz
    do j=1,ny
       energy_boundary_type%left(j,k)=cell_boundary_type_dirichlet
       temperature_boundary_value%left(j,k)=...
    enddo
enddo
```

Documentation - Doxygen

For writing software reference documentation

- Documentation is written within the code
- Open-source, generates html, pdf, latex files

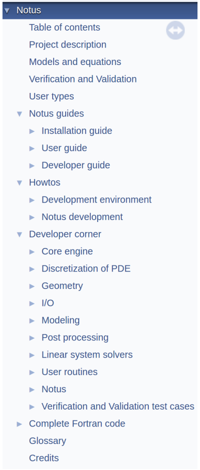
Doxygen and Notus

- https://doc.notus-cfd.org
- Upper level doc: installation, git, architecture, howtos, etc. (markdown format)
- One documentation group per src/lib subdirectories (physics, numerical_methods, io, etc.)

```
cat /src/lib/mesh/grid_generation/doc.f90
!> @defgroup grid_generation Grid Generation
!! @ingroup mesh
!! @brief Compute grid coordinates and spatial steps
```

- Documentation inside each Fortran files

```
cat /src/lib/mesh/grid_generation/create_regular_mesh.f90
!> Create a regular Cartesian mesh (constant step size per direction).
!! The mesh is created in two steps:
!! 1. Provide global face coordinates
!! 2. Compute local variables (coordinates and space steps)
!! The second step is automated in complete_mesh_structure
!! Require the number of points per directions
!! ingroup grid_generation
subroutine create_regular_mesh()
...
```



Contents

IO / Visualisation

Domain is partioned, data are distributed

$\rightarrow$ How to write and plot data efficiently on thousands of processors?

Use of ADIOS library (Oak Ridge National Laboratory)

- Open-source
- Adaptable IO System
- Simple and flexible way to describe the data
- Masks IO parallelism
- Different methods: POSIX, MPI-IO, aggregation
- From 1 to 100 000 processors

Notus IO

- A list of data is created, printed at the end of the time loop
- Add a field anywhere in the code:
  call add_field_to_list(print_list, enstrophy, 'enstrophy')

Visualisation of the results $\rightarrow$ VisIt (Lawrence Livermore National Laboratory)

- Open-source
- Sequential and Parallel
- ...

Verification and Validation V&V

Verification

- **proves that the continuous model is solved precisely by the discrete approach**
  - analyses the numerical solution of equations
  - quantifies and reduces of the numerical errors
  - computes spatial and temporal convergence orders
- $\rightarrow$ **mainly a mathematical and computing process, unlinked to physical problem**

Validation

- **analyses the capacity of a model to represent a physical phenomena**
  - compares numerical solution to experimental results
  - identifies and quantifies errors and uncertainties of continuous and discrete models, and experience

$\rightarrow$ **Accumulation of evidence that the code works!**

Verification

2 main steps

- no bug in the code or unconsistant solution
- quantify numerical errors
  - start from an exact (built) solution
  - compute errors, convergence order
  - compare the given order to the expected one

Error sources

- coding bug
- numerical stability condition not satisfied
- insufficiant spatial or temporal convergence
- iterative methods not converged
- rounding errors

Hypothesis: smoothed solution in the asymptotic convergence zone

N discrete solutions $f_k (1 \leq k \leq N)$

$$f_{h\to 0} = f_k + C h_k^p + \mathrm{O}(h_k^{p+1})$$

$$p_k = \frac{log(\frac{E_k}{E_{k-1}})}{log(\frac{h_k}{h_{k+1}})}$$

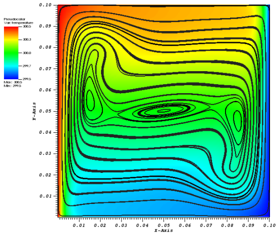
where $E_k = f_{exact} - f_k$

mesh	L_∞ error	Order	L_2 error	Order
10	2.53e-03	n/a	6.87e-04	n/a
20	6.49e-04	1.97	1.69e-04	2.02
40	1.63e-04	1.99	4.22e-05	2.00
80	4.08e-05	2.00	1.05e-05	2.00

Validation

Analyses the capacity of a model to represent a physical phenomena

- no exact solution
- post processing of physical parameter (velocity plot, Nusselt numbers, lift, drag, etc.)
- comparison with experience or other code
- quantify error and uncertainty
- 3 meshes → convergence order → Richardson extrapolation



Mesh	Nusselt nb.	Order	Velocity	Order
32	1.0490e+01	na	3.7921e-03	na
64	9.1842e+00	na	3.6811e-03	na
128	8.9013e+00	2.2070	3.6387e-03	1.3913
256	8.8424e+00	2.2635	3.6277e-03	1.9381
512	8.8292e+00	2.1622	3.6249e-03	1.9957
Ext.	8.8254e+00		3.6240e-03	
Réf.	8.8252e+00			

Notus V & V tools

1 - compute convergence order of a test case

Run the same case varying a parameter (mesh or time step)

- $\rightarrow$ *json* file

```
{"number_of_cells": [ 100, 25], "time_step": 0.5},
{"number_of_cells": [ 200, 50], "time_step": 0.25},
{"number_of_cells": [ 400, 100], "time_step": 0.125},
{"number_of_cells": [ 800, 200], "time_step": 0.0625}
```

- Python script:

```
./notus_grid_convergence -np 8 --doxygen test_case_name
```

  - run (interactivly or submission) the test case with different meshes
  - collect the results of the chosen quantities
  - compute convergence order and extrapolated values
  - output to doxygen format

2 - non regression

- **list of V&V test cases files**
- quick or full validation
- run the test cases with bash script
- results in *txt* file: OK, NO, FAIL, etc.
- commit the results (one per architecture) to Git repository

Exemple of Output of the non regression process

```
$ ./notus_validation.sh -h

  Usage : notus_validation.sh [OPTIONS]
  -s sequential validation (default: parallel)
  -d 2/3 2D or 3D validation (default: 2D and 3D)
  -l long validation (default: false); check for special keywords in case.nts and run the case several times
  -h print usage

$ cat notus_validation.txt
  Test case name                Validated    Converged    Time iteration             Error
  ibd_laplacian_dirichlet.nts     FAIL
  ibd_laplacian_neumann.nts       FAIL
  poiseuille.nts                   OK           OK             356          1.3877787807814457E-17
  poiseuille_periodic.nts          OK           OK              69          1.3877787807814457E-16
  poiseuille_viscosity.nts         OK           OK            2989          0.0000000000000000E+00
  ibd/ibd_poiseuille.nts          FAIL
  level_set_sheared_2D.nts         NO           N/A            200          3.8200452689984843E-08
  mof_analytic_periodic.nts        OK           N/A            141          2.2204460492503131E-16
  mof_analytic_sheared.nts         OK           N/A           1000          1.9984014443252818E-15
  mof_minimization_sheared.nts     OK           N/A           1000          2.2204460492503131E-16
  vof_plic_periodic.nts            OK           N/A            141          3.3306690738754696E-16
  vof_plic_sheared.nts             OK           N/A           1000          3.3306690738754696E-16
  ball_equilibrium.nts             NO           OK            1128          1.4963675386815269E-07
  square_cavity.nts                OK           OK             291          5.3942093847236805E-14
  driven_cavity.nts                OK           OK            3449          5.1625370645069779E-15
  dam_break_mof.nts                OK           N/A             50          2.5313084961453569E-14
  dam_break_vof_plic.nts           OK           N/A             50          3.3556490919295356E-14
  solitary_wav                     NO           N/A            450          5.1368178637115763E-04
  solitary_wav                     NO           N/A            500          7.6377097850394010E-03
  square_cavity.nts                NO           OK             235         3 .0898306135895837E-10
  ...
```

Check Portability and Performances

Portability

- Associated to V & V process
- Numerical solutions should be **independant of**:
  - compiler editors, compiler versions, MPI libraries, etc.
  - computer architectures and processor numbers
- Notus portable on:
  - GNU + OpenMPI; Intel + MPT; Intel + IntelMPI; Intel + BullXMPI
  - Sequential and Parallel versions
  - $\rightarrow$ “Same” results betwwen 10^{-8} and 10^{-15})

Performances

- Compare measured scalability to the expected one
- Identify and measure relevant parts of the code
  - partitiong
  - initialization
  - time loop: equation preparation, solvers (external), I/O
- Lot of functionalities: **identify the relevant test cases**
- Determine optimal use of supercomputers (nodes number per core)

Notus, performance tools

Most of CPU time in linear system solvers

$\rightarrow$ Third party libraries

HYPRE library (Livermore USA)

- BiCGStab, GMRES iterative solvers
- Geometric and algebraic preconditioners

LIS library (SSISC Japan)

- BiCGStab, GMRES iterative solvers
- ILU family preconditioners

MUMPS (Cerfacs / INRIA, France)

- Direct solver
- Mainly for 2D matrix
- PORD, Metis graph partitioners

Notus, performance tools

Objectives

- Verify weak and strong scalability
- Verify I/O performance
- Ensure non regression of these performances
- On several supercomputers (from local to PRACE one)

Step 1, scalability at test case level

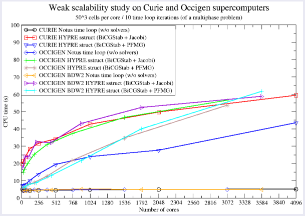
- Template directoy
  - notus template .nts file
  - submission template file (depending of the workload manager)
- Submission bash script
  - `./submit_jobs.sh -t weak -a 9 -c 40 -m 16 -s template_sub_curie -q ccc_msub`
  - `./submit_jobs.sh -t strong -i 3 -a 9 -c 512 -m 16 -s template_sub_curie -q ccc_msub`
  - `./submit_jobs.sh -t strong_node -c 100 -m 16 -s template_sub_curie -q ccc_msub`
  - $\rightarrow$ copy template directory
  - $\rightarrow$ adapt template files
  - $\rightarrow$ submit jobs
- Concatenation bash script
  - `./concatenate_cpu_times.sh -t weak -a 9 -c 40 -m 16`

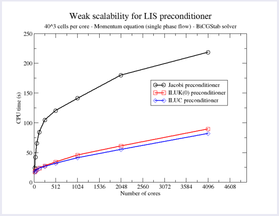
```
128     0.26000E+01    0.86140E+00    0.94443E+00    0.79417E+00
256     0.29297E+01    0.10660E+01    0.10462E+01    0.81751E+00
512     0.30754E+01    0.11369E+01    0.11025E+01    0.83590E+00
1024    0.38859E+01    0.16025E+01    0.13959E+01    0.88751E+00
2048    0.43207E+01    0.18807E+01    0.15359E+01    0.90404E+00
4096    0.47281E+01    0.22302E+01    0.16268E+01    0.87108E+00
8192    0.65902E+01    0.32613E+01    0.23815E+01    0.94744E+00
```

Notus, performance tools

Weak scalability on Curie and Occigen supercomputers

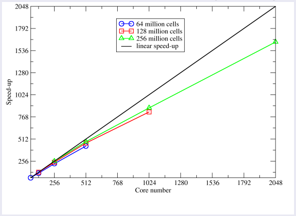
→ 50^3 cells per core, number of core increases, constant CPU time expected



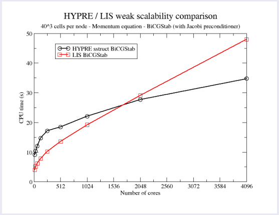


Strong scalability

→ constant number of global cells, number of core increases, linear speed-up expected



HYPRE / LIS comparison: BiCGStab + Jacobi



Notus, performance tools

Step 2 under progress, non regression list of representative test cases

- get reference times for each one and each target supercomputer
- bash script to run all the performance study
- comparison, OK, NO, FAIL
- commit the results (one per architecture) to Git repository

Conclusion

- Use of some standard development tools (Git, CMake, Doxygen)
- Use of specific libraries: IO, solvers
- Single Doxygen documentation: concepts, installation, modeling, subroutines
- Different users (from student to researcher, from modeling to numerical methods)
- Different computers
- A few scripts, easy to use and modify for:
  - installation
  - execution
  - V&V
  - scalability studies

$\rightarrow$ *ongoing project, version 0.2.0 only !*