Massively parallel solving of the Pressure-Poisson equation on unstructured meshes

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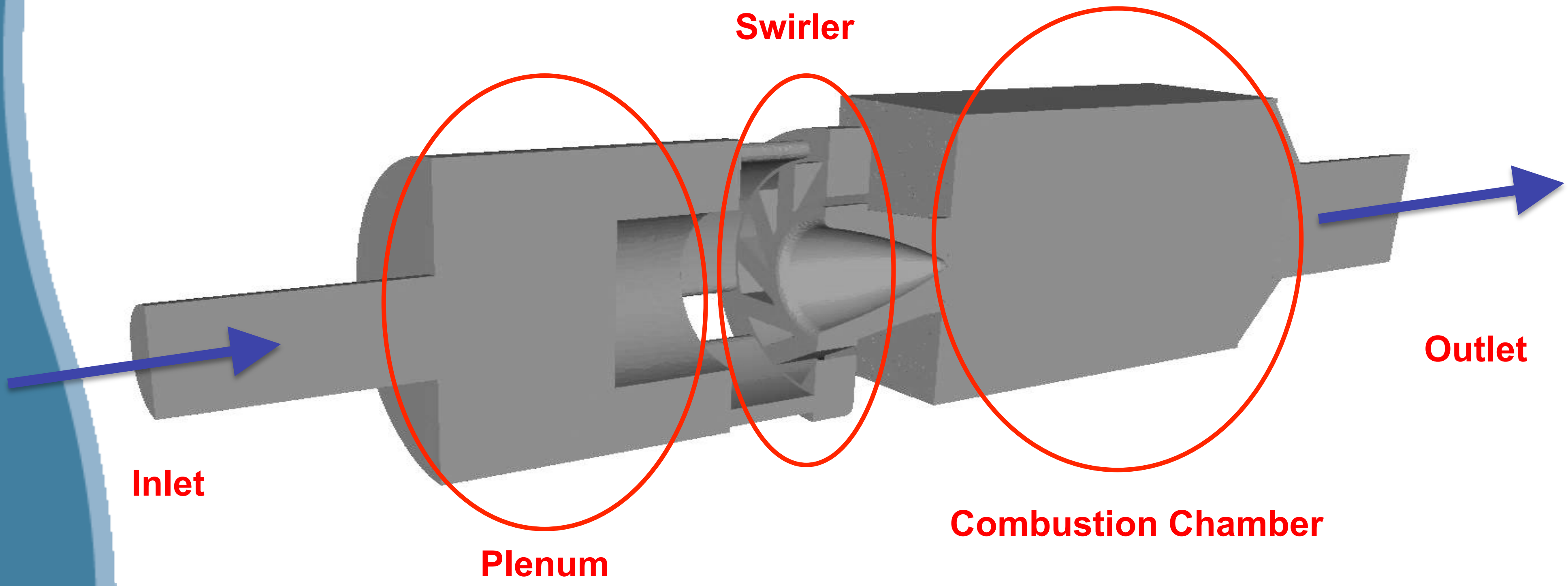
Simulation of the PRECCINSTA burner

- **PRECCINSTA burner :**



- Rectangular cuboid chamber : 110mm x 86mm x 86mm
- Air-methane mixture, Re=45000

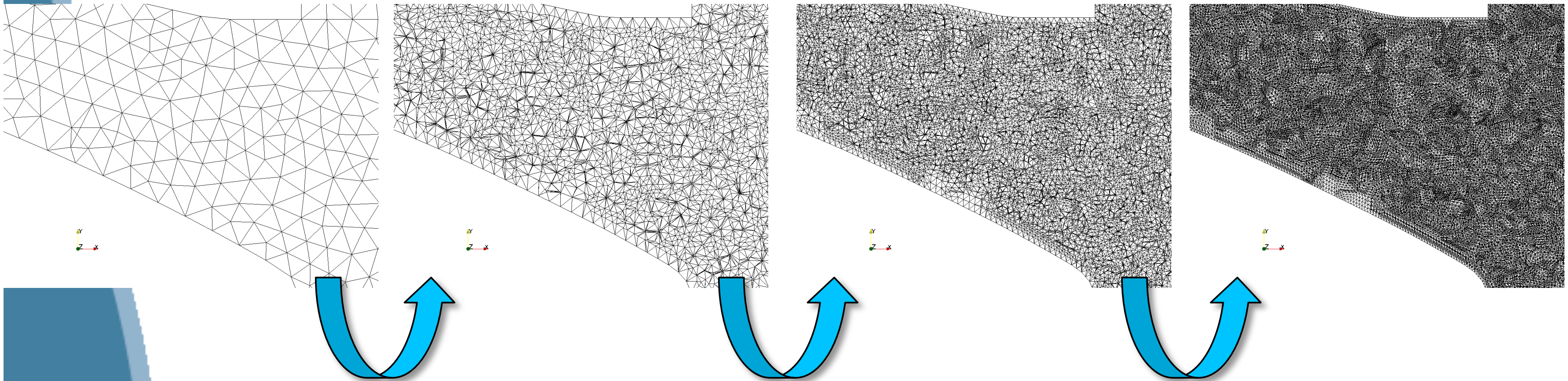
[1] Lartigue, Meier & Berat, « Experimental and numerical investigation of self-excited combustion oscillations in a scaled gas turbine combustor », 2004

[2] Galpin, Naudin, Vervisch, Angelberger, Colin & Domingo, « Large-eddy simulation of a fuel-lean premixed turbulent swirl burner », 2008

[3] Moureau, Bérat & Pitsch, « An efficient semi-implicit compressible solver for large-eddy simulations », 2007

Simulation of PRECCINSTA

- Successive **grid refinements** lead from 1.7 million cells to 2.6 billion[1] :



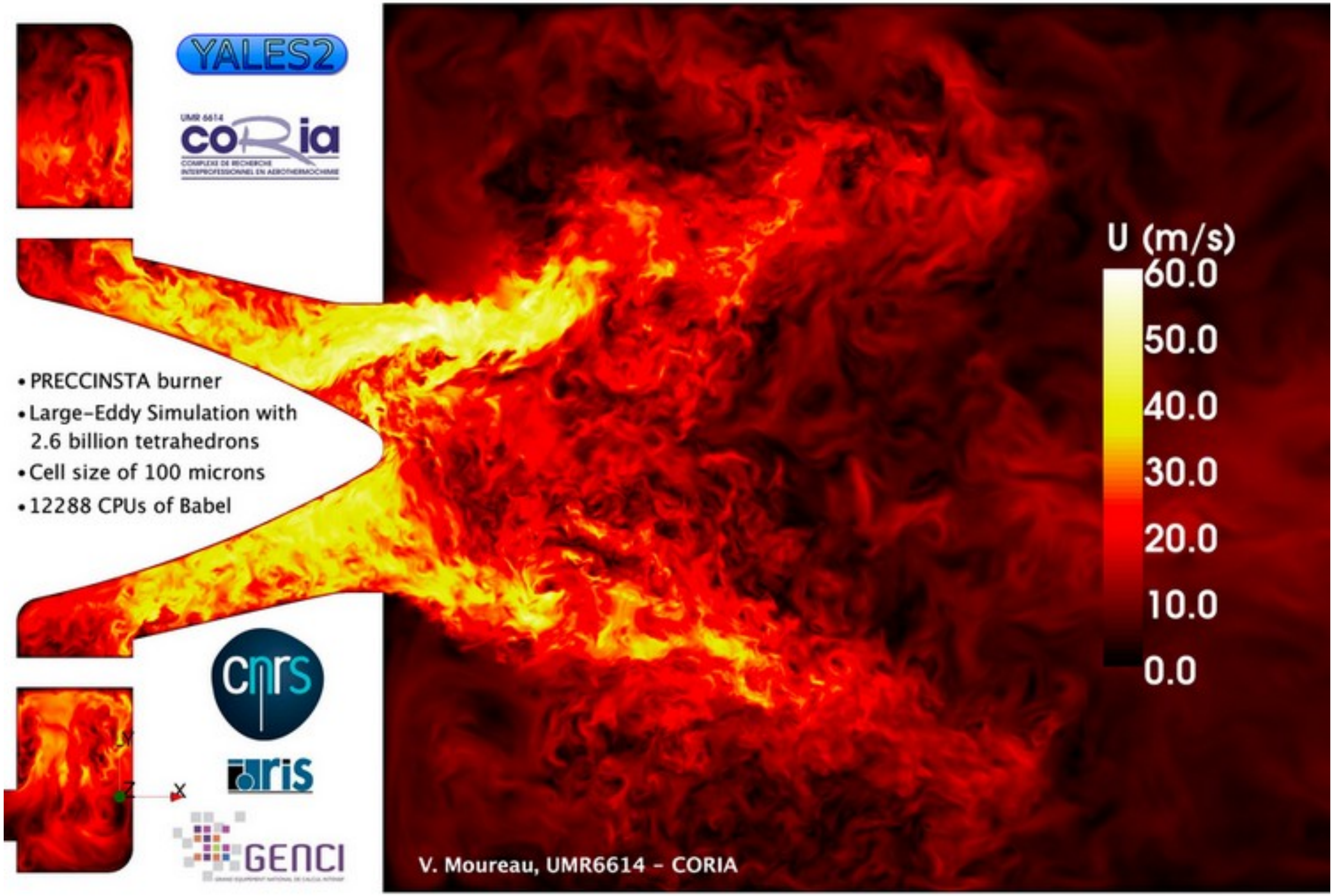
- Chosen among other possible solutions :

  - direct import of large meshes
  - reconstruction from partial meshes on the domain

[1] Rivara, « Mesh refinement processes based on the generalized bisection of simplices », 1984

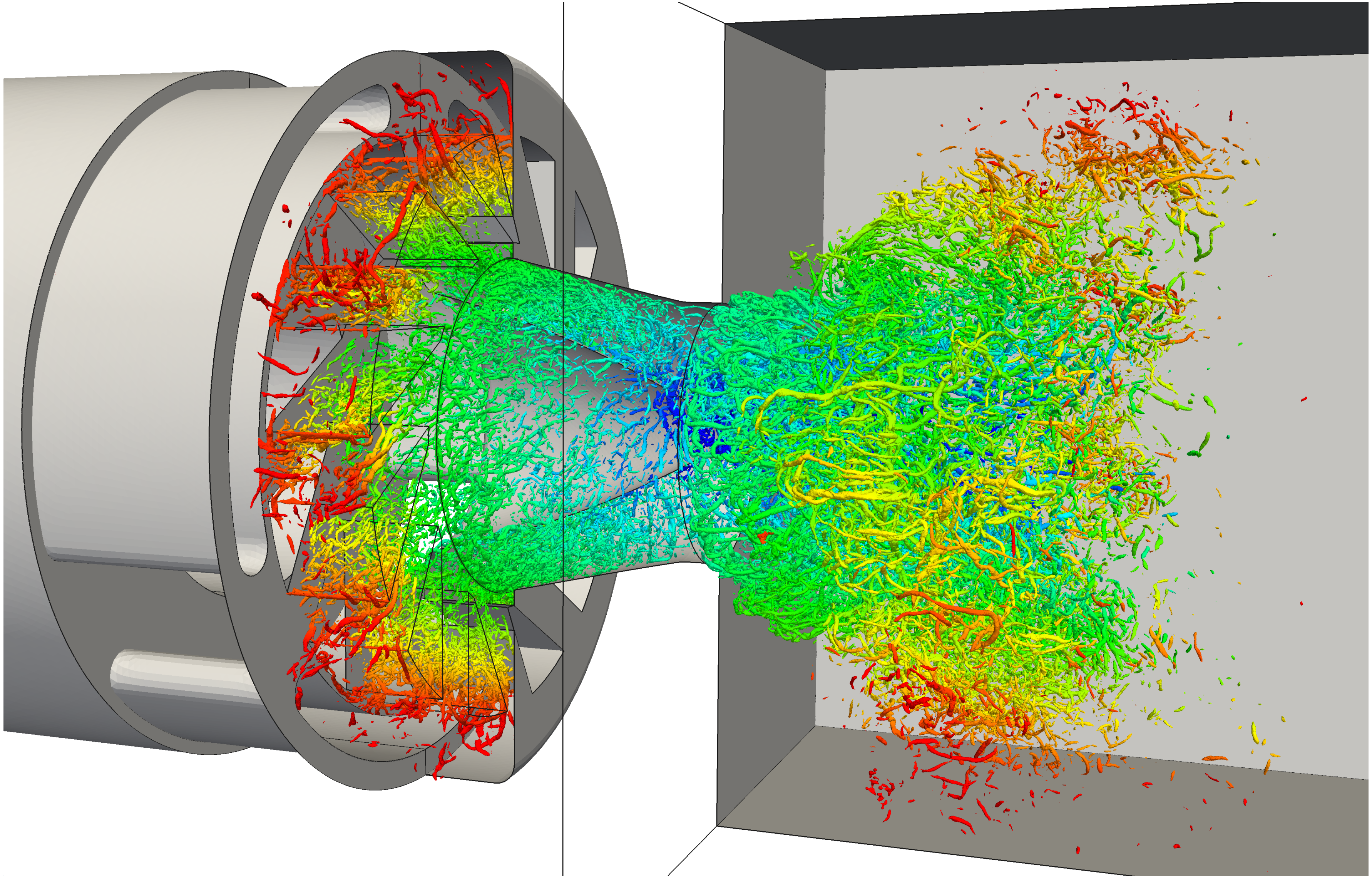
Simulation of PRECCINSTA (Large-eddy simulation)

- **Cold flow** :



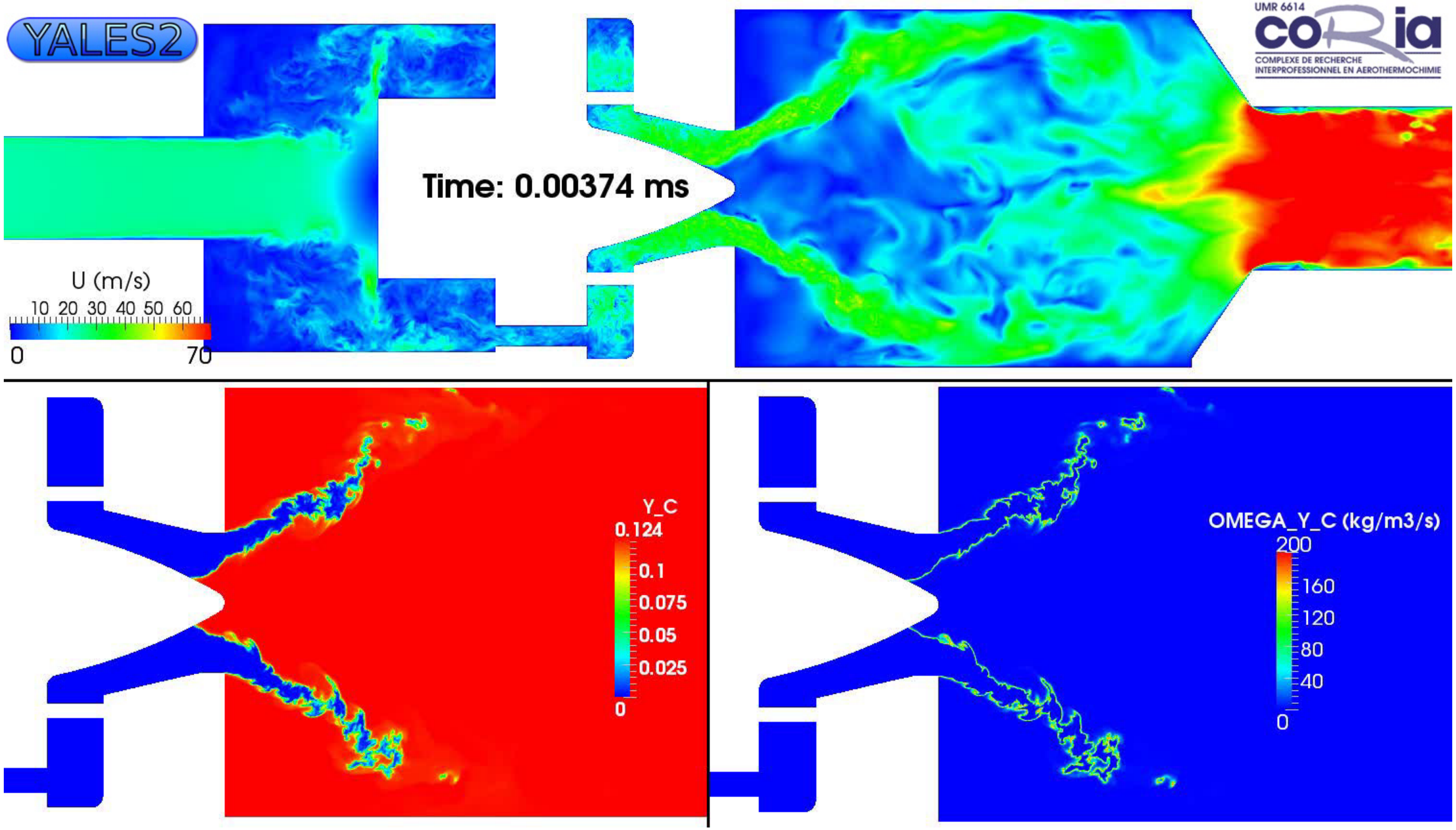
Simulation of PRECCINSTA (Large-eddy simulation)

- **Cold flow** :

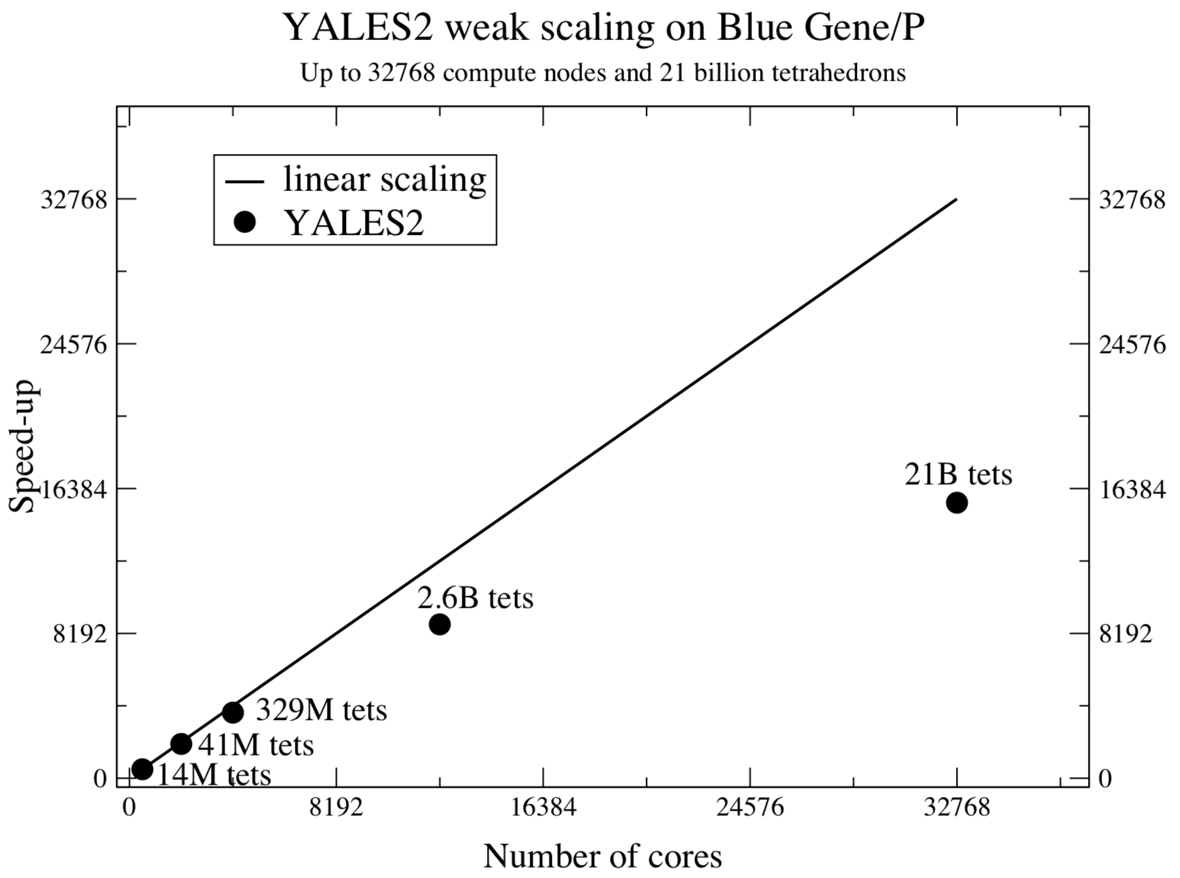


Simulation of PRECCINSTA (Large-eddy simulation)

- **Movie of a combustion** :



Speed-up on PRECCINSTA (solver used : Deflated PCG)



- Most of the computational time is spent in the Pressure-Poisson solver

Plan

- Numerical schemes

- **Double Domain Decomposition** methodology

- « Standard » domain decomposition **deflation**

- Improvements :

    - **linear/quadratic deflation** : idea, implementation and results
    - **stabilization** of PCG algorithm
    - **multi-level deflation** : concept, implementation of three-level deflation

- Conclusion and **perspectives**

Numerical schemes

- **Temporal scheme** : fourth order time integration

  - Runge-Kutta 4 (stable on a centered space discretization, provided that a CFL condition is satisfied)

  - **TRK4** (RK4 with tunable diffusion, obtained by combination of RK4 and Lax-Wendroff-type schemes)

    - Runge-Kutta schemes known to be unstable but non-dissipative, and Lax-Wendroff scheme known to be stable but dissipative
    - Idea : *creating an affine combination of RK and LW second-order spatial derivatives*, and adjusting the coefficients to tune the stability and diffusion of the scheme
    - High CFL numbers for TRK4 schemes can make up for the additional computational costs involved
    - Work to be published by Moureau and coworkers

Numerical schemes

- **Spatial scheme** : centered finite volume method of fourth order

  - conservative : ideal for discontinuities arising in compressible flows (Variable Density Solver) for instance

  - well-adapted to unstructured meshes : RHS computed as a sum of contributions on edges or faces

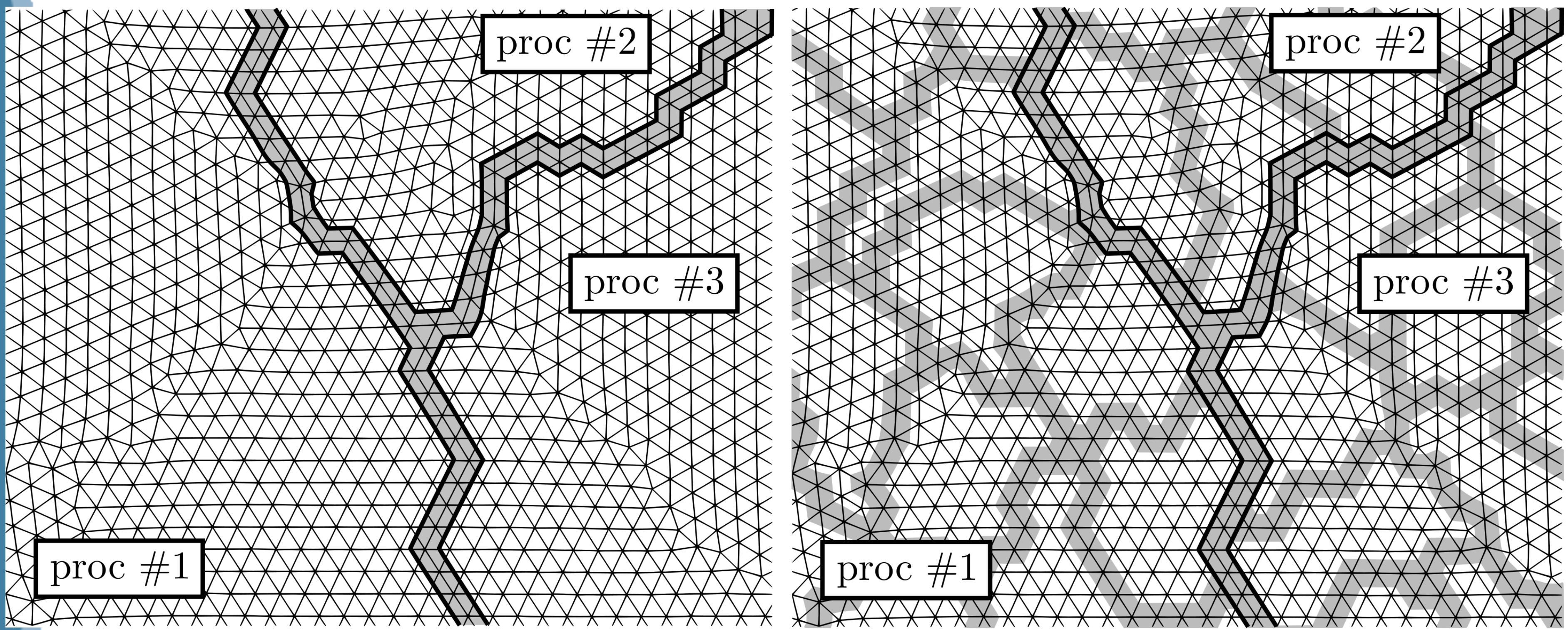
- **Stabilization** : Cabot & Cook fourth-order artificial viscosity

  - Will approximate the cusp in the turbulent energy spectrum induced by fourth-order error

Discretization : DDD

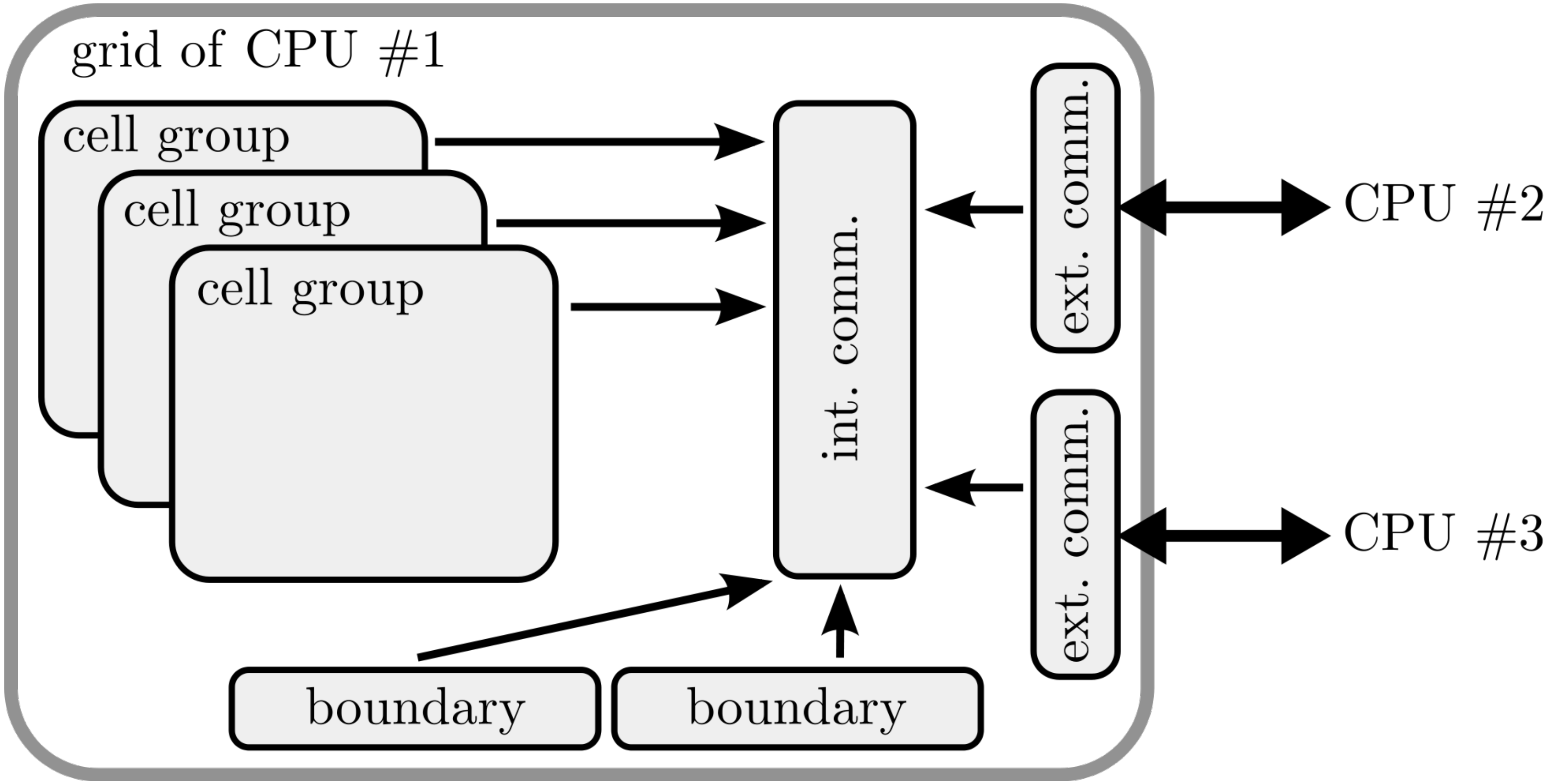
- Unstructured 1D, 2D and 3D solver with different cell geometries afforded (e.g., tetrahedra and hexahedra in 3D).

- **Double Domain Decomposition** methodology :



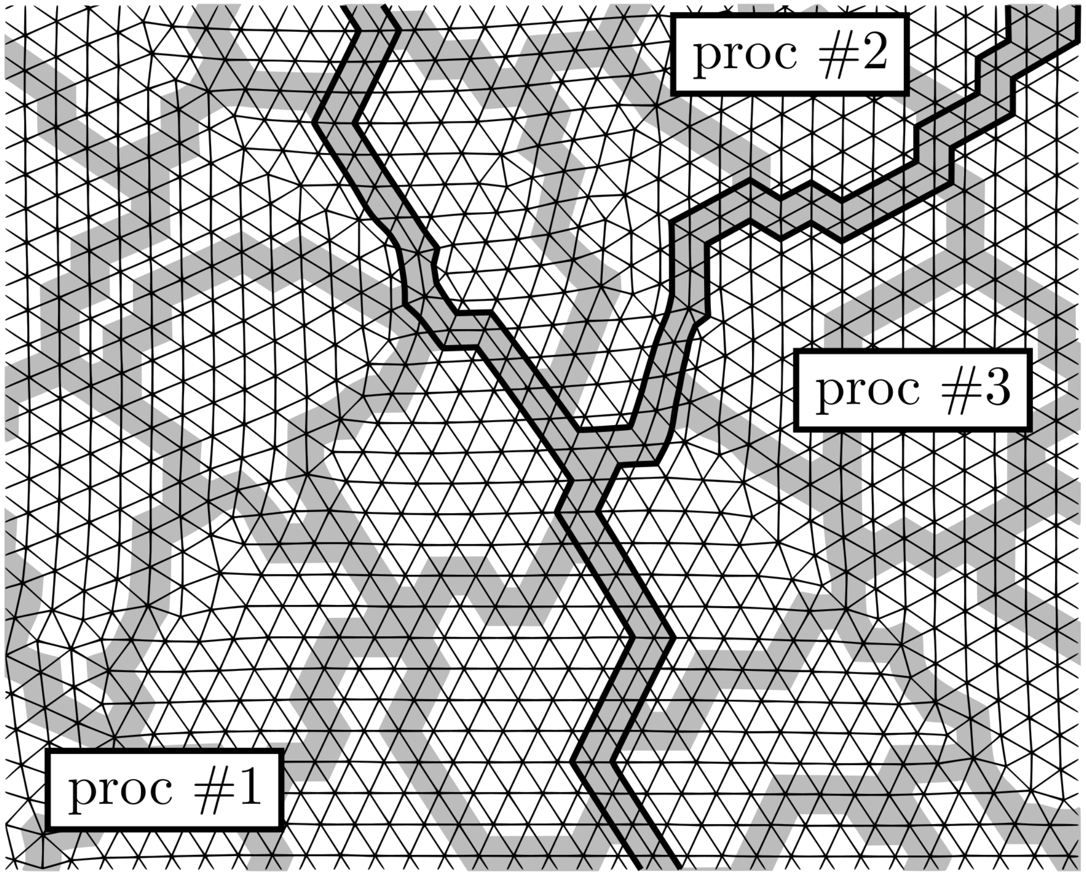
Discretization : DDD

- To deal with this structure, internal communicators are added to the « usual » external communicators



Discretization : DDD

- Advantages of DDD :
  - reduces costs related to parallel use
  - massively parallel comp. (load balancing, local mesh refinement)
  - well-adapted to preconditioned/deflated solvers



- **Deflated PCG** :

  - Preconditioner : inverse of the diagonal
  - Domain Decomposition deflation method on the cell groups

$$E=W^{T}AW \; ; \; Q=WE^{-1}W^{T} \; ; \; P=I-AQ$$

- Quite a common use of deflation (introduced with a mathematical idea of using eigenvectors[1], but widely used as a preconditioner on a coarse grid[2])

- **Deflated BiCGStab(2)** :

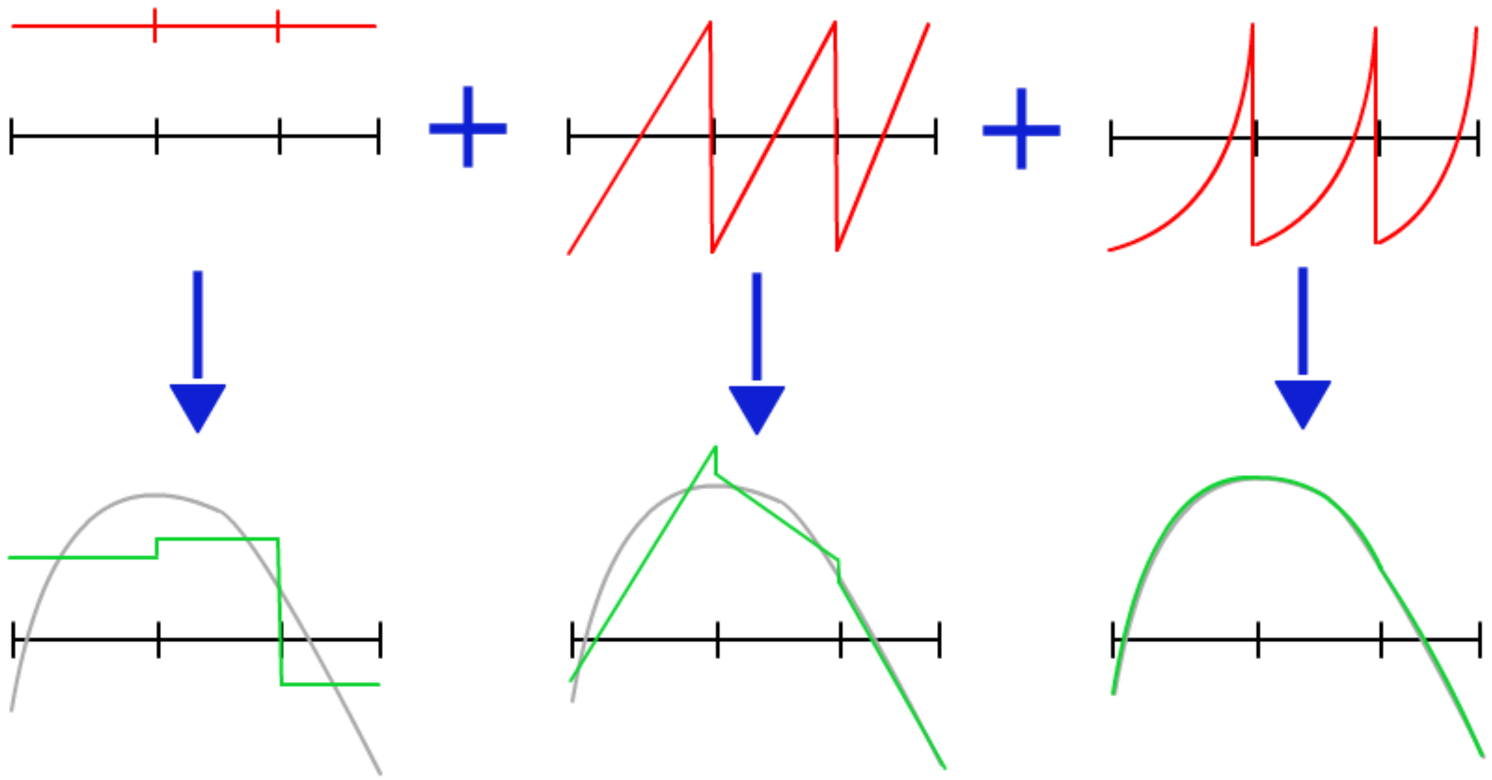
  - Family of BiCGStab(L) introduced in 1993[3] in order to overcome the BiCGStab2 algorithm[4]

[1] Nicolaides, « Deflation of Conjugate Gradients with Application to Boundary Value Problems », 1987
[2] Vermolen, Vuik & Segal, « Deflation in preconditioned conjugate gradient methods for Finite Elements Problems », 2002
[3] Sleijpen & Fokkema, « BiCGStab(L) for linear equations involving unsymmetric matrices with complex spectrum », 1993
[4] Gutknecht, « Variants of BiCGStab for matrices with complex spectrum », 1991

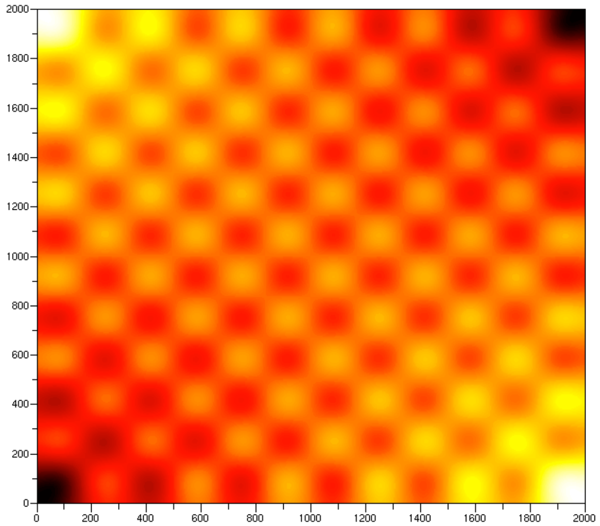
Linear and quadratic deflation

- *Idea :* adding deflation vectors changes the solution of the deflated system

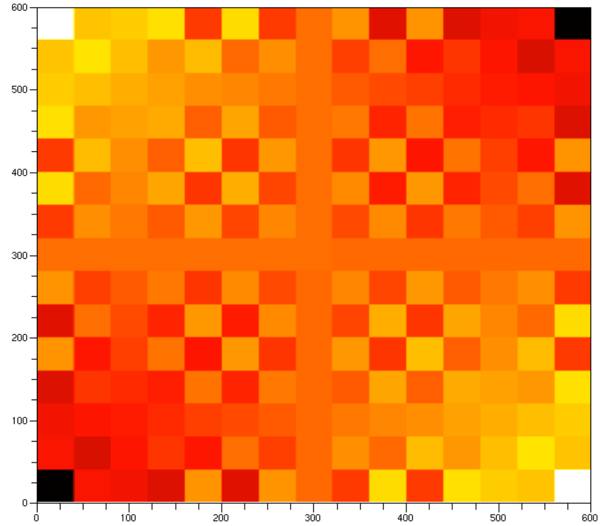
Constant *Linear* *Quadratic*



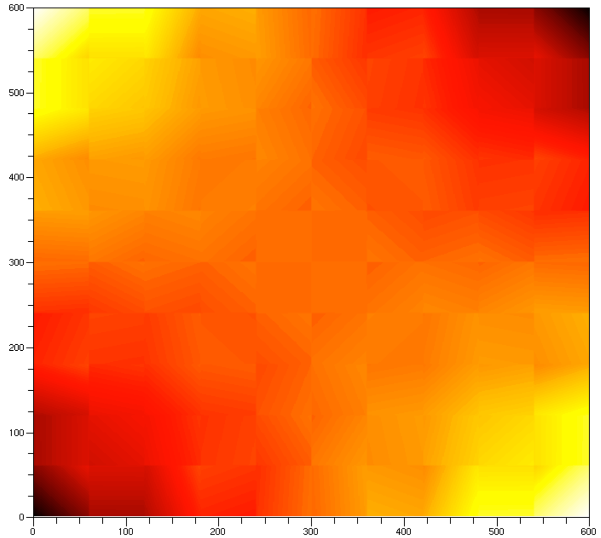
Linear and quadratic deflation : application (2D structured code)



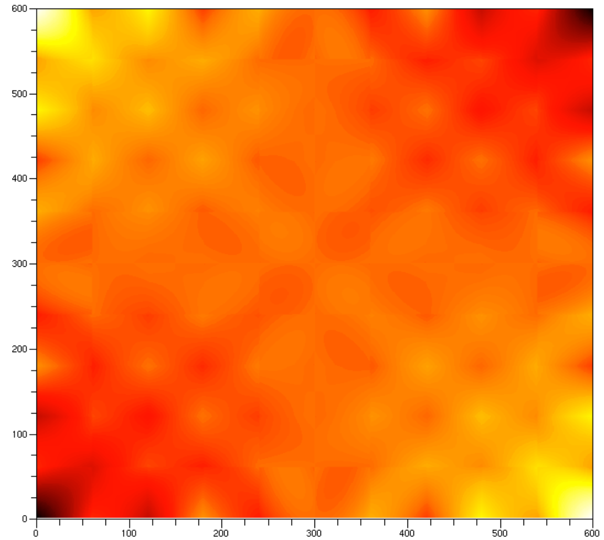
Expected solution



First solution of DD deflation



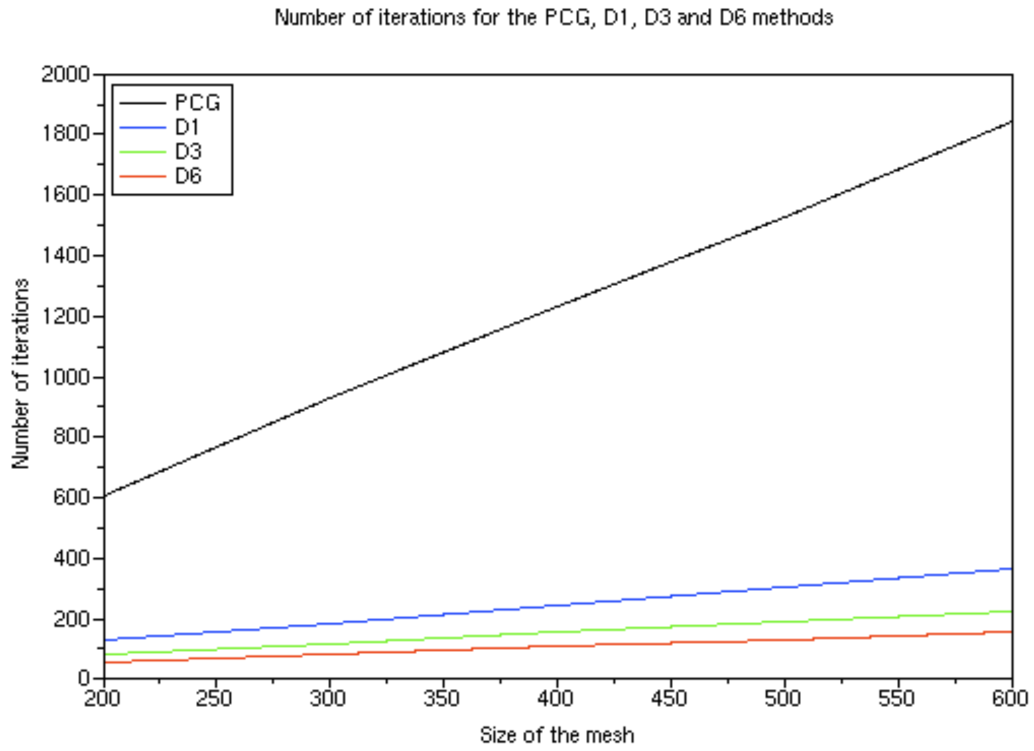
First solution of *linear deflation*



First solution of *quadratic deflation*

Linear and quadratic deflation

- Very promising : number of iterations substantially decreased



- Numerical instabilities in the 3D unstructured solver Yales2 → divergences

- Attempts to stabilize the deflated algorithm (*A-DEF2*)

Improvement of the DPCG algorithm

- Stabilization of Deflated PCG thanks to a 2009 article from Tang and coworkers[1]

  - Deflation, Domain Decomposition and Multigrid Methods are written as preconditioners

  - Multiplicative combination : C_1 and C_2 two preconditioners, then $x^{i+1/2}=x^i+C_1(b-Ax^i)$ and $x^{i+1}=x^{i+1/2}+C_2(b-Ax^{i+1/2})$ give :

$$x^{i+1}=x^i+(\mathbf{C_1+C_2-C_2AC_1})(b-Ax^i)$$

  - Applied to the « usual » inverse of the diagonal M^{-1} and the deflation matrix Q gives birth to the adapted deflations ($P_{A\text{-}DEF1} = M^{-1}P+Q$; $P_{A\text{-}DEF2} = P^T M^{-1}+Q$)

  - The *A-DEF2*, although being quite costly, is shown to be the most stable among nine different methods on a porous media problem and a bubbly flow problem

[1] Tang, Nabben, Vuik & Erlangga, « Comparison of Two-Level Preconditioners Derived from Deflation, Domain Decomposition and Multigrid Methods », 2009

Multi-level deflation

- **3-Level Deflated PCG** :

- Inspired from the multigrid conception, with the benefits of deflation (for unstructured meshes)

  - Thanks to the METIS library, every cell group is split into « subgroups », thus providing an intermediate level between the fine mesh and the coarse mesh

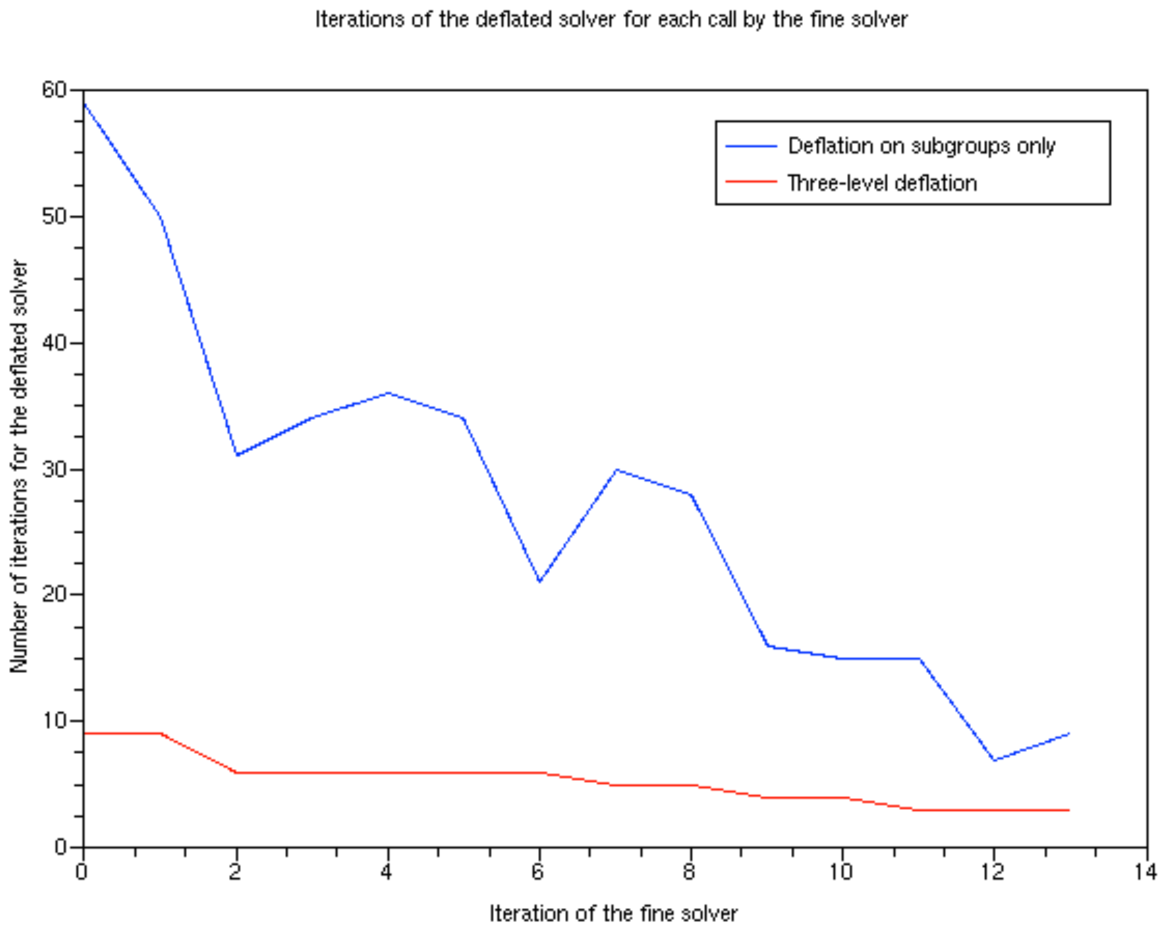
  - The solver on the fine mesh uses deflation on the intermediate mesh, whose solver uses deflation on the coarse mesh

- Aims at reducing the time spent on the deflation on the cell groups

  - Size of cell groups to be adapted carefully, in order not to spend too much time in communications

Multi-level deflation

- Number of iterations of the deflated solver at each call, for identical cell group sizes (3D cartesian grid) :



Conclusion and perspectives

- *Encouraging results* obtained on the multi-level deflation when applied to test-cases

- Evolution of the existing Conjugate Gradient solvers

- Exposed weaknesses on PCG solvers that are to be corrected

- **Next perspective** : recycling the residuals at each iteration

  - Sequence of linear systems $Ax_n=b_n$ to be solved (*n* stands for a time step e.g.)
  - b_n is a linear combination of the vectors $\{b_{n-l},\ldots,b_{n-1}\}$ and an additional vector $ß_n$
  - Projection technique : assured not to deteriorate the system to be solved (contrarily to the standard change $A(x_n-x_{n-1})=b_n-b_{n-1}$)

[1] Fischer, « Projection techniques for iterative solutions of *Ax=b* with successive right-hand sides », 1996

Thank you for your attention !

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