



EUROPEAN CENTRE FOR RESEARCH AND ADVANCED TRAINING IN SCIENTIFIC COMPUTING

Numerics

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Theoretical insights

- Mathematical background
- Numerical methods

Description of AVBP schemes

- Lax Wendroff
- Two-step Taylor Galerkin schemes
- Properties of AVBP schemes

Practical elements

- Wiggles
- Issues at corners
- Artificial viscosity
- *Shock sensors*

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Mathematical background

- Conservation law (conservative formulation)

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial}{\partial x} f(\mathbf{u}) = 0 \quad \text{with}$$

$$\mathbf{u} = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho E \end{pmatrix}$$

- Non-conservative formulation

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{a}(\mathbf{u}) \frac{\partial \mathbf{u}}{\partial x} = 0 \quad \text{with} \quad \mathbf{a}(\mathbf{u}) = \frac{\partial f(\mathbf{u})}{\partial \mathbf{u}} \text{ Jacobian}$$

- The Cauchy problem (initial value problem)

$$\begin{cases} \frac{\partial \mathbf{u}}{\partial t} + \frac{\partial}{\partial x} f(\mathbf{u}) = 0 \\ \mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0 \end{cases}$$

- A solution $\mathbf{u}(x, t), \forall (x, t)$ satisfying the Cauchy problem is called a “**Strong**” solution (or “**Classical**”).
- Such solution **may not exist** (if discontinuity in the initial solution).
→ For this reason, “**Weak**” solutions are of interest.



Weak solutions for conservation equations

Will be of interest for finite-elements ...

Let's consider a function $\phi(\mathbf{x}, t)$ defined on a compact support.

- Let's multiply the conservation equation :

$$\left(\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial}{\partial x} f(\mathbf{u}) \right) \cdot \phi(\mathbf{x}, t) = 0$$

- Integration over space-time: *(Scalar product)*

$$\int_{\mathbb{R}} \int_0^{\infty} \left(\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial}{\partial x} f(\mathbf{u}) \right) \cdot \phi(\mathbf{x}, t) \, d\mathbf{x} \, dt = 0$$

- Provided $\phi(\mathbf{x}, t)$ nullifies on the support boundaries, after **integration by parts**:

$$\int_{\mathbb{R}} \int_0^{\infty} \left(\mathbf{u} \frac{\partial \phi}{\partial t} + f(\mathbf{u}) \frac{\partial \phi}{\partial x} \right) \, dx \, dt + \int_{\mathbb{R}} \mathbf{u}_0 \phi(\mathbf{x}, 0) \, dx = 0$$

Variational formulation for the conservation equation

→ No longer derivatives of $\mathbf{u}(\mathbf{x}, t)$!

→ Derivatives of $\phi(\mathbf{x}, t)$ instead (mass-matrix in the FE formalism...)

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Finite Volumes and Finite Elements

Finite-volume is based on the **strong formulation** of the conservation equation

- **Conservation** of transported quantities in a **control volume**
- The unknown is approximated by the **mean** over the control volume

Finite elements rely on the concept of **variational formulation**, and **weak solutions**

- **Shape functions** are defined within each cell.
- Unknowns are determined at the **node** (*instead average value in cell for FV*)

Both approaches rely on :

- Space and time **discretization of the conservation equation**
- Integration over a control volume, **fluxes balance** over the control volume

$$\frac{\partial U}{\partial t} = - \frac{1}{V_\Omega} \int_{\Omega} \underbrace{\vec{\nabla} \cdot \vec{F}}_{R_\Omega}_{\text{Residual}} dV$$

→ Requires to the computation of a **residual**



Let's focus on space and time discretization...

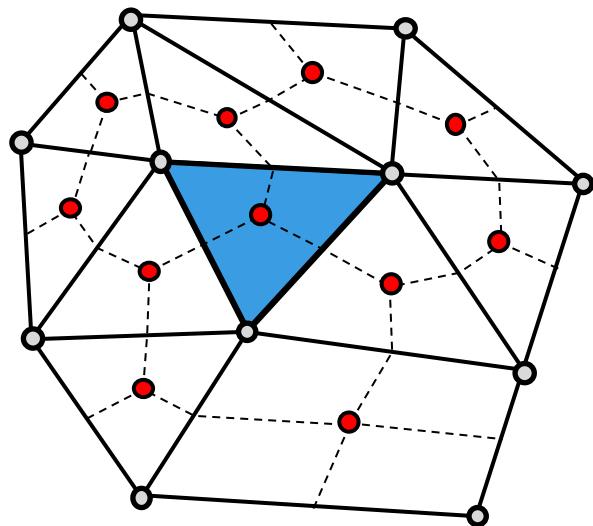
$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial}{\partial x} f(\mathbf{u}) = 0$$

- The continuous conservation equation is discretized **on a mesh**
 - Allows to store variables at each iteration
 - Allows to define control volumes

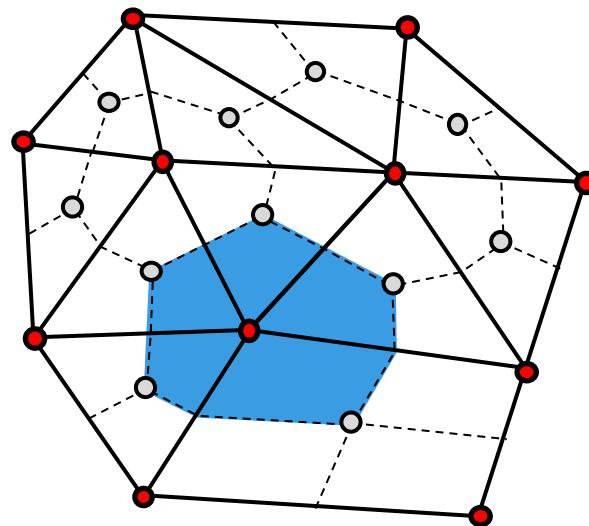
- The continuous conservation equation is discretized **in time**

Spatial discretization

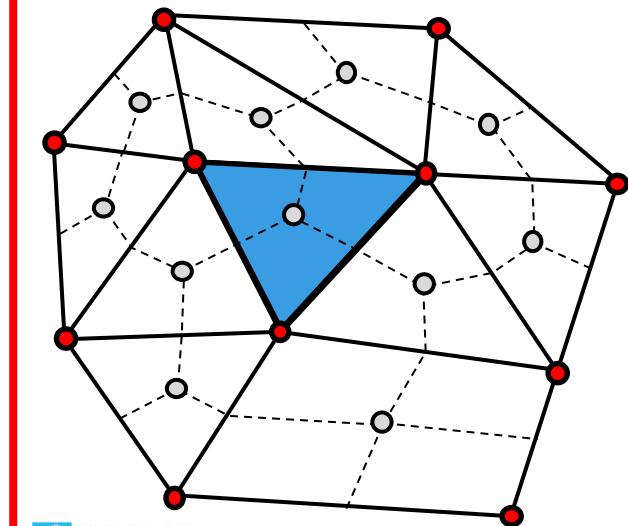
Cell-centred



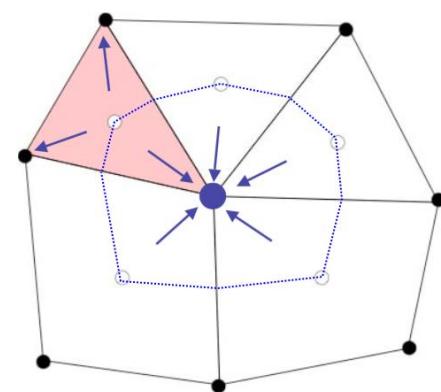
Vertex-centred



Cell-vertex



AVBP
Variables are stored at the nodes
Control volumes are primal cells



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Presentation of 2 main Numerical schemes of AVBP

- **Lax-Wendroff (LW)**
- **Two-Step Taylor Galerkin (TTG) schemes**


$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial}{\partial x} f(\mathbf{u}) = 0$$

Summary

In summary, two families of schemes are available in AVBP:

- LW *Finite Volume*
 - second order accurate in space and time
 - + not expensive
- TTG4A and TTGC *Finite Element*
 - + third order accurate in space and time
dissipation and dispersion properties meeting LES requirements
 - - ~ 2.5 times more expensive than LW

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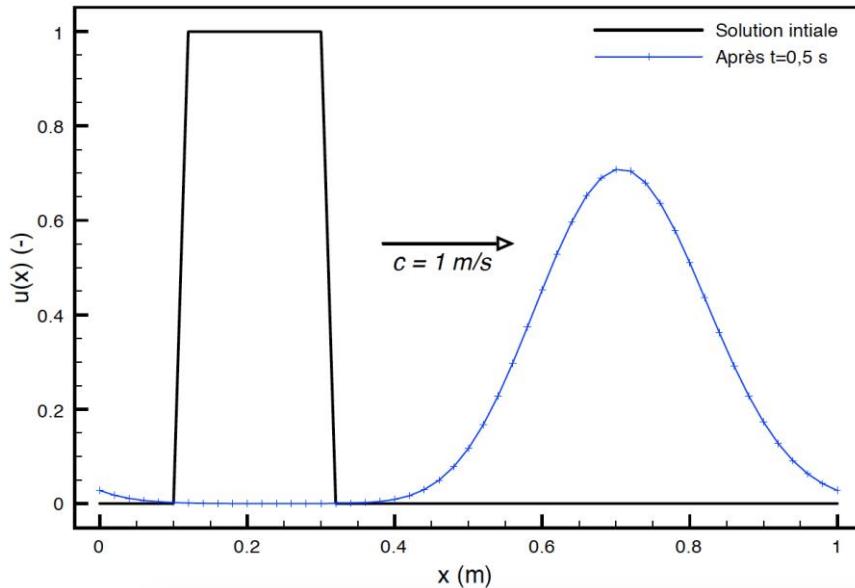
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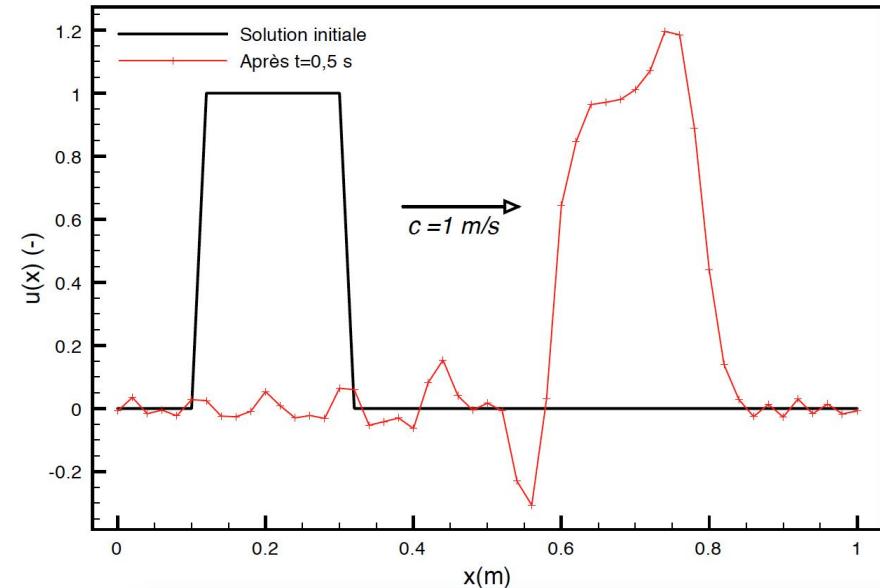
Properties of AVBP schemes

Mesh discretization introduces errors:

Dissipation error



Dispersion error



- Decrease of the wave amplitude
- Smoothing of its gradients

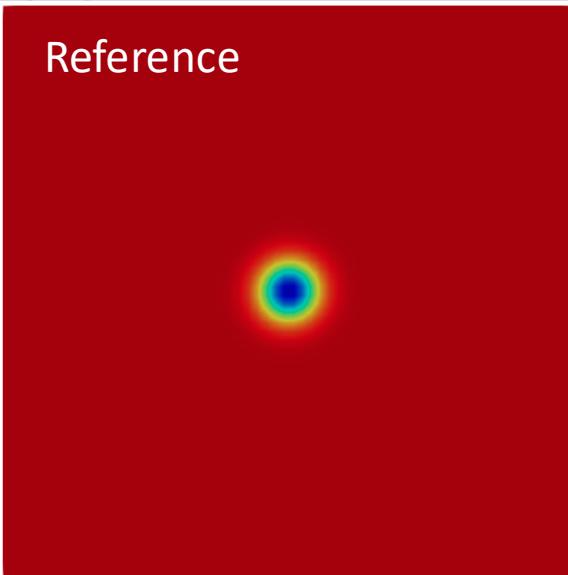
Dispersive medium:

A medium in which wave velocities depend on the wave frequency

➔ Harmonics of the initial solution are not transported at the same speed

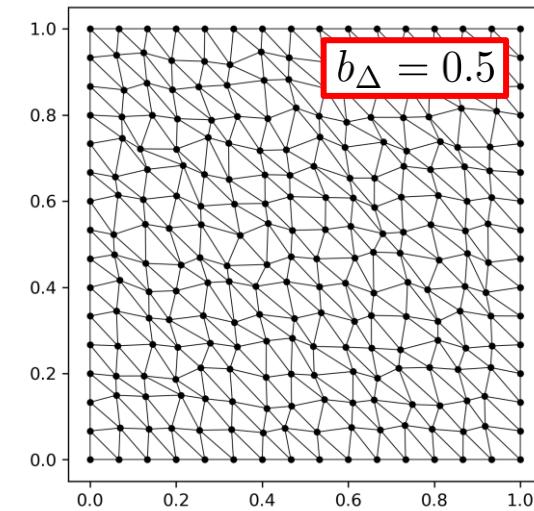
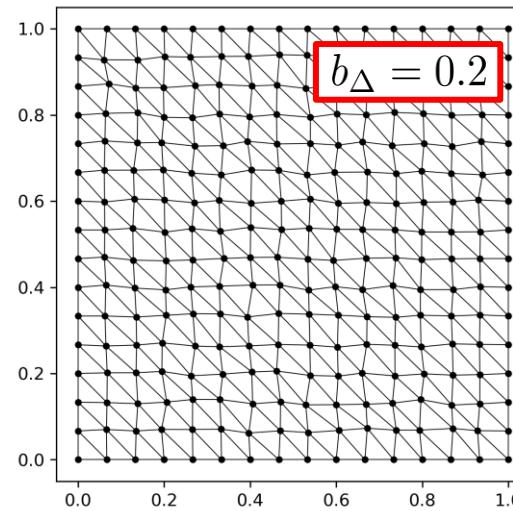
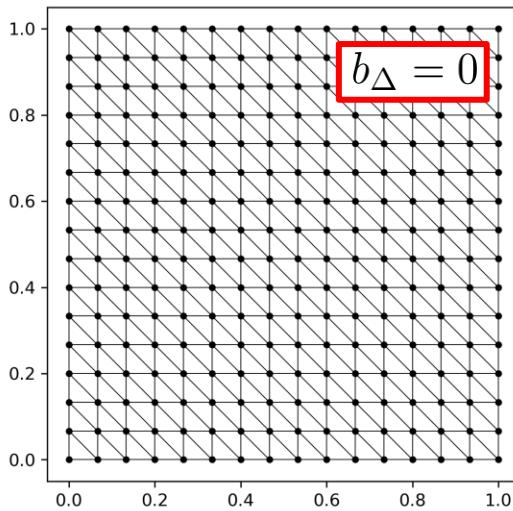
Application

Reference



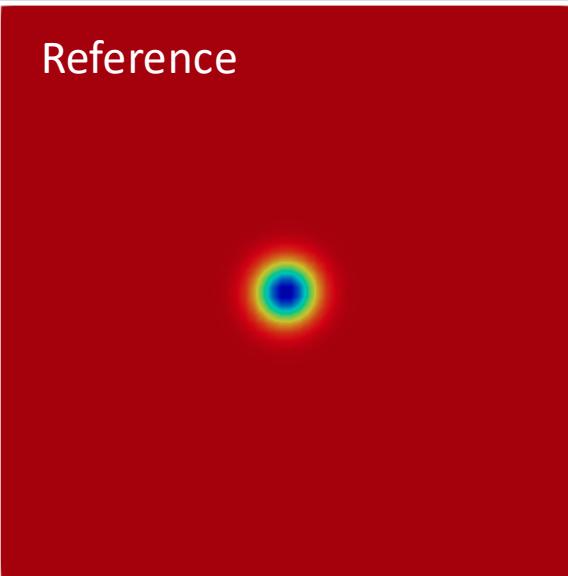
Let's consider the advection of a 2D isentropic vortex...

Let's try several schemes, and several mesh qualities



Reference

Lax-Wendroff

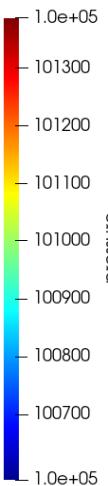
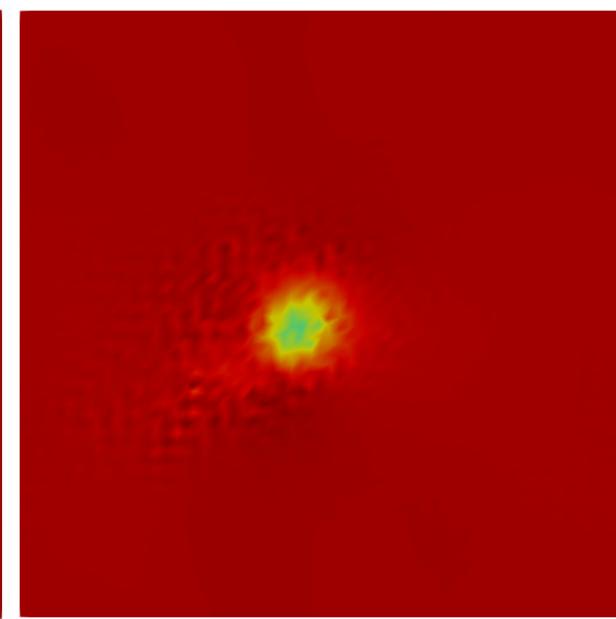
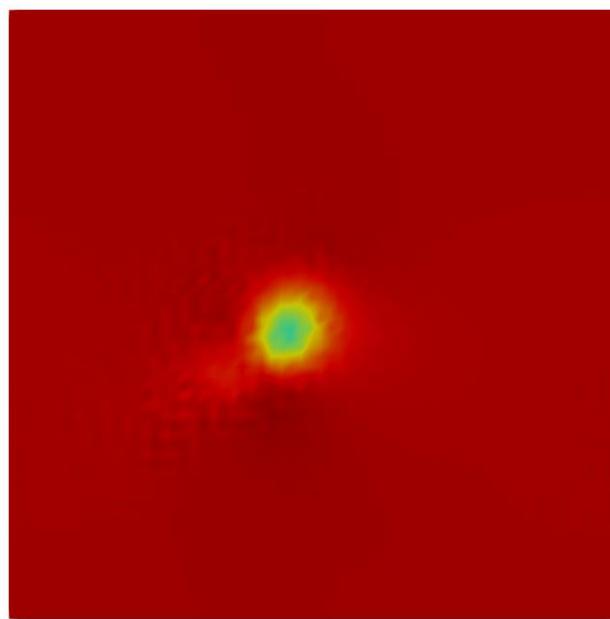
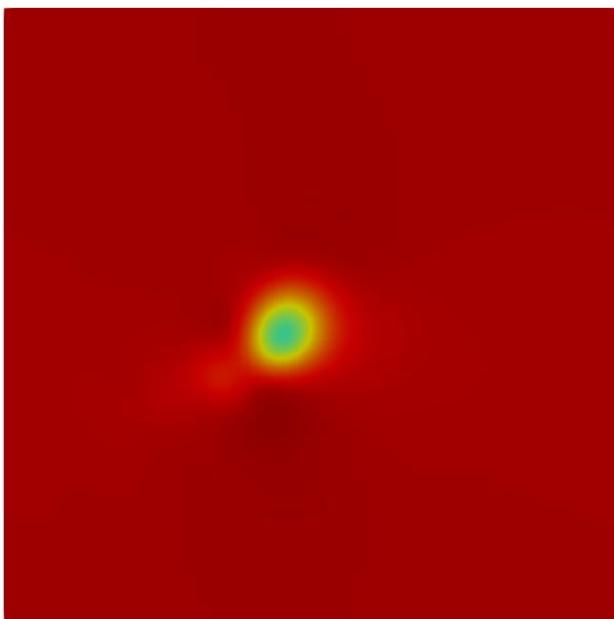


⇒ Dissipative
⇒ Some dispersion

$b_\Delta = 0$

$b_\Delta = 0.2$

$b_\Delta = 0.5$



Reference

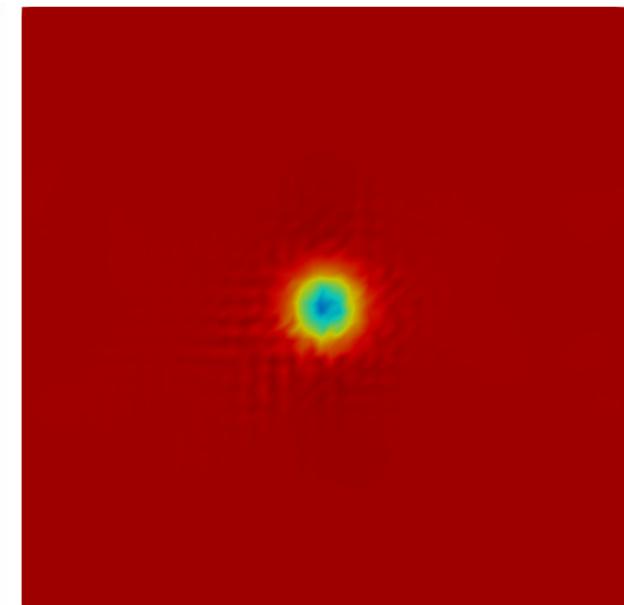
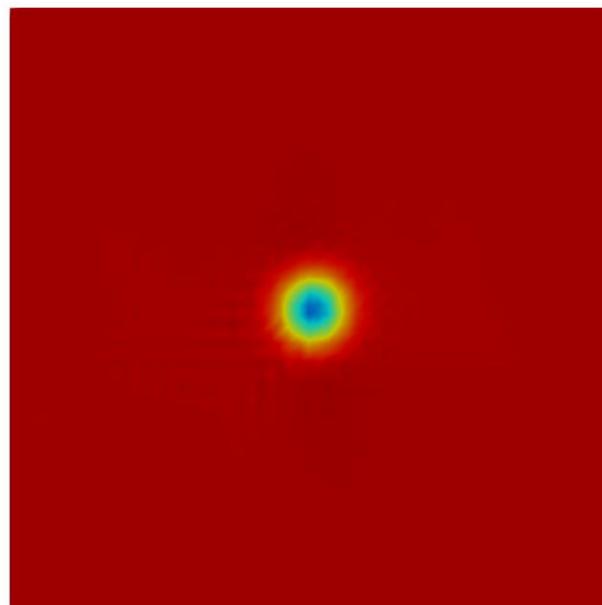
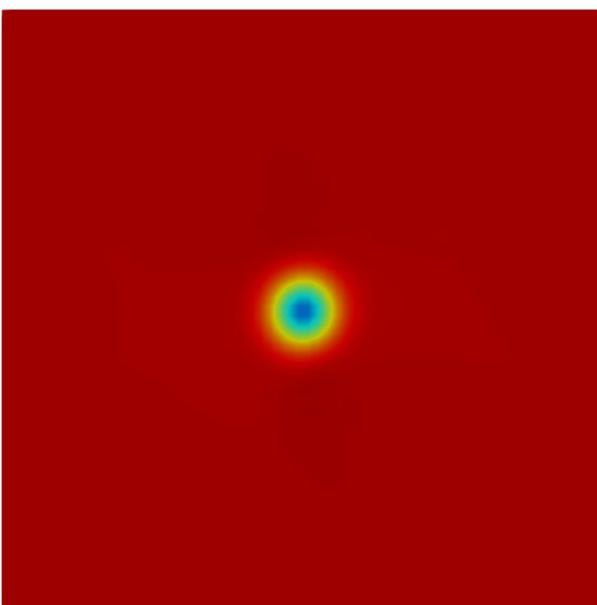
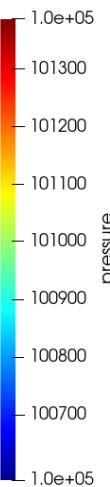
TTG4A

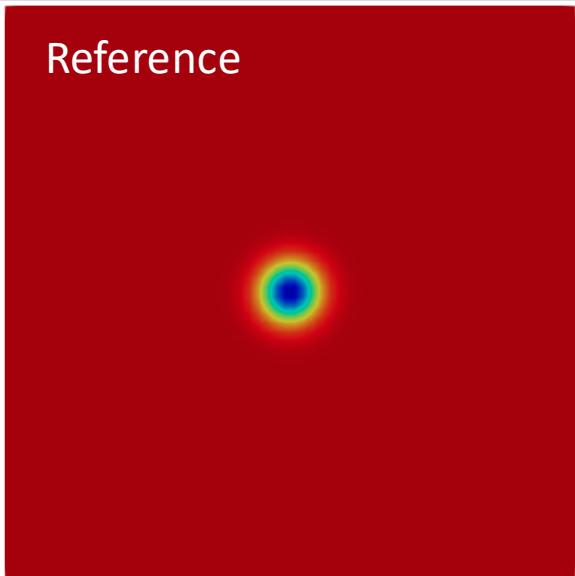
⇒ Still dissipation
⇒ Smaller dispersion

$b_\Delta = 0$

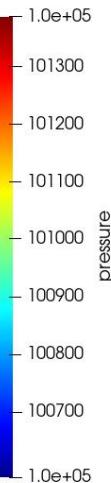
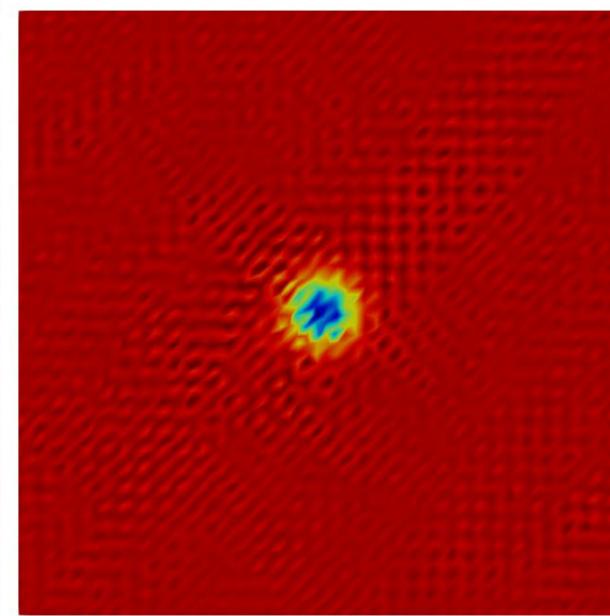
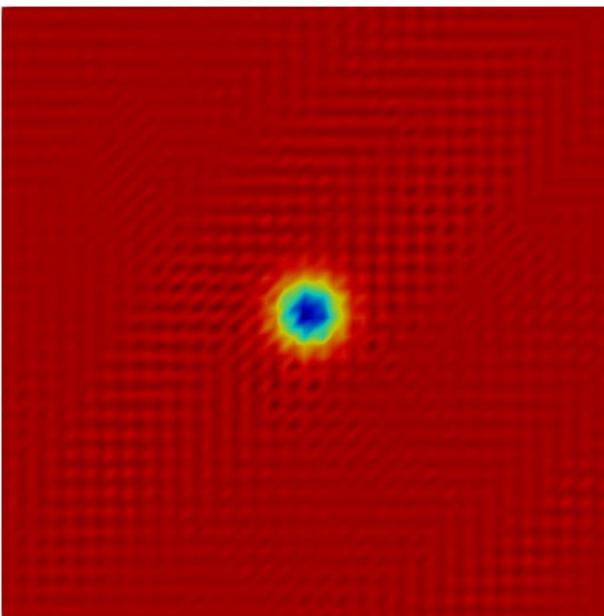
$b_\Delta = 0.2$

$b_\Delta = 0.5$



 $b_{\Delta} = 0$ $b_{\Delta} = 0.2$ $b_{\Delta} = 0.5$

⇒ Very few dissipation
⇒ Large dispersion





Partial conclusion

- Lax Wendroff is dissipative
- TTG4A is also dissipative, but induces small dispersion
- TTGC very accurate on perfect grids. Dispersion errors however occur for distorted grids
- TTG scheme ~ 2.5 times more expensive

⇒ No scheme is perfect !

LW is of interest for LES initialization.

TTG schemes better suited for statistics.

Errors decrease with increasing:

- Mesh quality
- Mesh resolution
- Order of numerical scheme
- Lower CFL





A simple tip...

HIP allows mesh adaptation thanks to the MMG3D library.

"Mmg3d isofactor -f 1"

Can significantly improve your initial Centaur / Ansys mesh !

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Wiggles

- AVBP schemes are **centred schemes**.
- In case of **discontinuity in the discrete approximation** of the hyperbolic equation (e.g. mesh **refinement interface**, mesh **boundary**):

→ Creation of a **spurious wave**, with a wavelength $\lambda = 2\Delta x$:
“Wiggles”, “q-waves”

Wiggles move forward at a group velocity -c

Vichnevetsky/Boyles, 1982

Vichnevetsky Comp. Math. Appls 1985

Vichnevetsky Int. J. Num. methods Fluids 1987

Sengupta App. Maths. Comp. 2012



Centred schemes and q -waves

It can be showed that: when **using centred schemes** i.e. $\left[\frac{du_n}{dt} + \left(\frac{u_{n+1} - u_{n-1}}{2h} \right) = 0 \right]$

to discretize a continuous **wave equation** $\frac{\partial^2 u}{\partial t^2} - c^2 \frac{\partial^2 u}{\partial x^2} = 0$

leads to a **numerical** (discrete) solution consisting in **2 waves** :

$$\begin{cases} "p\text{-waves}" \\ p(\mathbf{x}, t) = \frac{u + v}{2} \\ "q\text{-waves}" \\ q(\mathbf{x}, t) = \frac{u - v}{2} \end{cases}$$

satisfying

$$\begin{cases} \frac{\partial p}{\partial t} + c \frac{\partial p}{\partial x} = 0 \\ \frac{\partial q}{\partial t} - c \frac{\partial q}{\partial x} = 0 \end{cases}$$

$\xrightarrow{+c}$
Moving **forward**
 $\xleftarrow{-c}$
Moving **backward**



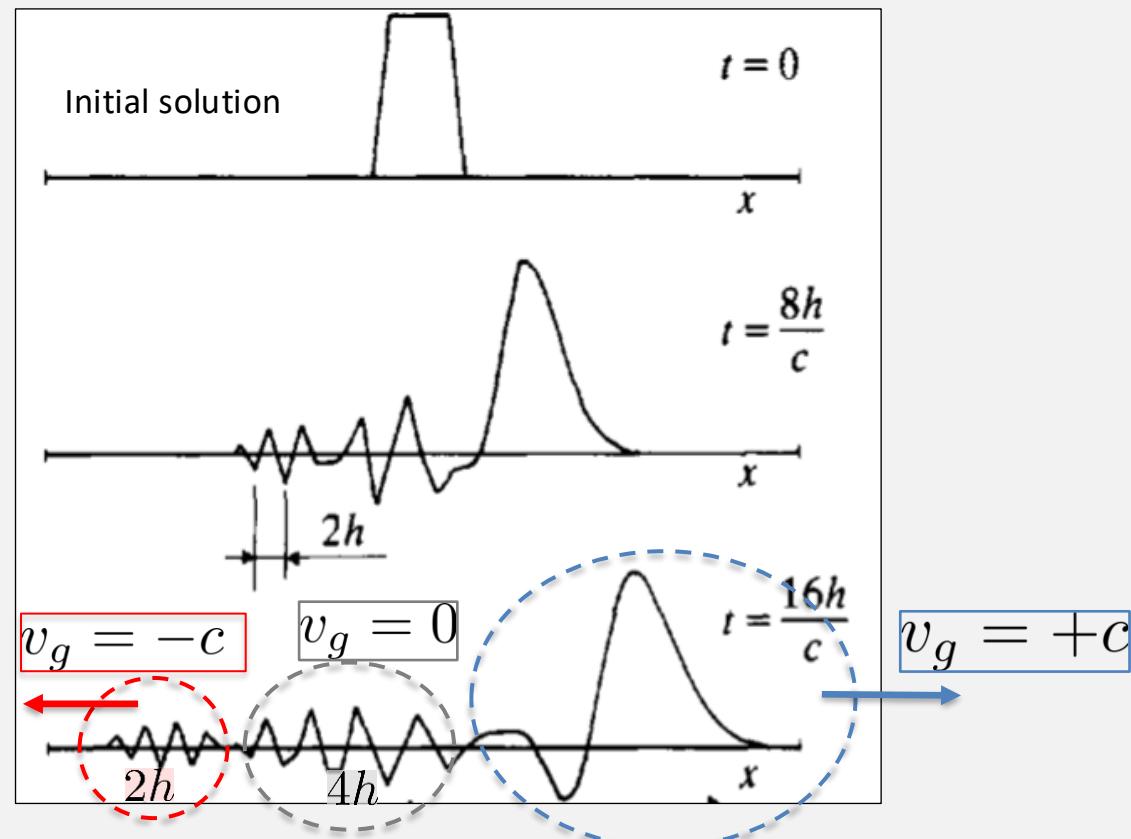
Centred schemes and q -waves

“Smooth” part

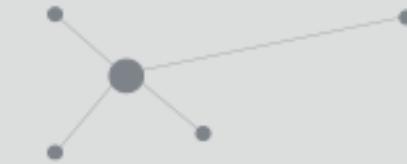
$$p(\mathbf{x}, t) = \frac{u + v}{2}$$

“Oscillatory” part

$$q(\mathbf{x}, t) = \frac{u - v}{2} = u$$

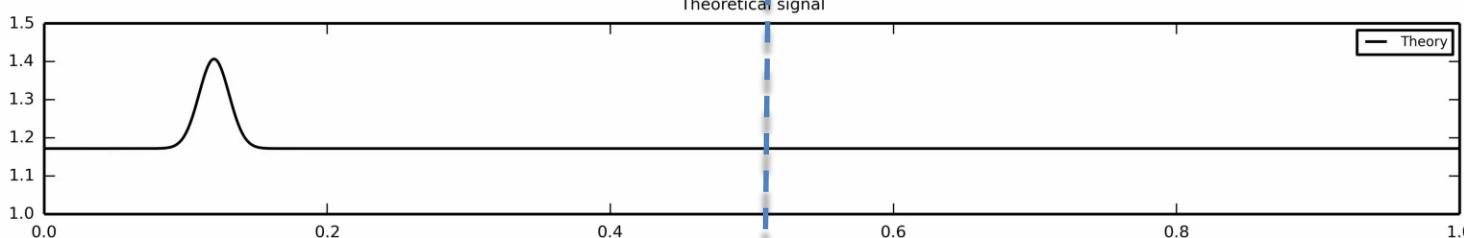


Wiggles: illustration



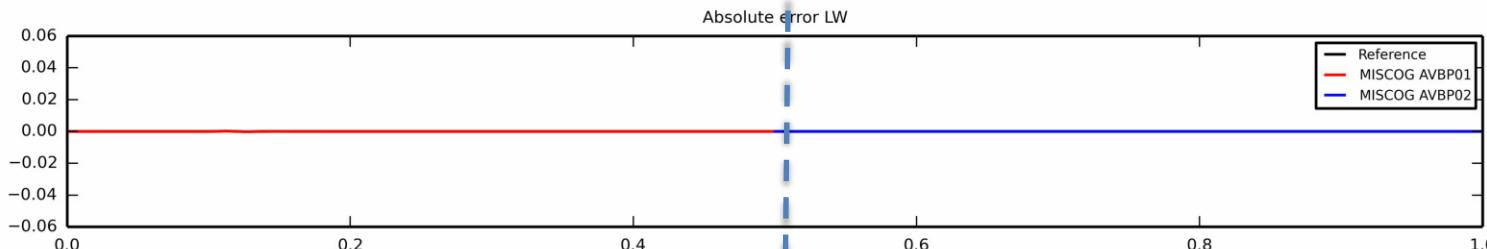
Mesh interface

Boundary condition

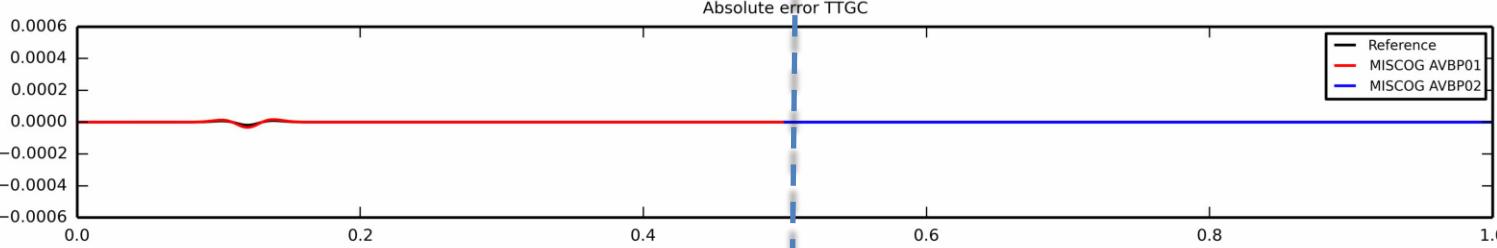


Theoretical signal

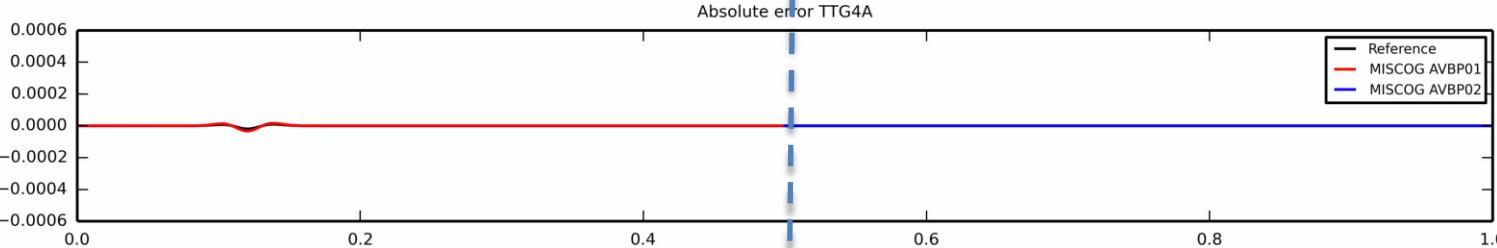
Boundary condition



Absolute error LW



Absolute error TTGC



Absolute error TTG4A

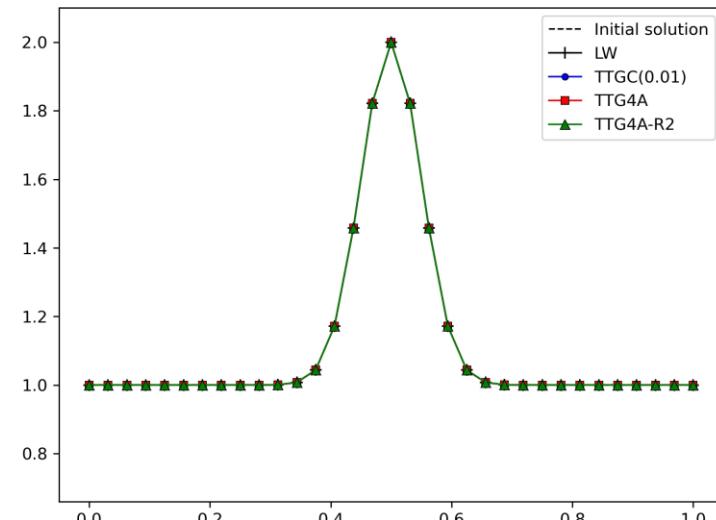
q-waves
generate
p-wave !



Dispersion errors and q -waves

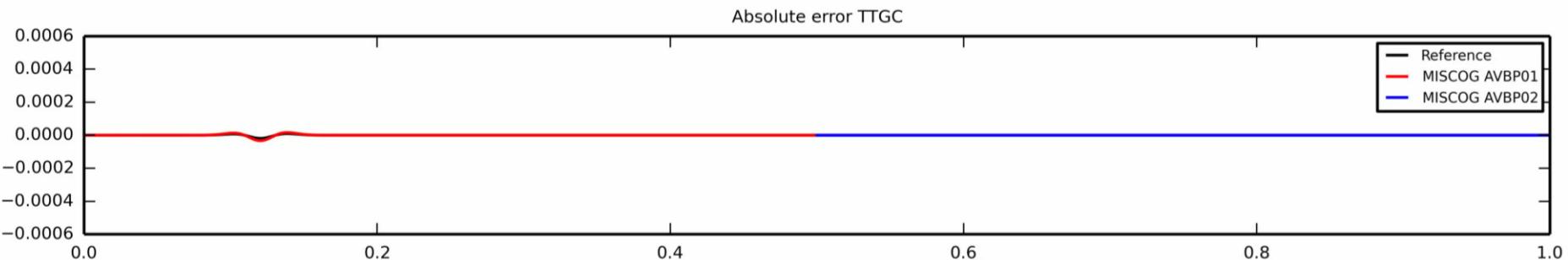
Dispersion error

Mostly convected at the phase velocity $u+c$, along with the physical wave



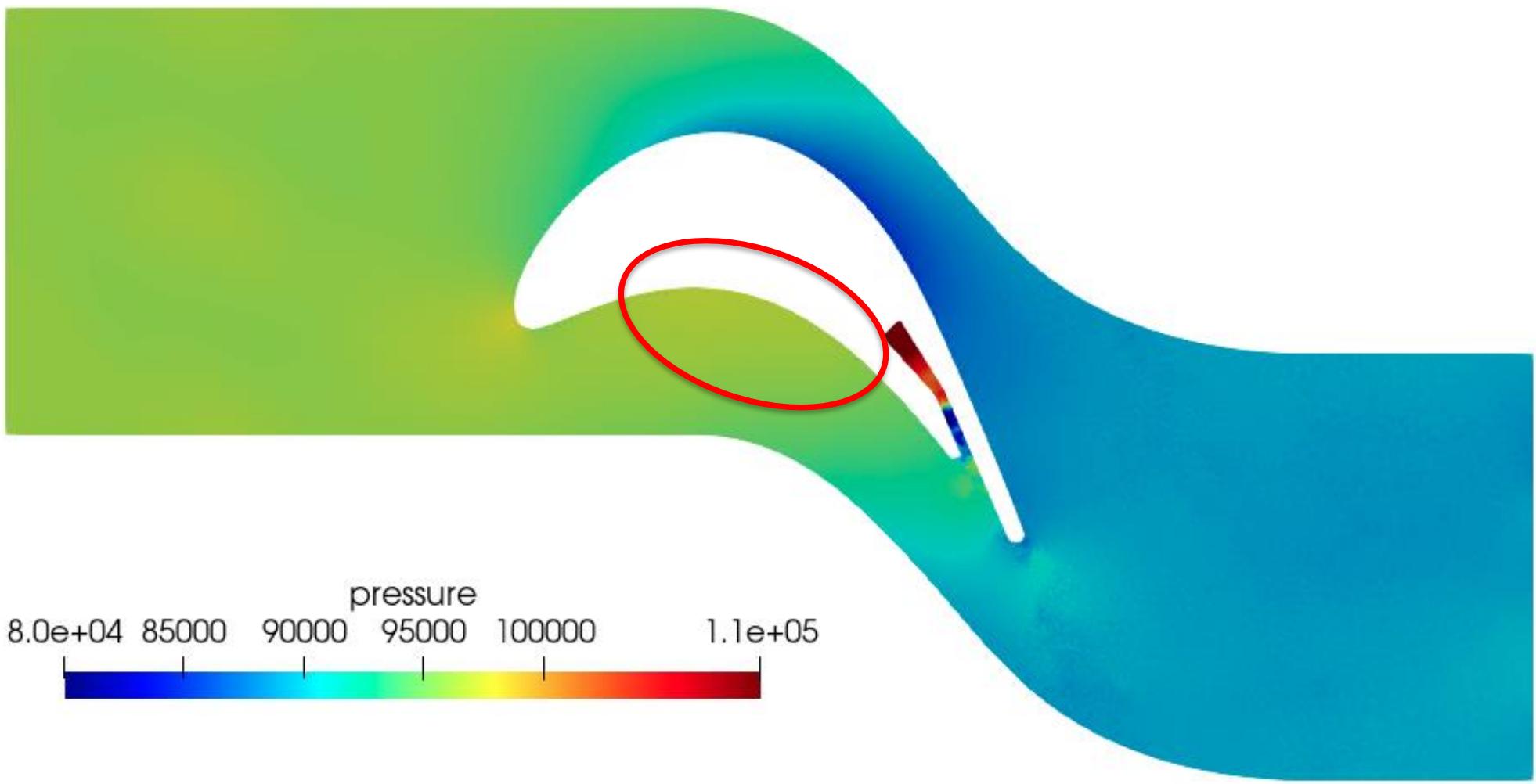
q -waves (wiggles)

Convected with a group velocity $-c$, as physical wave interacts with a boundary
 q -waves may generate p-waves (physical waves) when interacting back the other boundary



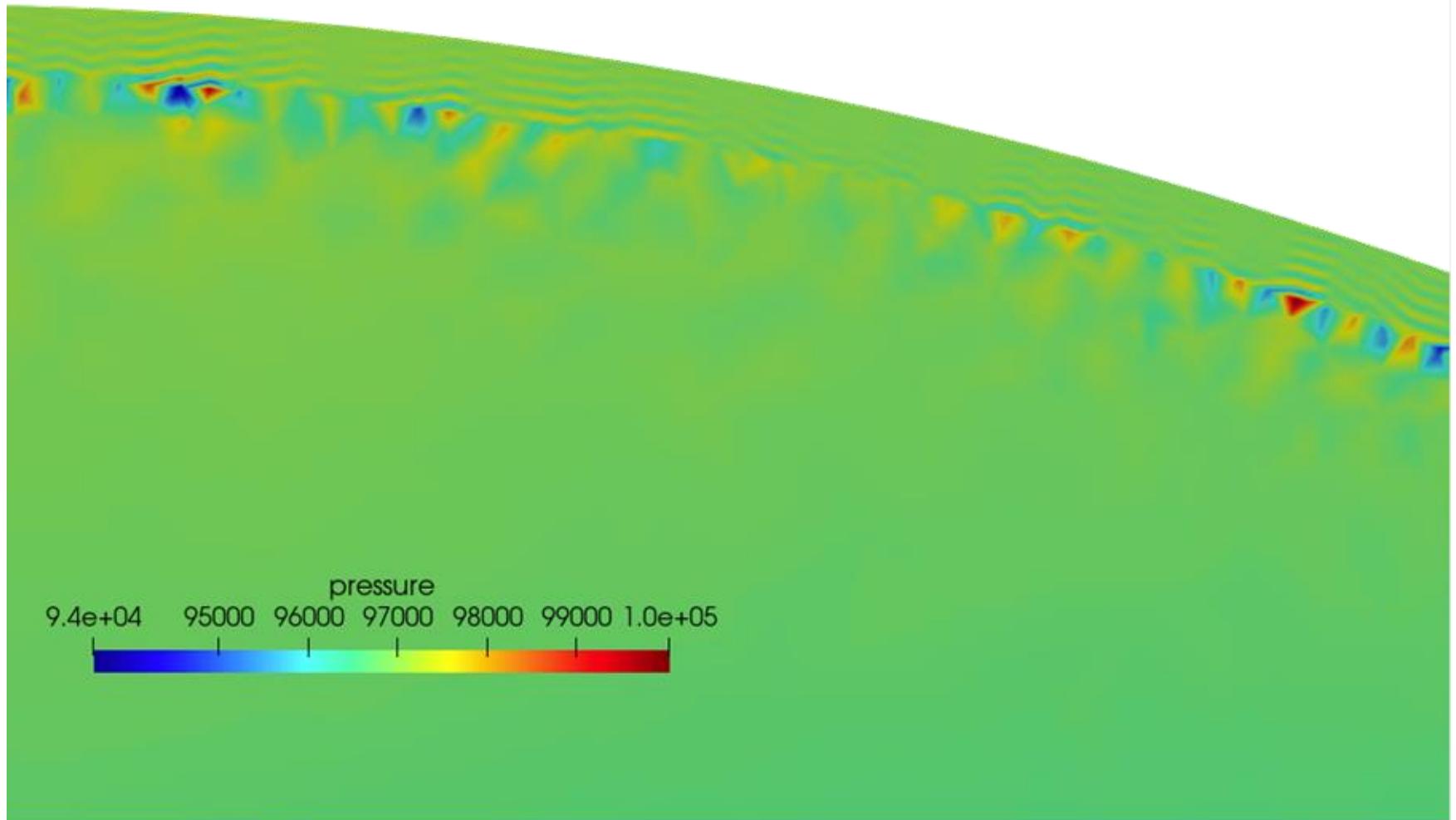


Issue at mesh interface



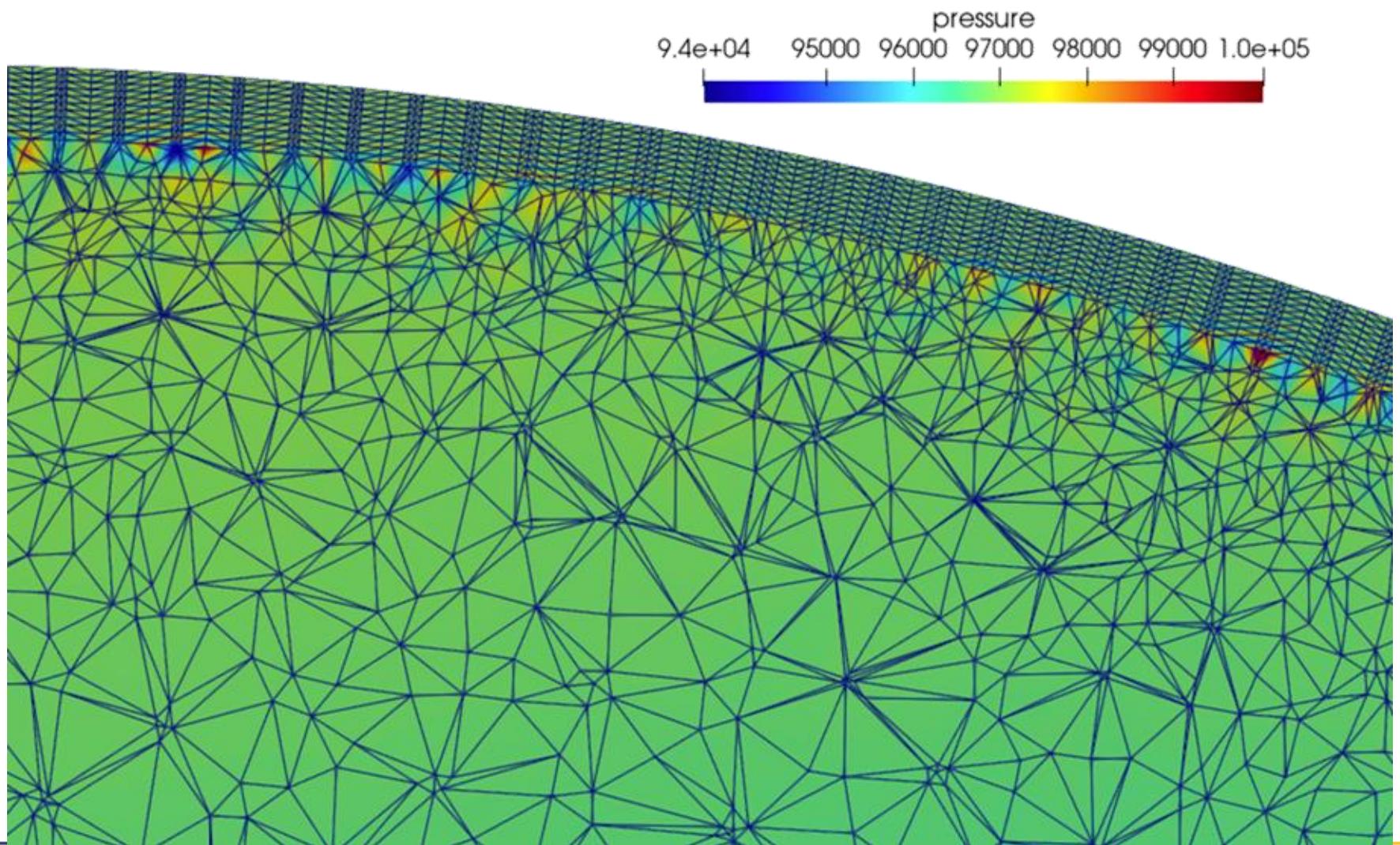


Issue at mesh interface



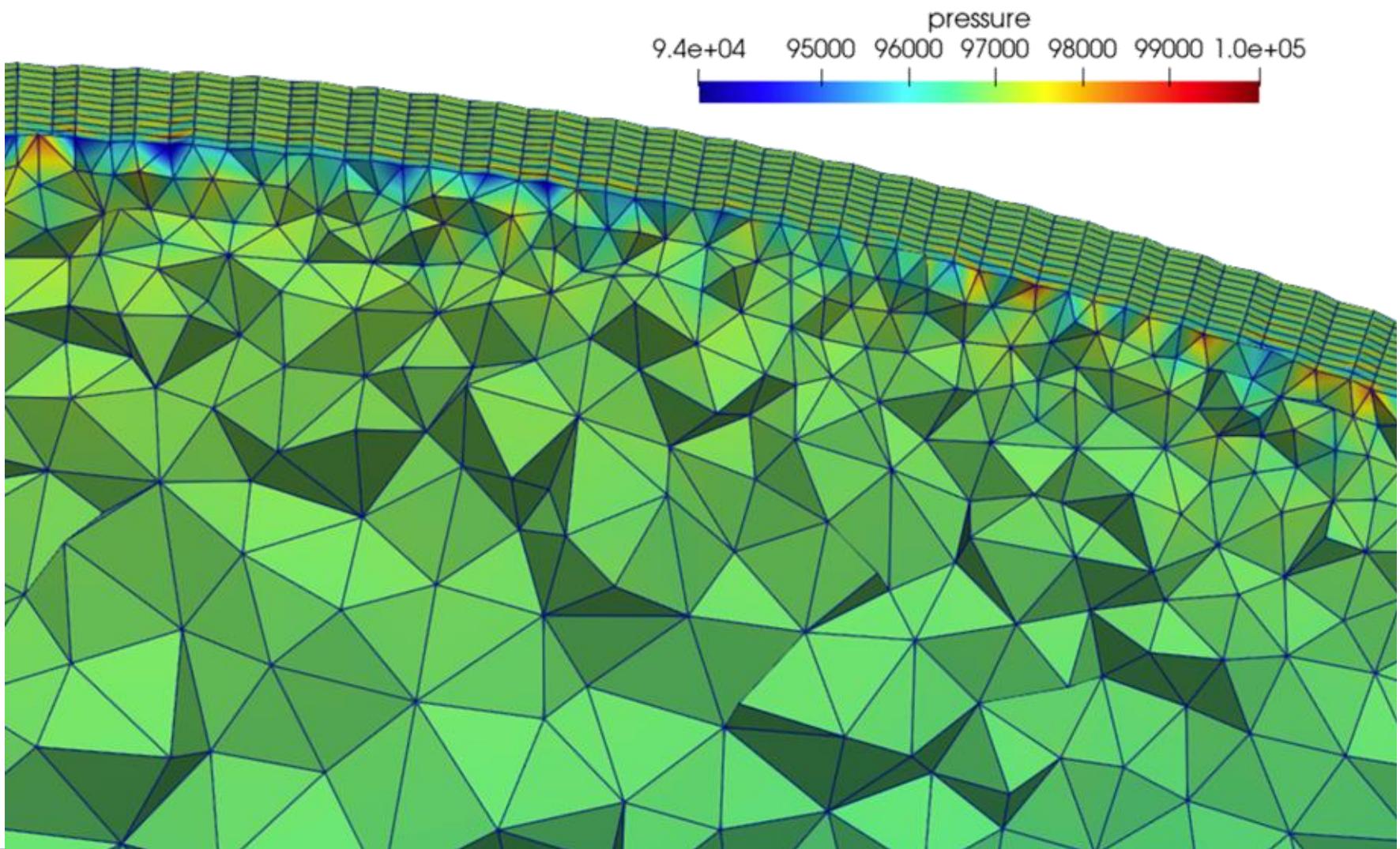


Issue at mesh interface





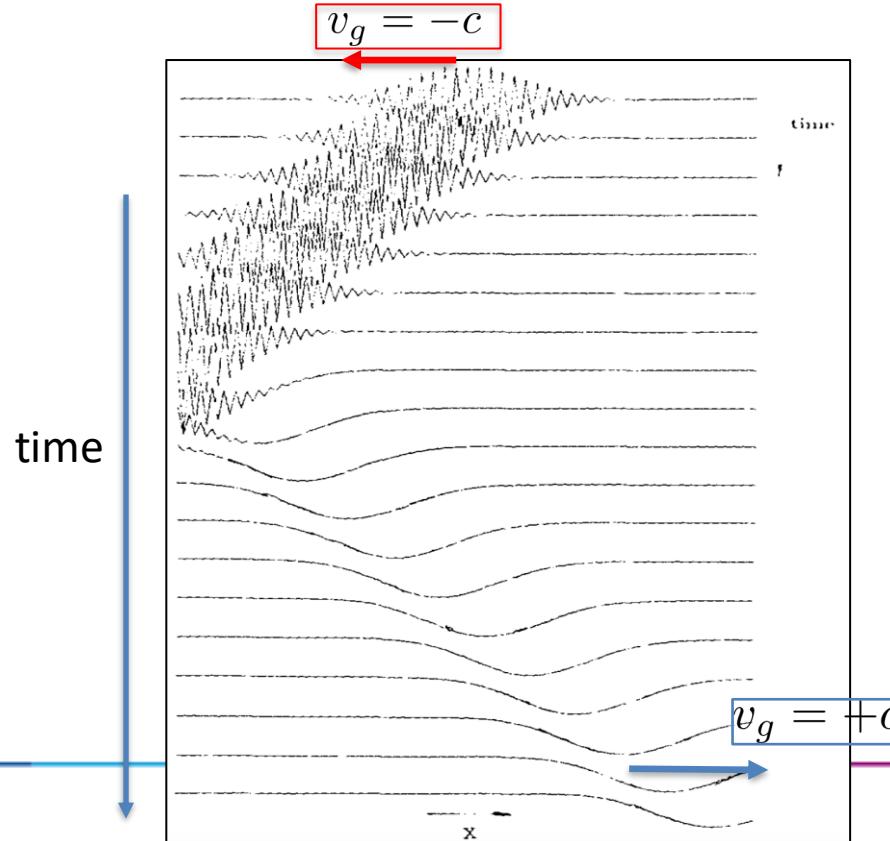
Issue at mesh interface





Partial conclusion on Wiggles

- Wiggles are not just dispersion error downstream of physical waves
- Wiggles are actual waves, propagating into the domain, at a group velocity $-c$
- Wiggles can generate physical waves when interacting with a BC !



See
Vichnevsky Bowles, SIAM 1982
Poinsot Veynante Ch.9
Sengupta et al. App. Math. Comp. 2012

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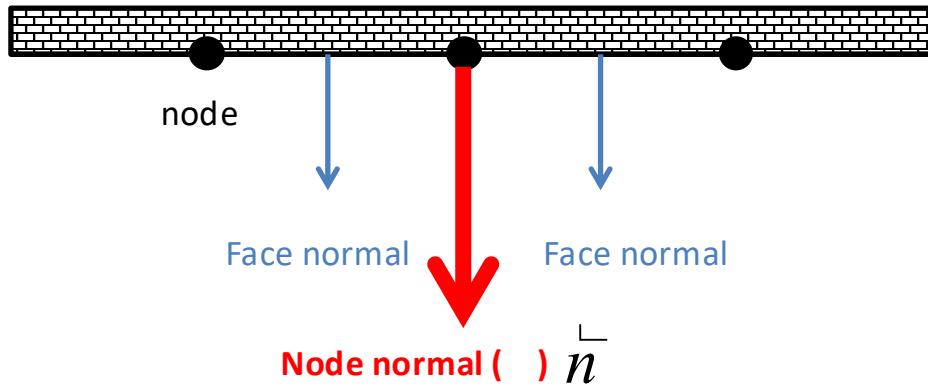


WALL/ WALL interaction : critical issue on corner

To ensure **mass conservation**, the normal (to the wall) velocity is cancelled:

$$U \cdot n = 0$$

Node normals are an average of normals on neighboring surfaces:



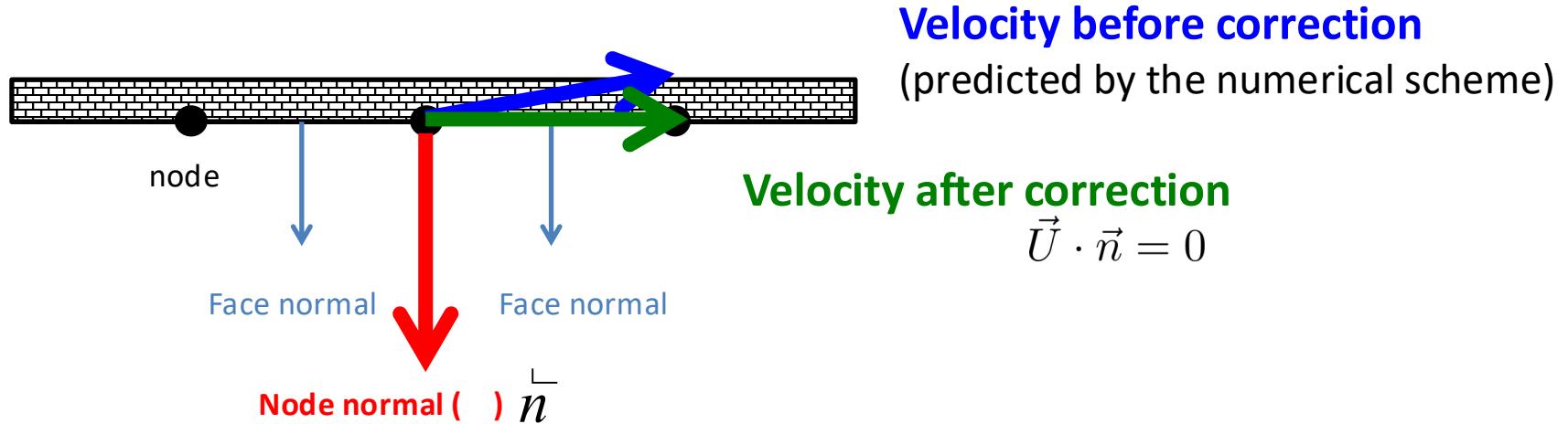


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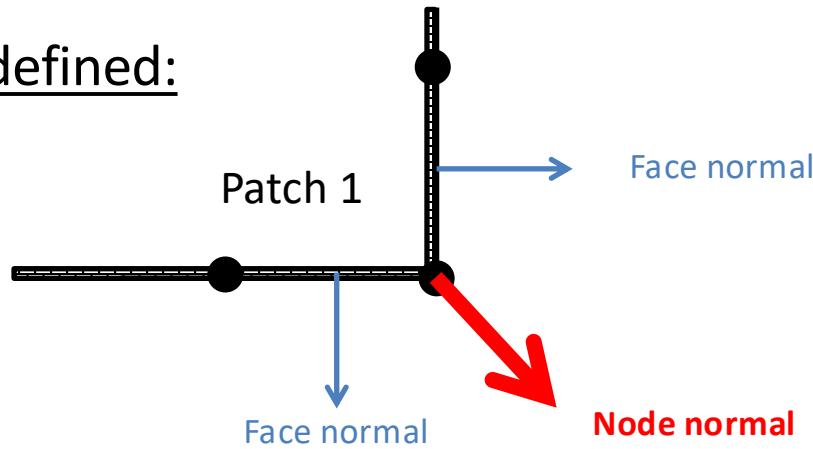


WALL/ WALL interaction : critical issue on corner

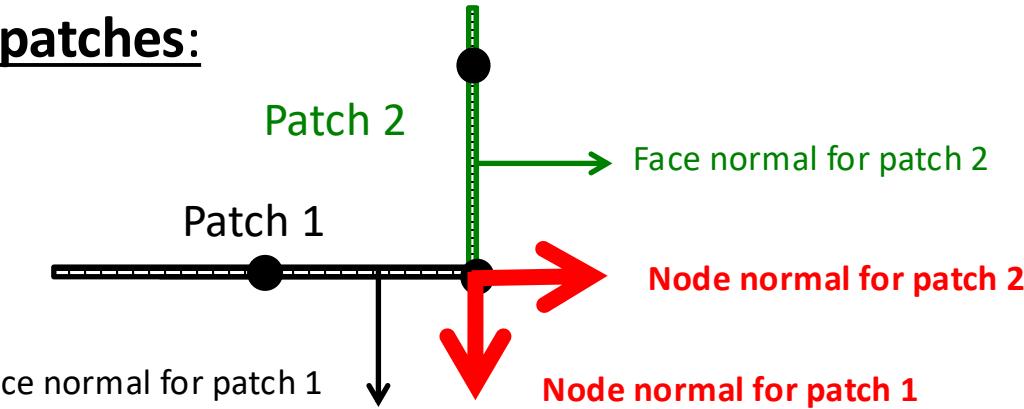
Wall normal direction at corners is an **ambiguous quantity!**

It depends on how patches are defined :

- If only 1 wall patch is defined:



- If the wall is split in 2 patches:



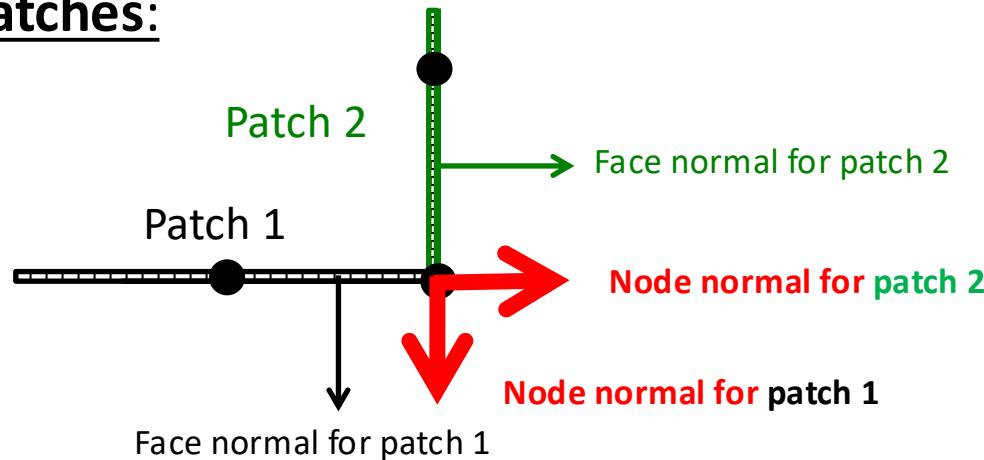


WALL/ WALL interaction : critical issue on corner

Wall normal direction at **corners** is an **ambiguous quantity!**

It depends on how patches are defined :

- If the wall is **split in 2 patches**:



→ Two normals are defined for the same node !

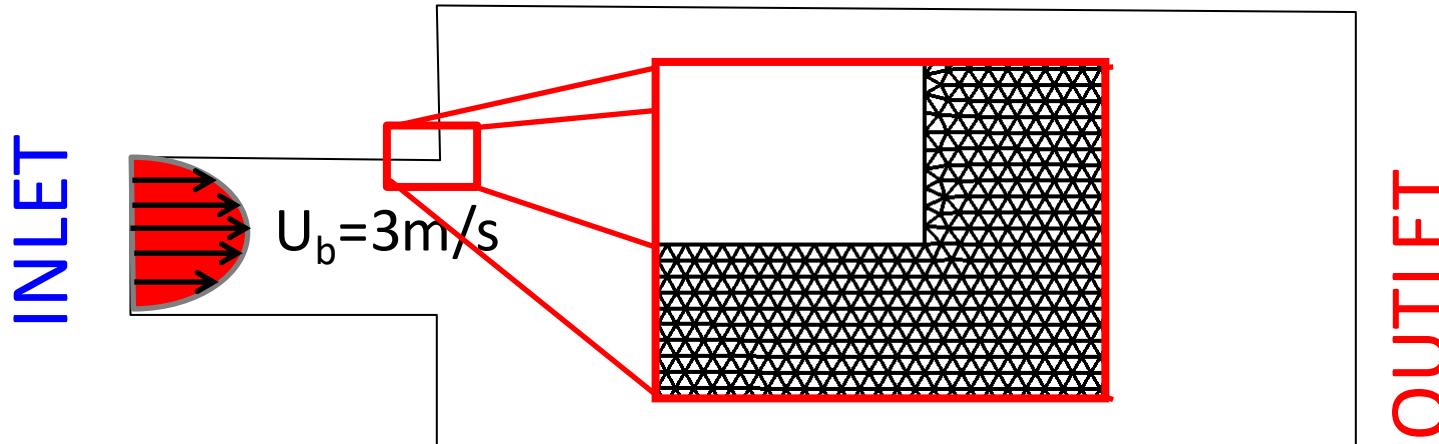
→ Two treatments are successively applied



Wall corners

Example : sudden expansion

WALLS (Law)



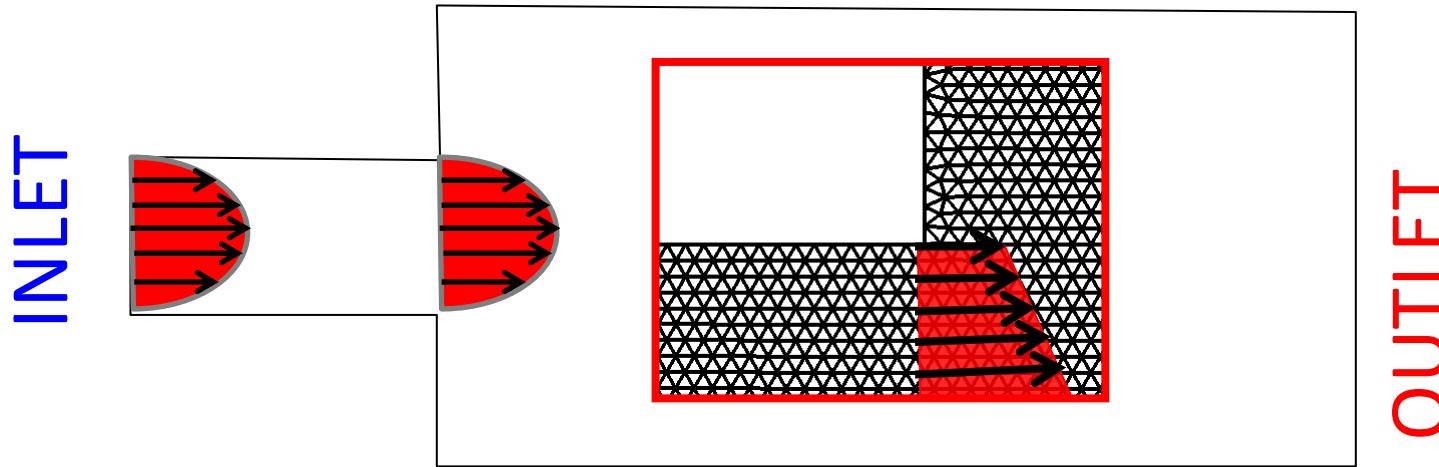
WALLS (Law)

WHAT HAPPENS AT THE CORNER ?



Wall corners
Example : sudden expansion

WALLS (Slip or Law)



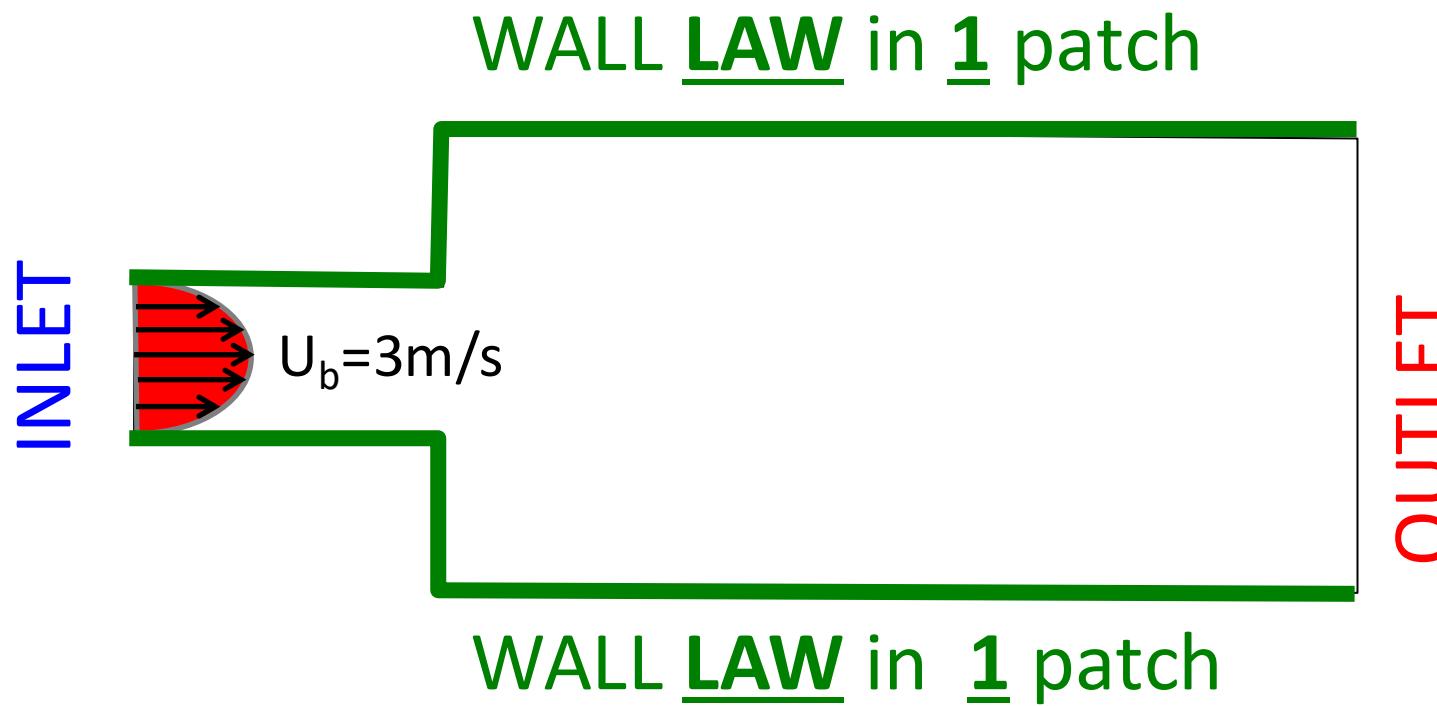
WALLS (Slip or Law)

Expected solution: the **flow** should go **straight**



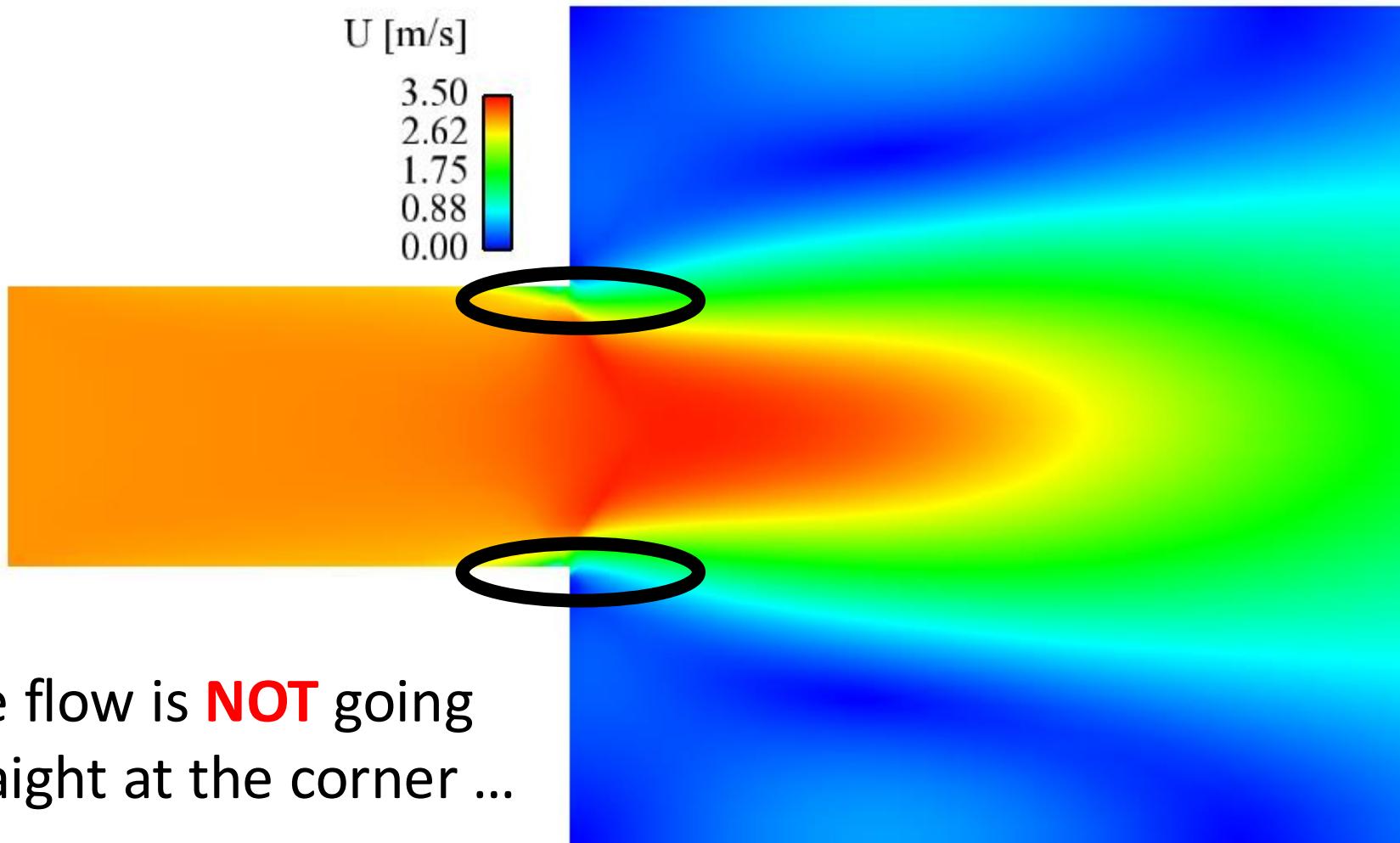
Joint patches test case

→ First, let's consider **wall Law** using one single patch





Joint patches test case

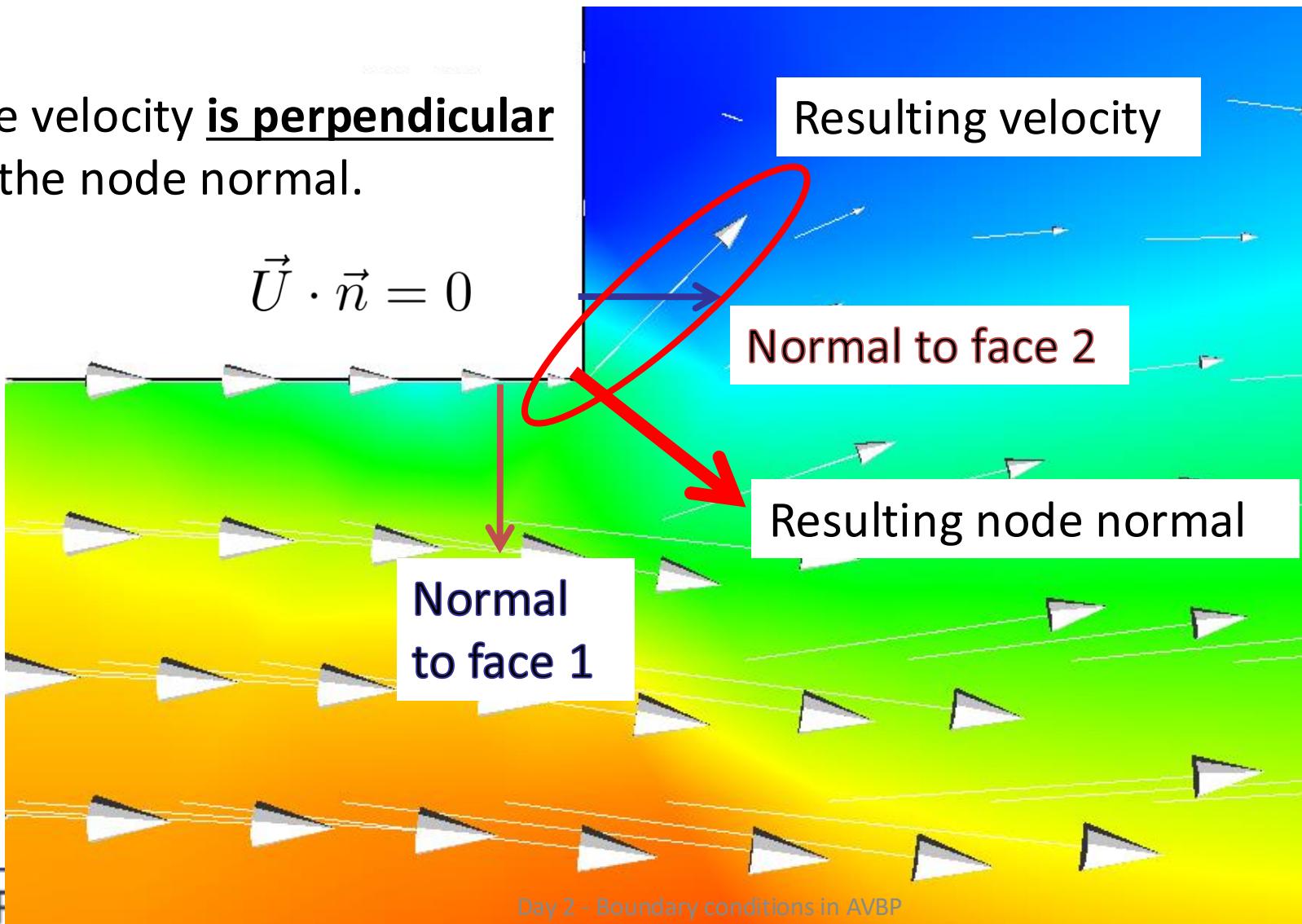


Joint patches test case



The velocity is perpendicular to the node normal.

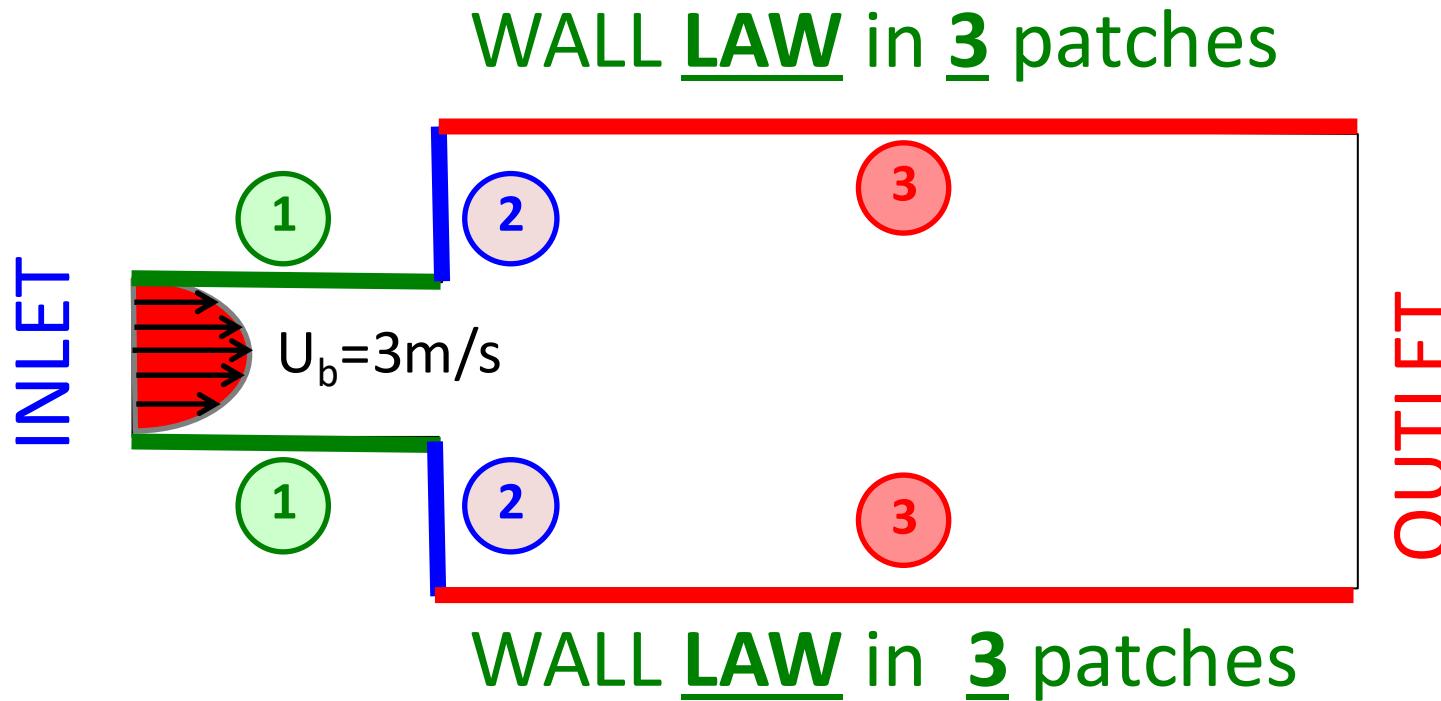
$$\vec{U} \cdot \vec{n} = 0$$



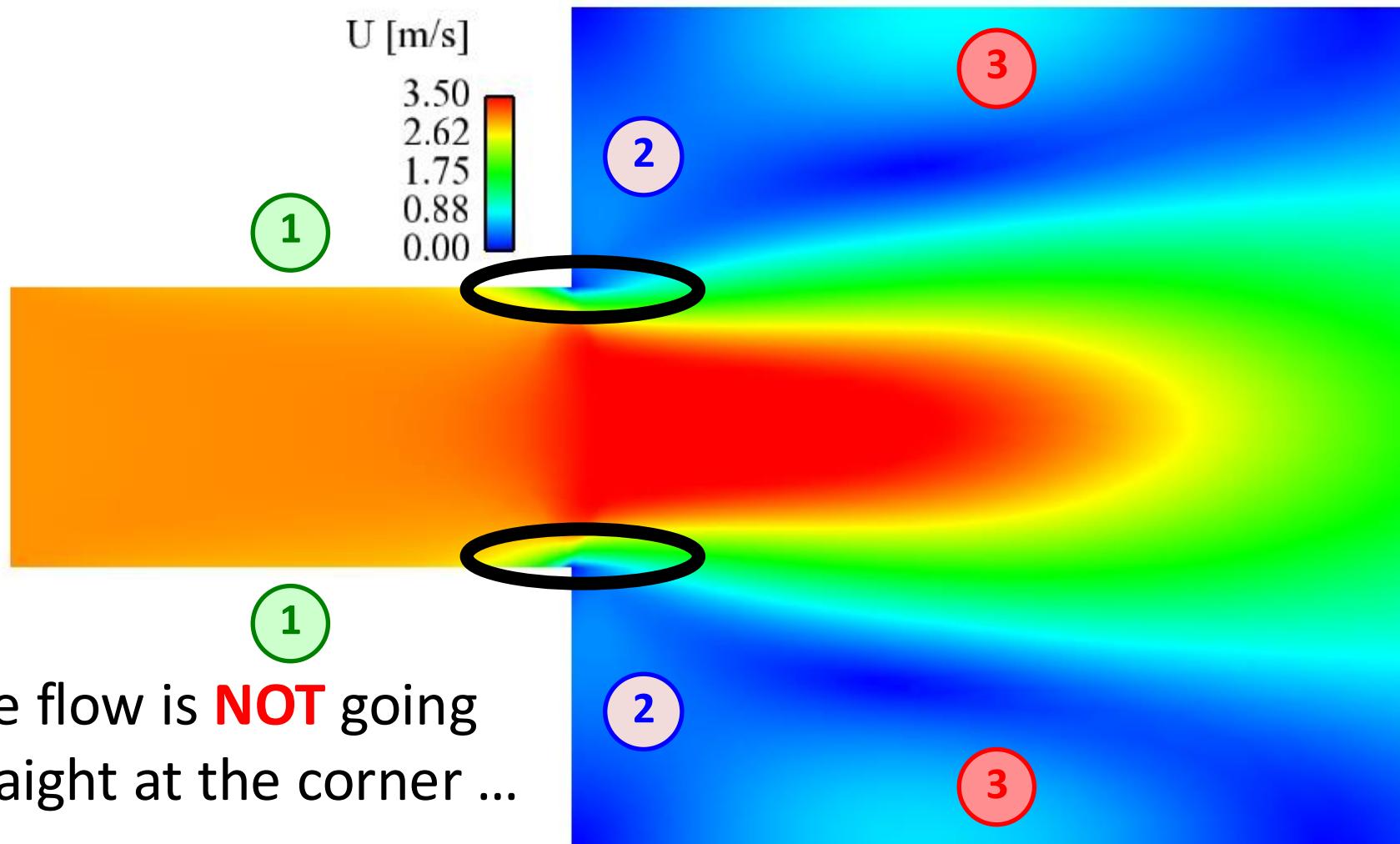
Wall corners

Example : sudden expansion

→ Let's consider **wall Law** using **2 separated** at the corner



Separated patches test case



Separated patches test case

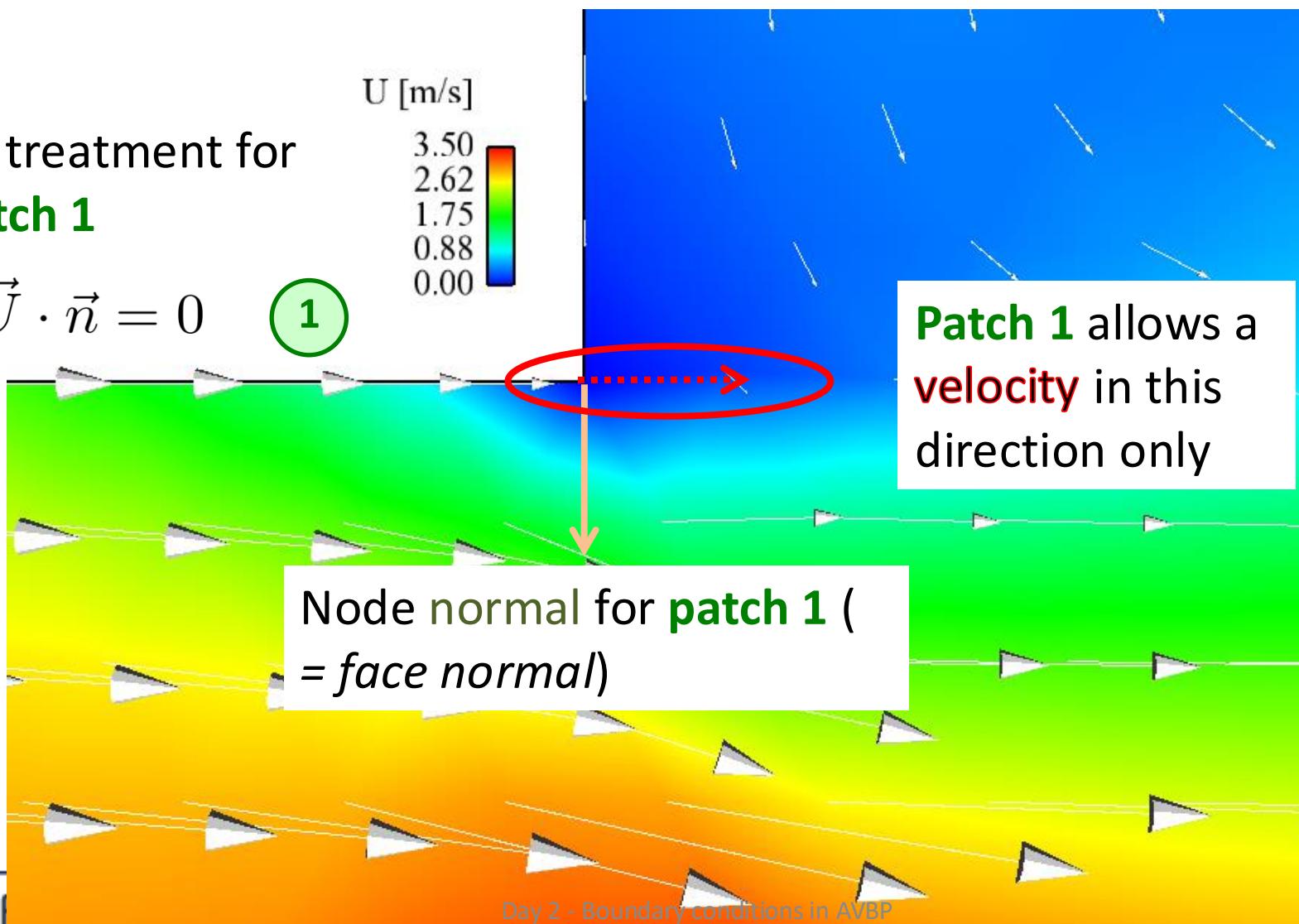
BC treatment for
patch 1

$$\vec{U} \cdot \vec{n} = 0$$

1

U [m/s]

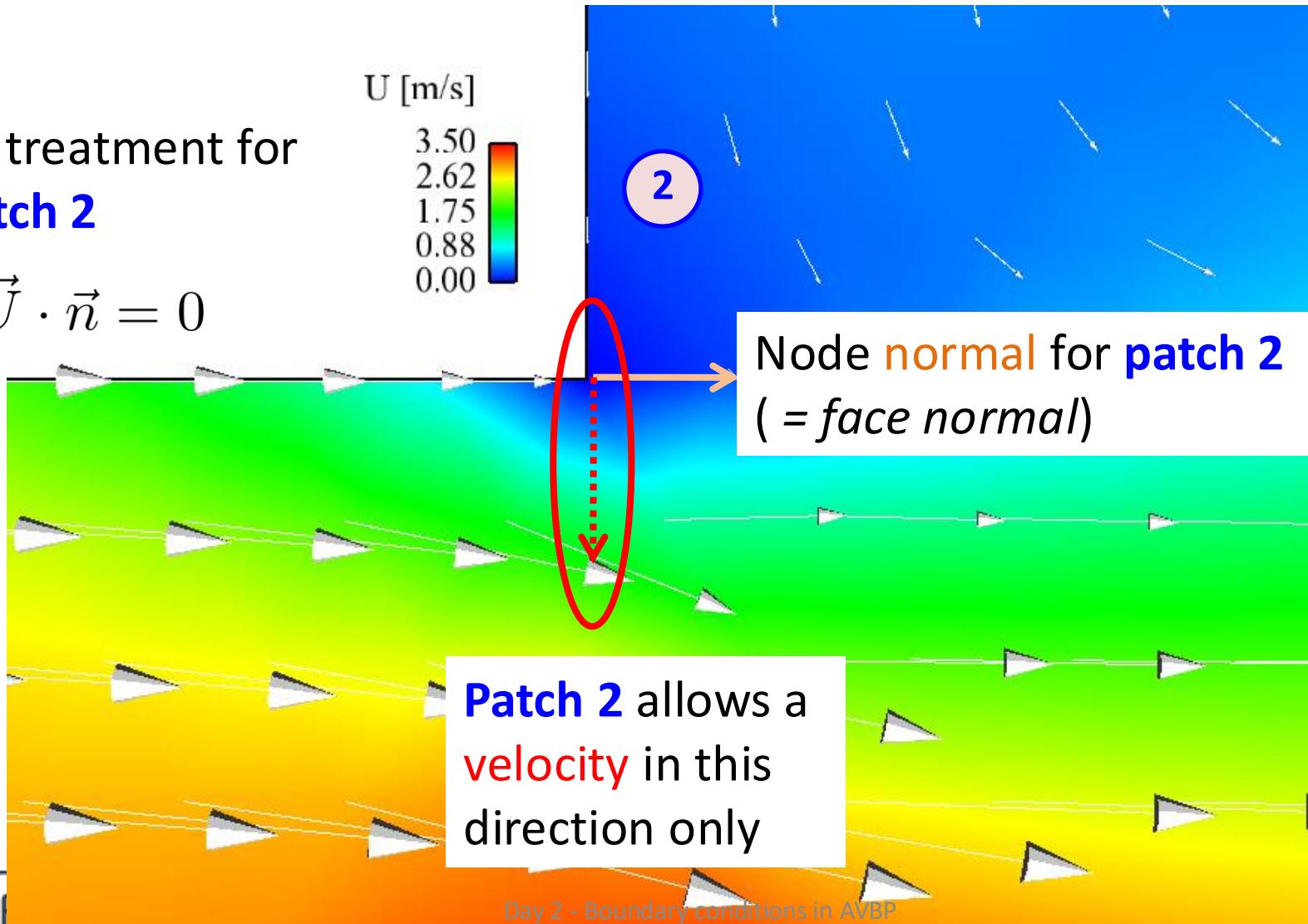
3.50
2.62
1.75
0.88
0.00



Separated patches test case

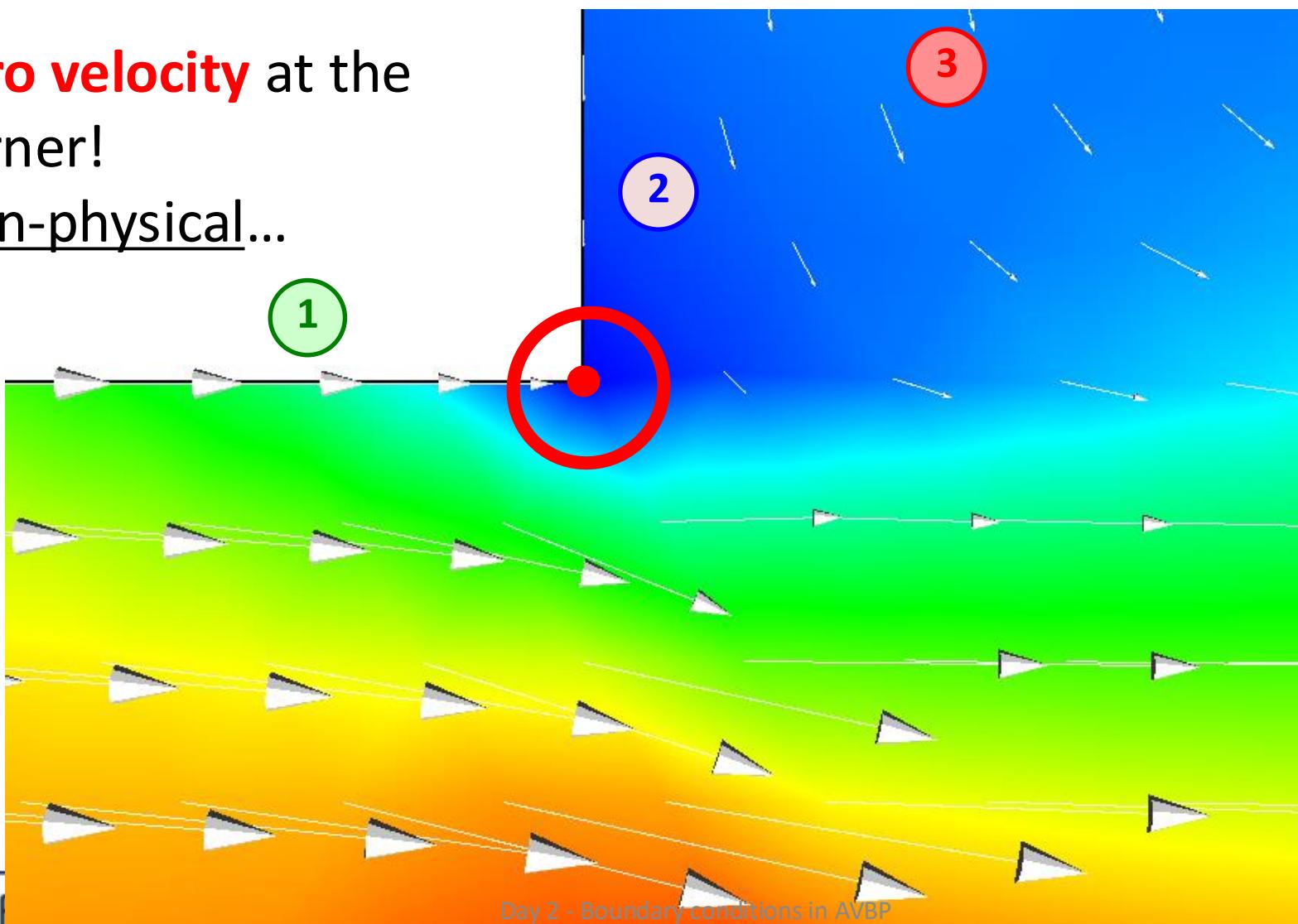
BC treatment for
patch 2

$$\vec{U} \cdot \vec{n} = 0$$



Separated patches test case

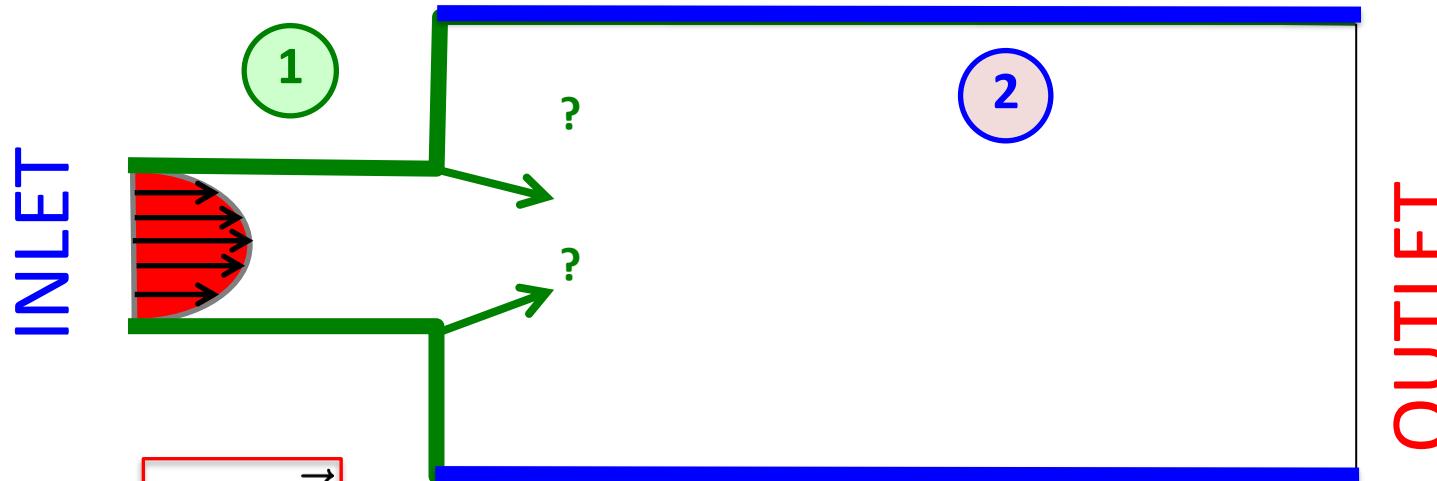
Zero velocity at the corner!
Non-physical...



The free corner method

What is the solution ?

→ The free-corner procedure !



Let's impose $\vec{n} = \vec{0}$:

→ $\vec{U} \cdot \vec{n} = 0$ is always satisfied.

→ The flow **direction** is let **free**

→ Additional treatments are imposed to enforce mass conservation
(*PhD P. Schmitt*)



Asciibound file

- You must enforce a single patch

```
!-----  
patch_name = wall_carter  
boundary_condition = WALL_LAWADIAB  
free_corner_min_angle = 60.0D00  
!-----
```



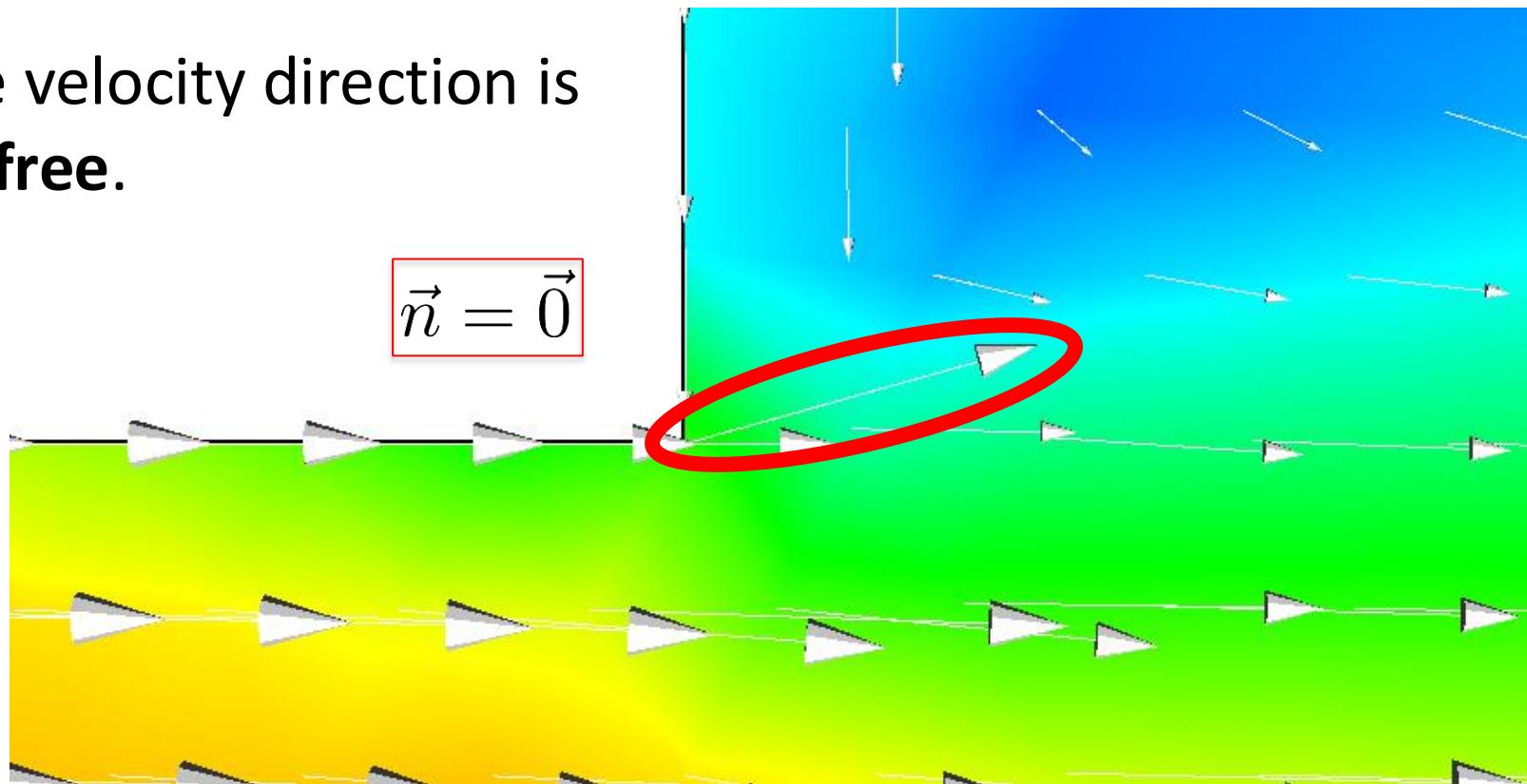
Activates free-corner procedure for angle between face normals > 60°



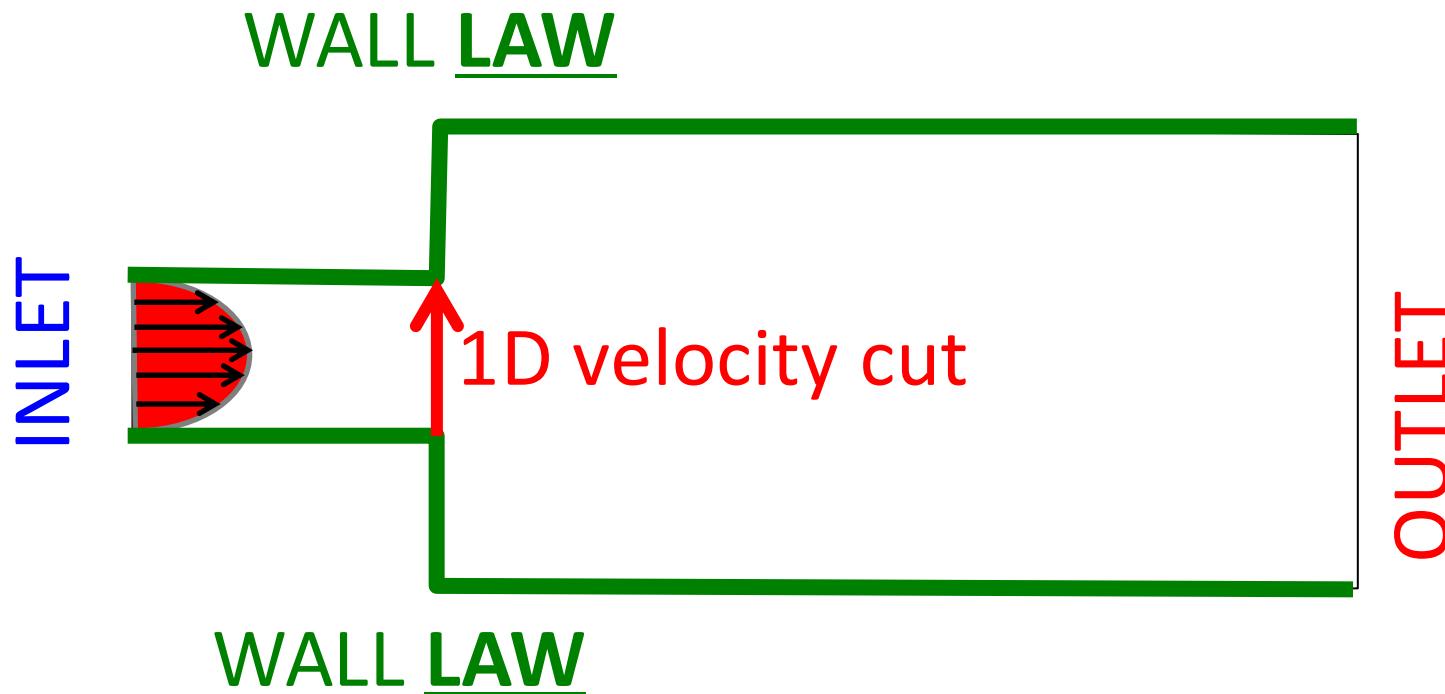
Example of corner treatments : 1 single patch + free corner

The velocity direction is let **free**.

$$\vec{n} = \vec{0}$$



In that case, an **additional correction** ensures the **mass conservation**

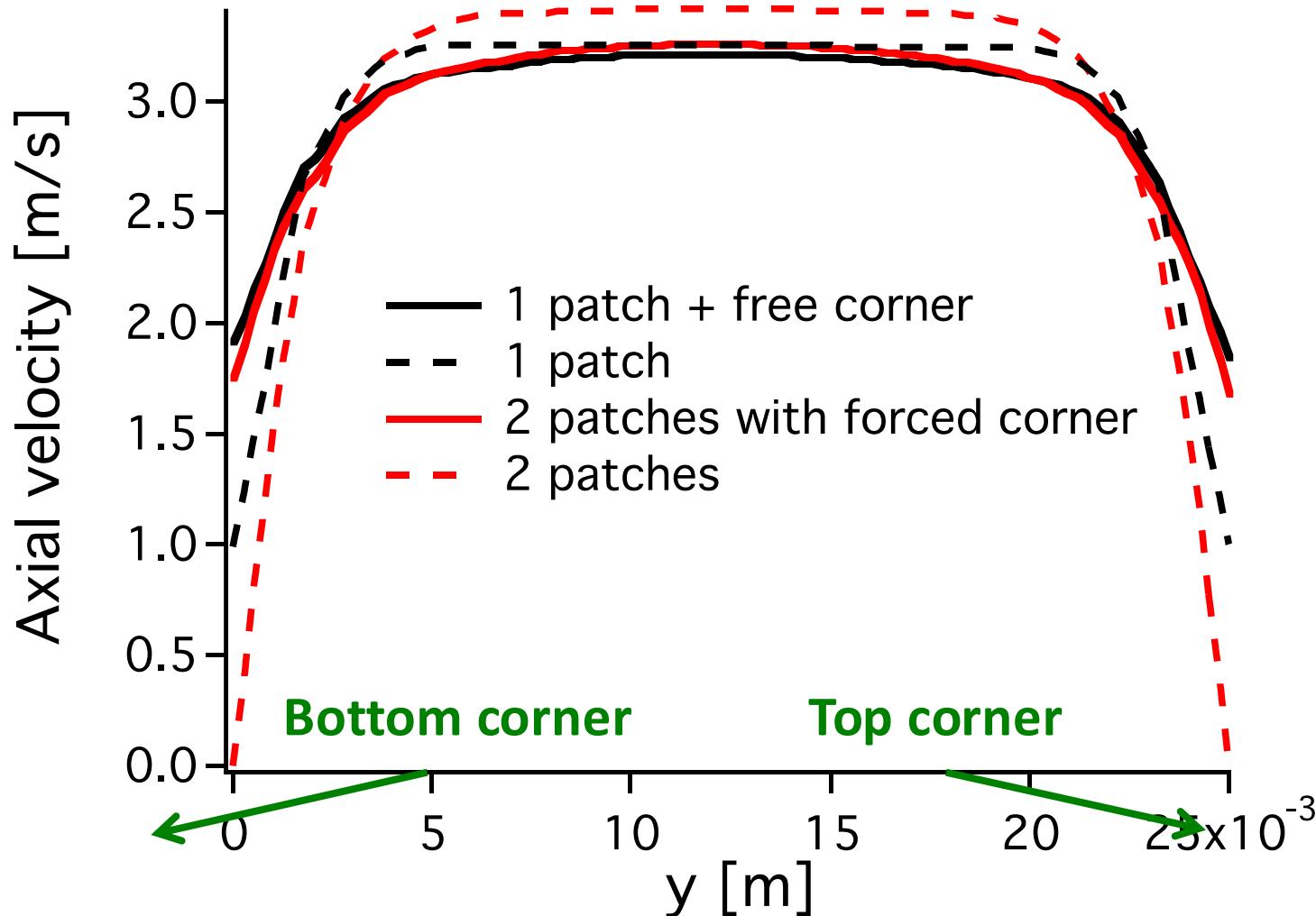


Velocity profiles at the cut position ?

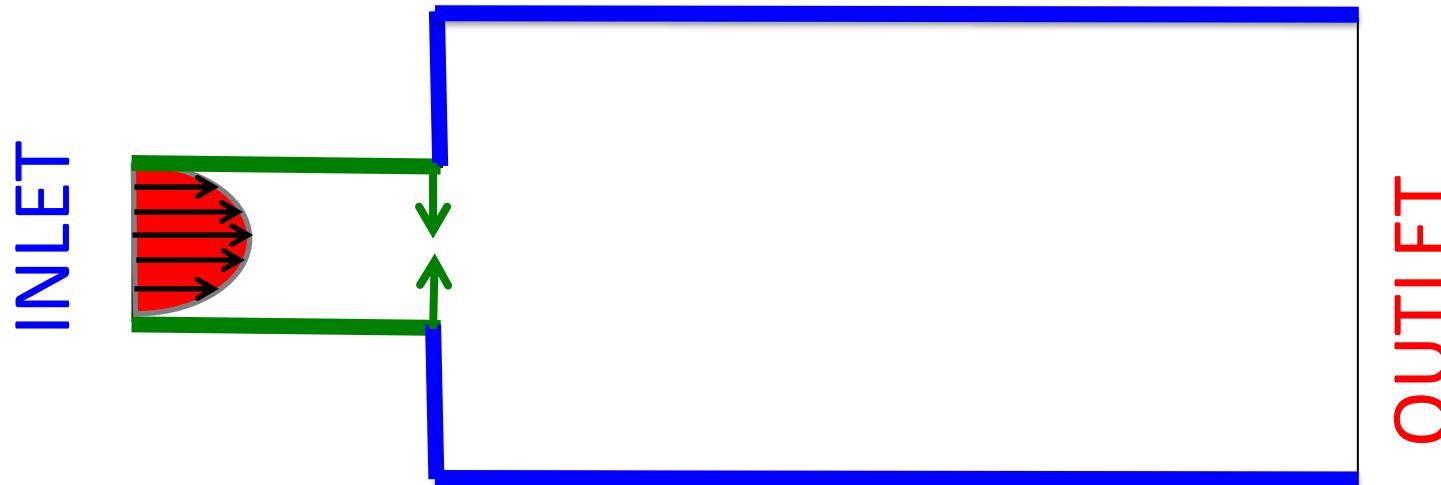




Example of corner treatments : summary



Sometimes, we may want to **enforce** the flow direction



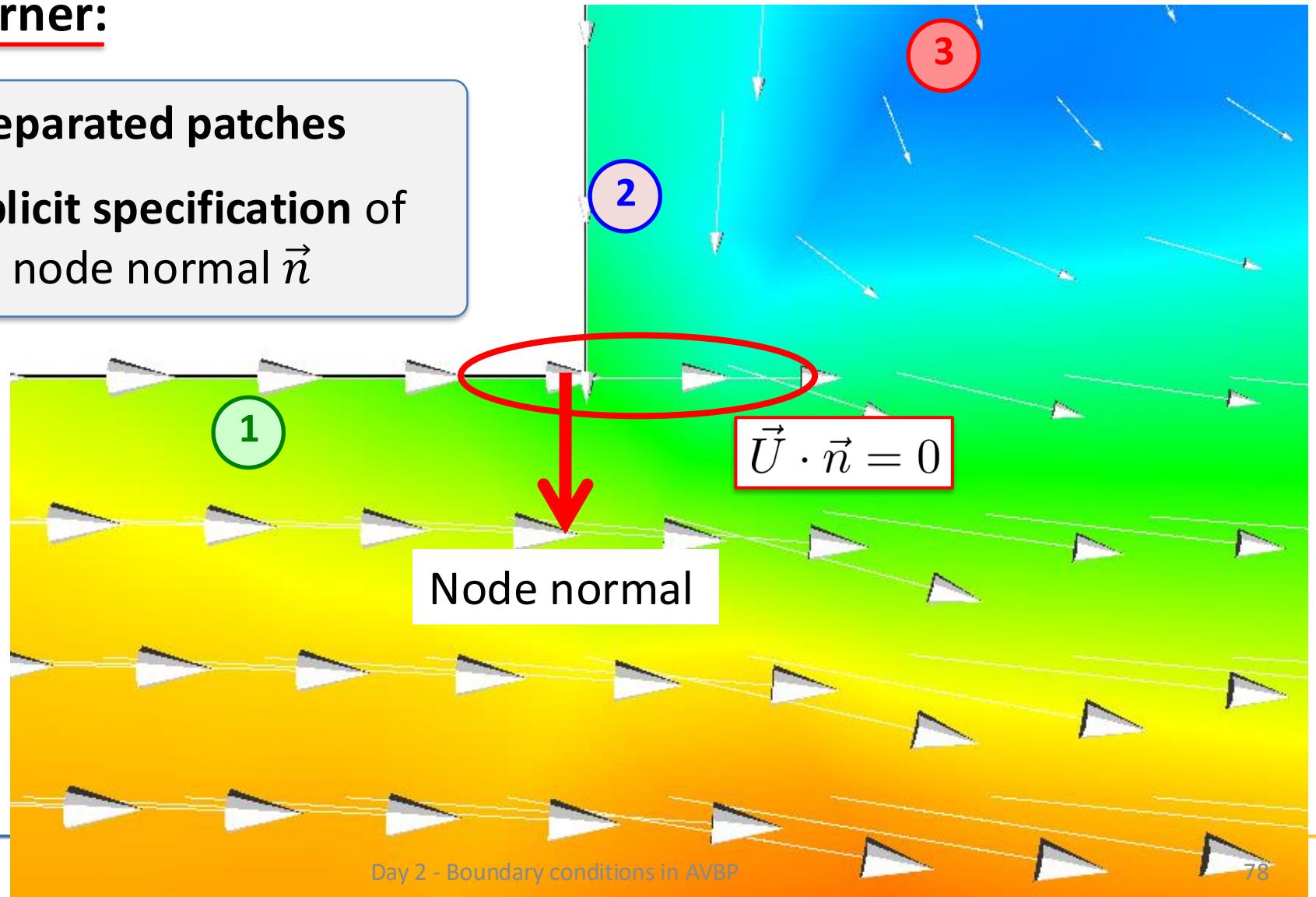
→ The **forced-corner procedure** !



Example of corner treatments : 2 patches with forced corner

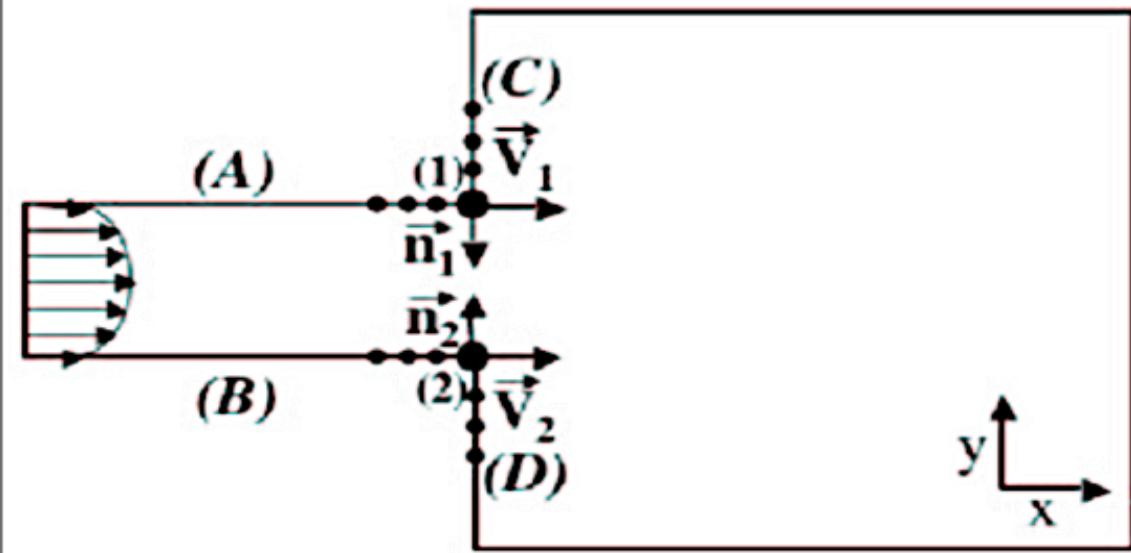
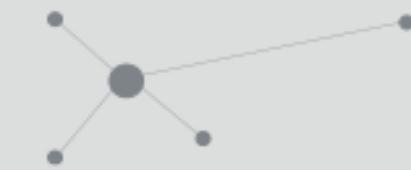
Forced-corner:

- **2 separated patches**
- **Explicit specification of the node normal \vec{n}**



Issues on corners

Forced corner method



Separated patches A and B

```
$BOUNDARY-PATCHES
patch_name = Patch_A
boundary_condition = WALL_LAW_ADIAB
free_corner_min_angle = 0.60D+02
forced_corner_associated_patch = Patch_C
```

**Patch_A imposes its normal to
Patch_C**
=> Enforce the velocity direction

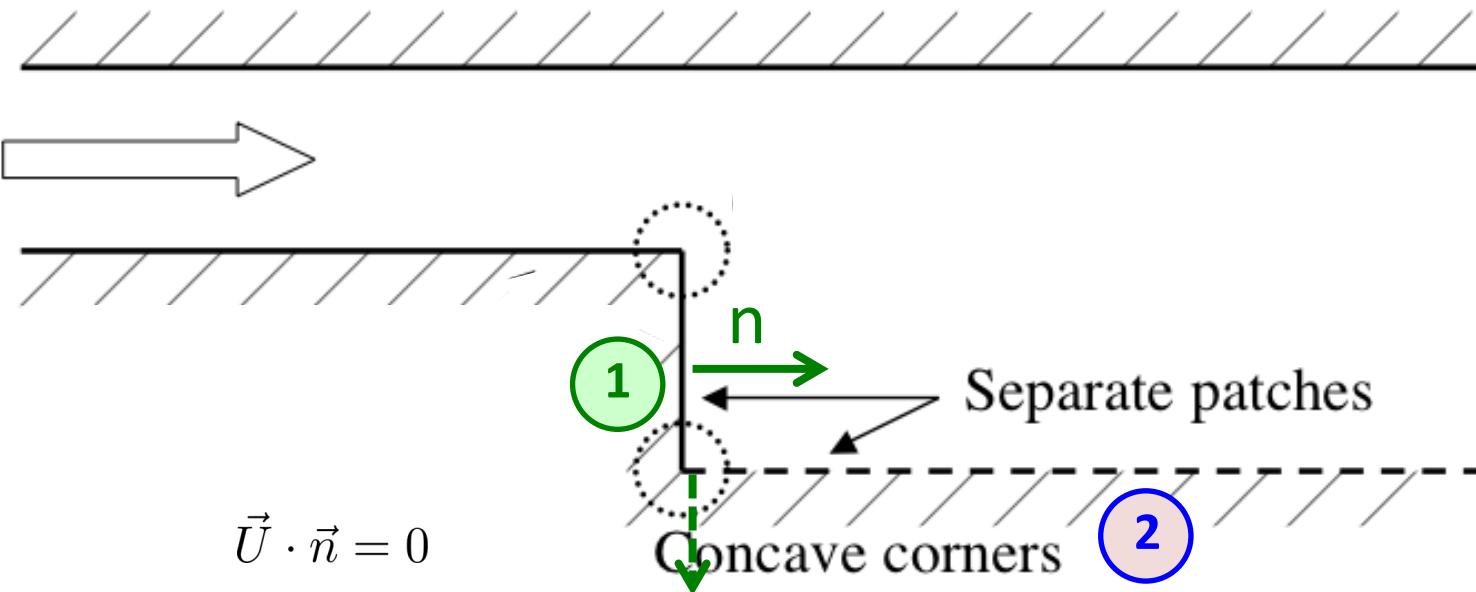


Issues on corners

Concave corners

For **concave corners**, the situation is simpler:

→ The two patches (1 and 2) **must be separated**.



- The first treatment (**patch 1**) implies that the **velocity normal to 1** is **zero**.

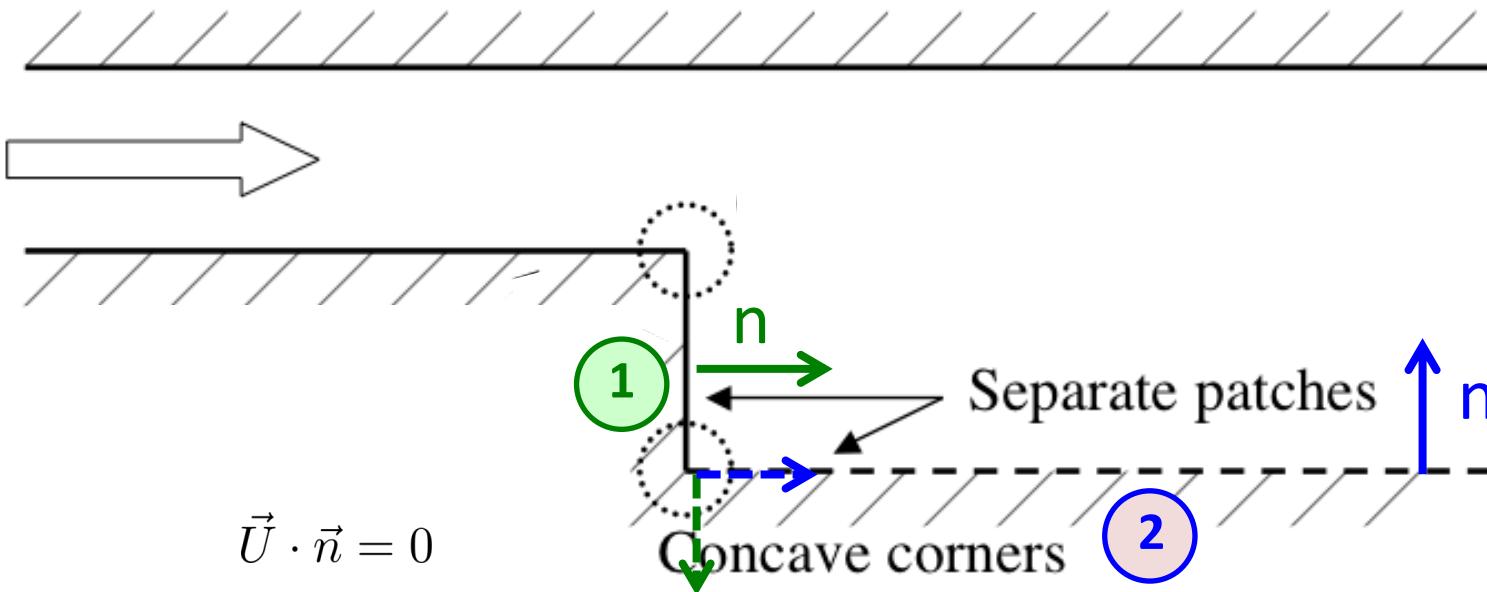


Issues on corners

Concave corners

For **concave corners**, the situation is simpler:

→ The two patches (**1** and **2**) **must be separated**.



- The first treatment (**patch 1**) implies that the **velocity normal** to **1** is **zero**.
- The second treatment (**patch 2**) implies that the **velocity normal** to **2** is **zero**.

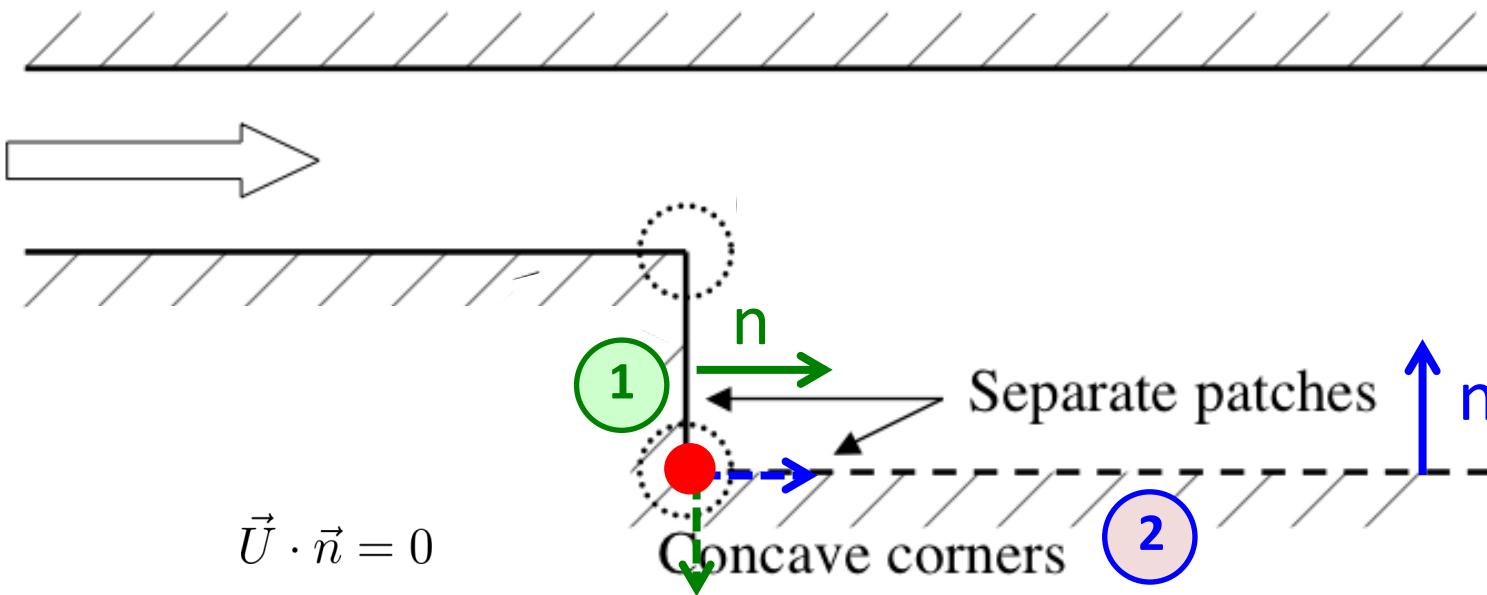


Issues on corners

Concave corners

For **concave corners**, the situation is simpler:

→ The two patches (**1** and **2**) **must be separated**.

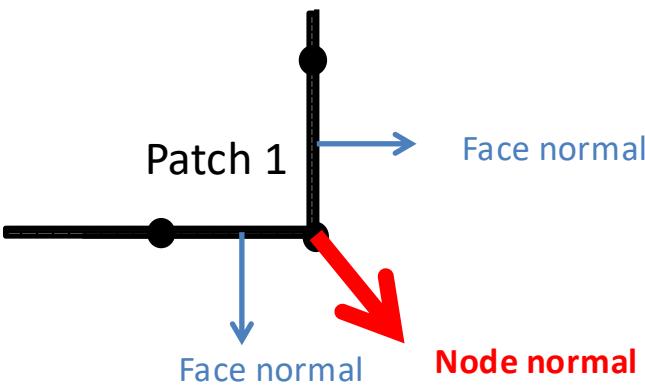


- The first treatment (**patch 1**) implies that the **velocity normal** to **1** is **zero**.
 - The second treatment (**patch 2**) implies that the **velocity normal** to **2** is **zero**.
- $\vec{U} = \vec{0}$ at the corner (●), which is physical.

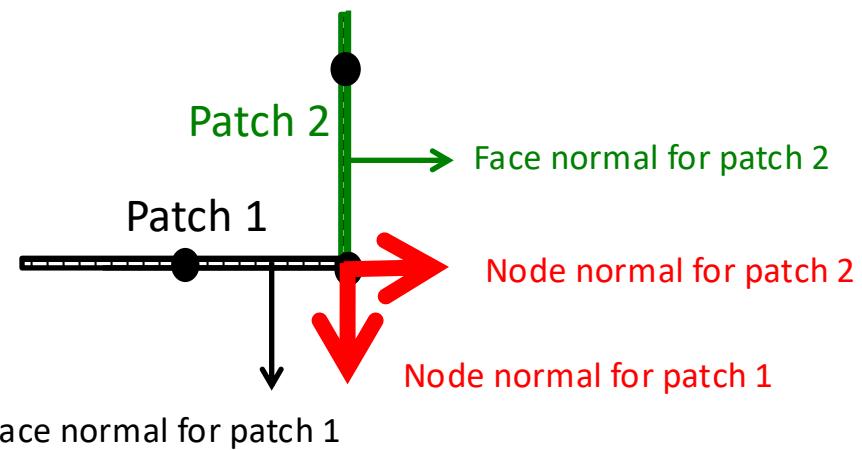


Partial conclusion on corners

One single patch



Separated patches



→ Recommended solution : free-corner approach

```
!-----  
patch_name = wall_carter  
boundary_condition = WALL_LAWADIAB  
free_corner_min_angle = 60.0D00
```

Theoretical insights

- Mathematical background
- Numerical methods

Description of AVBP schemes

- Lax Wendroff
- Two-step Taylor Galerkin schemes
- Properties of AVBP schemes

Practical elements

- Wiggles
- Issues at corners
- Artificial viscosity
- Shock sensors



Artificial viscosity

- Numerical schemes in AVBP are **centred schemes**. They are designed to be **low-dissipative**
- They however suffer from **dispersion errors** (as any numerical scheme)
- When Reynolds number increases, **dissipation operators may not allow to damp spurious errors**

→ Solution adopted in AVBP: artificial viscosity.



Artificial viscosity

Artificial viscosity in AVBP combines **two different types of operators** :

$$\frac{d\mathbf{U}_j}{dt} = \mathbf{R}_j + \mathbf{D}_j^{(2*)} + \mathbf{D}_j^{(4*)}$$

residual

2nd order artificial
viscosity

4th order artificial
viscosity

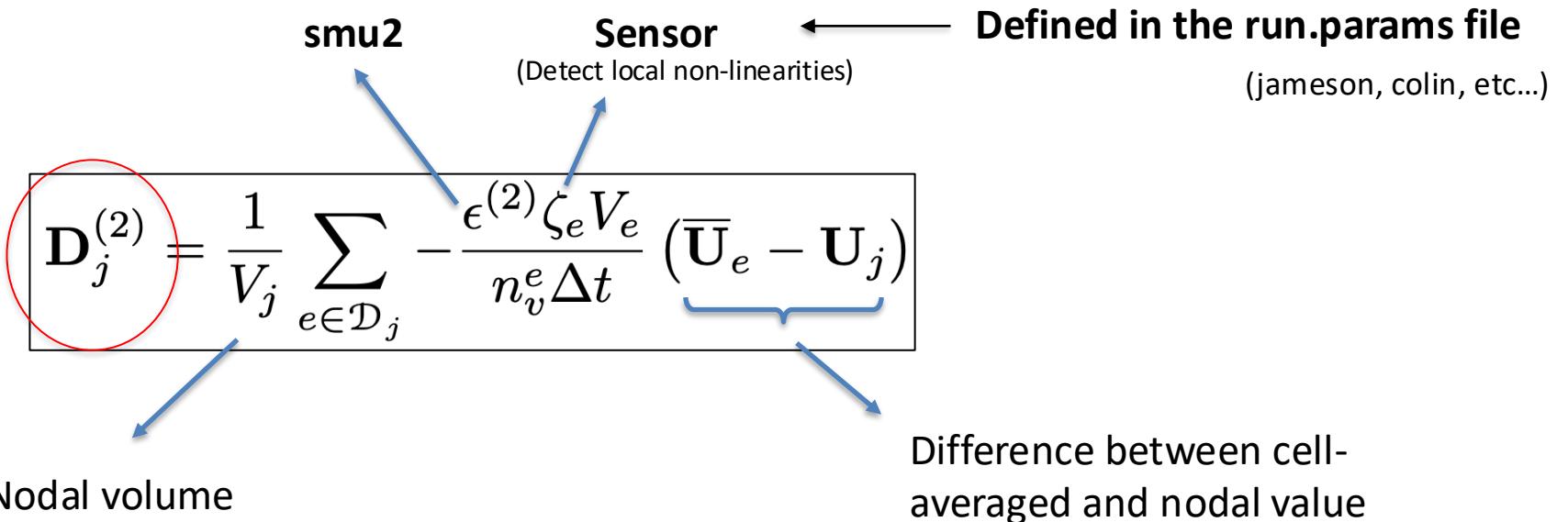
2nd and 4th order operators rely on **sensors**

→ Let's have a look in these operators, and sensors...

$$\frac{d\mathbf{U}_j}{dt} = \mathbf{R}_j + \mathbf{D}_j^{(2*)} + \mathbf{D}_j^{(4*)}$$

Second order AV

- 2nd order viscosity is based on a pseudo-Laplacian formulation
- Allow to damp **non-linearities**, stiff gradients



```
artificial_viscosity_model = colin
artificial_viscosity_2nd_order = 0.01D+00
artificial_viscosity_4th_order = 0.005D+00
```

$$\frac{d\mathbf{U}_j}{dt} = \mathbf{R}_j + \mathbf{D}_j^{(2*)} + \mathbf{D}_j^{(4*)}$$

Fourth order AV

- Contrarily to 2nd order operator, 4th order operator **operates in the entire domain**
- Allows to damp **node-to-node oscillations**

Smu4 **Sensor**

$$\epsilon_e^{(4*)} = \max \left(0, \epsilon^{(4)} - \zeta_e \epsilon^{(2)} \right)$$

$$\mathbf{D}_j^{(4)} = \frac{1}{V_j} \sum_{e \in \mathcal{D}_j} \frac{\epsilon_e^{(4*)} V_e}{n_v^e \Delta t} \left[\left(\frac{1}{n_v^e} \sum_{k \in K_e} \vec{\nabla} \mathbf{U}_k \right) \cdot (\vec{x}_e - \vec{x}_j) - (\mathbf{U}_e - \mathbf{U}_j) \right]$$

Nodal volume **Bi-Laplacian operator
(approximates a 4th-order derivatives)**

→ AV4 is applied everywhere, excepted in region where AV2 occurs



Sensors: Jameson

Jameson sensor at node k :

$$\zeta_k = \frac{|\Delta_1^k - \Delta_2^k|}{|\Delta_1^k| + |\Delta_2^k| + |\phi_k|}$$

With:

ϕ_k : nodal scalar quantity the sensor is based on
 $\Delta_1^k = \bar{\phi}_C - \phi_k$
 $\Delta_2^k = \nabla \phi_k \cdot (\mathbf{x}_C - \mathbf{x}_k)$

In AVBP, sensor applied on all conservatives variables, excepted species

Sensor at cell

$$\zeta_C^{Jameson} = \max_{k \in C} \zeta_k$$

Operators equivalence for a 1D regular mesh:

$$\Delta_1^k = \frac{\phi_{k+1} - \phi_k}{2}$$

$$\Delta_2^k = \frac{\phi_{k+1} - \phi_{k-1}}{4}$$

$$|\Delta_1^k - \Delta_2^k| = \left| \frac{1}{4} (\phi_{k+1} - 2\phi_k + \phi_{k-1}) \right|$$

- Proportional to 2nd order derivative of ϕ .
- Detect variations of $\vec{\nabla} \phi$ (wiggles). **Varies linearly with the perturbation**
- **However, also dissipates small scales of turbulence.**
- Not so adapted for LES. May be useful for initialization.



Sensors: Colin

Colin sensor:

$$\zeta_C^{Colin} = \frac{1}{2} \left(1 + \tanh \left(\frac{\Psi - \Psi_0}{\delta} \right) \right) - \frac{1}{2} \left(1 + \tanh \left(\frac{-\Psi_0}{\delta} \right) \right)$$

with

$$\begin{aligned}\Psi &= \max_{k \in C} \left(0, \frac{\Delta^k}{|\Delta^k + \epsilon_1 \phi_k|} \zeta_C^{Jameson} \right) \\ \Delta^k &= |\Delta_1^k - \Delta_2^k| - \epsilon^k \max(|\Delta_1^k|, |\Delta_2^k|) \\ \epsilon^k &= \epsilon_2 \left(1 - \epsilon_3 \frac{\max(|\Delta_1^k|, |\Delta_2^k|)}{|\Delta_1^k| + |\Delta_2^k| + |\phi_k|} \right)\end{aligned}$$

$$\begin{array}{lll}\Psi_0 = 2.10^{-2} & \delta = 1.10^{-2} \\ \epsilon_1 = 1.10^{-2} & \epsilon_2 = 0.95 & \epsilon_3 = 0.5\end{array}$$

- ζ_C^{Colin} **small for:** low amplitude errors, or stiff gradients well resolved by the scheme
- ζ_C^{Colin} **large for:** high amplitude numerical oscillation

→ Colin sensor works more in a on/off way than Jameson

AV2, AV4 applied on $(\rho, \rho E, \rho Y_k)$

- **Colin sensor is better suited for LES than Jameson**
- In AVBP, variables considered for AV with Colin allows good LES of reacting flows



Artificial Viscosity, summary

Reminder on Artificial Viscosity

- Choices for the sensor (Jameson, Colin, Colin_rhou (SLK), ...)
 - Choice for the level of 2nd order and 4th order applied (smu2, smu4)
 - Choice for the variable on which AV applies
-
- **AV is required** for LES of actual configurations...
... but an **inaccurate AV can lead to physical issues** (wrong operating point, ...)
 - **Do not confuse:** *subgrid-scale* viscosity and *artificial* viscosity !

See AVBP website (dedicated page) for recommendations !

Available AV options in ABVP

At present time, one can chose between 8 values for the keyword `artificial_viscosity_model` :

- `no`: no A.V. ("Academic" LES or true DNS).
- `honey`: "honey" mode, sensor fully active (equal to 1), the flow is very viscous, should only be used for transients (Initialization of the computation).
- `Jameson`: A.V. for "aerodynamics" (based on Jameson sensor).
- `Jameson_species`: A.V. for "aerodynamics" (based on Jameson sensor). An additional sensor is applied for the species mass fractions.
- `Colin`: A.V. for LES and/or combustion (based on Colin sensor).
- `Colin_species`: A.V. for LES and/or combustion (based on Colin sensor). An additional sensor is applied for the species mass fractions.
- `Colin_rhou`: A.V. for LES and/or combustion (based on Colin sensor), applying besides artificial viscosity upon ρu .
- `Colin_rhou_species`: A.V. for LES and/or combustion (based on Colin sensor), applying besides artificial viscosity upon ρu . An additional sensor is applied for the species mass fractions.



AVBP run.params file

```
$RUN-CONTROL
solver_type = ns
diffusion_scheme = FE_2delta
simulation_end_time = 1.0000000d-03
mixture_name = AIR
reactive_flow = no
combustion_model = no
two_phase_flow = no
real_gas = no
LES_model = sigma
prandtl_turb = 0.6000000D+00
schmidt_turb = 0.6000000D+00
convection_scheme = LW
CFL = 0.9000000D+00
Fourier = 0.1000000D+00
compute_chemical_timestep = no
artificial_viscosity_model = colin
artificial_viscosity_2nd_order = 0.01D+00
artificial_viscosity_4th_order = 0.005D+00
clip_species = no
$end_RUN-CONTROL
```

Euler / Navier-Stokes

Diffusion scheme.

(*FE_2delta* only choice since AVBP_7.7)

LW / TTG4A / TTGC (+ many others !)

CFL number, if time-step is not imposed

AV Sensor model

smu2

smu4

You should be able to understand, and accurately
set these parameters for your case !

AVBP WEBSITE

The image shows the homepage of the AVBP website. The top navigation bar includes links for Home, Input (circled in red), Output Tools, Docs, Install, Tutorials, and FAQ. A sidebar on the left lists General, Versions, Handbook, QPF table, HIP, Chemistry, Movie, Gallery, Bug store, and Training. The main content area features a title "THIS IS THE WEBSITE OF THE AVBP CODE OF CERFACS" and a description of the code's capabilities. Below this are two sections: "AVBP: a leader in the field of simulation of turbulent reacting flows" and "AVBP: a leader in the field of High Performance Computing". The "Gallery" section contains four images illustrating the code's output: a 3D simulation of a flame kernel, a 2D color map of turbulent structures, a 3D simulation of a flame front, and a 2D cross-section of a flame front.

THIS IS THE WEBSITE OF THE AVBP CODE OF CERFACS

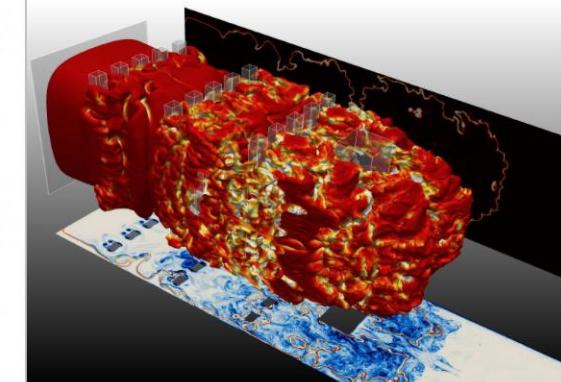
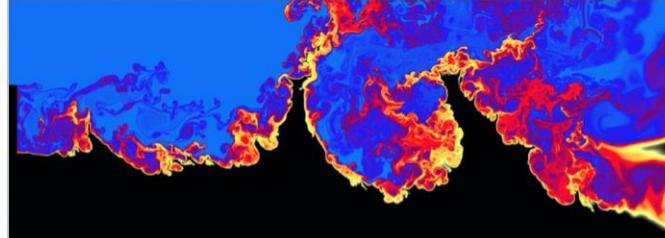
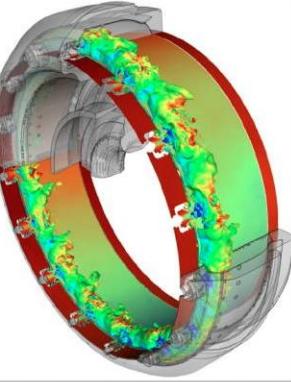
You can find here examples of simulations as movies or images (in the [Gallery](#)). You can also have information on AVBP trainings. If you are an AVBP user, you can also find here information on the AVBP input files, on the scientific manual, the list of test cases (QPFs), the chemistry site of CERFACS and the bug store.

AVBP: a leader in the field of simulation of turbulent reacting flows

AVBP is a suite of CFD tools to perform DNS and LES of compressible, reacting, turbulent, multispecies flows, on massively parallel CPU and GPU architectures. AVBP is widely used for basic research in multiple laboratories. It is also the design CFD tool for many french companies using LES. The AVBP project is one of the largest CFD teams worldwide focusing on reacting flows with more than 60 researcher scientists and engineers.

AVBP: a leader in the field of High Performance Computing

AVBP is at the forefront of HPC developments. It is a reference code in the HPC community, used today in the [COEC](#) European Center for Excellence. AVBP is also used for LES of non-reacting flows (turbomachinery), safety CFD (pollution dispersion, virus airborne transport) and environmental problems (solar, wind farms). AVBP is also applied to multiphysics problems in collaboration with ONERA using the [CWIP1](#) coupler technology.



This is what a typical AVBP simulation looks like:

```
graph TD; AVBP_CASE[AVBP CASE] --> RUN[RUN]; AVBP_CASE --> MESH[MESH]; AVBP_CASE --> SOLUTBOUND[SOLUTBOUND]; AVBP_CASE --> INIT[INIT]; RUN --> run_params["run.params"]; RUN --> keywords_in["keywords.in"]; RUN --> species_database_dat["species_database.dat"]; RUN --> mixture_database_dat["mixture_database.dat"]; RUN --> command_dat["command.dat"]; RUN --> injection_EL_dat["injection_EL.dat"]; RUN --> turboavbp["TurboAVBP"];
```

Several files are mandatory to perform a run with AVBP, others are optional. The following sections and links describe how to generate or fill in these files.

The parameter files

Four parameter files are needed to parametrize a computation with AVBP (two are dedicated to Euler-Lagrange simulation) :

- **keywords.in**: this file is the rule file. It specifies the name of the main input file of your computation (default name = 'run.params') and it also contains a list of keyw all the options available for a computation in AVBP.
This file is specific to a given version of AVBP and may be retrieved for each distribution of AVBP in the directory `$AVBP_HOME/WORK/INPUT`.
For a technical description of this file, see [this page](#).

<code>convection_scheme.boundary_terms</code>	character	closed unclosed	<p>Controls the boundary term treatment. Only valid for convective schemes based on a Lax-Wendroff-like method (total discretization). Default values are:</p> <ul style="list-style-type: none"> • closed if <code>convection_scheme</code> = 'TTGC' or 'TTG4A'. • unclosed if <code>convection_scheme</code> = 'LW' or 'LW_FE'. • Not used otherwise. <p>More information is available in this document .</p>
<code>diffusion_scheme</code>	character	FV_4delta FE_2delta	<p>The diffusion scheme:</p> <ul style="list-style-type: none"> • FV_4delta : the original finite volume 4Δ diffusion scheme. • FE_2delta : the finite element 2Δ diffusion scheme developed by O. Colin. <p>More information is available in this document .</p> <p>Default: FE_2delta if <code>solver_type</code> = 'NS'. Not used otherwise.</p>
<code>CFL</code>	double	-	The CFL number used to compute the convective time-step.

Very interesting pdf files are available on the website through [this document](#)  !



Good readings

PhD thesis

- AVBP-Website
 - AVBP Handbook
 - AVBP QPF
- N. Lamarque
 - L.M Segui-Troth
 - B. Martin

<https://elearning.cerfacs.fr>

Books:

- Hirsch, C. (1990) Numerical Computation of Internal and External Flows. Wiley, Hoboken.
- G. Allaire. Analyse numérique et optimisation. Les Editions de l'Ecole Polytechnique, 2012
- J. Donea and A. Huerta. *Finite Element Methods for Flow Problems*. Wiley–Blackwell, 2003
- T. Poinsot and D. Veynante. Theoretical and Numerical Combustion. R.T. Edwards Inc., 2005. Ch. 9
- R. Vichnevetsky and J. Bowles. Fourier analysis of numerical approximations of hyperbolic equations. SIAM, 1982.
- B. Després, F. Dubois. Systèmes hyperboliques de lois de conservation. Les Editions de l'Ecole Polytechnique, 2005
- Godlewski, E., and Raviart, P. A., *Numerical Approximation of Hyperbolic Systems of Conservation Laws*, Springer-Verlag, New York, 1996
- *Numerical Recipes in FORTRAN: The Art of Scientific Computing*

