High-order flux reconstruction schemes for combustion and AMR

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Work join with

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CONTEXT

- The modeling of turbulent combustion requires an accurate numerical method and modeling of the effects of turbulence

- For Large Eddy Simulation, it is necessary to use high-order methods in order to reduce numerical dissipation

Objectives of the thesis:

Developing high-order numerical methods for LES modeling of low-dispersion/dissipation combustion

Leonard de Vinci

HIGH-ORDER METHODS: STATE OF THE ART

$$\|U_{approx} - U_{exact}\|_{L^2} = \mathcal{O}(\Delta x^{p+1})$$

- Discontinuous Galerkin by Reed and Hill 1973
  - weak formulation, mass matrix bloc-diagonal
  - expensive if standard Gaussian quadrature rules are employed
- Spectral Difference by Kopriva and Kolias 1996
  - strong formulation, exponential convergence for smooth solutions
  - difficult to implement on complex geometries
- Flux Reconstruction by Huynh 2007
  - strong formulation
  - set of schemes including collocation-based nodal DG and SD schemes in linear cases with many properties (stability, dissp, CFL)

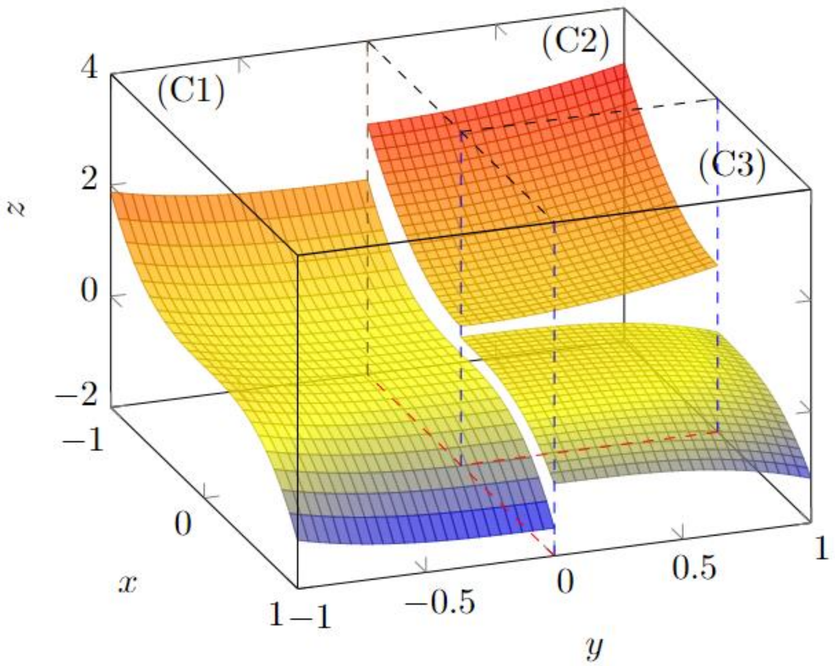


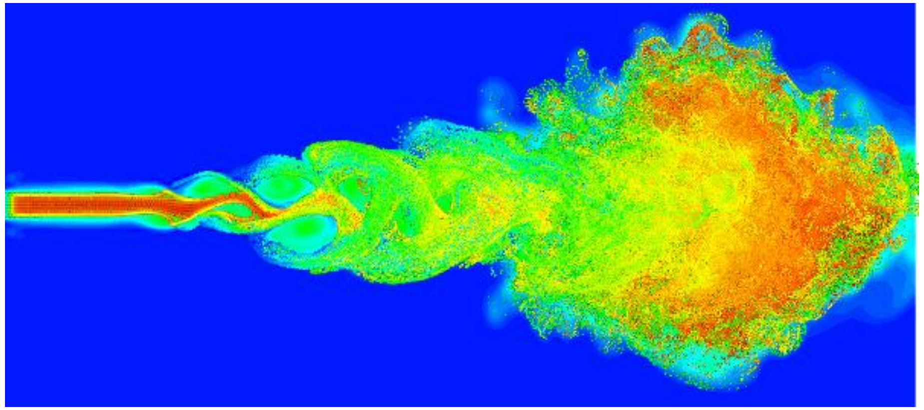
Figure 2 : Representation of a discontinuous solution over three cells

HIGH-ORDER METHODS: APPLICATIONS

- Discontinuous Galerkin by Reed and Hill 1973
  - turbulent jets, Anghan et el.[1]
  - laminar-turbulent transition, Beck et al. [2]

- Spectral Difference by Kopriva and Kolias 1996
  - turbulent flows limited to the walls, Chapelier et al.[3]
  - shocks and detonations, Gupta et al. [4]
  - SD method for laminar and turbulent combustion,T. Marchal et al [5]

- Flux Reconstruction by Huynh 2007
  - flows in turbomachines, flow around a wing and a cylinder Vincent, Jameson et al [6]
  - double flux method to the FR discretization of the multi-species Euler equations, Peyvan et al [7]
  - no work on combustion



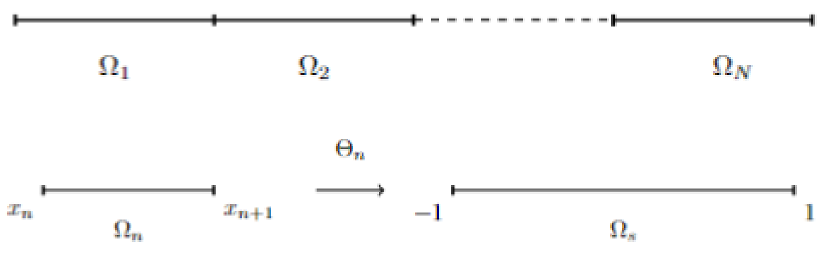
Development of turbulent flow in a jet

OUTLINE

- **Principles of Flux Reconstruction method**
- Development of FR schemes for non-reactive 3D flows in AEROSOL
- Development of FR schemes for non-reactive and reactive 3D flows in CONVERGE
- Development of a coupling methodology for FR schemes and AMR in CONVERGE
- Conclusion and future works

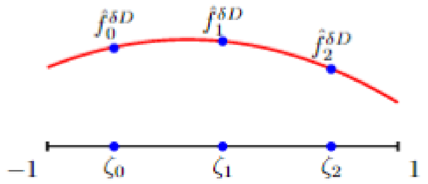
PRINCIPLES OF FLUX RECONSTRUCTION METHOD FOR $\partial_t u + \partial_x f(u) = 0$

1. Write conservation laws on each Ω_n, $\Omega = \cup_{n=1}^{N} \Omega_n$
   - $\partial_t u_n^{\delta D} + \partial_x f_n^{\delta}(u_n^{\delta}) = 0$



2. Isoparametric map $\Theta_n: \Omega_n \longrightarrow \Omega_s$
   - $\partial_t \hat{u}_n^{\delta D} + \partial_\zeta \hat{f}_n^{\delta}(\hat{u}_n^{\delta}) = 0$
   - $\hat{u}_n^{\delta D} = J_n u_n^{\delta D}, \quad \hat{f}_n^{\delta} = f_n^{\delta}$

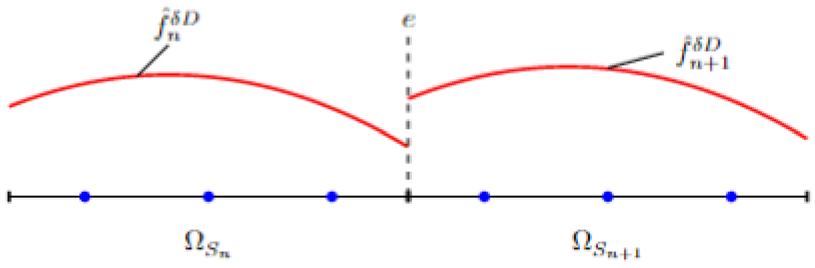
3. Polynomial approximation
   - $p + 1$ solution points $\zeta_k \ / \ k = 0, \dots, p$
   - Interpolation $\left(\zeta_k, \hat{u}^{\delta D}(t, \zeta_k)\right) = \left(\zeta_k, \hat{u}_k^{\delta D}\right)$



$\hat{u}^{\delta D}(\zeta) = \sum_{0 \leqslant k \leqslant p} \hat{u}_k^{\delta D}\, l_k(\zeta)$ (degree p), $\quad \hat{f}^{\delta D}(\zeta) = \sum_{0 \leqslant k \leqslant p} \hat{f}_k^{\delta D}\, l_k(\zeta)$ (degree p)

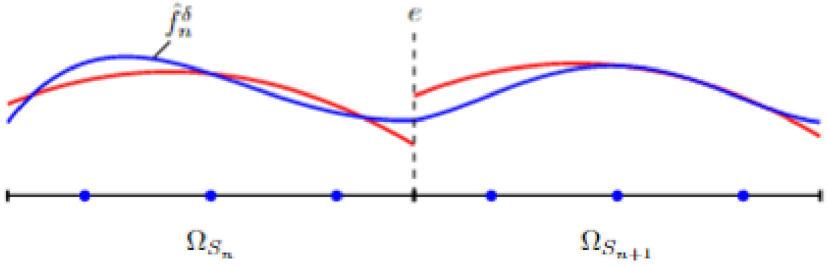
PRINCIPLES OF FLUX RECONSTRUCTION METHOD

- $\hat{u}^{\delta D}$ and $\hat{f}^{\delta D}$ may be discontinuous at the interfaces



- The transfer of information is ensured by flux reconstruction

$$\hat{f}_n^{\delta}(\zeta) = \underbrace{\hat{f}_n^{\delta D}(\zeta) + \hat{f}_n^{\delta C}(\zeta, g_L, g_R)}_{\text{degree } p+1}$$



PRINCIPLES OF FLUX RECONSTRUCTION METHOD

- Vincent-Castonguay-Jameson-Huynh VCJH correction functions
  - $g_L = \frac{(-1)^p}{2}\left(L_p - \frac{\eta_p L_{p-1} + L_{p+1}}{1+\eta_p}\right), \; g_R = \frac{1}{2}\left(L_p + \frac{\eta_p L_{p-1} + L_{p+1}}{1+\eta_p}\right)$
    - L_p : Legendre polynomial of degree p
    - $\eta_p = \frac{c(2p+1)(a_p p!)^2}{2}, \; a_p = \frac{2p!}{2^p\,(p!)^2}$
- Set of schemes parameterized by c : $\frac{-2}{(2p+1)(a_p p!)^2} < c < +\infty$
  - $c = 0$: Nodal Discontinuous Galerkin scheme
  - $c = \frac{2p}{(2p+1)(p+1)(a_p p!)^2}$: Spectral Difference scheme
  - $c = \frac{2(p+1)}{(2p+1)p(a_p p!)^2}$: Huynh scheme

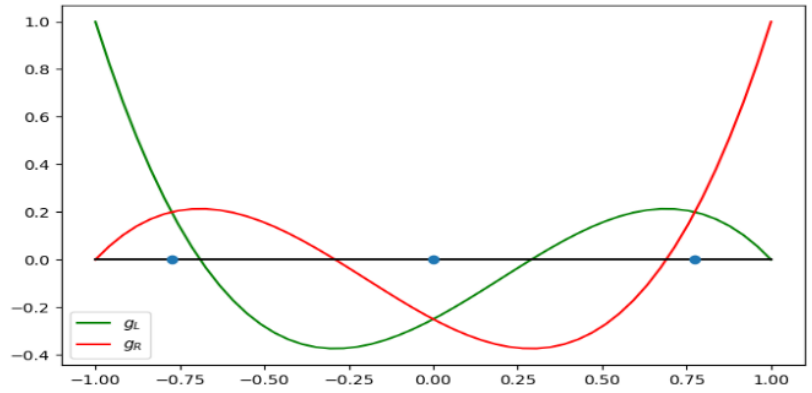


Figure 3 : VCJH Correction functions for $c = 0$ and $p = 2$

OUTLINE

- Principles of Flux Reconstruction method
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General form of the Navier-Stokes equations

$$\partial_t \boldsymbol{U} + \nabla \cdot \boldsymbol{F}_{\text{conv}}(\boldsymbol{U}) + \nabla \cdot \boldsymbol{F}_{\text{vis}}(\boldsymbol{U}, \nabla \boldsymbol{U}) = \boldsymbol{S}, \qquad (t, x) \in [0; T_f] \times \Omega$$

$$\boldsymbol{U} = \mathbf{g}, \qquad (t, x) \in [0, T_f] \times \Gamma$$

$$\boldsymbol{U} = (\rho, \rho \boldsymbol{V}, \rho E)$$

$$\boldsymbol{F}_{\text{conv}} = (\rho \boldsymbol{V}, \rho \boldsymbol{V} \otimes \boldsymbol{V} + pI, \rho E \boldsymbol{V} + p \boldsymbol{V})$$

$$\boldsymbol{F}_{\text{vis}} = (0, -\nabla \cdot \boldsymbol{\tau}, -(\nabla \cdot (\boldsymbol{\tau} \cdot \boldsymbol{V}) + \nabla \cdot (\kappa \nabla T)))$$

$$\tau_{ij} = \nu(\partial_{x_i} V_j + \partial_{x_j} V_i + \lambda \, \delta_{ij} \nabla \cdot \boldsymbol{V})$$

$$E = \frac{P}{\rho(\gamma - 1)} + \frac{1}{2}(V_1^2 + V_2^2 + V_3^2)$$

NUMERICAL EXPERIMENTS: NAVIER-STOKES EQUATIONS 2D

Poiseuille Flow

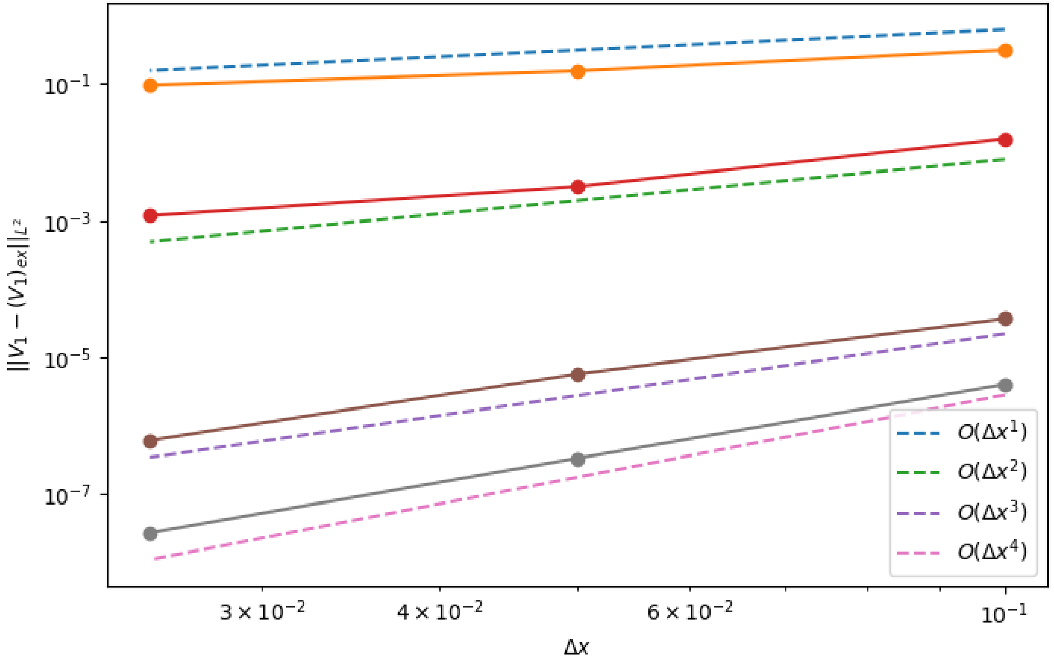
- Source term: $\mathbf{S} = (0, F_V, F_V \cdot V)$
  - $F_V = (8\, \nu u_c, 0)$
  - $F_V \cdot V = 32\, \nu u_c^2 y(1-y)$
- Isothermal boundary conditions : $(V_1, V_2, T) = (0,0,T_W)$
  - $g = \left(\rho_{ref}, 0,0, \rho_{ref}\, c_v T_W\right)$
- Exact solution
  - $V = (4u_c y(1-y), 0\,)$
  - $T(x,y) = T_w\left[1 + \frac{16\, Pr\, Ma^2\,(\gamma-1)}{3} y(1-y)\left(y^2 - y + \frac{1}{2}\right)\right]$
- Discretisation
  - $\Omega = [0,1] \times [0,1], T_W = 1, \mathrm{u}_c = 1, \rho_{ref} = 0.001, \nu = 0.001, Pr = 0.7, Ma = 0.2, Re = 1$
  - Numerical flux Lax-Friedrichs (advective), LdG (viscous); RK45, DG via FR
  - $CFL = \frac{\delta_t \nu}{\delta_x^2}, p \in \{0,1,2,3\}, N^2 \in \{10^2, 20^2, 40^2\}$

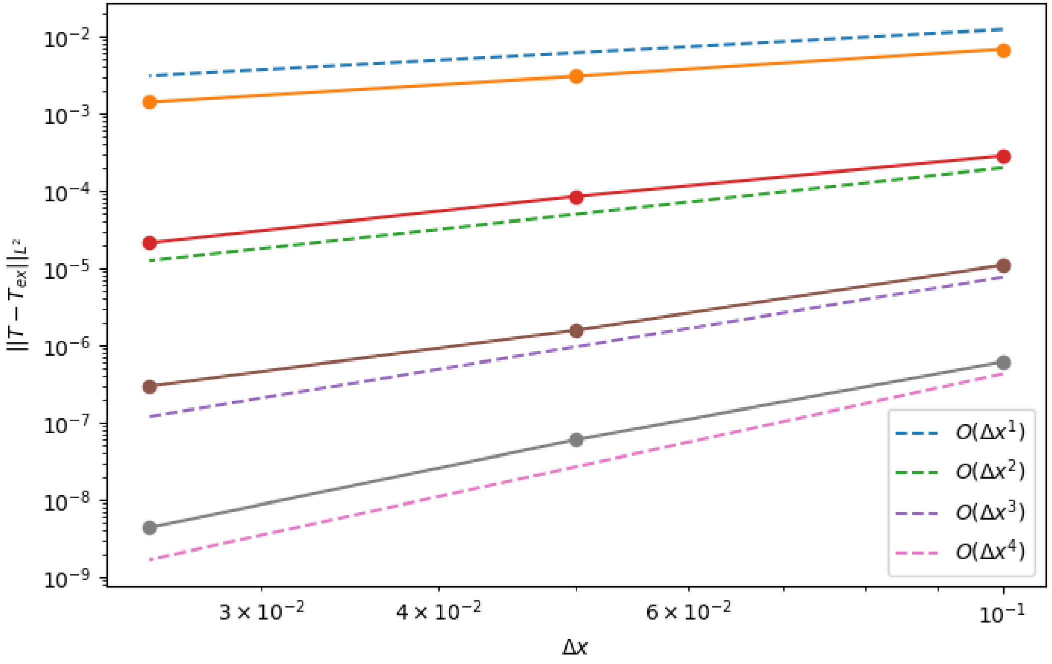
C. Brun, M. Petrovan Boiarciuc, M. Haberkorn, and P. Comte, Large eddy si-mulation of compressible channel flow, Theor. Comput. Fluid Dyn., 22 (2008)

NUMERICAL EXPERIMENTS: NAVIER-STOKES EQUATIONS 2D

Convergence curves with DG via FR

- $p \in \{0,1,2,3\}$
- $N^2 \in \{10^2, 20^2, 40^2\}$





$$\left\|U - U^\delta\right\|_{L^2} = \mathcal{O}(\Delta x^{p+1})$$

NUMERICAL EXPERIMENTS: NAVIER-STOKES EQUATIONS 3D

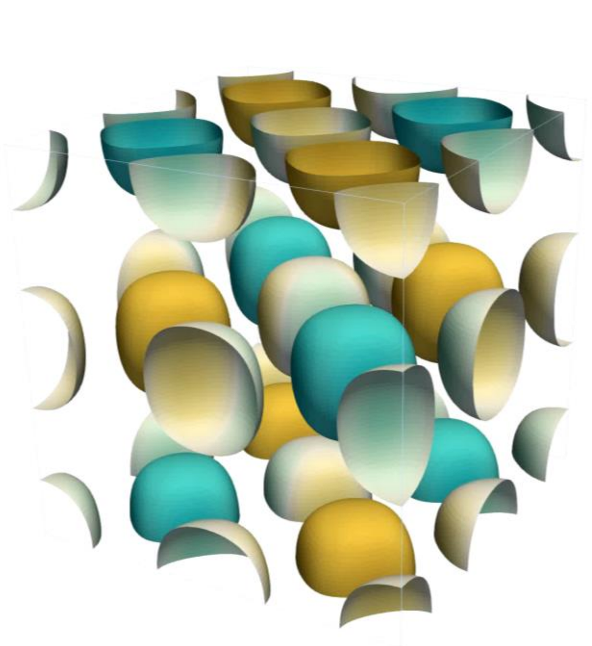
Taylor-Green Vortex (TGV)

- Initial condition
  - $V_1 = u_0 \sin\left(\frac{x}{L_0}\right) \cos\left(\frac{y}{L_0}\right) \cos(\frac{z}{L_0})$
  - $V_2 = -u_0 \cos\left(\frac{x}{L_0}\right) \sin\left(\frac{y}{L_0}\right) \cos(\frac{z}{L_0})$
  - $V_3 = 0$
  - $P = P_0 + \frac{\rho_0 V_0^2}{16}(\cos\left(\frac{2x}{L_0}\right) + \cos\left(\frac{2y}{L_0}\right))(\cos\left(\frac{2z}{L_0}\right) + 2)$
- Boundary condition
  - Periodic
- Discretisation
  - Numerical flux Lax-Friedrichs (advective), LdG (viscous); RK45, DG via FR
  - $\Omega = [-\pi \mathrm{L}_0, \pi L_0] \times [-\pi \mathrm{L}_0, \pi L_0] \times [-\pi \mathrm{L}_0, \pi L_0],\ T_f = 12\mathrm{s}.$
  - $L_0 = \frac{1}{\pi}, u_0 = \frac{1}{\pi}, \rho_0 = 1, T_0 = 1, Pr = 0.71,\ Ma = 0.1,\ Re = 1600.$

Chapelier J. B., De La Llave Plata M., Renac F. & Lamballais E., Evaluation of a high-order discontinuous Galerkin method for the DNS of turbulent flows, *Computers & Fluids* **95**, 210–226 (2014).

NUMERICAL EXPERIMENTS: TGV at Re = 1600

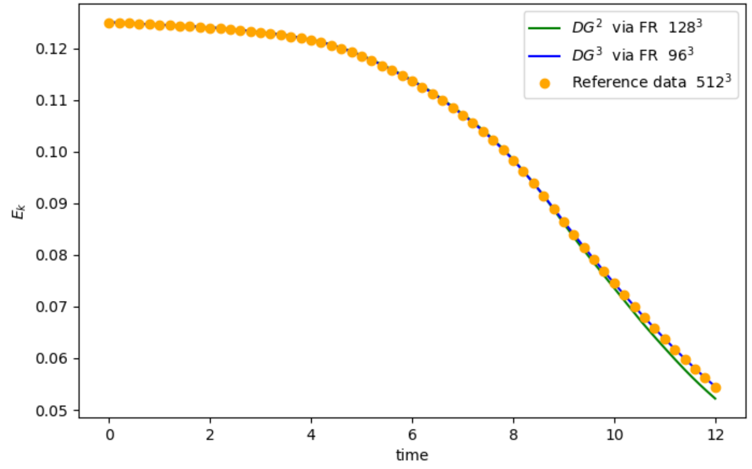
Isosurface of Q criterion colored by the *z*-vorticity
- Order $= 4$
- $N^3 = 96^3$



h,*p*-refinement
- Order $\in \{3,4\}$
- $N^3 \in \{96^3, 128^3\}$

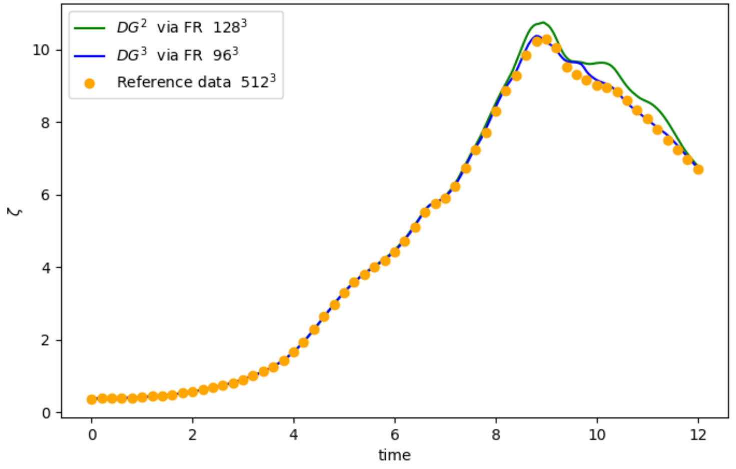
Kinetic Energy

$$E_k = \frac{1}{K}\int_K \frac{V\cdot V}{2}$$



Enstrophy

$$\zeta = \frac{1}{K}\int_K \frac{(\nabla\times V)\cdot(\nabla\times V)}{2}$$



- Good agreement with reference data and with less DoF
- The results are better with high-order for constant number of DoF

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Cant R., *FERGUS, A user guide*, technical report, Cambridge University Engineering Department.

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NAVIER-STOKES EQUATIONS: GLOBAL CONSERVATION OF MASS

General form of Navier-Stokes equations

- $\partial_t \rho + \nabla \cdot (\rho \boldsymbol{u}) = 0, \quad (t, x) \in [0; T_f] \times \Omega$
- $\partial_t (\rho \boldsymbol{u}) + \nabla \cdot (\rho \boldsymbol{u} \otimes \boldsymbol{u} + PI) + \nabla \cdot (-\boldsymbol{\tau}) = 0, \; (t, x) \in [0; T_f] \times \Omega$
- $\partial_t (\rho E) + \nabla \cdot (\rho E \boldsymbol{u} + P \boldsymbol{u}) + \nabla \cdot \left(-\left((\boldsymbol{\tau} \cdot \boldsymbol{u}) + (\kappa \nabla T) - \rho \sum_k h_{sk} Y_k \boldsymbol{V}_k \right) \right) = \dot{\omega}_T, \; (t, x) \in [0; T_f] \times \Omega$
- $\partial_t \rho_k + \nabla \cdot (\rho_k \boldsymbol{u}) = \nabla \cdot \left(\rho D_k \frac{W_k}{W} \nabla X_k - \rho_k \boldsymbol{V}^c \right) + \dot{\omega}_k, \quad (t, x) \in [0; T_f] \times \Omega, \quad k \in \{1, 2, \cdots, N_s\}$

$$Y_k \boldsymbol{V}_k = -D_k \frac{W_k}{W} \nabla X_k$$

$$\boldsymbol{V}^c = \sum_j \frac{D_j W_j}{W} \nabla X_j$$

$$\frac{W_k}{W} \nabla X_k = \nabla Y_k - Y_k W \sum_s \frac{\nabla Y_s}{W_s}$$

$$E = e_s + \frac{1}{2} \boldsymbol{u}^2,$$

$$h_s = \sum Y_k h_{sk}$$

$$h_{sk} = \Delta h_{f,k}^0 + \int_{T_0}^{T} C_{pk}(T') dT'$$

CHALLENGES OF FR SCHEMES IN MULTI-SPECIES SIMULATION

HOW TO COMPUTE NUMERICAL FLUXES $F^{\delta I}$?

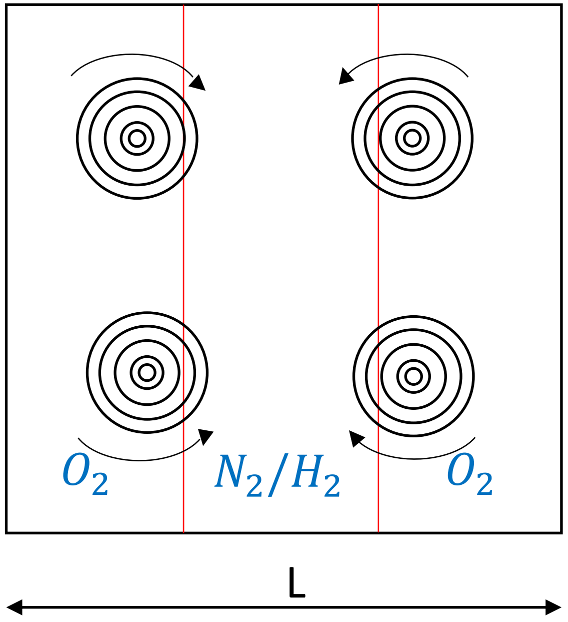
- Conservative variables: $U = (\rho, \rho V_1, \rho V_2, \rho V_3, \rho E, \rho Y_1, \rho Y_2, \cdots, \rho Y_{N_s})$
- Primitives variables: $Q = (P, V_1, V_2, V_3, T, Y_1, Y_2, \cdots, Y_{N_s})$
- CONS approach $U_{SP} \longrightarrow U_{FP} \longrightarrow F^{\delta I}$
  - Extrapolate the conservative variables to the flux points: $U_{SP} \longrightarrow U_{FP}$
  - Compute $F^{\delta I}$ from U_{FP}.
- TUPY approach $U_{SP} \longrightarrow Q_{SP} \longrightarrow Q_{FP} \longrightarrow U_{FP} \longrightarrow F^{\delta I}$
  - Compute the primitive variables from the conservative variables at the solution points: $U_{SP} \longrightarrow Q_{SP}$
  - Extrapolate the primitive variables to the flux points: $Q_{SP} \longrightarrow Q_{FP}$
  - Compute the conservative variables from the primitive variables at the flux points: $Q_{FP} \longrightarrow U_{FP}$
  - Compute $F^{\delta I}$ from U_{FP}.

Thomas Marchal et al, Extension of the Spectral Difference method to combustion, *Journal of Computational Physics*, 2023.

NUMERICAL EXPERIMENTS: REACTIVE NAVIER-STOKES EQUATIONS 2D

H2/O2 combustion kinetic scheme Boivin et al. (9 species | 12 reactions)
SAGE is used to solve kinetic chemistry.

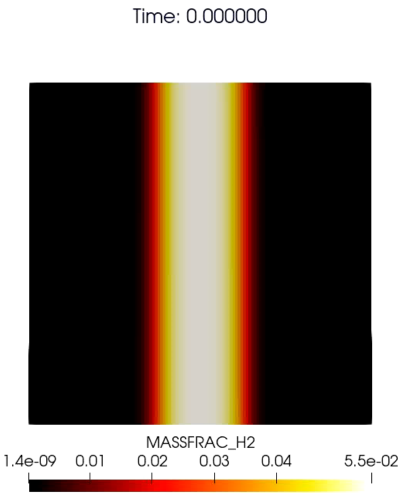
- $Y^0_{O_2}, \quad Y^0_{N_2}, \quad Y^0_{H_2}, \; P = 101325 \text{ Pa}, \;\; T = 300 \text{ K}, \;\; T_f = 1910 \text{ K}$ at the interface between the O_2 and $H_2 + N_2$
- $V_1 = u_0 \sin\left(\frac{x}{L_0}\right) \cos\left(\frac{y}{L_0}\right), \quad V_2 = -u_0 \cos\left(\frac{x}{L_0}\right) \sin\left(\frac{y}{L_0}\right)$
- Boundary condition
  - Periodic
- Discretisation
  - Time: Explicit RK45, four order DG via FR vs PISO
  - Numerical flux Lax-Friedrichs, LdG (viscous)
- Setup
  - $\Omega = [-\pi L_0, \pi L_0] \times [-\pi L_0, \pi L_0], \quad L_0 = 1\text{mm}, L = 2\pi L_0, \;\; u_0 = 4,$
  - $\tau_{ref} = \frac{L_0}{u_0} = 0.25\text{ms}, \;\; T_{\text{end}} = 10 \times \tau_{ref}, \;\; Ma = 0.1, \;\; Re = 267, \;\; N^2 \in \{64^2, 128^2\}$, CFL=0.2

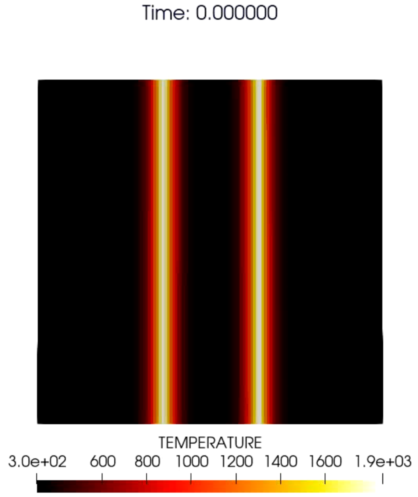


Ghislain Lartigue et al, The Taylor–Green vortex as a benchmark for high-fidelity combustion simulations using low-Mach solvers, *Computers & Fluids* **95**, 223(2021).

CHEMICAL REACTION: TRANSPORT - COMBUSTION

- The simulation is stable $\forall t \geq 0$
- We observe the consumption and production of chemical species
- $\sum_k Y_k(t,\cdot) = 1, \ \forall t \geq 0$
- $Y^0_{k,min} \leq Y_k(t,\cdot) \leq Y^0_{k,max}, \ \ \forall\, k \in [\![1, N_s]\!], \ t \geq 0$





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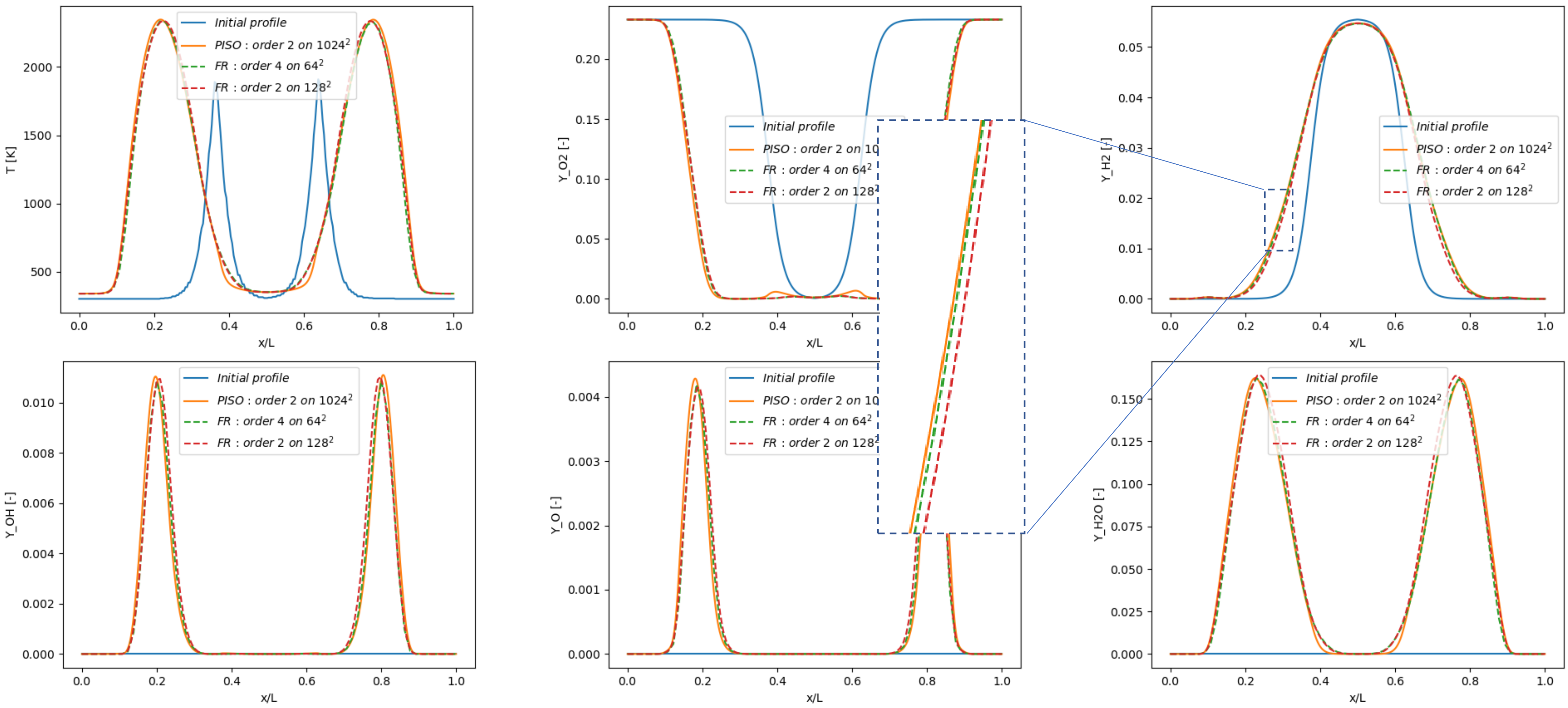
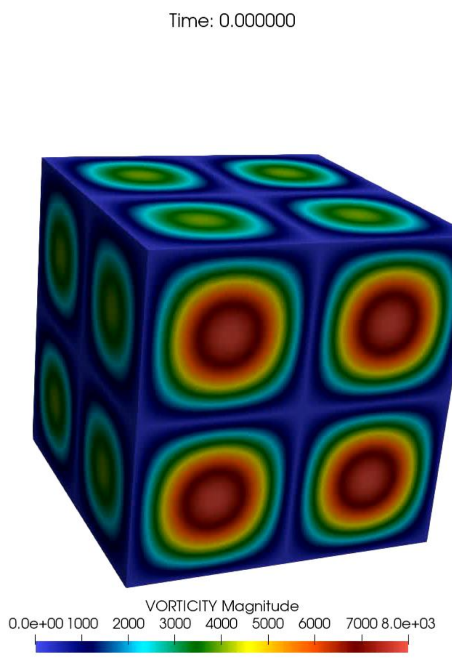
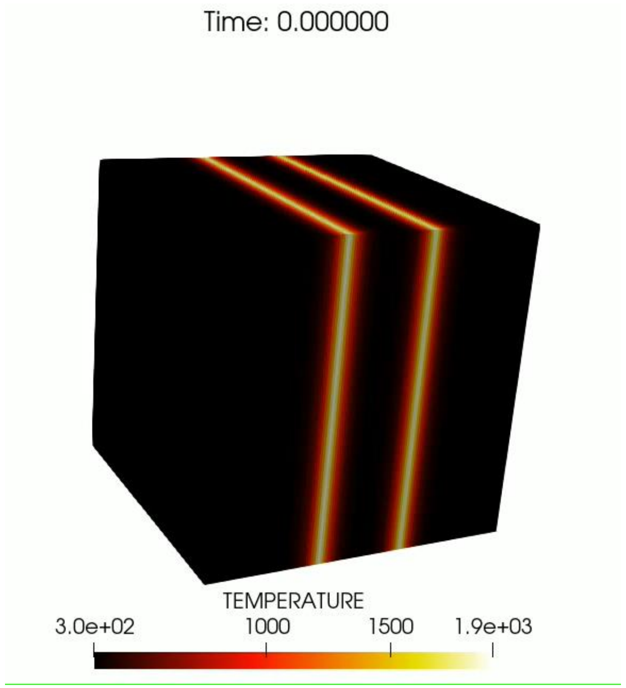
NUMERICAL EXPERIMENTS: 1D profiles at $t = \tau_{ref},\ y = 0.5L$

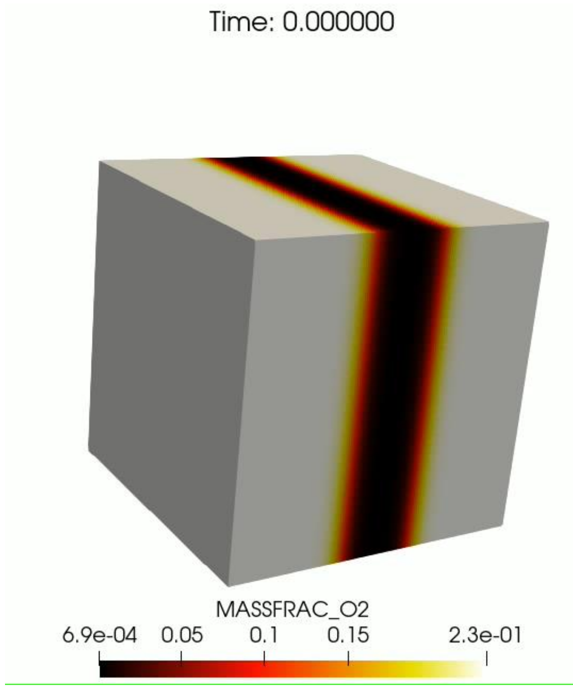


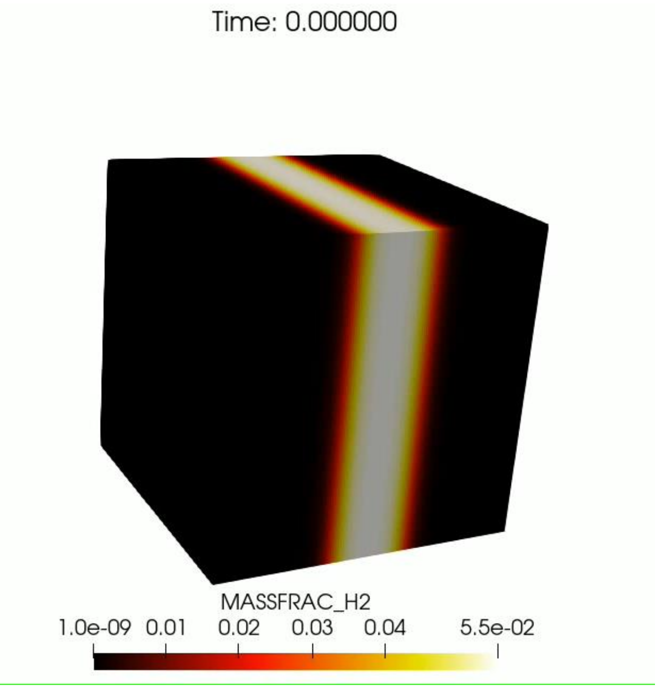
The results are better with high-order for constant number of DoF

NUMERICAL EXPERIMENTS: TUPY APPROACH IN 3D

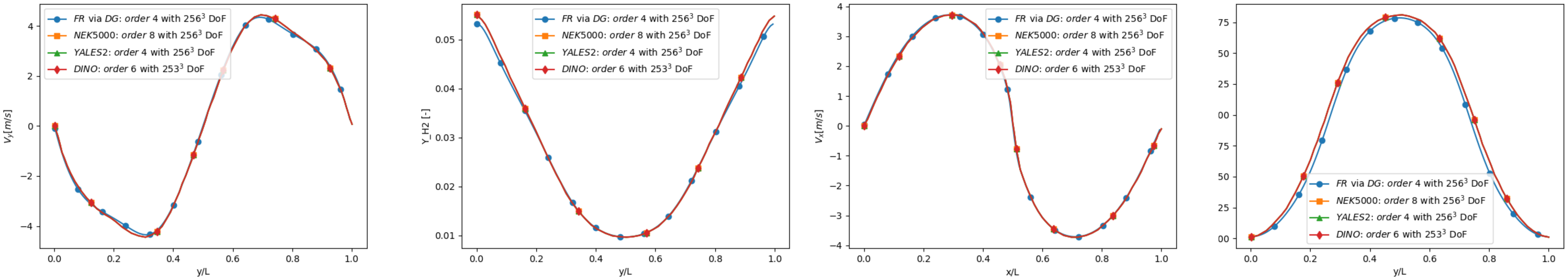








NUMERICAL EXPERIMENTS: TUPY APPROACH IN 3D



$x = 0.5\,L$, and $z = 0.5\,L$ for 3-D non-reacting multi-species flow at $t = 2\,\tau_{ref}$

Ghislain Lartigue et al, The Taylor–Green vortex as a benchmark for high-fidelity combustion simulations using low-Mach solvers, *Computers & Fluids* **95** 223(2021).

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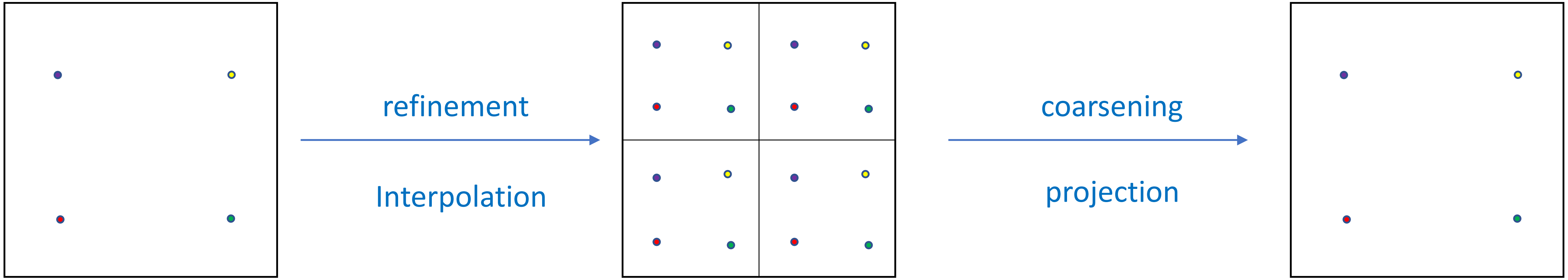
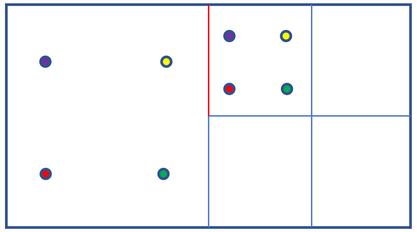
HIGH ORDER INTERPOLATION AND PROJECTION OPERATORS FOR AMR

- To ensure the conservativeness of the scheme, we need to define the high-order operators
  - To transfer data after refinement or coarsening



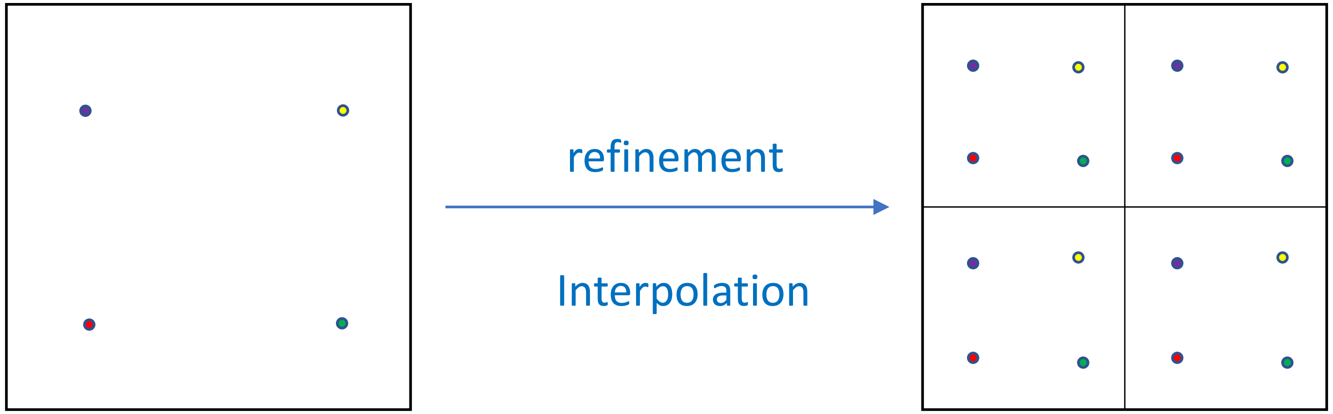
Example $p = 1$

- To calculate the numerical flux on the faces separating two cells of different sizes



David A. Kopriva A Conservative Staggered-Grid Chebyshev Multidomain Method for Compressible Flows. II. A Semi-Structured Method, JCP, 1996.

HIGH ORDER INTERPOLATION AND PROJECTION OPERATORS FOR AMR



$$\boldsymbol{u}^P(\zeta) = \sum_{i=1}^{N_p} l_i(\zeta)\boldsymbol{u}_i^P$$

$$\boldsymbol{u}_m^K(\zeta) = ?$$

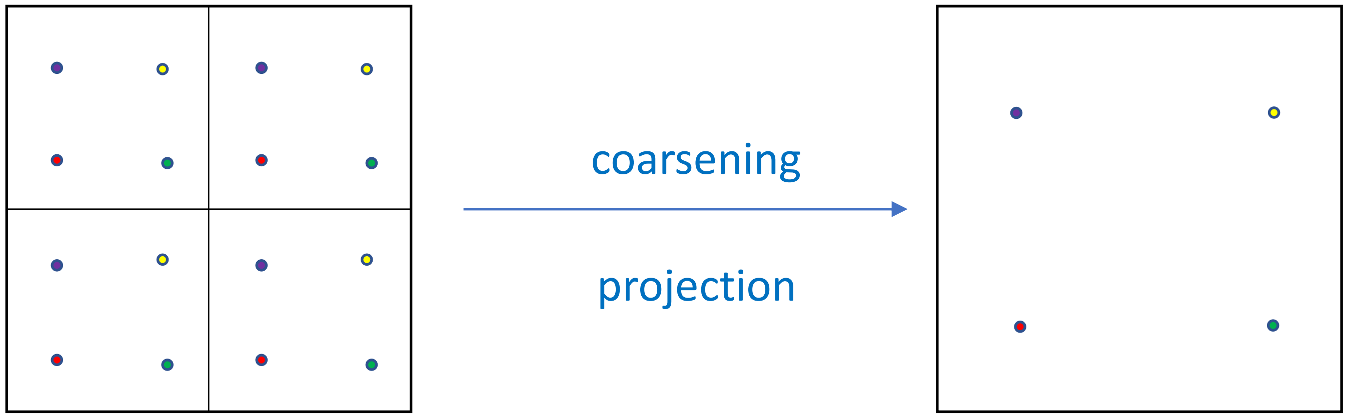
Interpolation operator:

$$\boldsymbol{u}_m^K(\zeta) = I^c(\boldsymbol{u}^P)(\zeta) = \sum_{i=1}^{N_p} l_i\big(\Phi^m(\zeta)\big)\boldsymbol{u}_i^P, \qquad m \in \{1,2,\cdots,2^D\}$$

With isoparametric map:

$$\Phi^m(\zeta) = \left(\frac{\zeta_1 - o_1^{(m)}}{s}, \frac{\zeta_1 - o_2^{(m)}}{s}\right), \qquad m \in \{1,2,\cdots,2^D\}$$

HIGH ORDER INTERPOLATION AND PROJECTION OPERATORS FOR AMR



$$\boldsymbol{u}_m^K(\zeta) = \sum_{i=1}^{N_p} \hat{l}_i^m(\zeta)\boldsymbol{u}_{m,i}^K$$

$$\boldsymbol{u}^P(\zeta) = ?$$

Projection operator:

$$\boldsymbol{u}^P = argmin_{\{V \in \hat{L}_p\}} \left\| V - \sum_{m=1}^{2^D} \boldsymbol{u}_m^K \right\|_{L^2} \Rightarrow \boldsymbol{u}^P = \Pi^c(\boldsymbol{u}_m^K) = \sum_{m=1}^{2^D} \boldsymbol{M}^{-1}\boldsymbol{S}_m \boldsymbol{u}_m^K$$

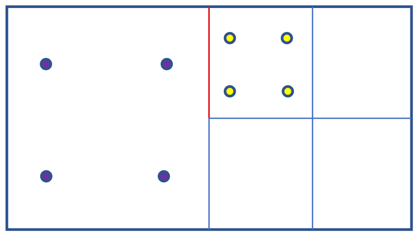
With mass matrix:

$$M_{ji} = \int_{\hat{\Omega}} l_j l_i \, d\zeta \qquad S_{m,ji} = \int_{\hat{\Omega}} l_j \, \hat{l}_i^m \, d\zeta$$

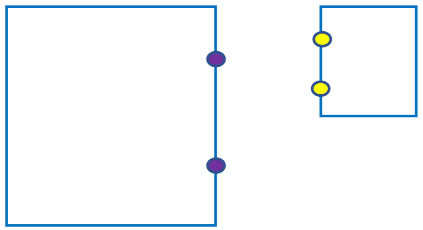
David A. Kopriva A Conservative Staggered-Grid Chebyshev Multidomain Method for Compressible Flows. II. A Semi-Structured Method, JCP, 1996.

HIGH ORDER INTERPOLATION AND PROJECTION OPERATORS FOR AMR

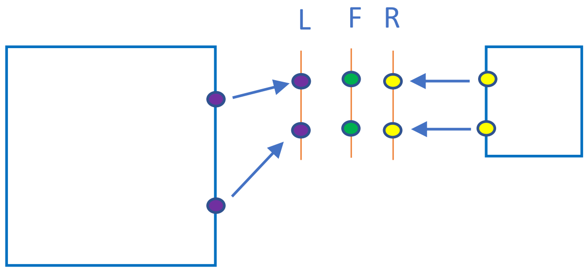
- The numerical flux on the faces separating two cells of different sizes



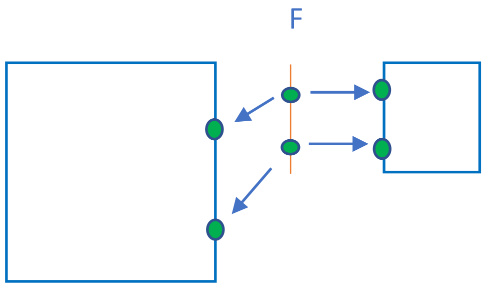
- Interpolation on the real faces of each element: I^f



- Projection on mortar face: $(\Pi^f)^{-1}$



- Projection from mortar face: Π^f

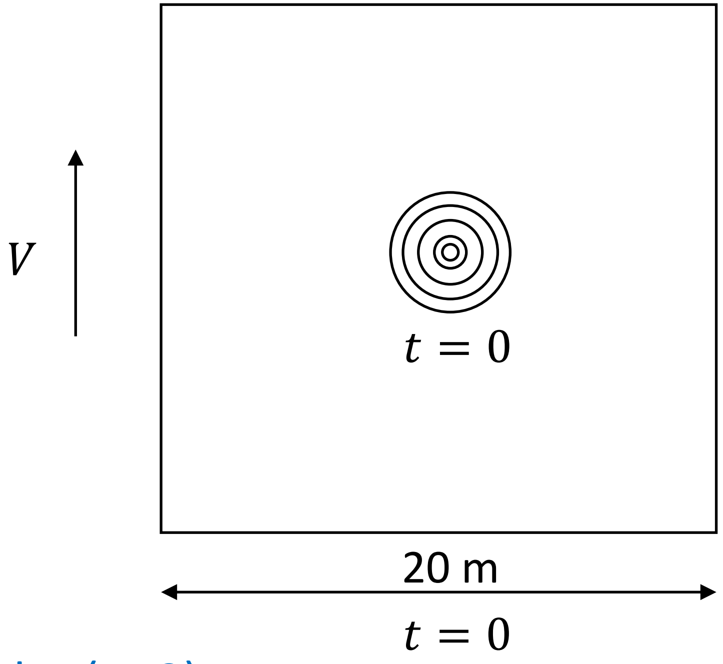


David A. Kopriva A Conservative Staggered-Grid Chebyshev Multidomain Method for Compressible Flows. II. A Semi-Structured Method, JCP, 1996.

NUMERICAL EXPERIMENTS: EULER EQUATIONS 2D

Vortex convection

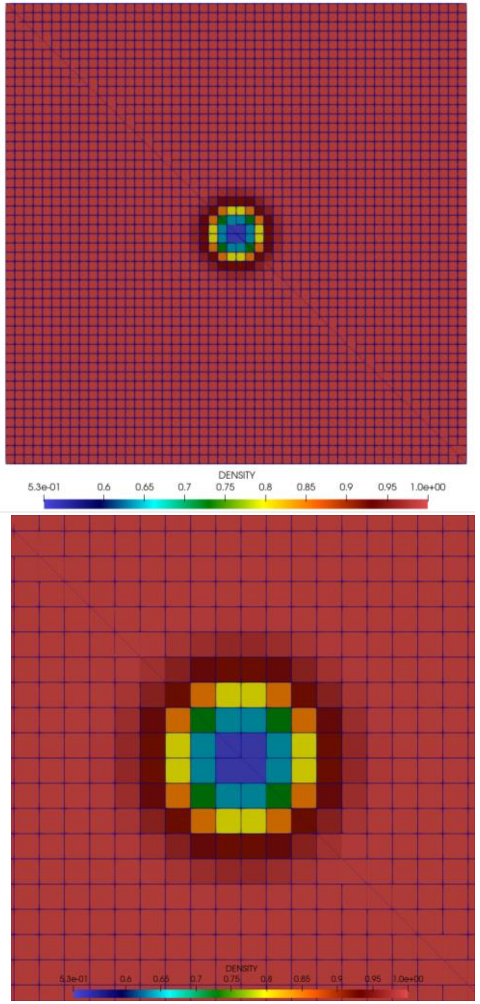
- Initial condition
  - $\rho = 1,\ V = (0,1),$
  - $\delta V = \frac{\beta}{2\pi}(-(\mathrm{y}-\mathrm{y_c}), (\mathrm{x}-\mathrm{x_c}))\exp(0.5(1-r^2))$
  - $\delta T = -\frac{(\gamma-1)\beta^2}{8\gamma\pi^2}\exp((1-r^2))$
  - $E = \frac{P}{\rho(\gamma-1)} + \frac{1}{2}(V_1^2+V_2^2),\ \gamma = 1.4$
- Boundary condition
  - Periodic



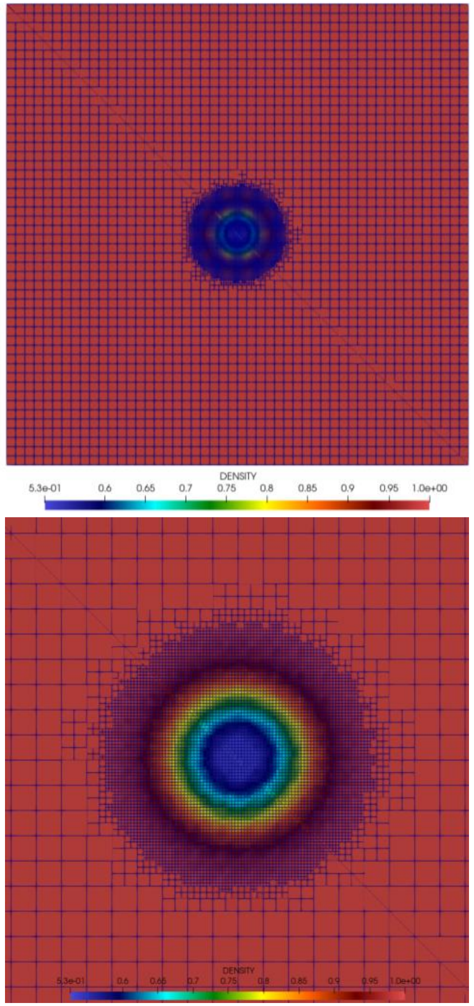
- Discretisation
  - Numerical flux Lax-Friedrichs (advective) , RK33, **DG** via FR second order (p=3)
  - $\Omega = [-10,10]\times[-10,10],\ \ N^2 = 50^2,\ \ T_f = 20\mathrm{s},\ \ \mathrm{CFL}(p) = \frac{1}{p+1}$

Shu C. W., *Essentially non-oscillatory and weighted essentially non-oscillatory schemes for hyperbolic conservation laws*, vol. **1697** of Lecture notes in Mathematics, 325–432, 1998.

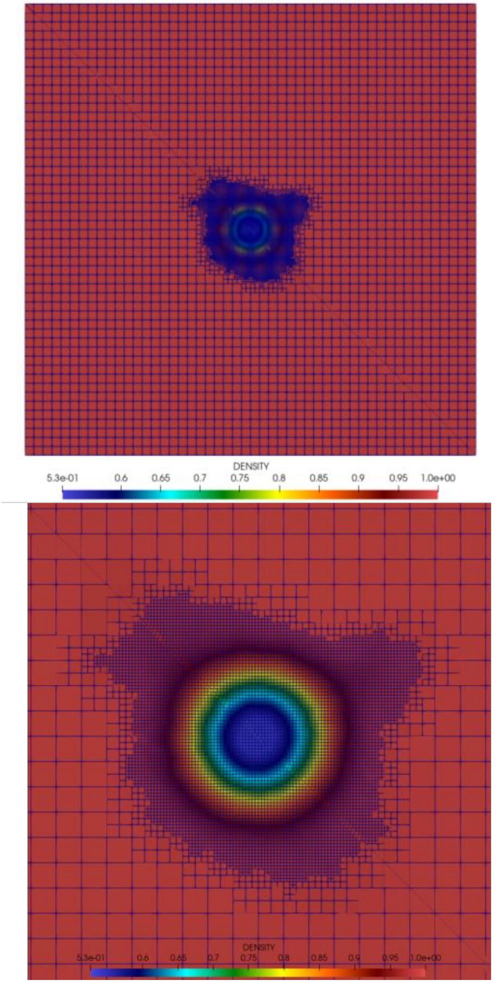
NUMERICAL EXPERIMENTS: EULER EQUATIONS 2D



Density profile at $t = 0$ sec
without AMR



Density profile at $t = 0$ sec
with AMR



Density profile at $t = 20$ sec
with AMR

Solution with four order accuracy, amr criterion based on density, level = 3

OUTLINE

- Principles of Flux Reconstruction method
- Development of FR schemes for non-reactive 3D flows in AEROSOL
- Development of FR schemes for non-reactive and reactive 3D flows in CONVERGE
- Development of a coupling methodology for FR schemes and AMR in CONVERGE
- **Conclusion and future works**

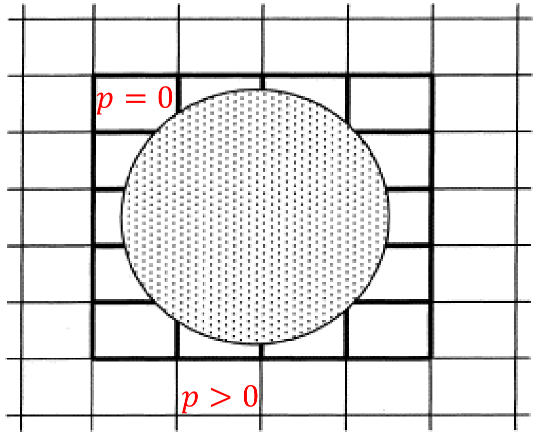
CONCLUSION AND FUTURE WORKS

During this work we have:

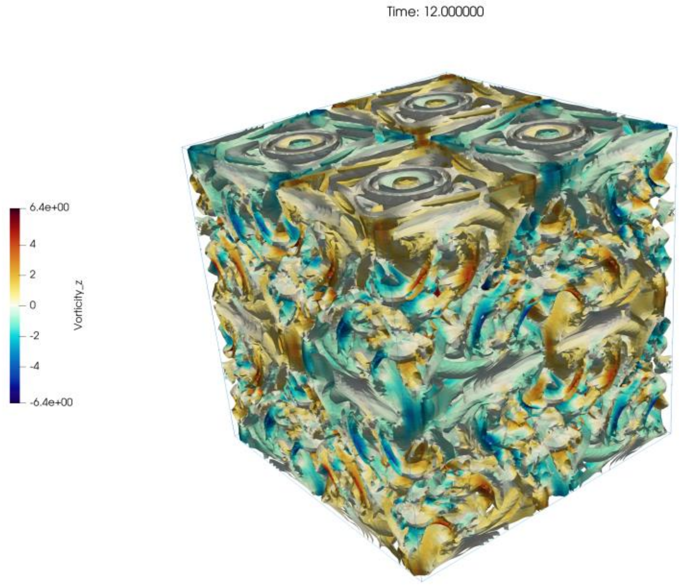
- Developed up to the sixth order of accuracy of Flux Reconstruction scheme for 3D non-reactive Navier-Stokes equations (AEROSOL CFD)
- Developed up to the sixth order of accuracy of Flux Reconstruction scheme for 3D multispecies reactive Navier-Stokes equations (CONVERGE CFD Version 3.1 and 3.2)
  - TUPY approach is stable, preserves global mass conservation and the positivity of mass fractions
- Developed high order Galerkin projection for AMR (h-refinement) coupled with FR Schemes (CONVERGE CFD Version 3.2)

Future work :

- Adapt FR schemes for order refinement: *h,p*-refinement
- Adapt FR Schemes for CutCells method: Add wall / inlet / outlet BC (p=0)



Cut Cells on the surface of a cylinder



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