Development of an integral formulation for flows in media cluttered with obstacles in an open-source CFD code

C. Colas, M. Ferrand, J.M. Hérard, X. Martin,
E. Le Coupanec
and also S. Benhamadouche, J. Bonelle, Y. Fournier and O. Hurisse

Fluid Mechanics, Energy and Environment department, EDF R&D

Workshop Industry and Mathematics, November 22^{nd}, 2016

Outlines

Overview

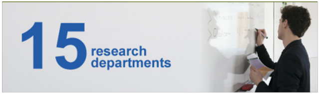
1. Introduction

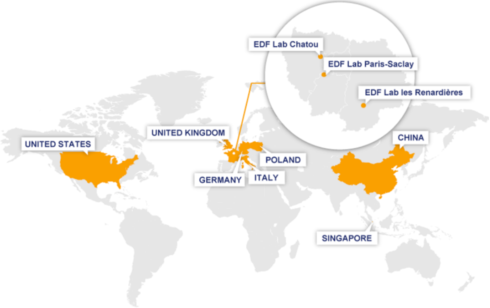
2. Numerical modelling of compressible flows in variable cross section ducts (1D)
   - The standard Well-Balanced approach
   - An alternative semi-discrete approach
   - Inviscid 1D unsteady test case

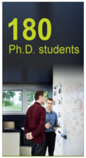
3. Numerical modelling of compressible flows in porous media (3D)
   - Integral formulation applied to implicit time scheme
   - Space discretisation with obstacles
   - Inviscid 2D steady test case

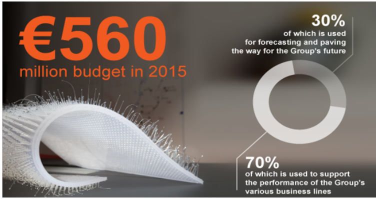
4. Conclusions and perspectives

EDF's R&D Key figures (2015)









EDF's R&D Strategic Priorities

CONSOLIDATE AND DEVELOP COMPETITIVE AND ZERO-CARBON PRODUCTION MIXES

- Consolidate the nuclear assets of the Group and build its future
- Control and anticipate environmental impacts
- Contribute to the success of renewable energy projects and prepare tomorrow's technologies
- Ensure a flexible articulation in the nuclear and renewable mix

DEVELOP AND TEST NEW ENERGY SERVICES FOR CLIENTS

- Develop new offers for our customers
- Promote new uses of electricity
- Develop offers for cities and territories
- Develop energy efficiency services

PAVE THE WAY FOR ELECTRIC SYSTEMS OF THE FUTURE

- Optimize the life of network infrastructure to contribute to the success of smart meter projects
- Contribute to the success of smart meters project
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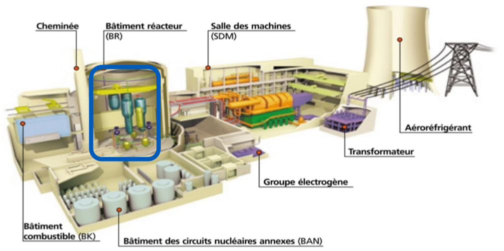
Computational Fluid Dynamics in Nuclear Power Plants

Few applications for safety or design



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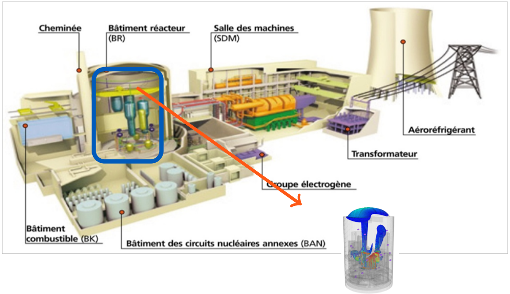

H^2 risk in reactor building

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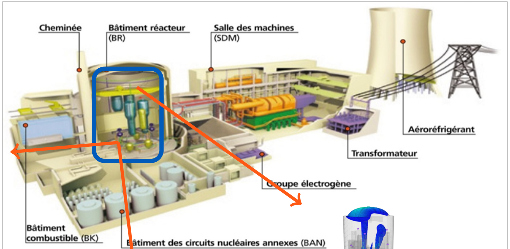
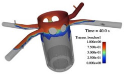
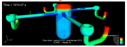
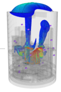




Boron dilution *scenarii*



Pressurised thermal shock



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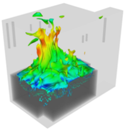
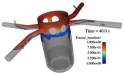


Fuel pool issue



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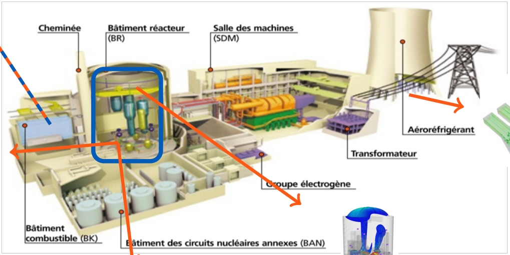
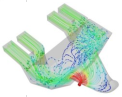
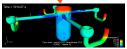




Heat sink



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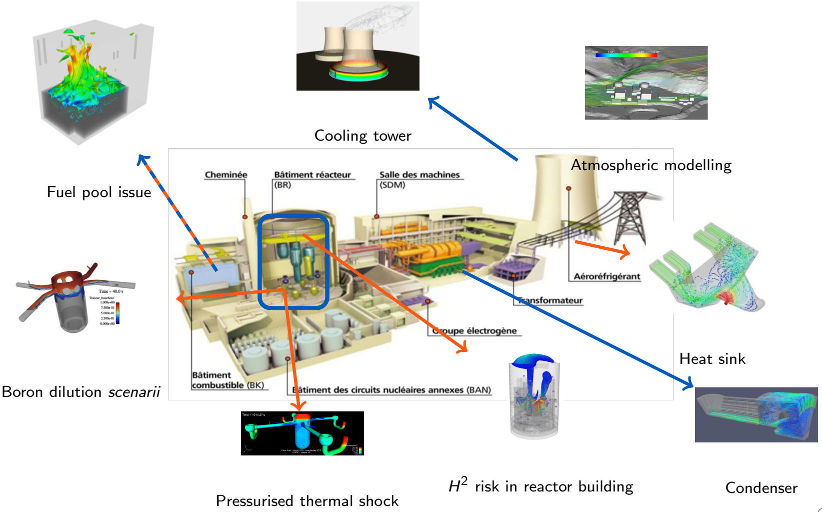

Inhouse CFD code: *Code_Saturne*

development under Quality Insurance

open-source:

`www.code-saturne.org`

- Transparency

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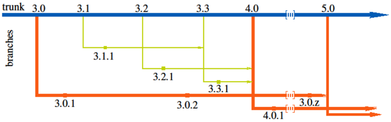

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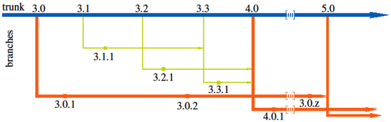

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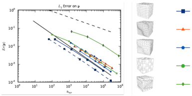

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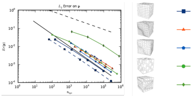
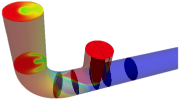
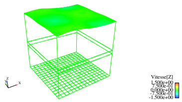




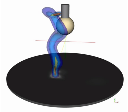
Development of *Code_Saturne* at EDF

Multiphysics modules fused into *Code_Saturne* framework

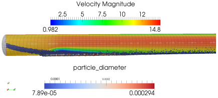
Arbitrary Lagrangian Eulerian (ALE)



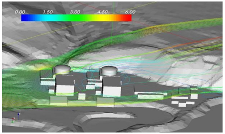
Electric Arc



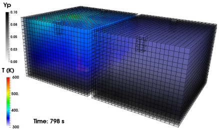
Lagrangian particle tracking



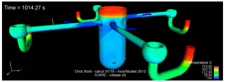
Atmospheric flows



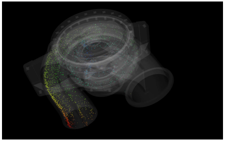
Fire modelling



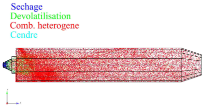
Thermohydraulics for Nuclear applications



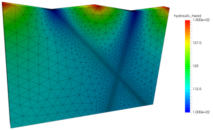
Turbomachinary



Combustion (fuel, coal, gas)



Geological flows



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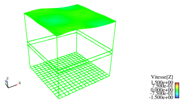

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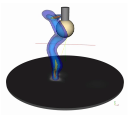

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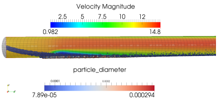

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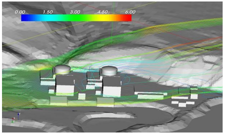

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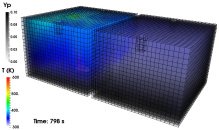

$$
\begin{cases}
\dfrac{\partial \rho}{\partial t} + \text{div}\,\rho \underline{u} = 0 \\
\dfrac{\partial \rho \underline{u}}{\partial t} + \underline{\text{div}}\,(\underline{u} \otimes \rho \underline{u}) = -\underline{\nabla} P \\
+\underline{\text{div}}\left(\mu\left(\underline{\nabla}\,\underline{u} + \underline{\nabla}\,\underline{u}^T\right)\right) + \rho \underline{g}
\end{cases}
$$

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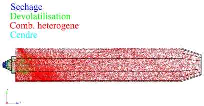

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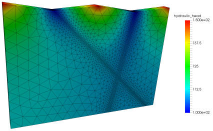

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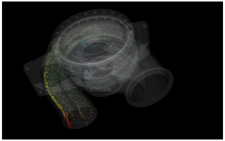
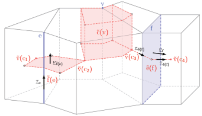
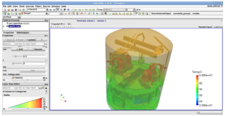


Axes of research and development

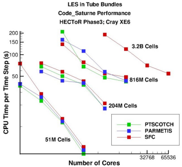
Numerics - Robustness[1,2]



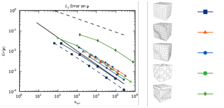
Ergonomic Plateform



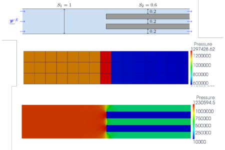
High Performance Computing[4]



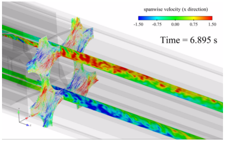
Verification and Validation



Multiscale applications and porous modelling[3]



Turbulence and thermal transfer[5]



A 5-years project is on the road until 2020!

1. J. Bonelle: Compatible Discrete Operator schemes on polyhedral meshes for elliptic and Stokes equations; PhD thesis, 2014.
2. P. Cantin and A. Ern: Vertex-Based Compatible Discrete Operator Schemes on Polyhedral Meshes for Advection-Diffusion Equations, Comput. Methods Appl. Math. 2016

Axes of research and development

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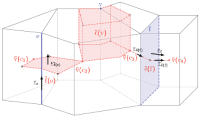

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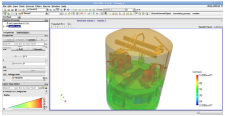

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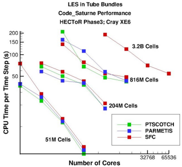

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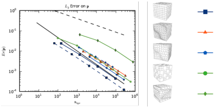

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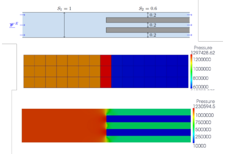

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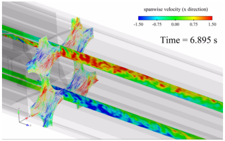

3. O. Hurisse: Verification of a two-phase flow code based on an homogeneous model; IJFV, 2016.

Axes of research and development

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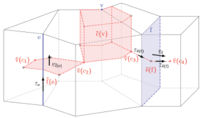

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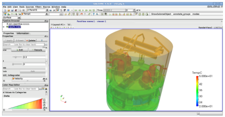

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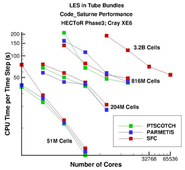

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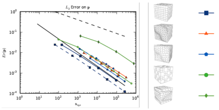

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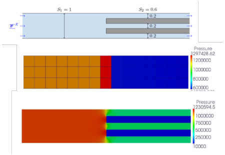

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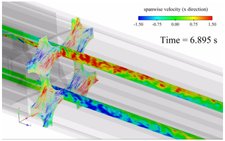

4. Y. Fournier, J. Bonelle, E. Le Coupanec, A. Ribes, B. Lorendeau and C. Moulinec: Recent and Upcoming Changes in *Code_Saturne*: Computational Fluid Dynamics HPC Tools Oriented Features, PARENG, 2015.

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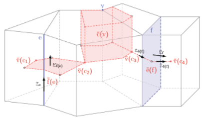

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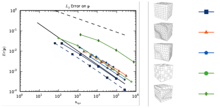
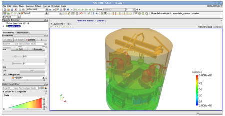
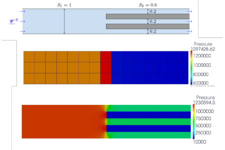


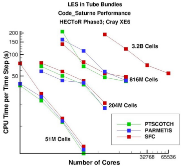
Ergonomic Plateform



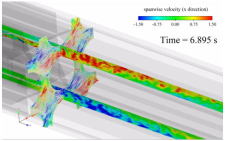
Multiscale applications and porous modelling[3]



High Performance Computing[4]



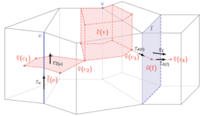
Turbulence and thermal transfer[5]



5. F. Dehoux, S. Benhamadouche, R. Manceau: An elliptic blending differential flux model for natural, mixed and forced convection; IJHFF, 2016.

Axes of research and development

Numerics - Robustness[1,2]



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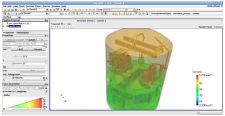

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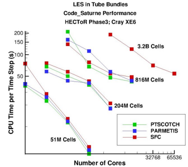

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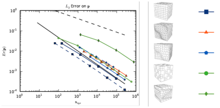

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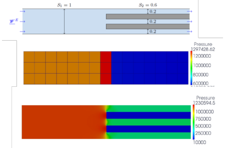

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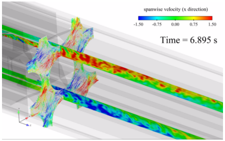
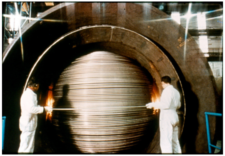


Three scales of modelling

System scale

- $0D$ modelling
- global mass/momentum/energy balances
- correlations
- the boilers, the vessel, ...



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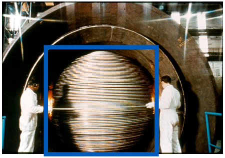

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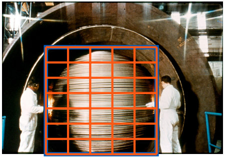
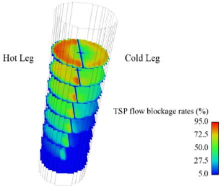


Component scale

- $1D$, $2D$, ($3D$) modelling
- mass / momentum / energy balances of mixture of fluid and solid
- correlations and *porous* approach for the core or the boilers



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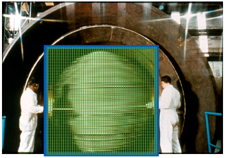

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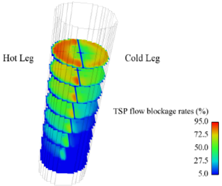

local CFD scale

- $3D$ local modelling
- explicit representation of solids
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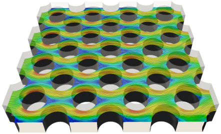

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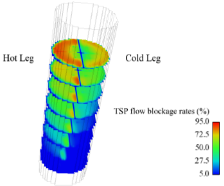

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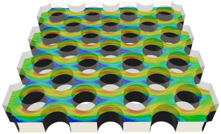

Introduction to porous modelling

Modelling fluid flows in large domains containing small obstacles (so-called "porous" scale) in Pressurized Water Reactors components

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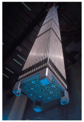

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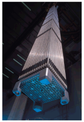

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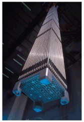

1. G. Le Coq, S. Aubry, J. Cahouet, P. Lequesne, G. Nicolas, S. Pastorini : Bulletin de la Direction des études et recherches - Electricité de France, 1989
2. I. Toumi, A. Bergeron, D. Gallo, E. Royer, D. Caruge : Nuclear Engineering and Design, 2000
3. F. Barre, M. Bernard : Nuclear Engineering and Design, 1990
4. M. Belliard : "Méthodes de décomposition de domaine et de frontière immergée pour la simulation des composants nucléaires." HDR 2014
5. M. Grandotto-Biettoli "Simulation numérique des écoulements diphasiques dans les échangeurs.": HDR 2006

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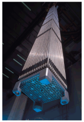

At least two fields of investigation seem mandatory:

Increase knowledge and propose new strategies to cope with flows in obstructed domains, that **degenerate** in a meaningful way when the mesh size tends to zero;

Propose relevant algorithms in order to tackle "low-Mach" number flows.

1. G. Le Coq, S. Aubry, J. Cahouet, P. Lequesne, G. Nicolas, S. Pastorini : Bulletin de la Direction des études et recherches - Electricité de France, 1989
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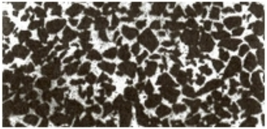
Context and objectives

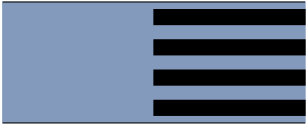
Objectives:

- Modelling viscous incompressible or weakly compressible flows in *media cluttered with obstacles*.
- Treat in the same formalism both fine scale simulations (CFD) and porous simulations at component scale.

Remark: porous media differs from cluttered media of interest



"Usual" porous medium[6]



Medium cluttered with obstacles

- Same ratio of fluid volume over total volume.
- But cluttered media of interest exhibit priviledged directions.

6. J. Bear : "Dynamics of fluids in porous media." Courier Corporation 1972

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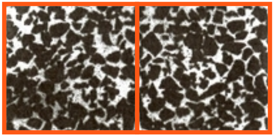

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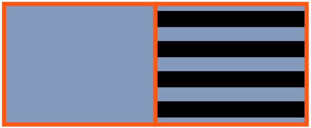

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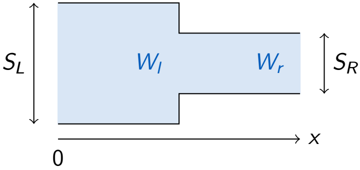
Overview

Classical Well-Balanced approach...

Compute approximations of the one-dimensional set of PDE:

$$\begin{cases} \dfrac{\partial S}{\partial t} = 0 \\ \dfrac{\partial \rho S}{\partial t} + \dfrac{\partial \rho u S}{\partial x} = 0 \\ \dfrac{\partial \rho u S}{\partial t} + \dfrac{\partial \rho u^2 S}{\partial x} + S\dfrac{\partial P}{\partial x} = 0 \\ \dfrac{\partial E S}{\partial t} + \dfrac{\partial u(E+P)S}{\partial x} = 0 \end{cases}$$



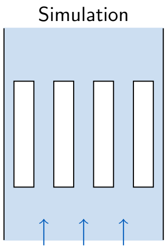
where ρ, u, P and S respectively stand for the density, the velocity, the pressure and the cross-section, and setting: $E = \rho(u^2/2 + \epsilon(P, \rho)))$.

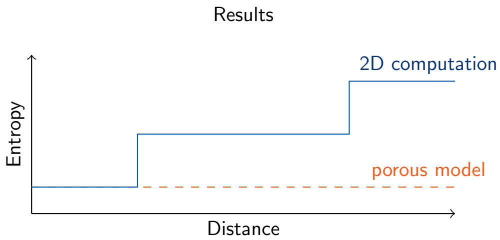
Well-Balanced Finite Volume schemes use an interface condition between cells to connect states between cells. The standard interface condition relies on the preservation of Riemann invariants of the steady contact discontinuity.

6. J.-M. Greenberg, A. Y. Leroux, SIAM J. Numer. Anal., 1996 // 7. L. Gosse, M3AS, 2001 // 8. F. Bouchut 's book, Birkhauser, 2004 // 9. D. Kröner, M.D.Thanh , SIAM J. Numer. Anal., 2006 // 10. D. Kröner, P.G. LeFloch, M.D. Thanh, M2AN, 2008, among many others....

... compared with the basic "numerical experiment"...

Full *n*D experiment with tubes *vs* standard WB 1D porous approach [11]:





The numerical solution preserves the total mass flux and total enthalpy flux; however, the entropy is not! Thus the numerical solution can be built, but is it physically relevant? Probably not!

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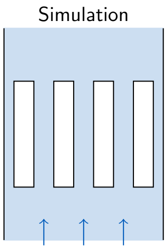

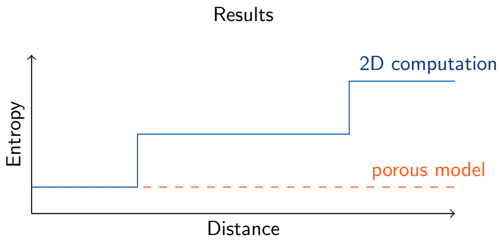

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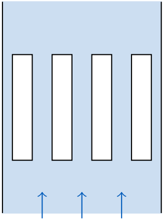
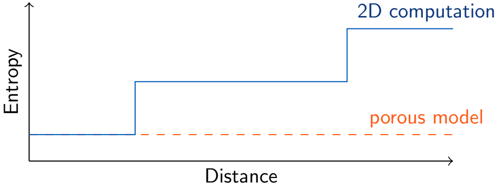
Simulation



Results



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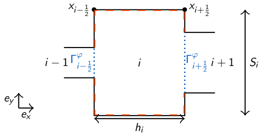
11. L. Girault, J.-M. Hérard, Int. J. Finite Volumes, 2010

A semi-discrete approach

Start with 2D Euler equations to simulate some compressible flow :

$$\begin{cases} \dfrac{\partial \rho}{\partial t} & + \quad \mathrm{div}(\underline{Q}) = 0 \\ \dfrac{\partial \underline{Q}}{\partial t} & + \quad \underline{\mathrm{div}} \left(\underline{Q} \otimes \underline{u}\right) + \underline{\nabla} P = \underline{0} \\ \dfrac{\partial E}{\partial t} & + \quad \mathrm{div}\left(\underline{Q} H\right) = 0 \end{cases}$$



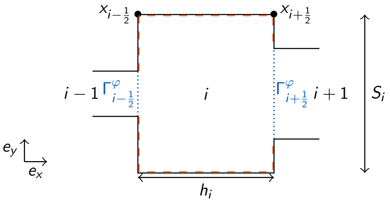
→ Total energy : $E = \rho \left(\left(\underline{u}\right)^2 /2 + \epsilon \left(P, \rho\right) \right)$,

→ Mean momentum: $\underline{Q} = \rho \underline{u}$,

→ Total enthalpy : $H = \dfrac{E+P}{\rho}$.

and integrate over time / space over fixed control volumes, using blue lines for fluid/fluid interfaces. Hence we get:

A semi-discrete approach...

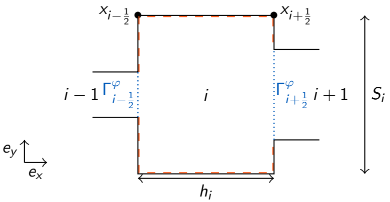


Natural integral formulation:

$$\begin{cases} \Omega_i^{\varphi}\left(\rho_i^{n+1}-\rho_i^n\right) + \displaystyle\int_{t^n}^{t^{n+1}}\int_{\Gamma(i)} \left(\underline{Q}\cdot\underline{n}\right)\left(\underline{x}_{\Gamma},t\right)d\Gamma dt = 0 \\ \Omega_i^{\varphi}\left(\underline{Q}_i^{n+1}-\underline{Q}_i^n\right) + \displaystyle\int_{t^n}^{t^{n+1}}\int_{\Gamma(i)} \left(\left(\underline{Q}\cdot\underline{n}\right)\underline{u}+P\underline{n}\right)\left(\underline{x}_{\Gamma},t\right)d\Gamma dt = \underline{0} \\ \Omega_i^{\varphi}\left(E_i^{n+1}-E_i^n\right) + \displaystyle\int_{t^n}^{t^{n+1}}\int_{\Gamma(i)} \left(\left(\underline{Q}\cdot\underline{n}\right)H\right)\left(\underline{x}_{\Gamma},t\right)d\Gamma dt = 0 \end{cases}$$

$\Omega_i^{\varphi} = S_i \times h_i$ and $\Gamma(i) = \partial\Omega_i^{\varphi}$

A naive explicit Finite Volume scheme



Finite Volume explicit scheme:

$$\left\{\begin{array}{lcl}
\Omega_i^{\varphi}\left(\rho_i^{n+1}-\rho_i^n\right) & + & \Delta t^n \displaystyle\sum_{j\in V(i)} (\underline{Q}\cdot\underline{n})_{ij}^{n,h}\Gamma_{ij} = 0 \\
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\end{array}\right.$$

where the numerical fluxes $(\Psi)^{n,h}$ have to be defined, and noting $V(i)$ the neighbouring cells for cell Ω_i, including mirror cells.

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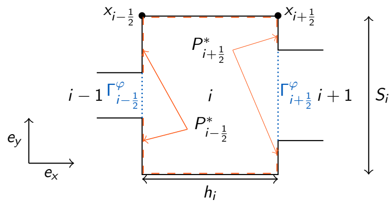
One straightforward result:

The discrete flow remains 1D, if the IC is such that: $u_y = 0$.
Thus the scheme simply computes ρ, E, u_x as follows:



Mass balance :

$$\Omega_i^{\varphi}\left(\rho_i^{n+1}-\rho_i^{n}\right)+\Delta t^n\left((\rho u_x)^{n,h}_{i+1/2}\Gamma^{\varphi}_{i+1/2}-(\rho u_x)^{n,h}_{i-1/2}\Gamma^{\varphi}_{i-1/2}\right)=0$$

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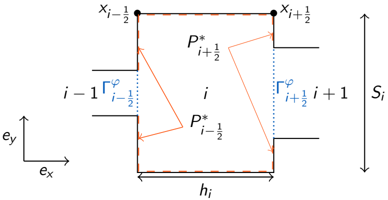

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Total energy balance :

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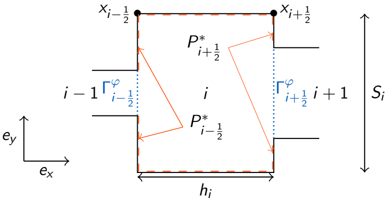

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X-momentum balance (in the $\underline{n}_x$ direction) :

$$\begin{aligned}\Omega_i^{\varphi}\left((\rho u_x)_i^{n+1} - (\rho u_x)_i^n\right) \quad &+ \quad \Delta t^n\left((\rho u_x^2 + P)^{n,h}_{i+1/2}\Gamma^{\varphi}_{i+1/2} - (\rho u_x^2 + P)^{n,h}_{i-1/2}\Gamma^{\varphi}_{i-1/2}\right) \\ &+ \quad \Delta t^n P^*_{i+\frac{1}{2},i}\left(S_i - \Gamma^{\varphi}_{i+1/2}\right) - \Delta t^n P^*_{i-\frac{1}{2},i}\left(S_i - \Gamma^{\varphi}_{i-1/2}\right) = 0\end{aligned}$$

We only need to give some approximation of the pressure $P^*_{.,i}$ at the walls.

Numerical results

We compare three distinct approaches:

A reference solution

which is obtained computing approximate solutions of the 2D Euler equations, using a very fine mesh and an approximate Godunov scheme at fluid/fluid interfaces (VFRoe-ncv[12] scheme, with symmetrizing variable $(\underline{u}, P, s)$).

The Well-Balanced scheme[13]

with the standard interface condition, and using fine meshes;

12. T. Gallouët, J.-M. Hérard, N. Seguin: "On the use of symetrizing variables for vacuums.", Calcolo 2003

13. D. Kröner, M.D.Thanh : "Numerical solutions to compressible flows in a nozzle with variable cross-section." SIAM 2006

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The proposed 1D+ approach:

relying on the previous scheme, using **coarse** or **fine** meshes, an approximate value of the wall pressure P^*, using the mirror state technique, and:

- either the exact value provided by the Riemann solution,
- or almost the same, though substituting the multi-D approximation "$M_i = \frac{\underline{u}_i \cdot \underline{n}}{c_i} = 0$" in the latter formula ($P^* = P_i$).

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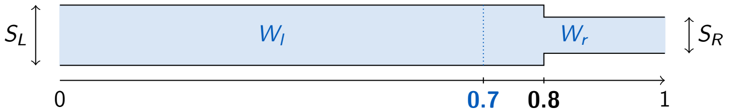
Numerical results...

We consider the following basic **unsteady** flow in a pipe:

- Two uniform pipes with a sudden contraction (or enlargement) : $S(x < x_s) = S_L; \quad S(x > x_S) = S_R$, with four distinct aspect ratios (S_L/S_R);
- IC: two distinct states W_L, W_R on each side of $x_{IC} = 0.7$, using "gentle" Sod data:
  - $W_L = (\rho_L, u_L, P_L) = (1, 0, 10^5)$
  - $W_R = (\rho_R, u_R, P_R) = (0.125, 0, 10^4)$

  with perfect gas EOS (setting $\gamma = 7/5$);
- Use 1D coarse or fine meshes (from 100 up to 10^5 uniform 1D cells), and 0.64×10^6 cells for the 2D reference solution.



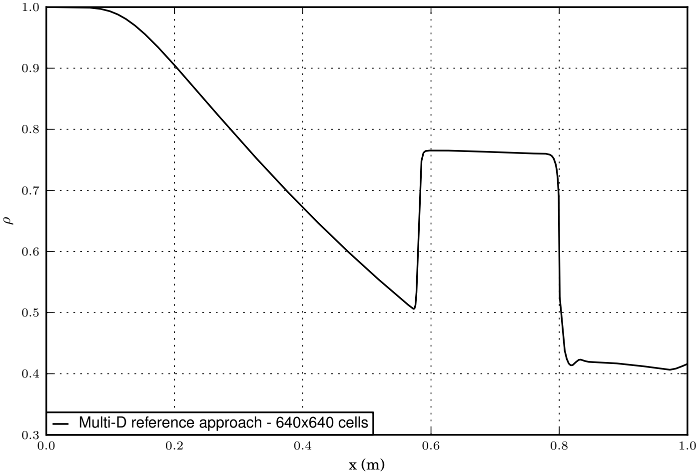
Numerical results...

Examine two cases among the 16 test cases below with different **aspect ratios** and **IC**:

	S_L	S_R	$\underline{W}(t=0.,x<0.7)$			$\underline{W}(t=0.,x>0.7)$		
	$x<0.8$	$x>0.8$	ρ	u	P	ρ	u	P
cas 1	1	**0.5**	1	0	10^5	0.125	0	10^4
cas 2	1	**0.01**	1	0	10^5	0.125	0	10^4
cas 3	1	0.5	0.125	0	10^4	1	0	10^5
cas 4	1	0.01	0.125	0	10^4	1	0	10^5
cas 5	0.5	1	1	0	10^5	0.125	0	10^4
cas 6	0.01	1	1	0	10^5	0.125	0	10^4
cas 7	0.5	1	0.125	0	10^4	1	0	10^5
cas 8	0.01	1	0.125	0	10^4	1	0	10^5
cas 9	1	0.1	1	0	10^5	0.125	0	10^4
cas 10	1	0.9	1	0	10^5	0.125	0	10^4
cas 11	1	0.1	0.125	0	10^4	1	0	10^5
cas 12	1	0.9	0.125	0	10^4	1	0	10^5
cas 13	0.1	1	1	0	10^5	0.125	0	10^4
cas 14	0.9	1	1	0	10^5	0.125	0	10^4
cas 15	0.1	1	0.125	0	10^4	1	0	10^5
cas 16	0.9	1	0.125	0	10^4	1	0	10^5

Numerical results...(test case 1: $S_L/S_R = 2$)

Density profile at time $T = 1.5 \times 10^{-3}$ using $CFL = 1/2$.



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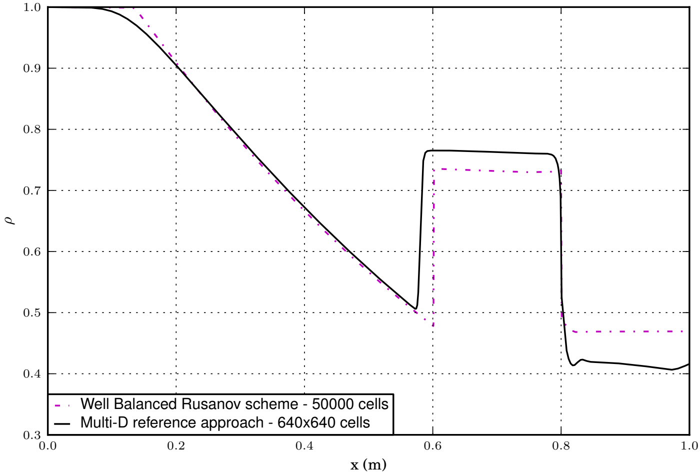

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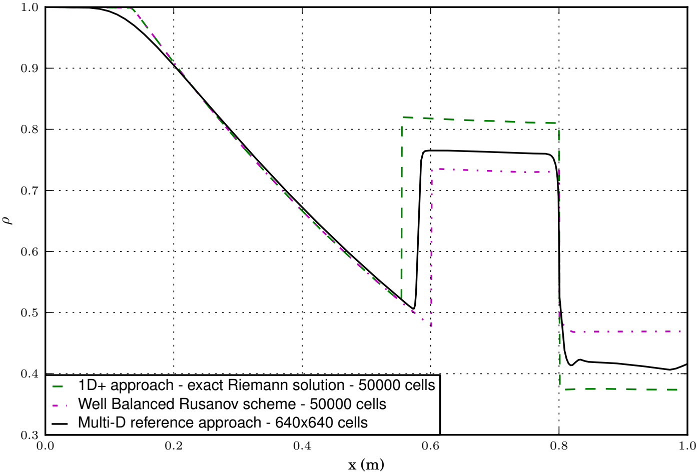

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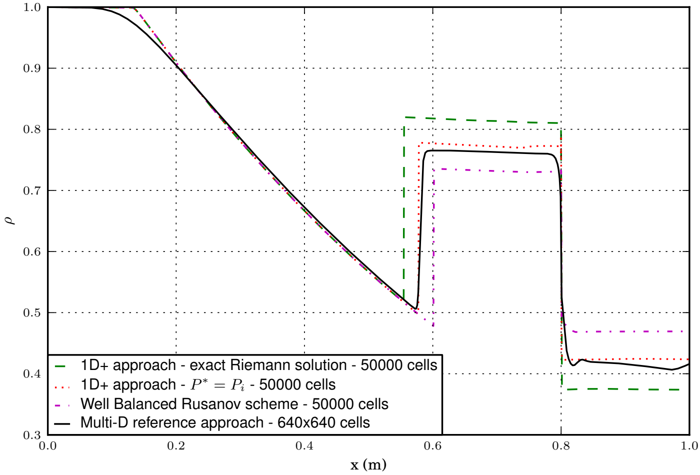

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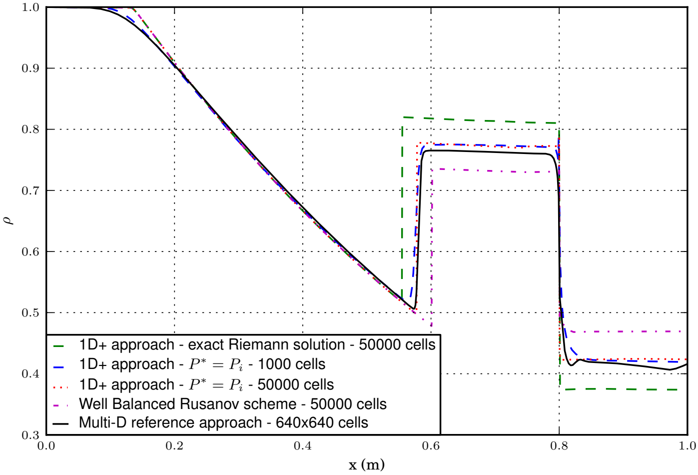
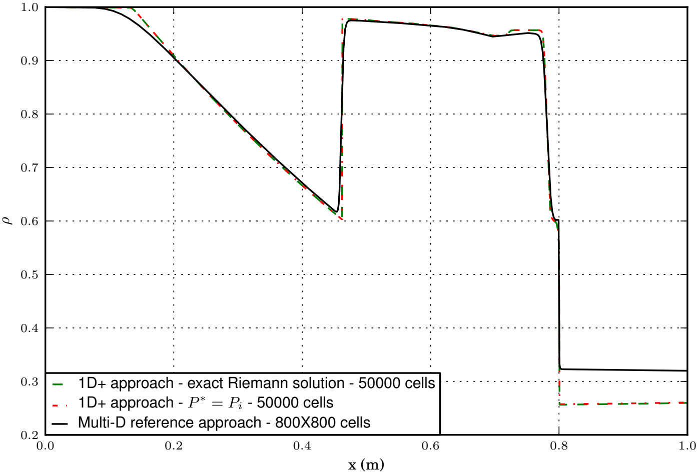


Numerical results...(test case 2: $S_L/S_R = 100$)

Density profile at time $T = 1.5 \times 10^{-3}$ using $CFL = 1/2$.

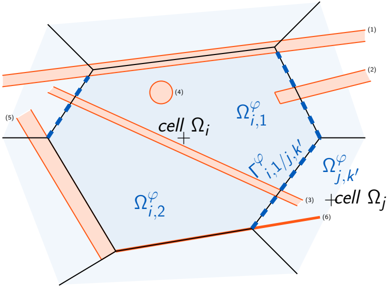


Overview

A semi-discrete approach
Some notations

Notations on an ordinary control volume Ω_i with internal elements

- $\Omega^{\varphi}_{i,k}$ fluid sub-cell of Ω_i.
- $\Omega^{\varphi}_{i} = \bigcup_k \Omega^{\varphi}_{i,k}$ total volume occupied by the fluid.
- $\Gamma^{\varphi}_{i,k/j,k'}$ fluid interface ("fluid passing" surface) between $\Omega^{\varphi}_{i,k}$ and $\Omega^{\varphi}_{j,k'}$.



Ferrand M., Hérard J.-M., Lecoupanec E., Martin X: Une formulation intégrale implicite pour la modélisation d'écoulements fluides en milieu encombré d'obstacles; EDF report H-I83-2015-05276-FR, in French, 2015.

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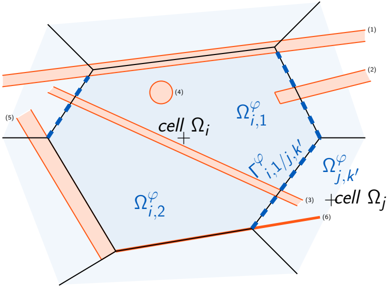

Characteristics of the internal elements (obstacles):

- Impermeable and steady.
- Typically plates or tubes.
- Totally or partially included in one control volume, or tangent to an interface between two control volumes.

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Governing equations for inviscid flows

System of Euler equations for a compressible flow

$$\begin{cases} \dfrac{\partial \rho}{\partial t} + \mathrm{div}(\underline{Q}) = 0 \\ \dfrac{\partial \underline{Q}}{\partial t} + \mathrm{div}(\underline{Q} \otimes \underline{Q}/\rho) + \underline{\nabla} P = \underline{0} \\ \dfrac{\partial E}{\partial t} + \mathrm{div}\left(\underline{Q}(E+P)/\rho\right) = 0 \end{cases}$$

The state vector $\underline{W}(\mathbf{x}, t) = \left(\rho, \underline{Q}, E\right)^t$ is the conservative variable.

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Mean value of $\underline{W}$ in the fluid sub-cell $\Omega^{\varphi}_{i,k}$ at time t:

$$\underline{W}_{i,k}(t) = \frac{1}{\Omega^{\varphi}_{i,k}} \left(\int_{\Omega^{\varphi}_{i,k}} \underline{W}(\mathbf{x}, t) dx \right)$$

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Mean value of $\underline{W}$ in the control volume Ω_i at time t with $\Omega^{\varphi}_i = \sum_k \Omega^{\varphi}_{i,k}$:

$$\underline{W}_i(t) = \frac{1}{\Omega^{\varphi}_i} \left(\sum_{k \in \{1, N(i)\}} \underline{W}_{i,k}(t) \Omega^{\varphi}_{i,k} \right)$$

Integral form

Starting from the following consise form of the conservation laws (Euler system):

$$\frac{\partial \underline{W}}{\partial t} + \underline{\mathrm{div}} \left(\underline{\underline{F}} \left(\underline{W} \right) \right) = \underline{0}$$

Integration over a fluid sub-cell $\Omega_{i,k}^{\varphi}$ of a control volume Ω_i and over a time interval $[t_1, t_2]$:

$$\int_{\Omega_{i,k}^{\varphi}} \left(\underline{W}(\mathbf{x}, t_2) - \underline{W}(\mathbf{x}, t_1) \right) d\Omega + \int_{t_1}^{t_2} \int_{\Omega_{i,k}^{\varphi}} \left(\underline{\mathrm{div}} \left(\underline{\underline{F}} \left(\underline{W} \right) \right) \right) d\Omega dt = \underline{0}$$

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Integration over the boundary $\Gamma_{i,k}$ of $\Omega^{\varphi}_{i,k}$ (Green formula):

$$\int_{\Omega^{\varphi}_{i,k}} \left(\underline{W}(\mathbf{x}, t_2) - \underline{W}(\mathbf{x}, t_1) \right) d\Omega + \int_{t_1}^{t_2} \int_{\Gamma_{i,k}} \left(\underline{\underline{F}}(\underline{W}(\mathbf{x}, t)) \cdot \underline{n} \right) d\Gamma dt = \underline{0}$$

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Splitting of the surface integral between fluid $\Gamma^{\varphi}_{i,k}$ and solid boundary $\Gamma^{w}_{i,k}$ so that:

$$\Gamma_{i,k} = \Gamma^{\varphi}_{i,k} \cup \Gamma^{w}_{i,k}$$

$$\emptyset = \Gamma^{\varphi}_{i,k} \cap \Gamma^{w}_{i,k}$$

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And finally summing over the $N(i)$ sub-cells of Ω_i:

$$\Omega_i^{\varphi} \left(\underline{W}_i(t_2) - \underline{W}_i(t_1) \right) + \sum_{k=1}^{N(i)} \left(\int_{t_1}^{t_2} \int_{\Gamma_{i,k}^{\varphi}} \left(\underline{\underline{F}}(\underline{W}(\mathbf{x}, t)) \cdot \underline{n} \right) d\Gamma dt \right)$$
$$+ \sum_{k=1}^{N(i)} \left(\int_{t_1}^{t_2} \int_{\Gamma_{i,k}^{w}} \left(\underline{\underline{F}}(\underline{W}(\mathbf{x}, t)) \cdot \underline{n} \right) d\Gamma dt \right) = \underline{0}$$

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$$\emptyset = \Gamma_{i,k}^{\varphi} \cap \Gamma_{i,k}^{w}$$

Time scheme: mass balance step

Integration over space and time:

$$\int_{t^n}^{t^{n+1}} \int_{\Omega\varphi} \left(\frac{\partial \rho}{\partial t} + \text{div}\underline{Q} \right) d\Omega dt = 0$$

Time scheme: mass balance step

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$$\int_{t^n}^{t^{n+1}} \int_{\Omega^\varphi} \left(\frac{\partial \rho}{\partial t} + \mathrm{div} \underline{Q} \right) d\Omega dt = 0$$

Time scheme:

$$\Omega_i^\varphi (\rho^{n+1,-} - \rho^n) + \Delta t^n \int_\Gamma \underline{Q}^* . \underline{n} d\Gamma = 0$$

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Time scheme:

$$\Omega_i^\varphi \underbrace{\left(\rho^{n+1,-} - \rho^n \right)}_{\delta \rho} + \Delta t^n \int_\Gamma \underline{Q}^* . \underline{n} d\Gamma = 0$$

Unsteady term linearisation:

Time scheme: mass balance step

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Unsteady term linearisation:

$$dP = \left. \frac{\partial P(\rho, s)}{\partial \rho} \right|_s d\rho + \left. \frac{\partial P(\rho, s)}{\partial s} \right|_\rho \underbrace{ds}_{=0}$$

.

Time scheme: mass balance step

Integration over space and time:

$$\int_{t^n}^{t^{n+1}} \int_{\Omega^\varphi} \left(\frac{\partial \rho}{\partial t} + \mathrm{div} \underline{Q} \right) d\Omega dt = 0$$

Time scheme:

$$\Omega_i^\varphi \frac{1}{(c^2)^n} \underbrace{\left(P^{n+1,-} - P^n\right)}_{\delta P} + \Delta t^n \int_\Gamma \underline{Q}^* . \underline{n} d\Gamma = 0$$

Unsteady term linearisation:

$$\delta P = c^2(P^n, \rho^n) \delta \rho$$

.

Time scheme: mass balance step

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$$\int_{t^n}^{t^{n+1}} \int_{\Omega^\varphi} \left(\frac{\partial \rho}{\partial t} + \text{div}\underline{Q} \right) d\Omega dt = 0$$

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Unsteady term linearisation:

$$\rho^{n+1,-} = \rho^n + \delta\rho = \rho^n + \frac{\delta P}{c^2}$$

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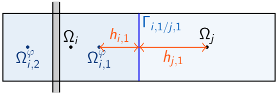
.

Convective mass flux computed with a simplified momentum balance:

$$\underline{Q}^* = \underline{Q}^n - \Delta t^n \nabla P^{n+1,-}$$

.

Space scheme: mass balance step (1)



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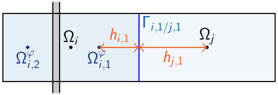

Splitting between fluid and solid boundary :

$$\Omega_i^{\varphi}\frac{1}{(c^2)^n}(P^{n+1,-}-P^n)+\Delta t^n\int_{\Gamma^{\varphi}}\underline{Q}^*.\underline{n}d\Gamma+\Delta t^n\int_{\Gamma^w}\underline{Q}^*\cdot\underline{n}d\Gamma=0$$

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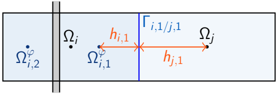

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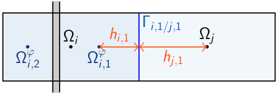

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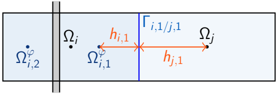

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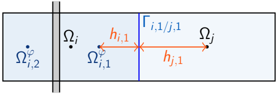

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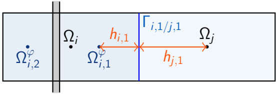
Evaluation of the 2 integrals over the fluid boundary:

Space scheme: mass balance step (1)



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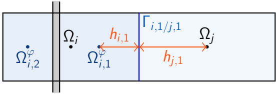
$$\Omega_i^{\varphi}\frac{1}{(c^2)^n}(P^{n+1,-}-P^n)+\Delta t^n\int_{\Gamma^{\varphi}}\underline{Q}^n\cdot\underline{n}d\Gamma-\Delta t^n\int_{\Gamma^{\varphi}}\underline{\nabla}P^{n+1,-}\cdot\underline{n}d\Gamma=0$$

Evaluation of the 2 integrals over the fluid boundary:

$$\int_{\Gamma_i^{\varphi}}\underline{Q}^n.\underline{n}d\Gamma=\sum_{k\in\{1,N(i)\}}\sum_{(j,k')\in V(i)}\rho^{n^{upw}}_{i,k/j,k'}(\underline{u}^n\cdot\underline{n})_{i,k/j,k'}S^{\varphi}_{i,k/j,k'}$$

With: $(\underline{u}^n\cdot\underline{n})_{i,k/j,k'}=\left(\alpha_{i,k/j,k'}\underline{u}_i+(1-\alpha_{i,k/j,k'})\,\underline{u}_j\right)^n\cdot\underline{n}_{i/j}$, $\alpha_{i,k/j,k'}=\frac{h_{j,k'}}{h_{i,k}+h_{j,k'}}$.

Space scheme: mass balance step (1)



Splitting between fluid and solid boundary :

$$\Omega_i^{\varphi}\frac{1}{(c^2)^n}(P^{n+1,-}-P^n)+\Delta t^n\int_{\Gamma^{\varphi}}\underline{Q}^n\cdot\underline{n}d\Gamma-\Delta t^n\int_{\Gamma^{\varphi}}\underline{\nabla}P^{n+1,-}\cdot\underline{n}d\Gamma=0$$

Evaluation of the 2 integrals over the fluid boundary:

$$\int_{\Gamma_i^{\varphi}}\underline{Q}^n.\underline{n}d\Gamma=\sum_{k\in\{1,N(i)\}}\sum_{(j,k')\in V(i)}\rho^{n^{upw}}_{i,k/j,k'}(\underline{u}^n\cdot\underline{n})_{i,k/j,k'}S^{\varphi}_{i,k/j,k'}$$

With: $(\underline{u}^n\cdot\underline{n})_{i,k/j,k'}=\left(\alpha_{i,k/j,k'}\underline{u}_i+(1-\alpha_{i,k/j,k'})\,\underline{u}_j\right)^n\cdot\underline{n}_{i/j},\ \alpha_{i,k/j,k'}=\frac{h_{j,k'}}{h_{i,k}+h_{j,k'}}.$

$$\int_{\Gamma_i^{\varphi}}\underline{\nabla}P^{n+1,-}\cdot\underline{n}d\Gamma=\sum_{k\in\{1,N(i)\}}\sum_{(j,k')\in V(i)}\frac{S^{\varphi}_{i,k/j,k'}}{h_{i,k}+h_{j,k'}}(P_j-P_i)^{n+1,-}$$

Space scheme: mass balance step (2)

Positivity of the pressure $P^{n+1,-}$ and the density $\rho^{n+1,-}$

Writing of the mass balance under its matrix form : $\underline{\underline{A}}\ \underline{X} = \underline{B}$ with $\underline{X} = \left(P_i^{n+1,-}\right)_{i\in\{1,N_{cells}\}}$, with $\underline{\underline{A}}$ **an M-matrix**.

Moreover, if $\forall i, |A_{ii}| - \sum_{j\neq i} \left|A_{ij}\right| > 0$, $\underline{\underline{A}}$ is inversible and $\underline{\underline{A^{-1}}}$ **is positive**.

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CFL-like condition:

$$\Omega_i^{\varphi} \geq \Delta t^n \sum_{k\in\{1,N(i)\}} \sum_{(j,k')\in V(i)} \beta_{i,k/j,k'} \left(\frac{\rho_i c_i^2}{P_i}\right)^n (\underline{u}^n \cdot \underline{n})_{i,k/j,k'} S_{i,k/j,k'}^{\varphi}$$

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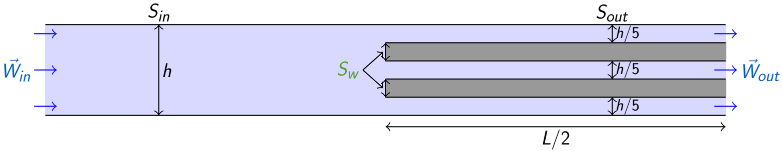
Property :

Let be $\rho_i^n > 0$ and $P_i^n > 0$. If the CFL condition is verified, then $\forall i, P_i^{n+1,-} > 0$.
Moreover, $P_i^{n+1,-} > 0 \Rightarrow \rho_i^{n+1,-} > 0$.

Test case: flow in a channel cluttered with obstacles (1)

Description:

- 2D steady flow at low Mach number.
- Inviscid compressible fluid.
- Infinite channel partially cluttered with impermeable tubes.



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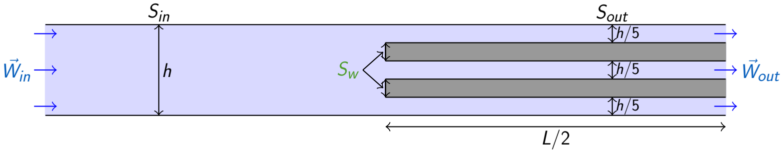

The time step is driven by the CFL condition.

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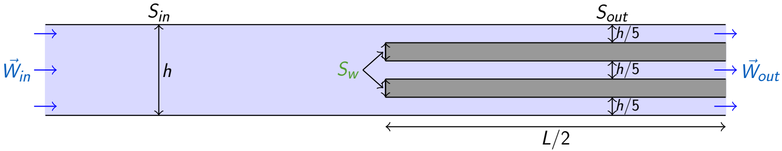


The time step is driven by the CFL condition.

Boundary conditions:

- **Symmetry** on bottom and top boundaries.
- **Half Riemann problem solving** at the inlet and outlet.

Test case: flow in a channel cluttered with obstacles (2)

Structured orthogonal mesh **adapted** to the fluid domain :
24×5, 48×10, 96×20, 192×40, 384×80, and 768×160 cells

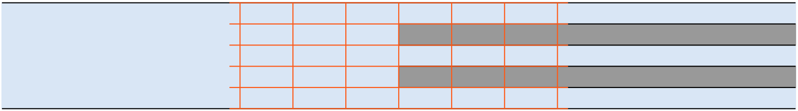


Figure: Adapted mesh composed of 24×5 cells

Structured orthogonal mesh with **porous** cells, **not adapted** to the fluid domain : 24×6, 48×12, 96×24, 192×48 cells

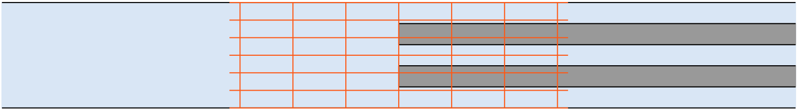


Figure: Not adapted mesh composed of 24×6 cells

Test case: flow in a channel cluttered with obstacles (3)

Steady flow, unidirectional at the infinite upstream and downstream:

$$\begin{aligned}(QS)_{in} &= (QS)_{out} \\ (QHS)_{in} &= (QHS)_{out} \\ ((QU+P)\,S)_{in} &= ((QU+P)\,S)_{out} + P^w S_w\end{aligned}$$

with P^w the **mean** pressure at the inlet of the cluttered zone,
and $S_w = S_{in} - S_{out}$ the surface of the inlet of the cluttered zone.

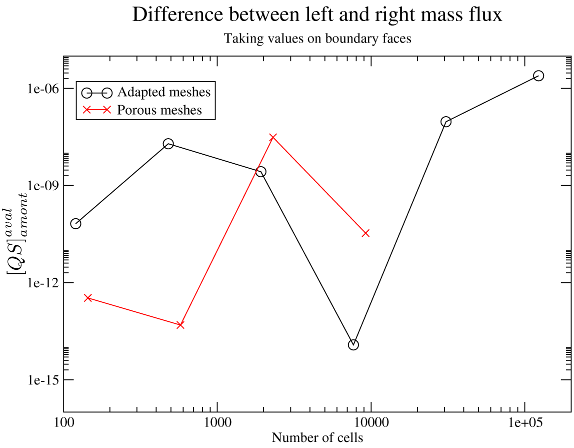
Difference between upstream and downstream flux deduced from the conservation laws:

$$e(\xi) = \frac{|\xi_{in} - (\xi_{out} + \Delta)|}{|\xi_{in}| + |\xi_{out}| + |\Delta|}$$

with $\xi = (QS, QHS, (QU+P)S)$ and $\Delta = (0., 0., P^w S_w)$

Test case: flow in a channel cluttered with obstacles (4)

Difference between upstream and downstream flux:



Test case: flow in a channel cluttered with obstacles (4)

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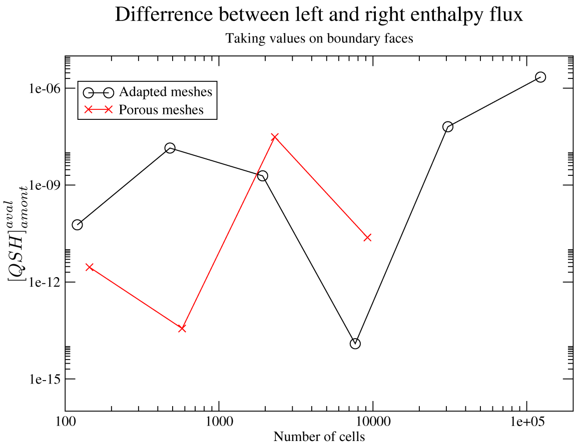

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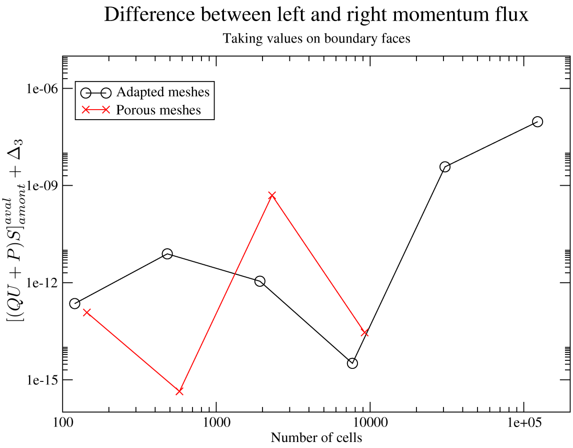
Difference between upstream and downstream flux:



Overview

Conclusions

Approach based on:

- an **integral formulation** over ordinary control volumes,
- and an estimation of the pressure at fluid/solid interfaces.

Reliable method for the future:

- Objectives reached on coarse structured meshes (components code scale),
- Adapted to the growing performances of computers,
- Convergence towards purely fluid simulation ("CFD" scale),
- Derived and tested with **implicit** and **explicit** schemes (not presented here).

Approach implemented in *Code_Saturne*:

- for compressible flows,
- using implicit schemes based on *Code_Saturne* compressible fractional step method.

Perspectives

in the starting thesis...

With different time schedules

- Propose a formulation to take correctly into account viscous shear stress and turbulence at “components” scale and at scales between the “components” and “CFD” ones.

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- Apply integral formulation to incompressible flow.

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- Comparison with porous codes on validation cases of THYC.
- Apply integral formulation to incompressible flow.
- Implement a generic pre-processor for ordinary meshes.
- Adapt the integral approach to multi-phase homogeneous models.

Thank you for your attention.
Any question?

Overview

5 Appendix
- Integral formulation applied to implicit time scheme
- Space discretisation with obstacles

Time scheme: momentum balance step

Integration over space and time :

$$\int_{t^n}^{t^{n+1}} \int_{\Omega\varphi} \left(\frac{\partial \underline{Q}}{\partial t} + \underline{\text{div}} \left(\underline{u} \otimes \underline{Q} \right) + \underline{\nabla} P \right) d\Omega dt = 0$$

Time scheme: momentum balance step

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Time scheme:

$$\Omega_i^\varphi \left(\underline{Q}^{n+1,-} - \underline{Q}^n \right) + \Delta t^n \int_\Gamma \underline{u}^{n+1,-} \left(\underline{Q}^* . \underline{n} \right) d\Gamma + \Delta t^n \int_\Gamma P^{n+1,-} \underline{n} d\Gamma = 0$$

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We obtain:

- The velocity $\underline{u}^{n+1,-}$.
- And $\underline{Q}^{n+1,-} = \underline{u}^{n+1,-} \rho^{n+1,-}$ (different from $\underline{Q}^*$!).

Time scheme: energy balance step

Integration over space and time :

$$\int_{t^n}^{t^{n+1}} \int_{\Omega\varphi} \left(\frac{\partial E}{\partial t} + \mathrm{div}(\underline{u}(E+P)) \right) d\Omega dt = 0$$

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Updates of the variables:

$$(\rho, \underline{u}, E)^{n+1} = (\rho, \underline{u}, E)^{n+1,-}$$

$$P^{n+1} = P\left(\rho^{n+1}, e^{n+1}\right) \text{ where } e^{n+1} = \frac{E^{n+1}}{\rho^{n+1}} - \frac{1}{2}\left(\underline{u}^2\right)^{n+1}$$

Positivity of the internal energy $e^{n+1,-}$ is checked (stop with an error otherwise).

Space scheme: momentum balance step

Splitting between fluid and solid boundary:

$$\begin{aligned}\Omega_i^{\varphi}\left(\underline{Q}^{n+1,-}-\underline{Q}^n\right) \quad &+ \quad \Delta t^n \int_{\Gamma\varphi} \left(\underline{u}\left(\underline{Q}^* \cdot \underline{n}\right)\right)^{n+1,-} d\Gamma + \Delta t^n \int_{\Gamma\varphi} P^{n+1,-} \underline{n} d\Gamma \\ &+ \quad \underbrace{\Delta t^n \int_{\Gamma w} \left(\underline{u}\left(\underline{Q}^* \cdot \underline{n}\right)\right)^{n+1,-} d\Gamma}_{=0} + \Delta t^n \int_{\Gamma w} P^{n+1,-} \underline{n} d\Gamma = 0\end{aligned}$$

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$$
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Evaluation of the three integrals:

Space scheme: momentum balance step

Splitting between fluid and solid boundary:

$$\Omega_i^{\varphi}\left(\underline{Q}^{n+1,-} - \underline{Q}^n\right) + \Delta t^n \int_{\Gamma^{\varphi}} \left(\underline{u}\left(\underline{Q}^* \cdot \underline{n}\right)\right)^{n+1,-} d\Gamma + \Delta t^n \int_{\Gamma^{\varphi}} P^{n+1,-} \underline{n} d\Gamma$$
$$+ \underbrace{\Delta t^n \int_{\Gamma^w} \left(\underline{u}\left(\underline{Q}^* \cdot \underline{n}\right)\right)^{n+1,-} d\Gamma}_{=0} + \Delta t^n \int_{\Gamma^w} P^{n+1,-} \underline{n} d\Gamma = 0$$

Evaluation of the three integrals:

$$\int_{\Gamma_i^{\varphi}} \left(\underline{u}\left(\underline{Q}^* . \underline{n}\right)\right)^{n+1,-} d\Gamma = \sum_{k \in \{1, N(i)\}} \sum_{(j,k') \in V(i)} \left(\underline{Q}^* . \underline{n}\right)_{i,k/j,k'} \left(\underline{u}^{n+1,-}\right)^{upw}_{i,k/j,k'} S^{\varphi}_{i,k/j,k'}$$

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$$\int_{\Gamma_i^{w}} P^{n+1,-}\underline{n} d\Gamma = P_i^{n+1,-} \sum_{w_i} \underline{S}_i^{w} = -P_i^{n+1,-} \sum_{k\in\{1,N(i)\}} \sum_{(j,k')\in V(i)} \underline{S}^{\varphi}_{i,k/j,k'}$$

Space scheme: energy balance step

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Evaluation of the integral over the fluid boundary:

$$\int_{\Gamma_i^{\varphi}} \left(\left(\underline{u}\cdot\underline{n}\right)(E+P)\right)^{n+1,-} d\Gamma =$$

$$\sum_{k\in\{1,N(i)\}} \sum_{(j,k')\in V(i)} \left(\underline{Q}^*\cdot\underline{n}\right)_{i,k/j,k'} \left(\frac{E^{n+1,-}}{\rho^{n+1,-}}\right)^{upw}_{i,k/j,k'} S^{\varphi}_{i,k/j,k'}$$

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