Notus CFD code presentation

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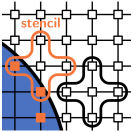
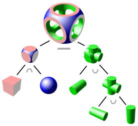
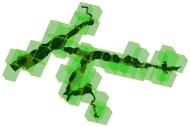
https://notus-cfd.org

Journées Calcul & Simulation - Dec. 2021

Presentation content

- The main features of Notus
- Short focus of some proposed numerical methods
- GENCI HPC challenge 2020 at TGCC

Notus code purposes

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

- Modeling and simulation of **incompressible fluid flows**, multiphysics
- 2D/3D Finite Volume/Difference methods on staggered grids, **massively parallel**
- **Still under development (version 0.5.0)**
- From 0.5.0 to 1.0.0, make all things work together!

Intended users

- **Mechanical community**: easy to use and adapt, proven state-of-the-art numerical methods, towards numerical experiments
- **Mathematical community**: develop new numerical schemes, fast and efficient framework for comparative and qualitative tests, benchmark methods on identified physical test cases, numerical toolbox
- Take advantage of **synergies between Research** / **Teaching** / **Industry** / **HPC**

What is not Notus

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

Supercomputers

- **GENCI/PRACE**: Joliot Curie at TGCC, Occigen at CINES, Jean-Zay at IDRIS
- Curta at mesocentre MCIA... *also on Linux laptop!*

Development environment

Modern development framework

- **Fortran 2008**
- **MPI** parallel coding library
- **OpenMP** share memory parallel coding library
- **Mask parallelism** complexities for easy programming
- **Git** distributed version control system
- **CMake** cross-platform build system → easy installation
- **Doxygen** documentation generator from source code
- **Linux only!**
- **Build scripts, Notus and third party libraries**
- A thoroughly **validated and documented code**, **non-regression** approach
- **Web sites**: general, doc, git
  https://notus-cfd.org, https://doc.notus-cfd.org, https://git.notus-cfd.org

Portability

- GNU + OpenMPI; Intel + IntelMPI
- Sequential and Parallel versions
- → "Same" results between 10^{-8} and 10^{-15})

Features - Modeling

Domain

- 2D/3D Cartesian, immersed sub-domains

Incompressible Navier-Stokes equations

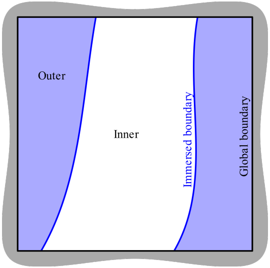
- Buoyancy force (Boussinesq approximation)
- Surface tension force (CSF model)
- Large Eddy Simulation (mixed scale model, WALE)
- RANS k-ω SST

Multiphase immiscible flows

- One-fluid model
- Volume-of-Fluid, Moment-of-Fluid, Level-Set interface representations

Energy equation, Species transport equations

- Free, mixed or forced convection, phase change liquid/solid
- Passive scalar, thermosolutal flows



Features - Numerical methods

Discretization

- **2D/3D Cartesian on staggered grids**, automatic partitioning
- **Implicit schemes**: up to O(2) implicit schemes (advection and diffusion)
- **Explicit schemes**: O(2) TVD LV Superbee, O(3) & O(5) WENO, HOUC (advection); O(2) & O(4) centered (diffusion)
- **Complex geometry**: Immersed Boundary Method (1^{st} & 2^{nd} order)

Navier-Stokes

- **Non conservative or momentum preserving approaches**
- **Velocity/pressure coupling**: time splitting methods (Goda, Timmermans)
- **Surface tension**: Height Function or Closest-Point methods to compute curvature

Fluid / fluid interface representation and transport

- **Volume-of-Fluid** method 2D-3D / PLIC (directional splitting)
- **Moment-of-Fluid** method 2D-3D / backward RK2 advection
- **Level-set** / WENO

HYPRE library (LLNL)

- BiCGStab, GMRES iterative solvers
- Preconditioners: **geometric & algebraic multigrid**

MUMPS direct solver

- Mainly for 2D linear systems
- PORD, Metis graph partitioners

Domain is partitioned, data are distributed

→ How to write and plot data efficiently on thousands of processors?

Use of ADIOS library (Oak Ridge National Laboratory)

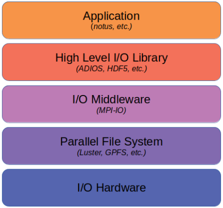
- Open-source
- Simple and flexible way to describe the data
- Masks IO parallelism, different methods: POSIX, MPI-IO, aggregation
- From 1 to 100 000 processors, around $50 GBs^{-1}$ on Joliot Curie Lustre file system

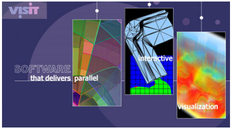
Visualisation of the results → VisIt (LLNL), Paraview

- With ADIOS file format, VisIt is limited to 2 billion cells, **sequential version only**!

Pixie

- Based on **HDF5 library** (`.h5` files)
- **Compatible with parallel VisIt** (automatic parallel domain decomposition)
- Non-uniform rectilinear grids
- Notus Pixie output less efficient then ADIOS, around $8 GBs^{-1}$ on Joliot Curie Lustre file system





Verification and Validation V&V

Notus V&V python script

Non-regression

- **list of V&V test cases files**
- quick or full validation (up to 1600 MPI jobs), **database of reference values for each case**
- validation runs on supercomputers thanks to slurm (2 pass script: submit jobs, collect and post-process)
- results in *txt* file: OK, NO, FAIL, difference to expected values. Summary.

Grid convergence: run the same case varying mesh or time step

- run (interactivly or submission) the test case with different meshes
- collect the results of the chosen quantities, compute convergence order and eventually extrapolated values
- **included into the non-regression process**

Performance python script

- Verify weak and strong scalability
- Identify and measure relevant parts of the code
- Verify I/O performance
- On several supercomputers (from local to GENCI/PRACE)
- Determine optimal use of supercomputers (number of cells per core)
- Compare measured scalability to the expected one
- Ensure non regression of these performances

User Interface: `.nts` file

Concept

- Text `.nts` files (unicode)
- Self-explanatory keywords, precise grammar
- Efficient parser that supports:
  - variable declaration
  - formula
  - 'include'
  - logical tests, loops
- **Associated documentation** → `test_cases/doc` directory

.nts file structure

- Physical fluid properties data base: `std/physical_properties.nts` file
- One `.nts` file per test case, block structure:
  - `include and variable declarations`
  - `system{}`
  - `domain{}`
  - `mesh{}`
  - `modeling{}`
  - `numerical_methods{}`
  - `post_processing{}`

User Interface: `.nts` file example

```
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 "water";}
  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;
}
```

Some development keys - Masking parallelism

Numerical domain and MPI process ghost cells

- The global domain is partitioned into subdomains
- Addition of a few layers of cells surrounding the local domain: $nx \times ny \times nz$ cells

MPI generic routines to exchange data

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

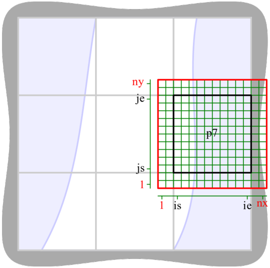
```
call mpi_exchange(pressure)
call mpi_exchange(velocity)
```

- Mandatory after any spatial derivative computations
- MPI Exchange + Fill boundary ghost nodes

```
call fill_ghost_nodes(scalar,
boundary_condition)
```

Global reduction routines

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



OpenMP generic algebraic operations for 3-dimensional arrays and face-fields

x = a + b

```
call field_operation_add(a, b, x)
```

a = a + b*c

```
call field_operation_add_mult(a,
b, c)
```

...

Presentation content

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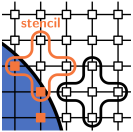
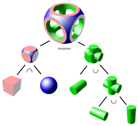
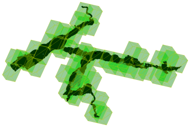






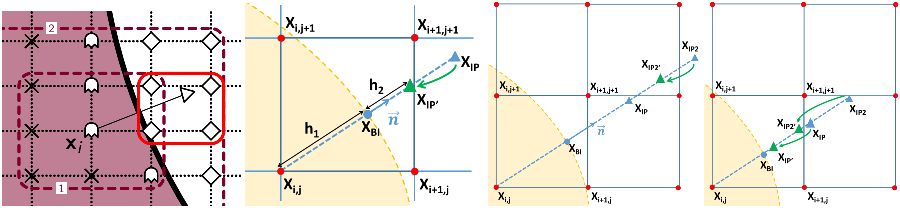
Direct forcing method of Mittal [JCP2008]

- **Extrapolate solution on the ghost nodes thanks a linear relation between the ghost nodes and their image nodes (△)**
  Interpolation of the solution on the image point, Lagrange interpolation, p=2 or p=3 (4 or 9 points in 2D)

  → **non-compact stencils** (loss of precision, non banded matrix, less efficient solver)

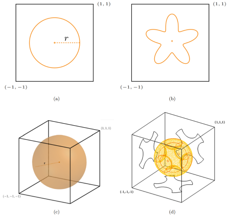
  Regular grid (square cells)
  Dirichlet : stencil size = 2, 2^{nd} order
  Neumann : stencil size = 2, 1^{st} order only → stencil size = 3 (2^{nd} order)

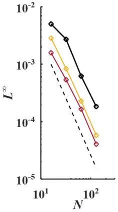
- **Improvements - through stencil size reduction - thanks to different class of shifting methods**
  Ghost node shifting method for irregular grids
  Square shifting methods for regular grid applied to linear interpolation and extended to quadratic one

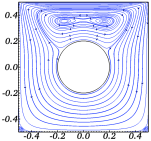


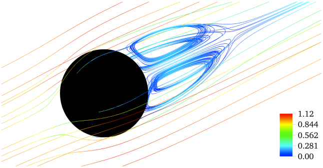
2D/3D verification and validation

- Laplacian: circle, 2D & 3D flowers
- Navier-Stokes: 3D channel, driven cavity with obstable, flow around a heated cylinder, around a sphere
- **Stencil 1:** 2^{nd} **order Dirichlet and** 1^{st} **order Neumann (with several shifting methods)**
- **Stencil 2:** 2^{nd} **order Neumann is possible with quadratic and double shifting method**
- **Conclusion : stencil size reduced, precision and regularity of the convergence also improved**







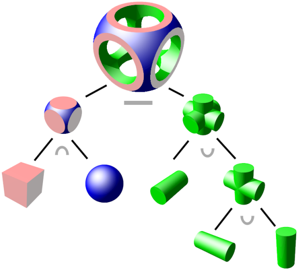


Performance analysis

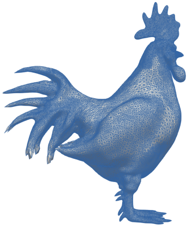
- CPU time. 3D pipe flow: x2.5 faster than original method. Flow past a sphere: x3 faster.

A. Jost, S. Glockner, Direct forcing immersed boundary methods: Improvements to the Ghost Node Method, *Journal of Computational Physics*, volume 438, 110371, 2021.

- Volumetric representation
- Boolean operations (CSG)
  - Union
  - Intersection
  - Difference
  - Complement
- Analytic shapes (primitives)
  - Half-space
  - Sphere
  - Box
  - Cylinder
  - Torus
- Surface mesh
  - Orientable
  - Inside/Outside
  - OBJ Wavefront format
- Transformations
  - Translation
  - Rotation
  - Scaling

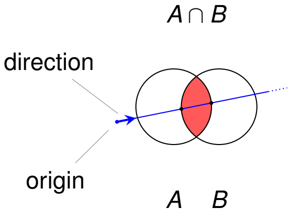


CSG tree (Wikimedia Commons)



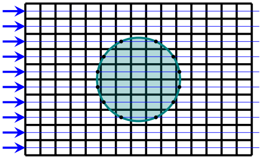
Surface mesh example

Ray-tracing (list of intersection points + distance + normal)

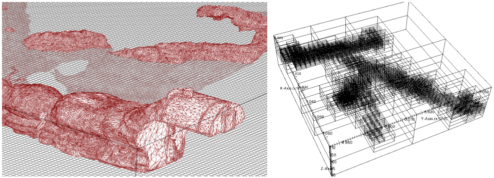


- Ray-tracing with $\cup$, $\cap$, and $\setminus$
- Jordan-Brouwer theorem
  $\rightarrow$ odd: inside
  $\rightarrow$ even: outside

Ray-trace once per row



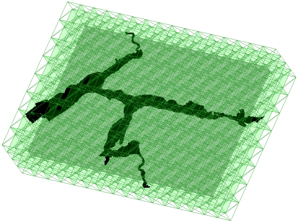
Space subdivision using octree (surface mesh only)

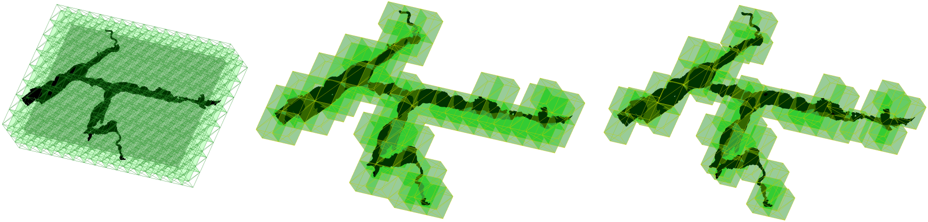


Cartesian grid partitioning and complex geometries

With immersed boundaries

- The number of inactive cells may be large
- Full inactive partitions
- $\rightarrow$ **Extra computational cost** (ex. Lascaux cave: 99% of inactive cells)
- **Solution**: remove inactive partitions and contract line or row of partitions (partition sliding)



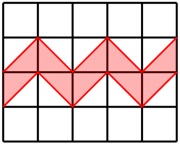


Lascaux cave example, 100 000 cells / core

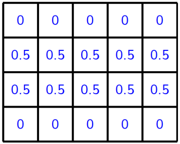
- **Global grid of 189 billion cells** - 99% of inactive cells
- Without sliding 3.2 billion cells - 35% of inactive cells
- **With sliding 3.0 billion cells - 31% of inactive cells**

Volume-of-Fluid - PLIC

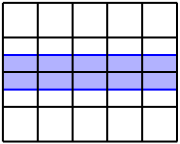
- Volume fraction + **normal** to the interface → linear construction of the interface
- Requires a **9 pts stencil** (2D)



Original interface



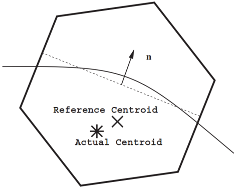
VOF representation



PLIC reconstruction

Moment-of-Fluid

- Volume fraction + **centroid** → linear reconstruction that:
  - matches the volume fraction
  - minimises the discrepancy between the specified centroid and the centroid of the reconstructed polygon
- → **1 pt stencil**, 2nd order
- Generalised to n materials



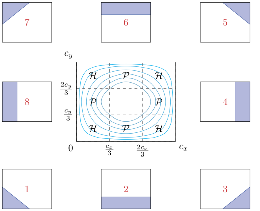
Source: Dyadechko & Shashkov (JCP 2006)

Moment-of-Fluid method

Remove minimisation for Cartesian grids in 2D

- analytic form of the centroid curve (for a given volume fraction)
- from 20% to 300% faster

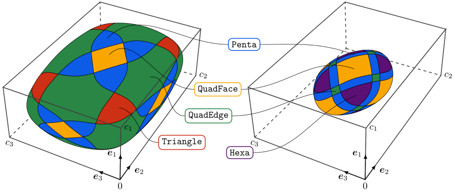
A. Lemoine, S. Glockner, J. Breil, Moment-of-Fluid Analytic Reconstruction on 2D Cartesian Grids, *Journal of Computational Physics*, vol. 328, pp. 131–139, 2017.



Extension to 3D hexahedral cells

- uses explicit analytic formulas of the objective function
- more robust and 100x faster

T. Milcent, A. Lemoine, Moment-of-Fluid Analytic Reconstruction on 3D Rectangular Hexahedrons, *Journal of Computational Physics*, 409, 109346, 2020



→ CPU time reduction as a source of motivation for new numerical methods

Level-set and closest point methods

Surface tension computation

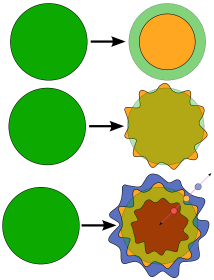
Context

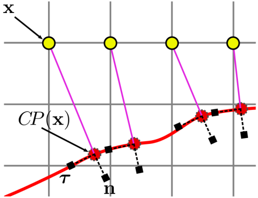
- Accurate computation of the curvature and precise transport of the interface is **still challenging**
- **Continuum Surface Force [Brackbill]**: $\sigma \kappa \nabla c$
- $\kappa = \nabla . (\frac{\nabla \phi}{|\nabla \phi|})$ on nodes where κ is not defined

Solution

- Curvature computation based on second derivatives of the surface/interface $\rightarrow$ **transport at least 4th order precise**
- WENO5/Level-Set framework
- Accurate κ computation
  - compared to exact curvature
  - with minimum variation along the surface
  - with minimum variation following the normal direction
- κ inside the domain = κ of the closest Γ point [Hermann, 2008]
- $\rightarrow$ **Extension of the curvature along the normal direction**

$$\kappa(\mathbf{x}) = \kappa\left(CP(\mathbf{x})\right)$$



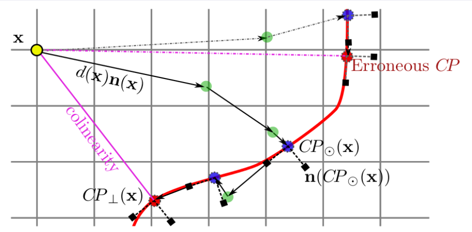


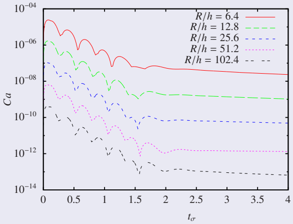
Level-set and closest point methods

Surface tension computation

Contribution

- Level-set $\neq$ distance function
- Improvement of the gradient descent to find the closest points to ensure **colinearity to the interface normal**





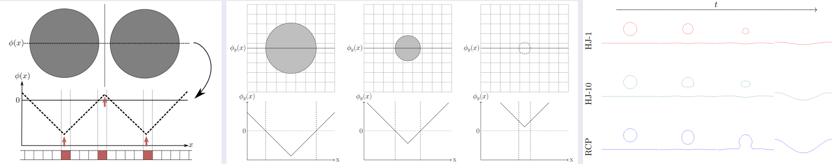
Results

- Viscous column equilibrium: 4th order decrease of spurious current
- **Advected** viscous column: 4th order (not even 1 for VOF method)

M. Coquerelle, S. Glockner, *A fourth-order accurate curvature computation in a level set framework for two-phase flows subjected to surface tension forces*, Journal of Computational Physics, 305, pp. 838-876, 2015.

Geometrical level set reinitialization method

- Use the CP approach to reinitialize and to detect precisely all the ill-defined points of the level set (kinks)
- Equivalent or even better results compared to solving the Hamilton-Jacobi equation



F. Henri, M. Coquerelle, P. Lubin, Geometrical level set reinitialization using closest point method and kink detection for thin filaments, topology changes and two-phase flows *Journal of Computational Physics*, vol. 448, 2022.

Hybrid advection scheme WENO5 / HOUC5

- Efficient HOUC5 in smooth level-set region
- Robust WENO5 where the spatial discretization of the advection equation is subject to large error, i.e. where level-set is ill-defined.
- $\rightarrow$ CPU lowered with a factor up to 2.

F. Henri, M. Coquerelle, P. Lubin, *An efficient hybrid advection scheme in a level set framework coupling WENO5 and HOUC5 schemes based on kink detection*, accepted in Journal of Computational Physics.

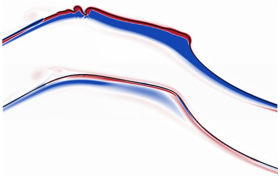
High order momentum preserving method

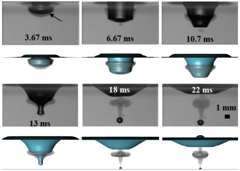
Context

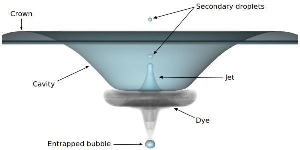
- Multiphase flows with high density ratio
- One-Fluid approach (VOF, MoF, Level-Set)
- Unconsistancy between mass and momentum flux can lead to instabilities and large errors

Solution

- Use the conservative momentum form
- Add a mass conservation equation to predict density for momentum equation
- Use of a synchronized temporal integration for the advective part of the momentum and mass equations.
- Use of consistent spatial conservative schemes for both
- $\rightarrow$ Discontinuity of the momentum is advected at the same speed as a discontinuity of the density
- $\rightarrow$ A high order approach (WENO5+RK2) proposed independent on the interface representation (VOF, MoF, Level-Set)



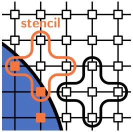


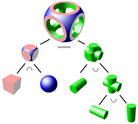
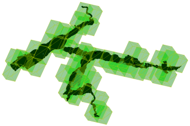


F. Desmons, M. Coquerelle, *A generalized high-order momentum preserving (HOMP) method in the one-fluid model for incompressible two phase flows with high density ratio*, Journal of Computational Physics, 437, 110322, 2021.

Presentation content

- The main features of Notus
- Short focus of some proposed numerical methods
- GENCI HPC challenge 2020 at TGCC

Continuous microfluidic process to generate nanoparticles
with A. Erriguible (I2M/ICMCB), S. Marre (ICMCB)

Macro-reactors *vs* micro-reactors. The scale-up challenge.

- Mixing of ethanol and supercritical CO2 in high pressure microfluidic system
  $\rightarrow$ Nucleation and growth of particles
- **Fast mixing reduces particle size**
  $\rightarrow$ **Turbulent flow in micro tubes (ICMCB experiments)**
  $\rightarrow$ **very good mixing (compare to larger reactor) and particle size around** $20nm$
- **Direct Numerical Simulation: all resolved mixing scale** (Kolmogorov $\approx$ Batchelor)
- **Limited production**. From lab to industrial scale? Sizing-up or numbering-up?
  $\rightarrow$ **Scale-up process, a pure numerical approach...**

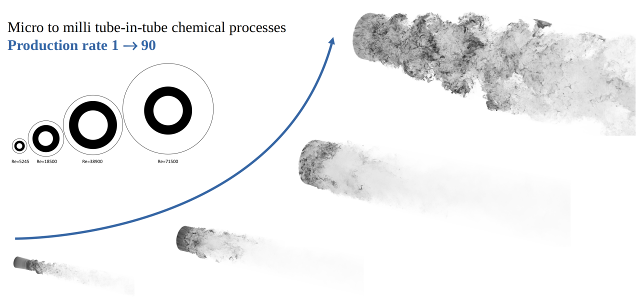
Large reactor (1cm). Injection velocity $3m.s^{-1}$, $R_{inj} = 90\mu m$, co-flow velocity $0.001m.s^{-1}$, $Re = 432$
Fully explicit (except pressure), 390.10^6 cells, 3584 processors

Micro reactor (0,3mm). Injection velocity $2.81m.s^{-1}$, $R_{inj} = 50\mu m$, co-flow velocity $3.97m.s^{-1}$, $Re = 5505$
Fully explicit (except pressure), 300.10^6 cells, 3584 processors

Process scale-up

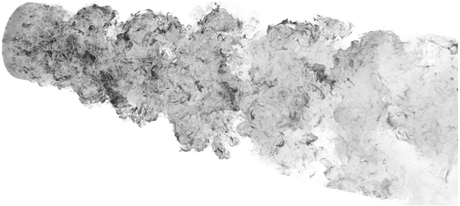
- Full explicit, Hybrid MPI/OpenMP version → **Improved strong and weak scalabilities**
- **From micro to milli tubes, TKE dissipation rate conserved**
- Re=5245 → **Re=71000**, all resolved mixing scale (DNS)
- GENCI HPC challenge (TGCC), 40 millions CPU hours
  from 300 million to 11 billion cells, up to 131 072 processors

→ **Still very fast mixing**
→ **Production x90**



S. Glockner, A.M.D. Jost, A. Erriguible, *Advanced petascale simulations of the scaling up of mixing limited flow processes for materials synthesis*, accepted in Chemical Engineering Journal.

HPC example: GENCI HPC challenge at TGCC



Concentration volume rendering, Kelvin-Helmholtz instabilities,
fast mixing, co-flow velocity effect, confinement effect