High-order Residual-Based Compact schemes on overset grids

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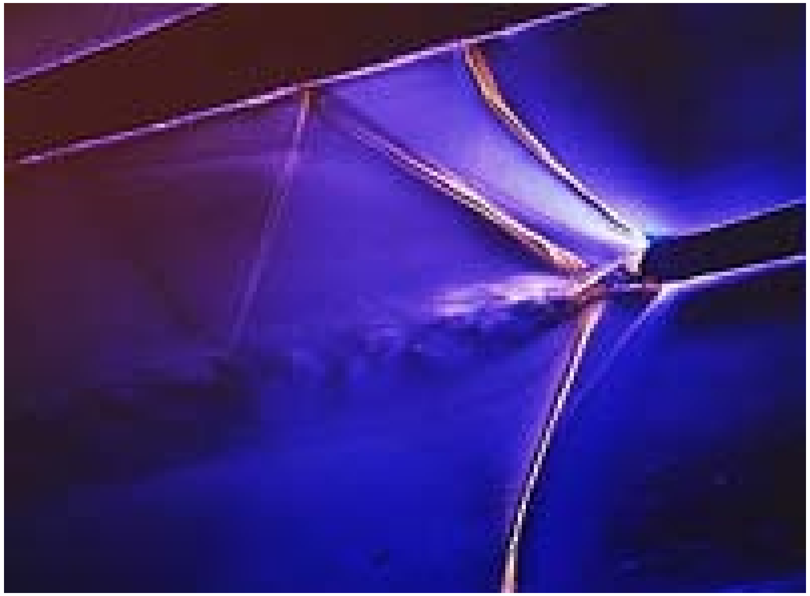
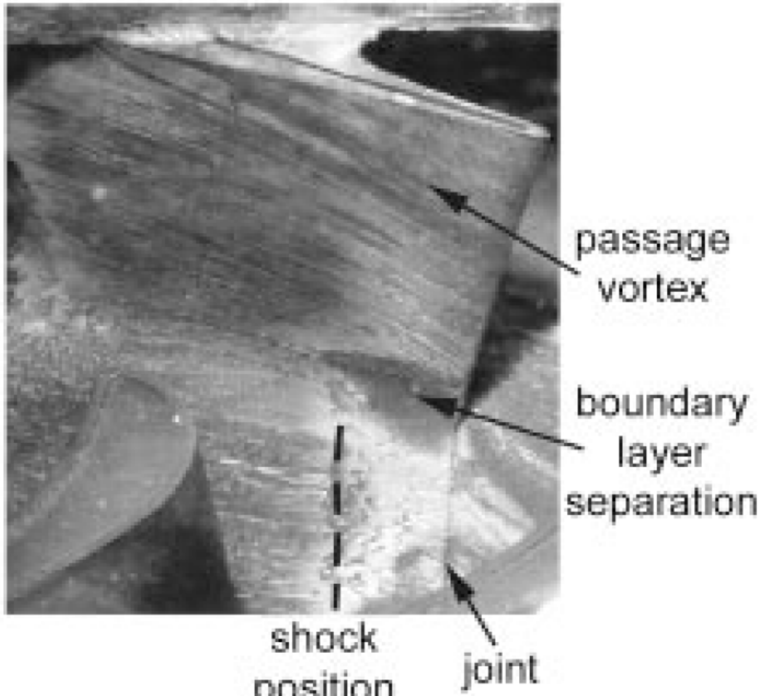
Introduction

- CFD applied to increasingly complex configurations (highly loaded components, off-design conditions, physically complex phenomena, unsteady flows), experimental campaigns reduced

→ **Need for high-fidelity industrial CFD**



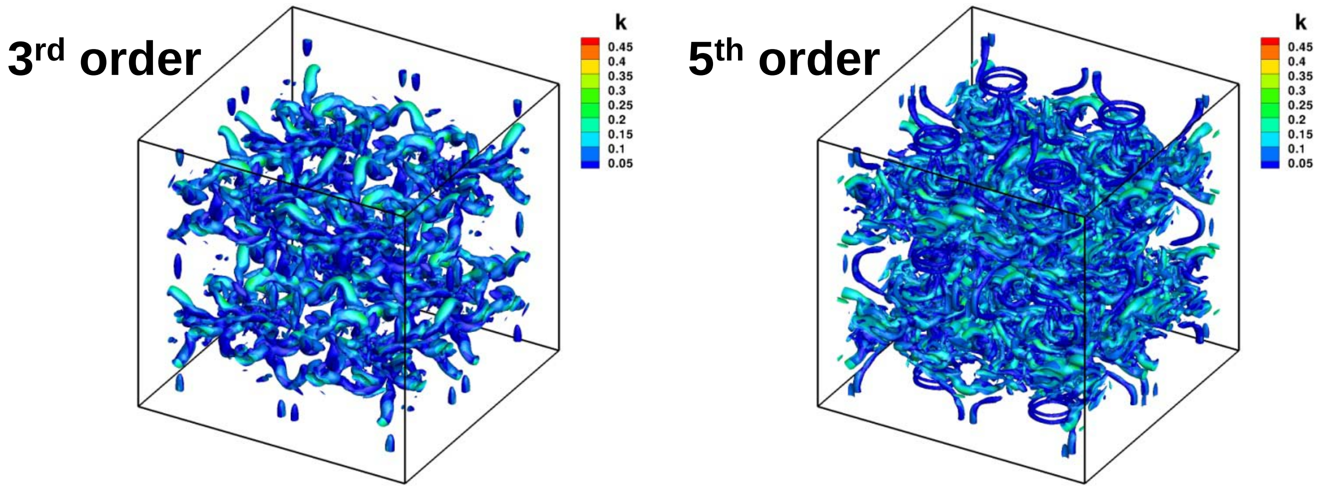
http://www.nrc-cnrc.gc.ca/eng/programs/iar/internal-aerodynamics.html



Gottlich et al. (2004), J. Turbom. 126:297-305.

Introduction

- Fundamental ingredients for HiFi CFD:
  - Improved unsteady physical models (e.g. LES or RANS/LES) : much more sensitive than RANS to numerical errors, which may be inextricably coupled to physical effects
  - High-accurate numerics
    - Large meshes + massive parallelism →memory, storage and post-treatment problems; massively parallel computer not always readily available in industry, high energy consumption
    - <u>High-accurate numerical schemes</u> → higher cost per mesh point, robustness, ability to handle complex geometries, parallel performance



Taylor-Green Vortex, 128^3 mesh, t=12, Q-criterion = 3: RBC3 left, RBC5 right

Objectives

- Develop a family of high-order schemes with the following characteristics
  - High resolvability
  - Good shock capturing capabilities
  - Ability to handle complex geometries
  - Robustness
  - Moderate computational cost and memory consumption requirements

- Design strategy
  - Structured grids → low memory, cost
  - Use of compact schemes → low error constants, spectral-like accuracy
  - Use of intrinsically dissipative schemes → stability and shock capturing without tuning parameters
  - Use of overset grids → complex geometries, parallelism

Context

- InDustrIalisation of High-Order Methods project:

IDIHOM

  - promotes the use of HO numerical methods by the European aerospace industry
  - 21 research groups, academic and industrial
  - from 10 European countries

- Our task: investigate the feasibility of Residual-Based Compact (RBC) schemes for challenging applications (FV framework)

Overview

- High-order Residual-based compact schemes
  - Design principles
  - Truncation error and spectral properties
  - Shock capturing properties
- Extension to complex geometries
  - Overset grid framework
  - High-order interpolations
- Numerical results
  - Preliminary validations
  - Application examples

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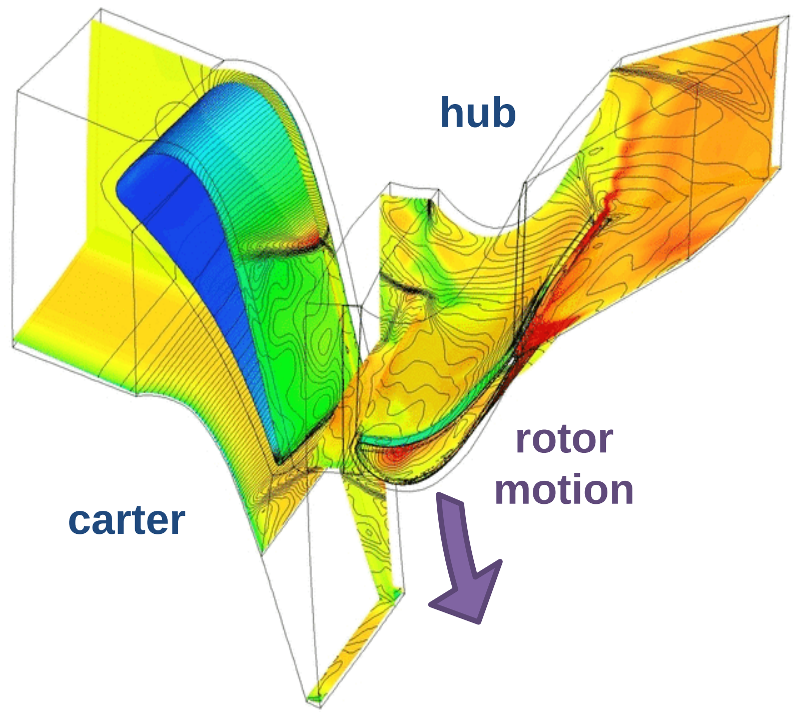
A little history…

- Residual-Based Compact (RBC) schemes (order 2,3,5 and 7)
  - derived in the finite-difference (FD) framework by Lerat and Corre [JCP 2001]
  - straightforward extension of the FD numerical fluxes to the FV framework for the simulation of inviscid and viscous problems
  - nominal order of accuracy lost on non-Cartesian and non-uniform meshes
  - High accurate extension to curvilinear meshes (RBCi) possible but limited to order 3 up to now [Hanss et al., 2002; Grimich et al., 2013] → **applied to industrial configurations**



Rotor/stator interaction in the BRITE HP turbine

- Idea: maximize regions of high-order treatment, RBC schemes used in conjunction with an overset grid framework

High-order RBC schemes

Initial value problem
$$\begin{cases} w_t + f_x + g_y = 0 \text{ on } \mathbb{R}^2 \times \mathbb{R}^+ \\ w(x,y,0) = w_0(x,y) \end{cases}$$

$w \rightarrow$ state vector, $f(w), g(w) \rightarrow$ fluxes in x and y

$A = {\partial f}/{\partial w}$, $B = {\partial g}/{\partial w} \rightarrow$ Jacobian matrices

Discretize on a uniform mesh
$$\begin{cases} x_j = j\delta x, y_k = k\delta y \\ \delta x \approx \delta y \approx \mathcal{O}(h) \end{cases}$$

Mean and difference operators:

$$(\delta_1 v)_{j+\frac{1}{2},k} = v_{j+1,k} - v_{j,k} \qquad (\delta_2 v)_{j,k+\frac{1}{2}} = v_{j,k+1} - v_{j,k}$$

$$(\mu_1 v)_{j+\frac{1}{2},k} = \frac{1}{2}(v_{j+1,k} + v_{j,k}) \qquad (\mu_2 v)_{j,k+\frac{1}{2}} = \frac{1}{2}(v_{j,k+1} + v_{j,k})$$

High-order RBC schemes

- Define the exact residual as:

$$r := w_t + f_x + g_y$$

- Residual-based (RB) scheme : can be written only in terms of approximations of the exact residual and its derivatives
- General formulation of a RB scheme:

$$\left(\tilde{r}_0\right)_{j,k} = \tilde{d}_{j,k}$$

$\left(\tilde{r}_0\right)_{j,k} \rightarrow$ centered approximation of r at point $\left(j,k\right)$

$\tilde{d}_{j,k} = \tilde{d}\left(r_{j,k}\right) \rightarrow$ residual-based numerical dissipation

RB numerical dissipation

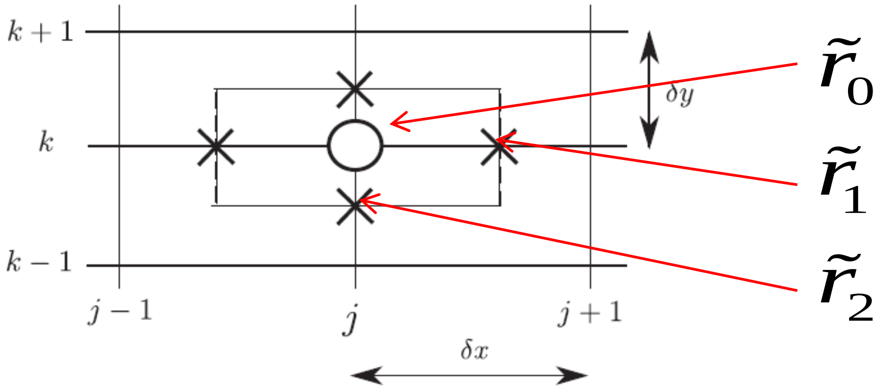
- A convenient expression for the dissipation operator is :

$$\tilde{d}_{j,k} = \frac{1}{2}\left[\delta_1\left(\Phi_1\tilde{r}_1\right)+\delta_2\left(\Phi_2\tilde{r}_2\right)\right]_{j,k} = \underbrace{\frac{1}{2}\left[\delta x\left(\Phi_1 r\right)_x+\delta y\left(\Phi_2 r\right)_y\right]_{j,k}}_{=0} + O\left(h^p\right)$$

$\tilde{r}_1, \tilde{r}_2 \longrightarrow$ midpoint residuals

centered approximations of *r*

$\Phi_1, \Phi_2 \longrightarrow$ dissipation matrices, depend on the eigenvalues of *A* and *B*; no tuning parameters



Compact approximations of the residuals

- RBC approach: compact centered difference(Padé) operators for the approximation of the main and midpoint residuals
  - RBC3 → 3rd-order on 3x3 points
  - RBC5 → 5th-order on 5x5 points
  - RBC7 → 7th-order on 5X5 points
  - RBC*q* → RBC scheme of order *q*

Main residual

Pade approximation of first order derivatives

$$f_x = (\overline{D_1})^{-1}\overline{N_1}\frac{\delta_1\mu_1 f}{\delta x} + \mathcal{O}(\delta x^{2p}) \quad g_y = (\overline{D_2})^{-1}\overline{N_2}\frac{\delta_2\mu_2 g}{\delta y} + \mathcal{O}(\delta y^{2p})$$

where $\overline{N_m} = I + \overline{a}\delta_m^2, \qquad \overline{D_m} = I + \overline{b}\delta_m^2 + \overline{c}\delta_m^4$

$$(\delta_m^p f)_{j,k} = \underbrace{\delta_m(\delta_m(...(\delta_m f)))}_{p \text{ times}} \qquad m = 1, 2$$

Applying $\overline{D_1}$ $\overline{D_2}$ to all terms at the left hand side gives

$$\boxed{(\tilde{r_0})_{j,k} = \left(\overline{D_1}\ \overline{D_2} w_t + \overline{D_2}\ \overline{N_1}\frac{\delta_1\mu_1 f}{\delta x} + \overline{D_1}\ \overline{N_2}\frac{\delta_2\mu_2 g}{\delta y}\right)_{j,k}}$$

Truncation error $\quad \varepsilon_{j,k} = \left[I + \mathcal{O}(h^2)\right]\left[r_{j,k} + \mathcal{O}(h^{2p})\right]$

Midpoint residuals

Mid-point residuals approximated by using the same technique as for the main residual

$$\boxed{\begin{aligned}(\tilde{r_1})_{j+\frac{1}{2},k} &= \left[N_1^{\mu}\mu_1\left(D_2 w_t + N_2\frac{\delta_2\mu_2 g}{\delta y}\right) + N_1^{\delta}D_2\frac{\delta_1 f}{\delta x}\right]_{j+\frac{1}{2},k}\\ (\tilde{r_2})_{j,k+\frac{1}{2}} &= \left[N_2^{\mu}\mu_2\left(D_1 w_t + N_1\frac{\delta_1\mu_1 f}{\delta x}\right) + N_2^{\delta}D_1\frac{\delta_2 g}{\delta y}\right]_{j,k+\frac{1}{2}}\end{aligned}}$$

→ Introduction of additional, face-centered Padé fractions + careful choice of common denominators

RBC spatial discretization

A peculiar feature of unsteady RBC schemes:

- A mass matrix appears due to difference operators applied to w_t.
- Not crucial for steady problems or slow unsteady problems solved using a sub-iteration technique (DTS or Newton)

$$(\tilde{r_0})_{j,k} = \left(\boxed{\overline{D_1}\;\overline{D_2} w_t} + \boxed{\overline{D_2}\;\overline{N_1}\frac{\delta_1\mu_1 f}{\delta x} + \overline{D_1}\;\overline{N_2}\frac{\delta_2\mu_2 g}{\delta y}} \right)_{j,k}$$

Operators applied to time derivatives

Operators applied to spatial derivatives

$$(\tilde{r_1})_{j+\frac{1}{2},k} = \left[N_1^{\mu}\mu_1 \left(D_2 w_t + N_2 \frac{\delta_2\mu_2 g}{\delta y} \right) + N_1^{\delta} D_2 \frac{\delta_1 f}{\delta x} \right]_{j+\frac{1}{2},k}$$

$$(\tilde{r_2})_{j,k+\frac{1}{2}} = \left[N_2^{\mu}\mu_2 \left(D_1 w_t + N_1 \frac{\delta_1\mu_1 f}{\delta x} \right) + N_2^{\delta} D_1 \frac{\delta_2 g}{\delta y} \right]_{j,k+\frac{1}{2}}$$

Truncation error analysis

$$\varepsilon_{j,k} = \mathcal{O}(h^{2p}) + \mathcal{O}(h^{2p-1})$$

main residual $\qquad = \mathcal{O}(h^{2p-1}) \qquad$ *dissipation*

The residual-based operator $\tilde{d}_{j,k}$ Taylor expansion expresses as:

$$\tilde{d}_{j,k} = \frac{\delta x}{2}(\Phi_1 r)_x + \frac{\delta y}{2}(\Phi_2 r)_y + \mathcal{O}(h^{2p-1})$$

For an exact solution the residual is null

$r = 0 \Rightarrow$ d consistent with a higher order term

Actually (Lerat et al., JCP 2013)

$$\tilde{d} = d_q + \mathcal{O}(h^{q+2}) \quad \text{with:} \quad q = 2p-1$$

$$\boxed{\begin{aligned} d_q = (-1)^{p-1}\kappa \{ & \delta x[\Phi_1(\delta x^{q-1} f_{qx} + \chi \delta y^{q-1} g_{qy})]_x \\ & + \delta y[\Phi_2(\delta y^{q-1} g_{qy} + \chi \delta x^{q-1} f_{qx})]_y \} \end{aligned}}$$

κ and χ functions of the Pade coefficients, $\qquad f_{qx}$ denotes $\dfrac{\partial^q f}{\partial x^q}$

Dissipation condition

- Operator $\tilde{d}$ is said <u>dissipative</u> if its (real) Fourier symbol is negative

The χ-criterion for dissipation [Lerat, Grimich, Cinnella, JCP 2013]**:**

<u>Theorem:</u> *The operator d_q is dissipative for any order q=2p-1, any pair (A,B) and any functions Φ_1 and Φ_2 such that*

$$\Phi_1 A \geqslant 0, \qquad \Phi_2 B \geqslant 0$$

$$\delta x \Phi_1 B = \delta y \Phi_2 A$$

if and only if $\boxed{\chi = 0}$

➢ Introduces an additional constraint on the choice of Pade coefficients

➢ Order conditions <u>and</u> the χ-criterion lead to :

✓ A unique set of coefficients for RBC3 and RBC7

✓ A one-parameter family of coefficients for RBC5

Similar results in 3D

Spectral properties

The RBC spatial discretization expresses as

$$\tilde{r_0}(w, w_t) = \tilde{d}(w, w_t)$$

and can be rewritten as

$$\mathfrak{J} w_t = -\mathfrak{R}(w)$$

Where $\mathfrak{J}$ is the operator applied to w_t and $\mathfrak{R}$ the operator applied to w.
In a more compact way:

$$\boxed{w_t = \mathcal{S}(w)}$$

with $\mathcal{S} = -\mathfrak{J}^{-1}\mathfrak{R}$

In the following, we compare the RBC operator to the exact transport operator for the multidimensional linear problem

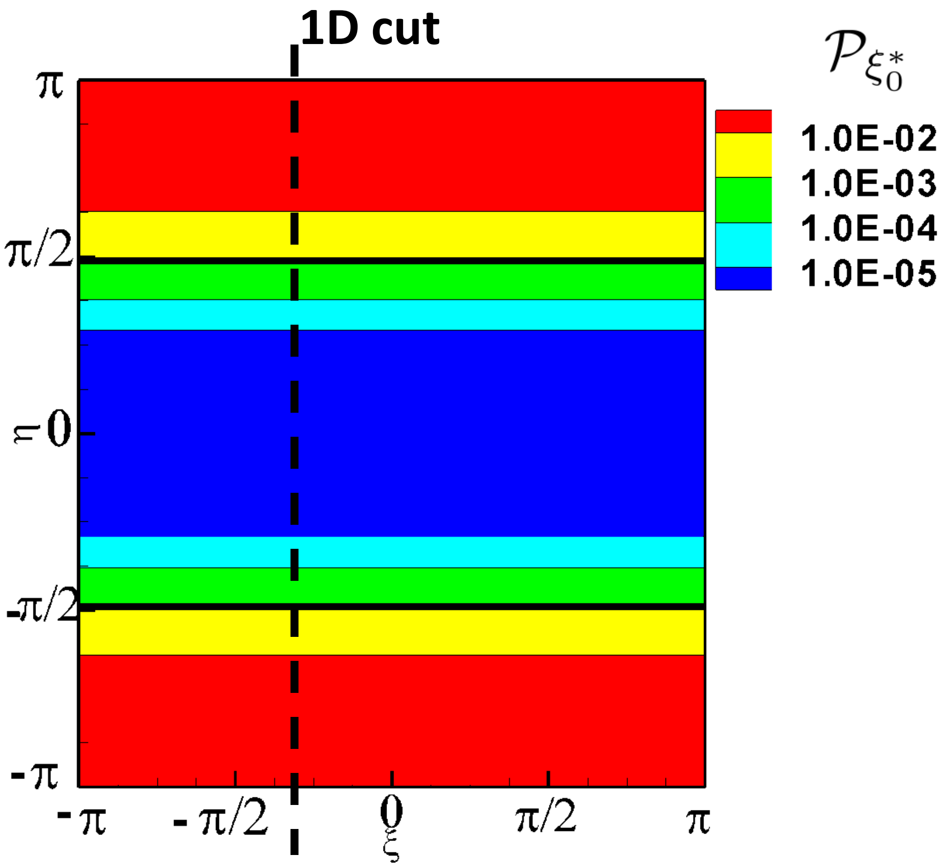
$$w_t + A w_x + B w_y = 0$$

and quantify the dissipation and dispersion errors

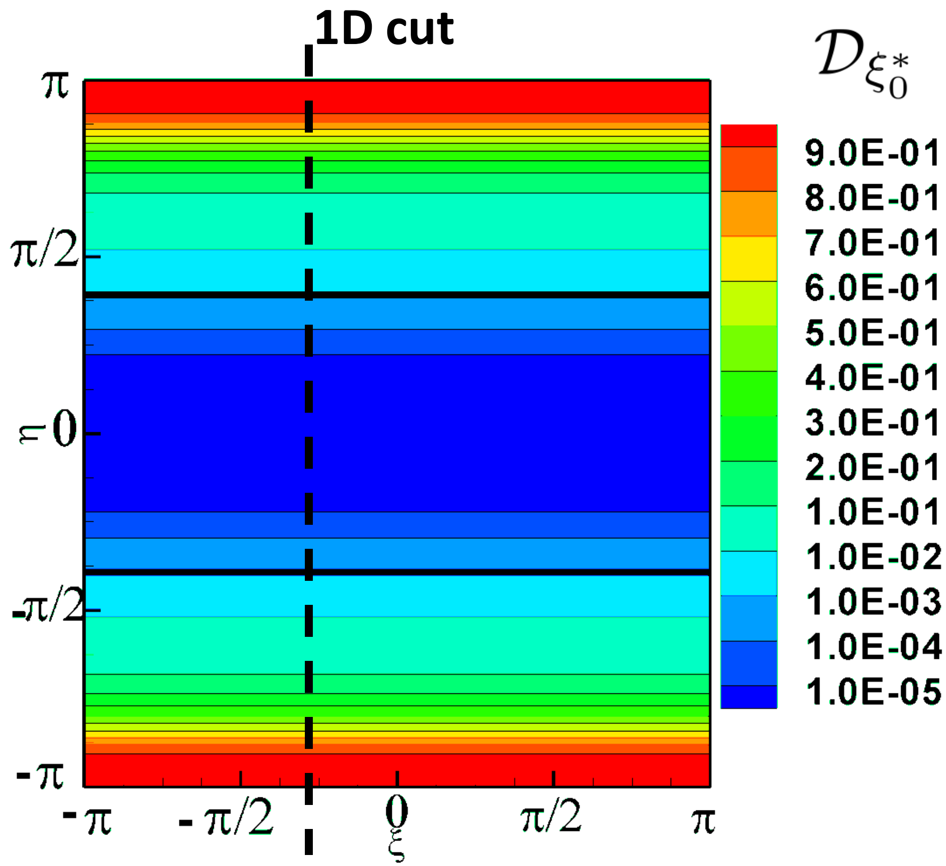
Spectral properties of RBC

Advection along a mesh direction

- ➢ **Dispersion and dissipation properties of RBC schemes (example of RBC7)**



Dispersion

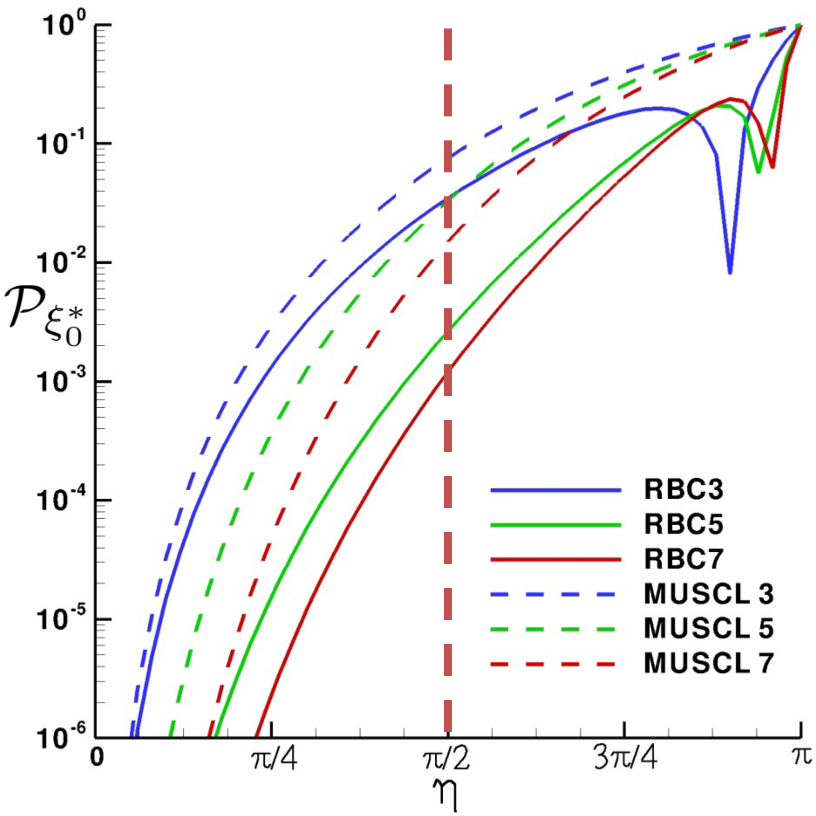


Dissipation

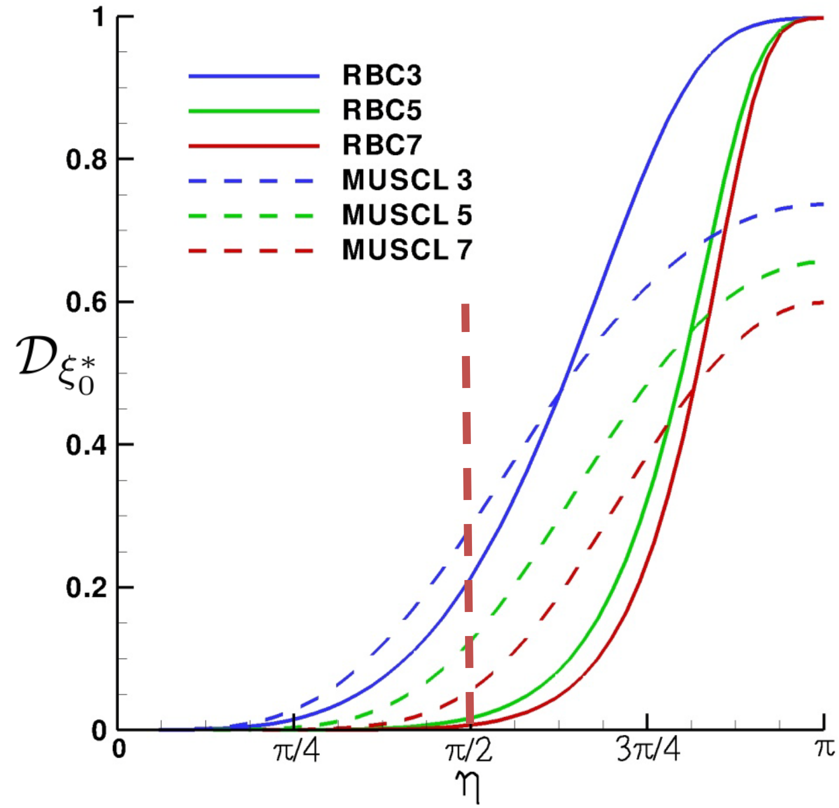
Spectral properties of RBC

Advection along a mesh direction

- 1D cut



Dispersion



Dissipation

Spectral properties of RBC

Resolvability

ξ_c : cutoff reduced wavelength for an error lower than 10^{-3}

$\lambda_c/\delta x$: minimum number of points per wavelength for an error lower than 10^{-3}

Dispersion accuracy limit

	ξ_c	$\lambda_c/\delta x$
RBC3	0.74	8.47
RBC5	1.39	4.53
RBC7	1.54	4.07

	$\lambda_c/\delta x$
MUSCL 3	10
MUSCL 5	7
MUSCL 7	5.5

Dissipation accuracy limit

	ξ_c	$\lambda_c/\delta x$
RBC3	0.40	15.56
RBC5	1.03	6.08
RBC7	1.24	5.06

	$\lambda_c/\delta x$
MUSCL 3	19
MUSCL 5	9
MUSCL 7	7

Shock capturing properties

- RBC schemes use no limiters or artificial viscosity
- They are intrinsically dissipative, odd order accurate → according to Thomée (1965), odd-order schemes are stable in the maximum norm
  - Oscillations generated near discontinuities remain bounded
- Lerat (JCP, 2013) proved, for 1D steady scalar problems, that RBC3 always provides non oscillatory exact shock profiles and RBC5 and 7 provide non oscillatory profiles if the discontinuity is aligned with a cell face

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Overset grid framework

- We consider computational grids made by several interconnected structured blocks
- Kinds of block joins:
  - **Conformal joins** → 1 to 1 or ‘point to point’ communication
  - **Non-conformal joins** → blocks share information on a variety of dimension *n*-1 (for a *n*-dimensional problem)
  - **Overset joins** → blocks share information on a *n*-dimensional variety; multiply defined points exist in the domain
    - Problems:
      - Mesh assembly
      - Cell blanking
      - Information exchanges through interpolation

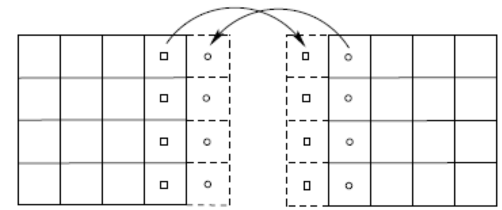


Figure: Example of a 2-D match join: use of dashed ghost-cells for the communication between grids.

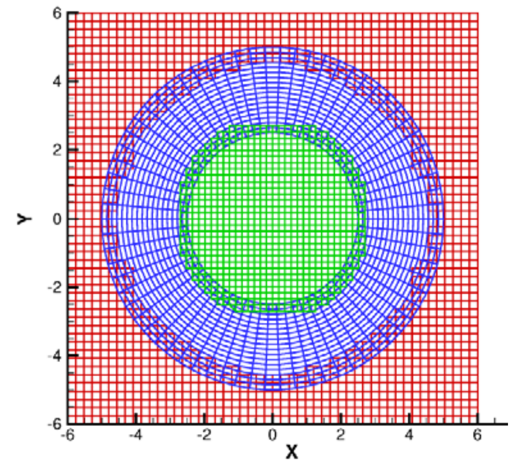
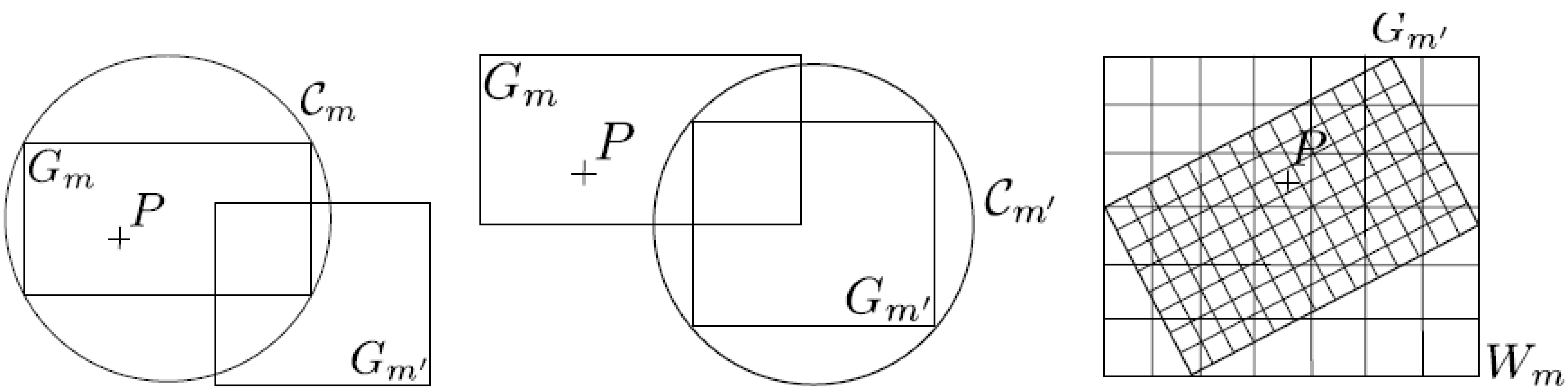


Figure: Example of an overset mesh (DynHoLab)

Overset grid framework

- Ingredients of grid assembly:
  - Grid ordering → assign levels of priority to different grid blocks
  - Compute grid connectivity → find neighbouring blocks
  - Mask overset grid points → exclude overlapped cells from calculations
  - Flag discretized and interpolated points
  - Compute interpolation coefficients



(a) First preconditioner (b) Second preconditioner (c) Third preconditioner

Interpolations

- High-order generalized Lagrangian interpolation of the field variables
  - Achieved through iso-parametric mapping
  - Solve the offsets of the receiver point in the reference Cartesian space with a Newton algorithm
  - Initialization with second-order offsets obtained through transfinite interpolation

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Numerical applications

- 2^{nd}-order accurate, A-stable Gear scheme
- 2^{nd}-order accurate viscous fluxes discretization
- Curvilinear blocks taken into account through a straightforward FV formulation
- Computational code: in-house code DynHOlab [Outtier, Content, Cinnella, Michel, AIAA 2013-2439]

Numerical applications

- RBC accuracy and shock capturing properties:
  - Inviscid and viscous Taylor-Green vortex
  - Converging cylindrical shock

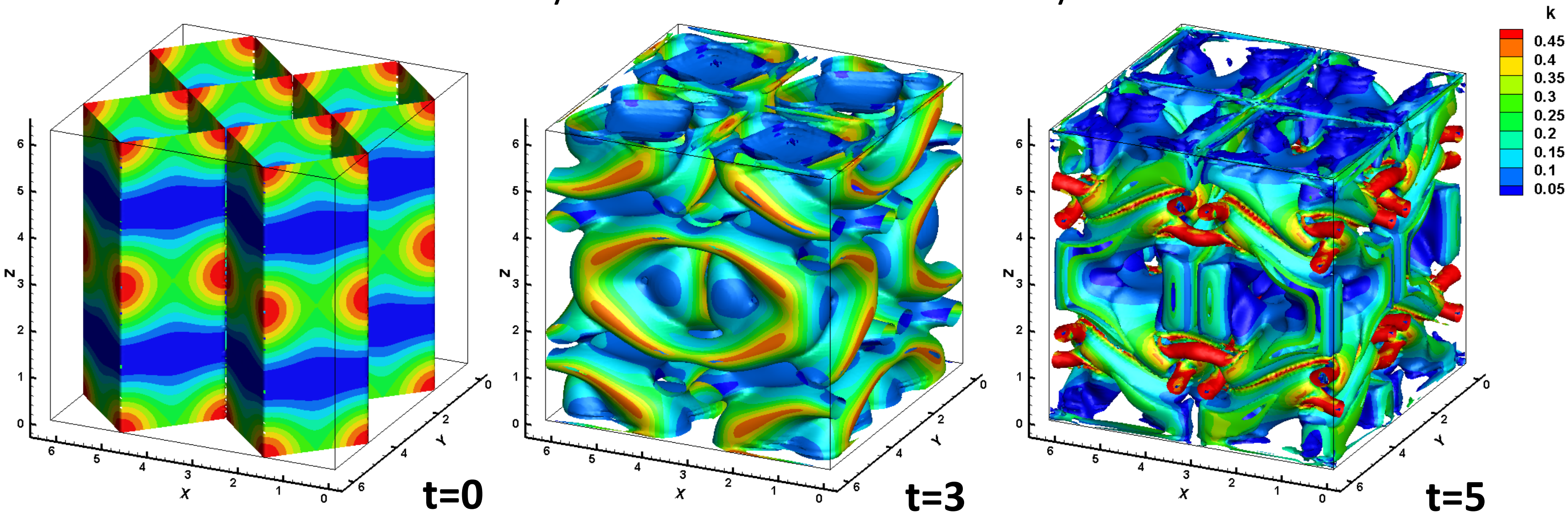
- Overset grid treatment:
    - Circular and helicoidal advection
    - Advection of a isentropic vortex
    - Transonic inviscid flow over a NACA0012

Inviscid Taylor-Green vortex

Code: DynHOlab

Inviscid approximation ➔ suitable to describe fine scale generation through the vortex stretching mechanism

Periodic boundary conditions + 3D initial velocity field



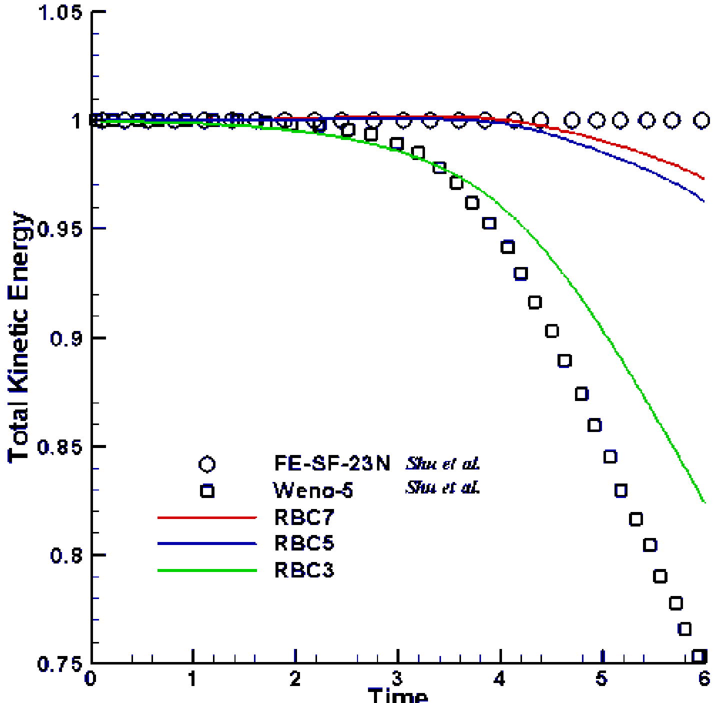
RBC5 scheme, 128^3 mesh, Q-criterion colored by kinetic energy

M=0.3 (Shu et al, J.Sci.Comput. 2005)

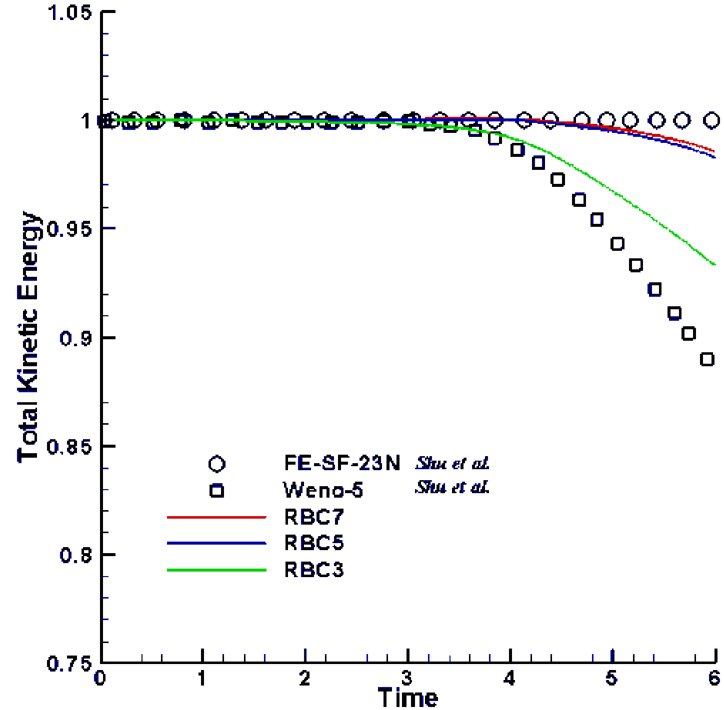
Inviscid Taylor-Green Vortex

Time evolution of the total kinetic energy

➔ quantify only the dissipation of the schemes



64^3 mesh



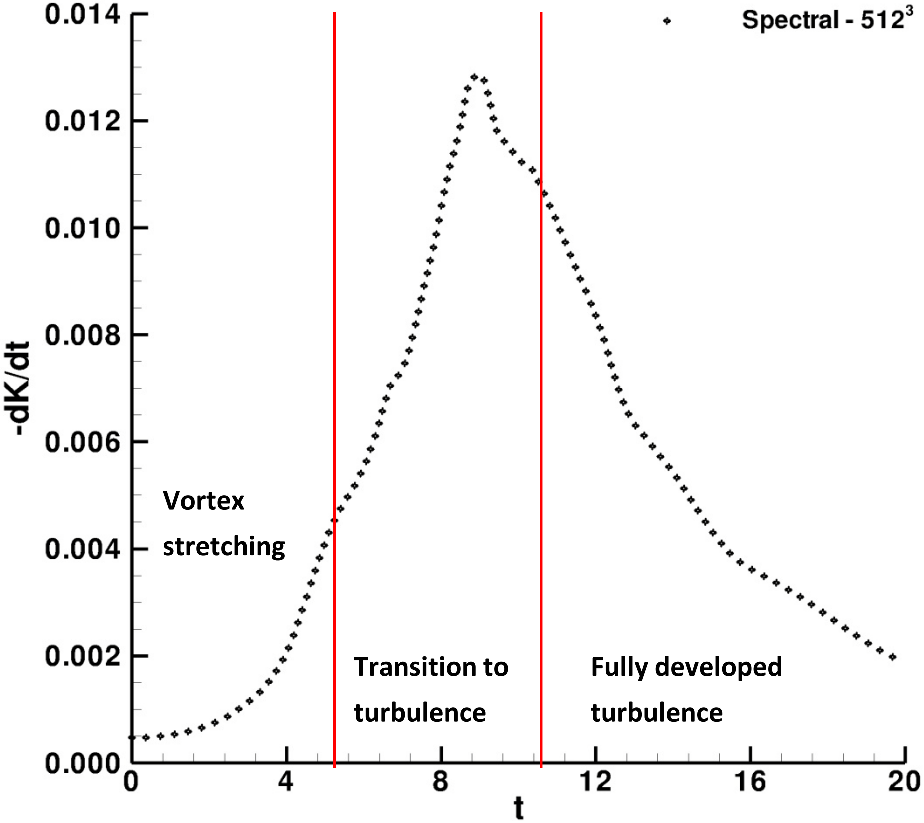
128^3 mesh

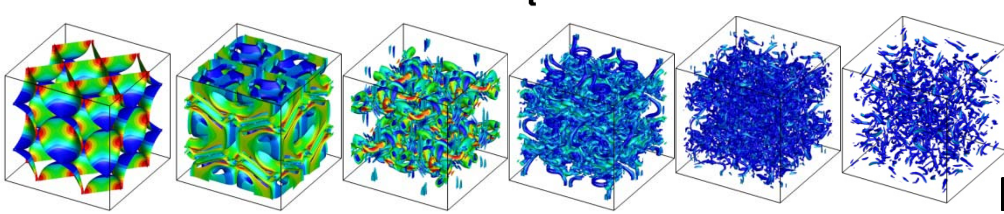
raw operation count for space discretization:

- Weno5 computational cost 75% higher than RBC3
- Weno5 computational cost 10% higher than RBC5 and RBC7

choice of time discretization

Viscous Taylor-Green Vortex





Code: DynHOlab

Viscous case, Re=1600

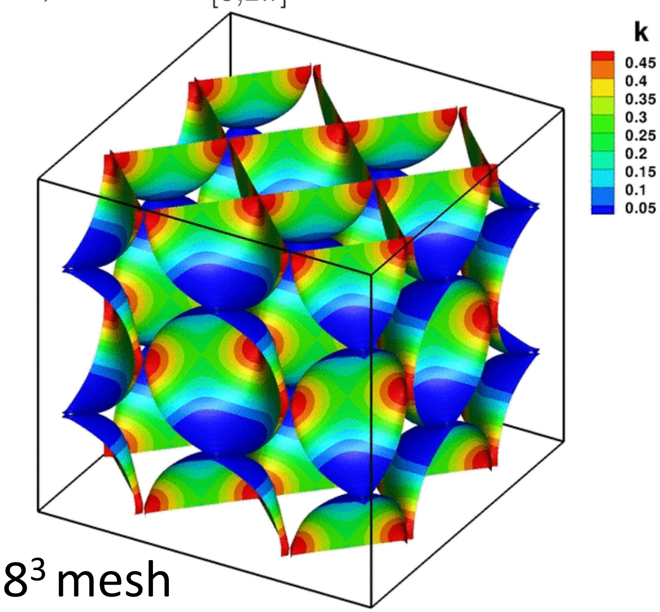
Model of transition to turbulence via vortex stretching mechanism

Integral quantities:

- kinetic energy

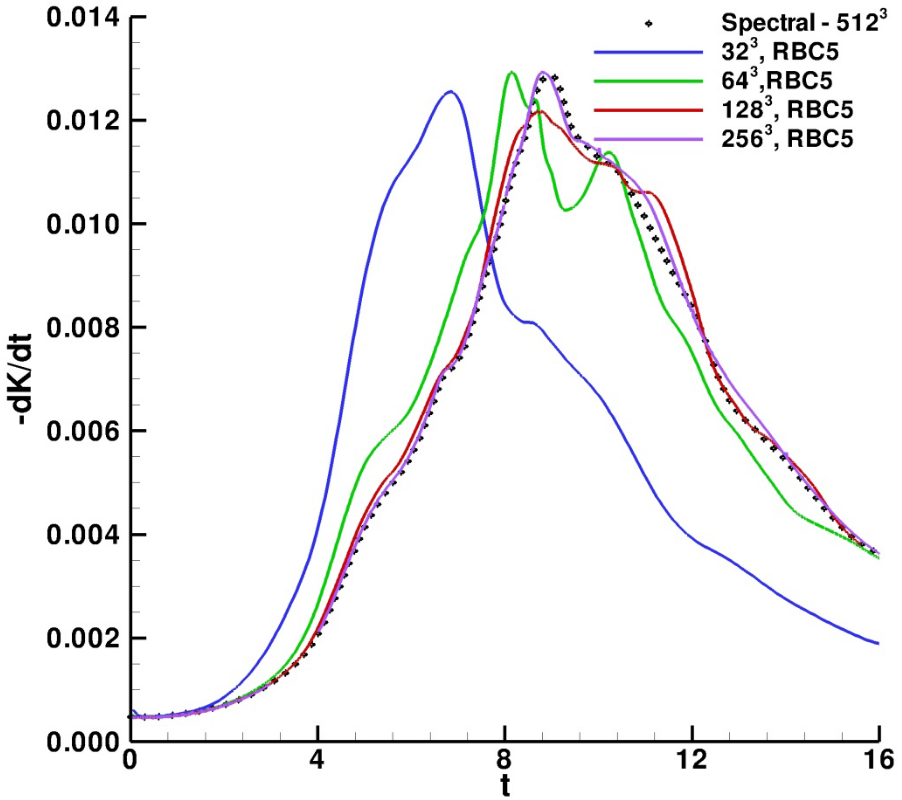
$$K = \frac{1}{(2\pi)^3} \int\int\int_{[0,2\pi]^3} \frac{1}{2}\rho||\boldsymbol{u}||^2 \; dxdydz$$

Q=0

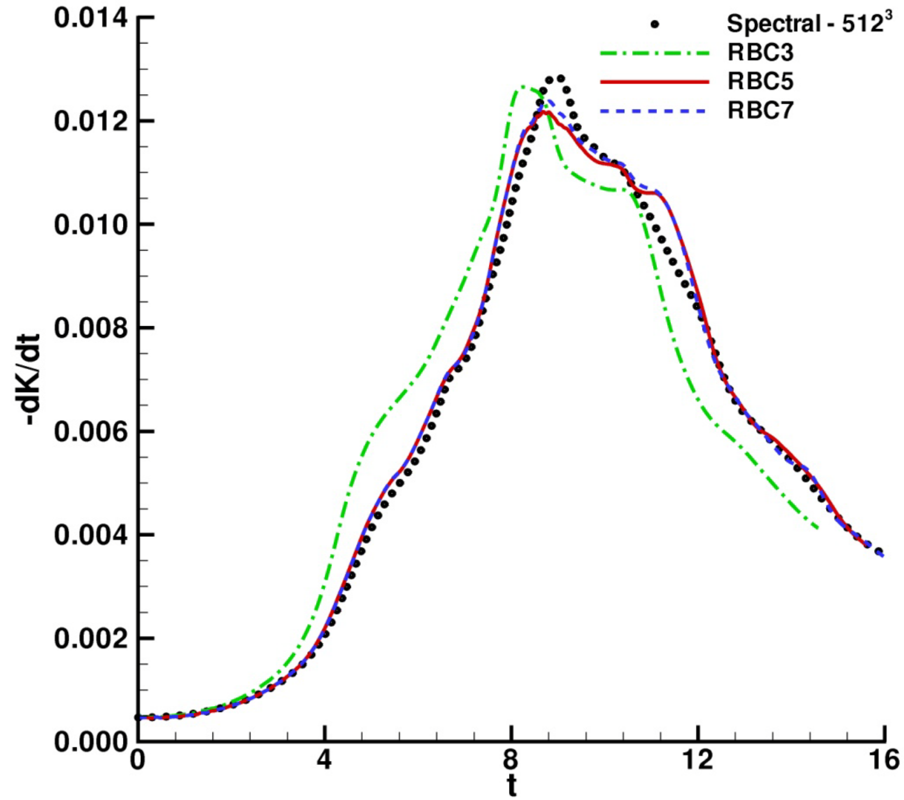


RBC5, 128^3 mesh

Viscous Taylor-Green Vortex

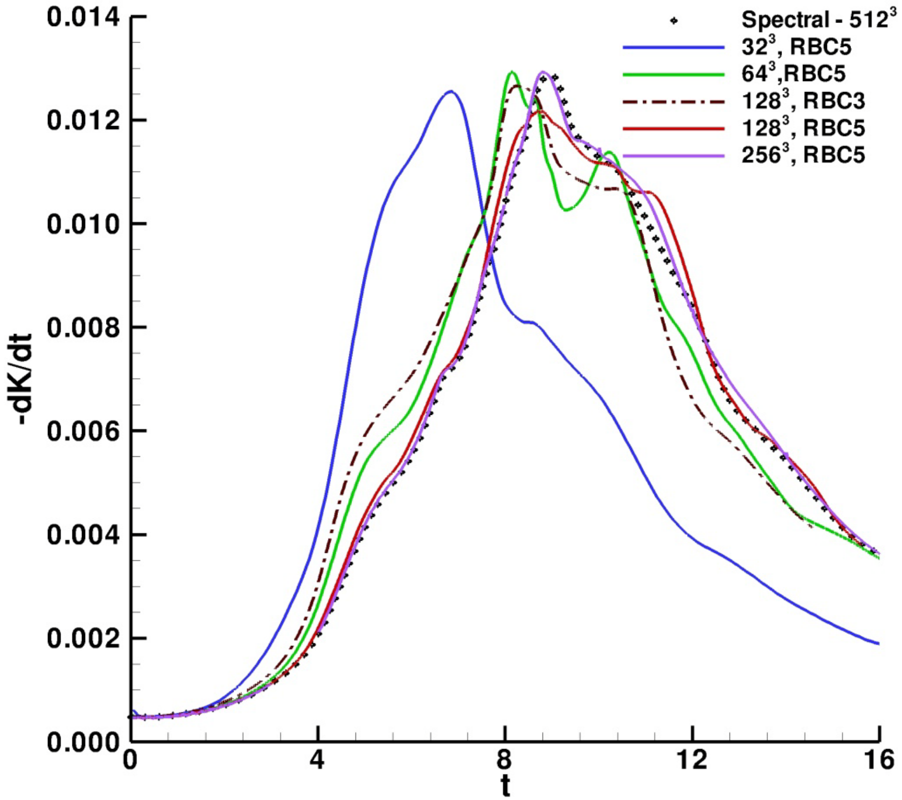


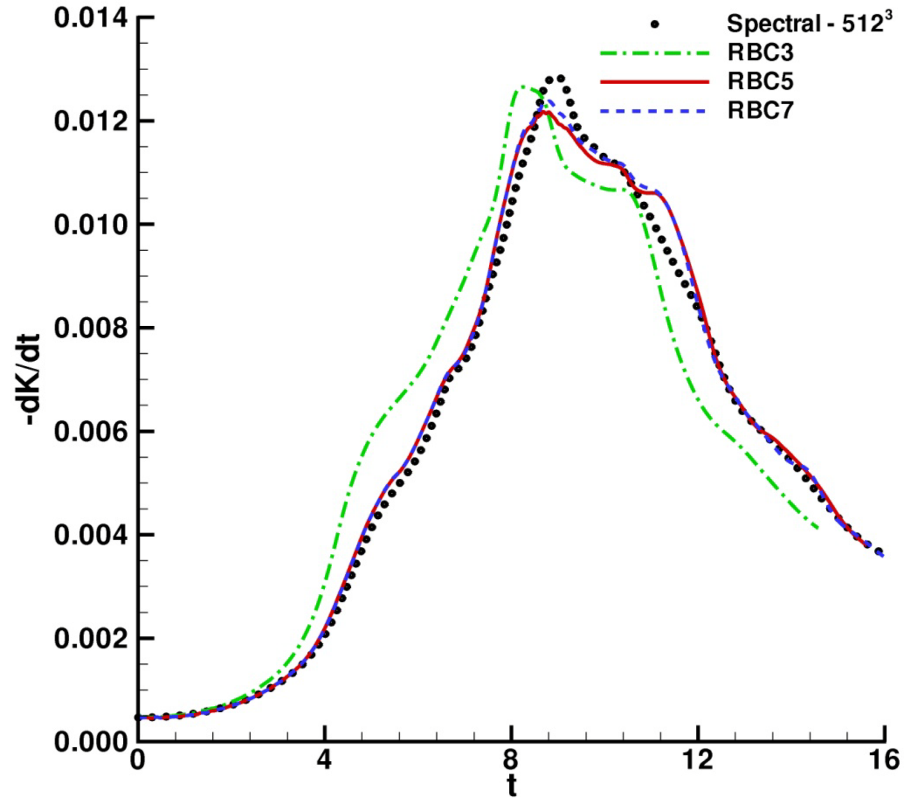
RBC5 scheme, different mesh resolutions



128^3 mesh, different RBC schemes

Viscous Taylor-Green Vortex





RBC5 scheme, different mesh resolutions
RBC3 scheme, 128^3 mesh

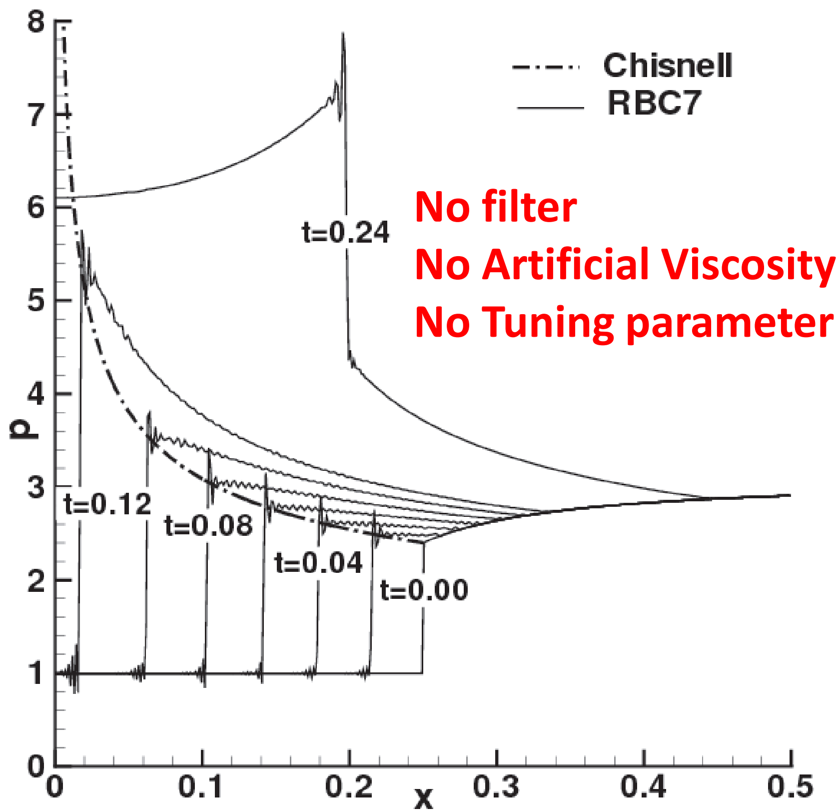
128^3 mesh, different RBC schemes

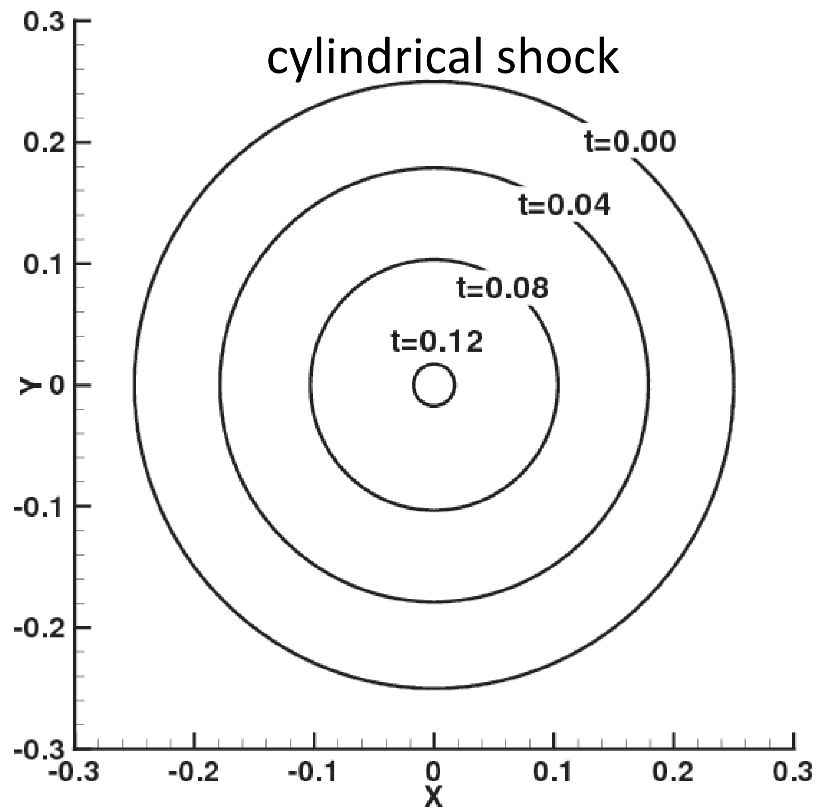
DynFluid Fluid Dynamics Laboratory

ARTS ET MÉTIERS ParisTech

Converging cylindrical shock

Converging cylindrical shock [Chisnell, JFM 1957] ➔ analytical estimation of the pressure behind a moving cylindrical shock

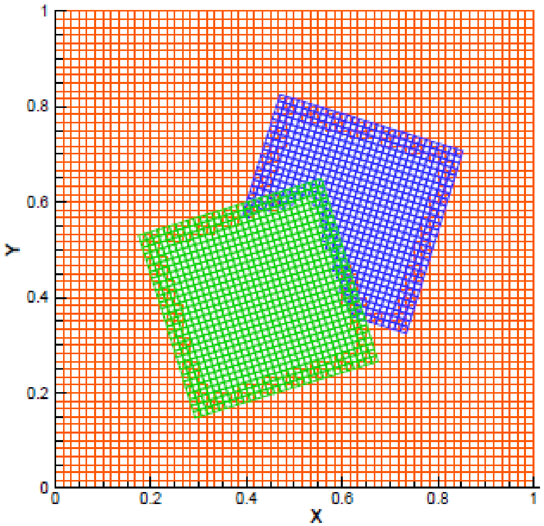


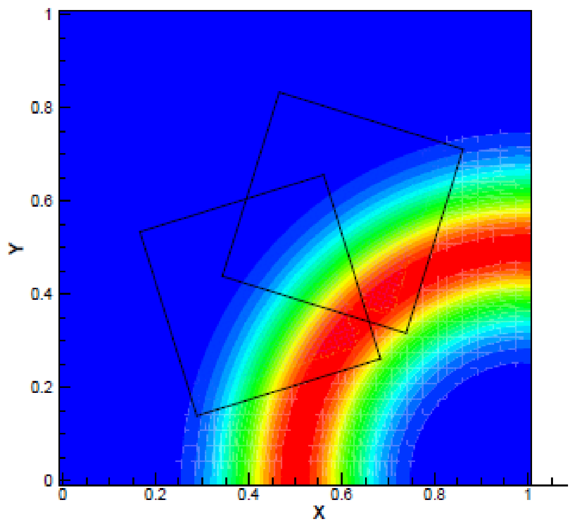


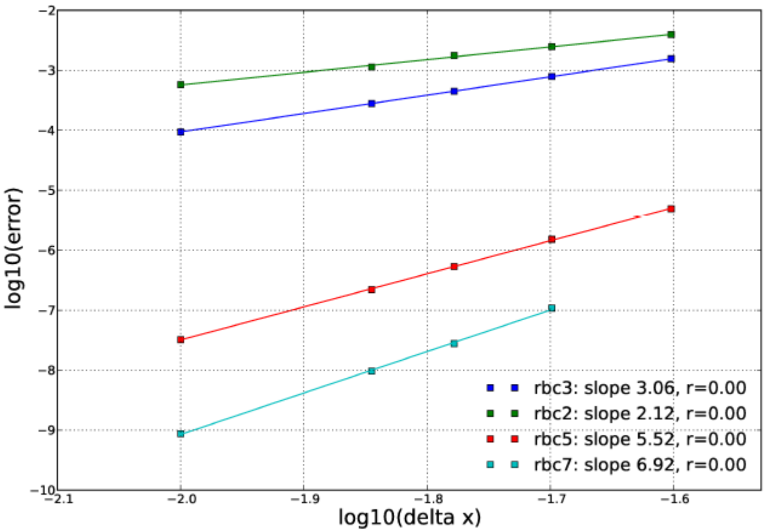
$p_1 = 2.4\, p_0$ at $t = 0$ Shock strength becomes infinite when it reaches the axis

Circular advection problem

- Gaussian function advected at constant speed along a circle
- Integration in the domain [0,1]x[0,1] by using an overset grid
- Comparison with the exact solution



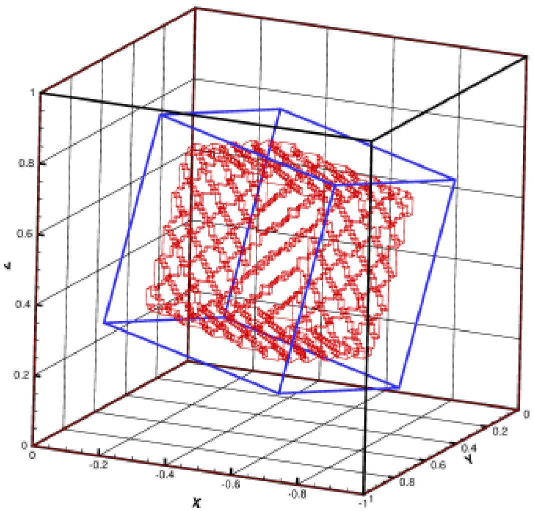


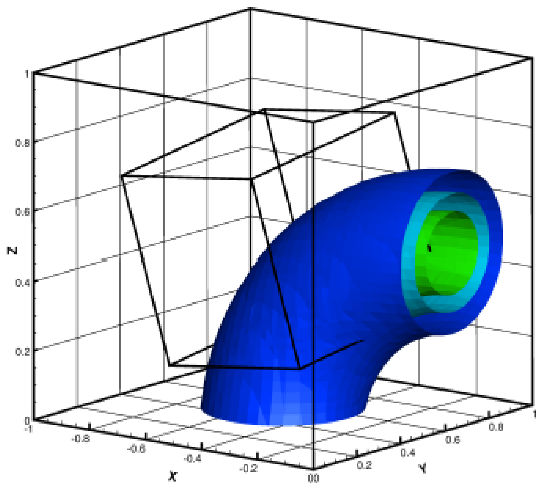


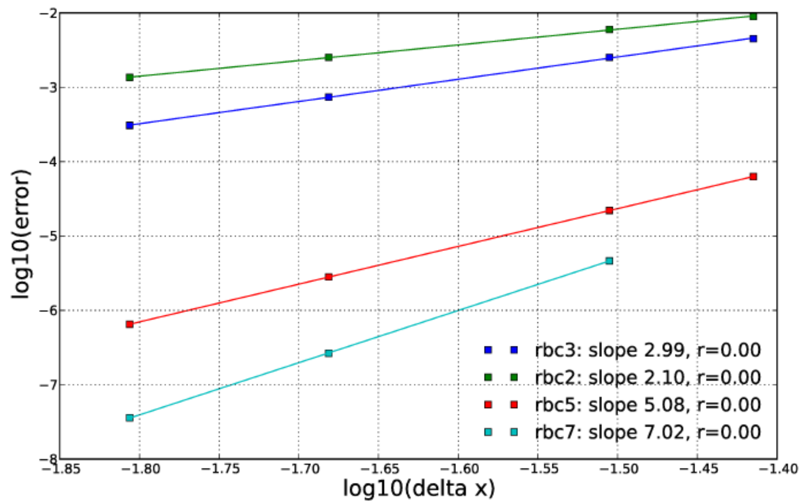
Overall convergence orders recovered when using interpolations of higher-order than the scheme in use

Helicoidal advection problem

- 3D counterpart of the preceding problem



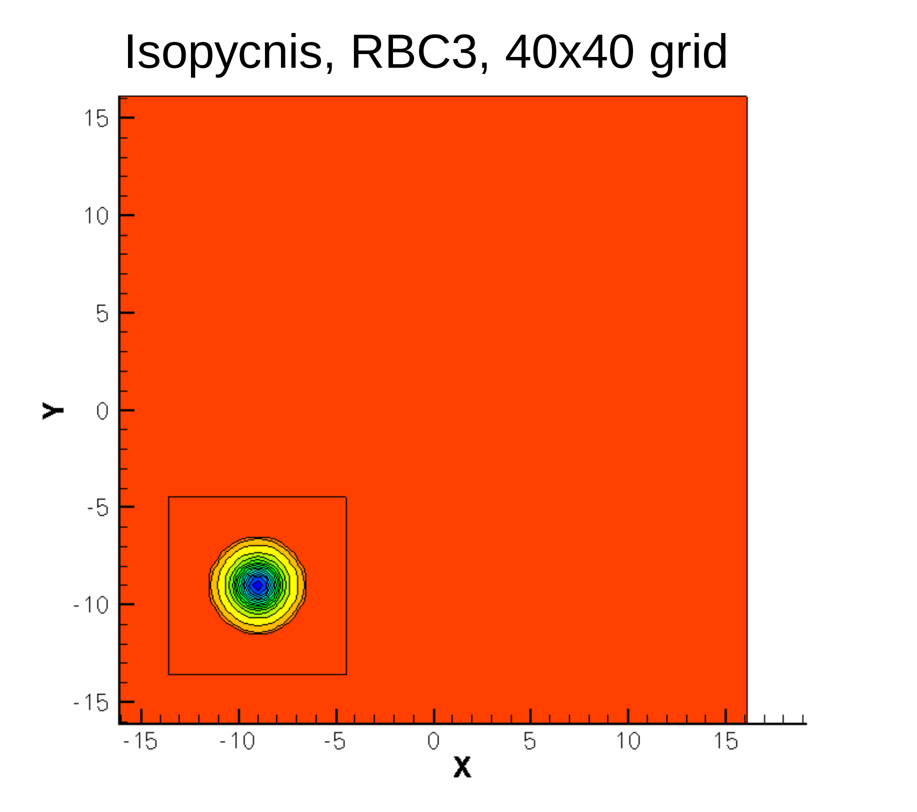




Similar results to the 2D case. It validates the 3D implementation.

Advection of an isentropic vortex

- Isentropic vortex (Yee et al., JCP 2000) diagonally advected by a M=0.5 stream
- Vortex initially located in (-9,-9) advected up to (9,9)
- 3 overset meshes: background meshes of 30x30, 40x40 and 50x50 cells; overset moving mesh 1.95 finer than the background

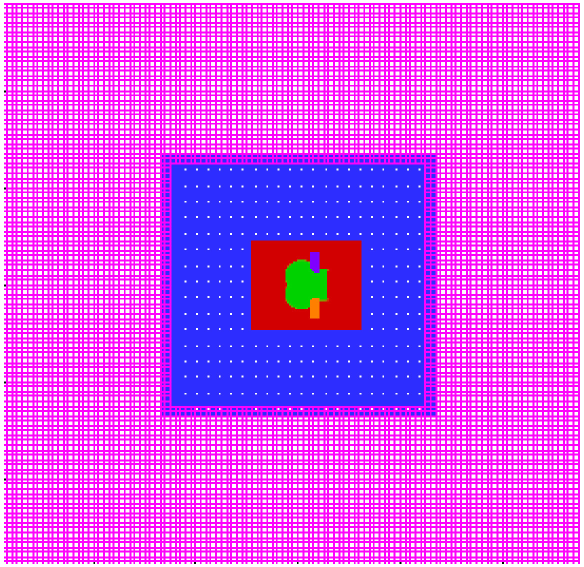


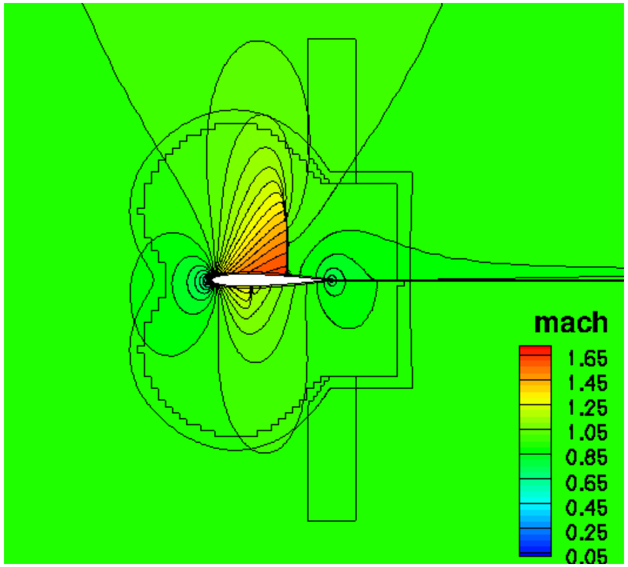
Error on the core density at final time

	RBC3	RBC5	RBC7
30x30	164%	84%	72%
40x40	52%	2.5%	2.1%
50x50	12%	2.5%	0.55%

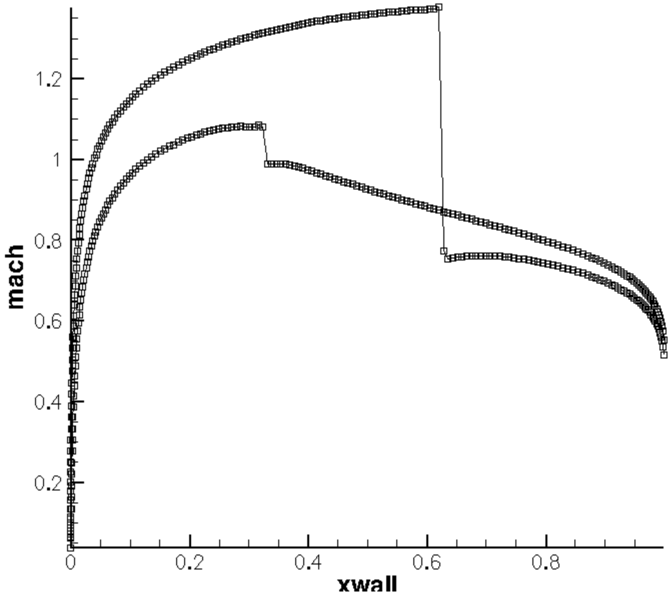
Inviscid flow over a NACA0012

- M=0.85, α=1° (ou alors M=0.8, a=1.25). RBC2 scheme


Grid



IsoMach lines



Wall Mach number

- Results in good agreement with the literature
  - Sharp and non-oscillatory shock profiles

Conclusions and perspectives

- Progress on the development of stable residual based compact schemes with good accuracy and shock capturing properties for unsteady compressible flows
- Preliminary steps toward their extension to complex geometries using an overset grid framework
  - Possibility of adaptive grid refinement

- Future steps
  - Validate the overset strategy on more complex configurations
  - FV vs FD with coordinate transformation for curvilinear blocks
  - Improve the accuracy and efficiency of the time integration method
  - Apply to scale-resolving simulations of compressible flows for industrial configurations