



Centre Tecnològic de Transferència de Calor
UNIVERSITAT POLITÈCNICA DE CATALUNYA

Preserving symmetries on unstructured grids

F.Xavier Trias

Heat and Mass Transfer Technological Center, Technical University of Catalonia (UPC)



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- 2 Soft landing...
- 3 Motivation
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About myself...

Professional...

- Current position (since 2018): **Associate Professor** at UPC
- Previous positions: PostDoc at University of Groningen (2007-2009) and UPC (2010-2013), and *Ramón y Cajal* Senior Researcher at UPC (2013-2018).
- My **research** focus is on fluid mechanics, turbulence modeling, physics and numerics of complex flows, applied mathematics and numerical methods.
- Some numbers: 48 papers, 125 conferences, 7 PhD's+7 (on-going)
- Stays and collaborations: Groningen (The Netherlands), UCLA, KIAM (Russian Academy of Sciences), Stanford, Manchester (UK), Tsinghua (China), TokioTech (Japan), Napoli (Italy)...
- More info: www.fxtrias.com

About myself...

... and more personal stuff

- My complete name: Francesc Xavier Trias Miquel
- Born in Barcelona
- My mother tongue is Catalan but I also speak Spanish at native level.
- Hobbies? I like my work but also sports. Most practiced ones are running and football (the one you play with your feet ;-)):



Groningen (2009?)

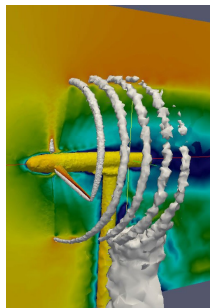
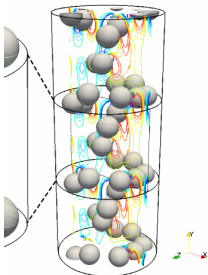
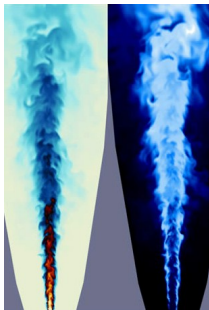


Barcelona (2019)

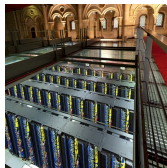
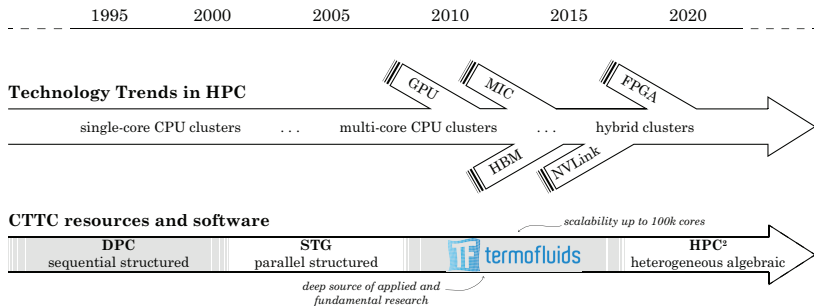
The CTTC research group

Heat and Mass Transfer Technological Center (Catalan: *Centre Tecnològic de Transferència de Calor*) has more than 25 years experience on CFD:

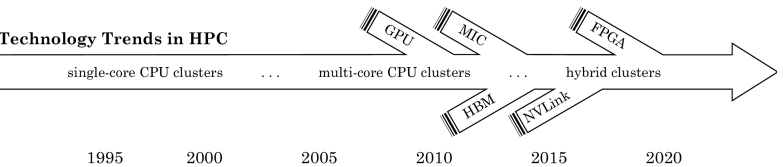
- **Fundamental research** on numerical methods, fluid dynamics and heat and mass transfer phenomena.
- **Applied research** on thermal and fluid dynamic optimization of thermal system and equipment.



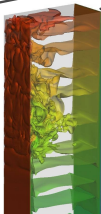
CTTC's historical background in HPC



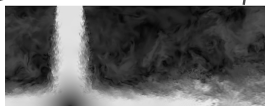
Technology Trends in HPC



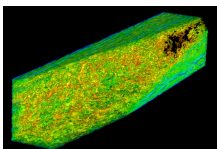
DHC
 $Ra=10^9$
 (3.2M)



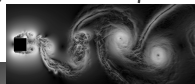
DHC
 $Ra=10^{11}$
 (111M)



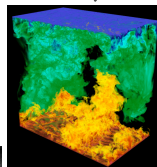
Impinging jet
 $Re=20000$
 (102M)



DUCT $Re_t=1200$ (172M)



SqCyl $Re=22000$ (324M)



RB
 $Ra=10^{10}$ (607M)
 $Ra=10^{11}$ (5600M)

Let's begin with some math...

$$\langle \nabla \cdot \vec{a} | \phi \rangle = -\langle \vec{a} | \nabla \phi \rangle$$

$$\langle \nabla^2 f | g \rangle = -\langle \nabla f | \nabla g \rangle = \langle f | \nabla^2 g \rangle$$

$$\langle C(\vec{u}, \phi_1) | \phi_2 \rangle = -\langle C(\vec{u}, \phi_2) | \phi_1 \rangle \quad \text{if } \nabla \cdot \vec{u} = 0$$

$$\langle \nabla \times \vec{a} | \vec{b} \rangle = \langle \vec{a} | \nabla \times \vec{b} \rangle$$

Notation:

$$\langle a | b \rangle := \int_{\Omega} a b \, d\Omega \quad C(\vec{u}, \phi) := (\vec{u} \cdot \nabla) \phi$$

REMEMBER: we always assume **no contribution from domain boundary, $\partial \Omega$**

Operator symmetries and conservation

$\langle \vec{u} | \vec{u} \rangle$ Kinetic energy (in 2D/3D)

$$\begin{aligned} \frac{1}{2} \frac{d \langle \vec{u} | \vec{u} \rangle}{dt} &= \left\langle \frac{\partial \vec{u}}{\partial t} \middle| \vec{u} \right\rangle = - \langle C(\vec{u}, \vec{u}) | \vec{u} \rangle + \nu \langle \nabla^2 \vec{u} | \vec{u} \rangle - \langle \nabla p | \vec{u} \rangle \\ &= -\nu \langle \nabla \vec{u} | \nabla \vec{u} \rangle = -\nu \|\nabla \vec{u}\|^2 \leq 0 \\ &= -\nu \langle \nabla \times \nabla \times \vec{u} | \vec{u} \rangle = -\nu \|\omega\|^2 \leq 0 \end{aligned}$$

If $\nu=0$, then $\langle \vec{u} | \vec{u} \rangle$ remains constant!!!

Also, if the flow is irrotational, $\vec{\omega} = \vec{0}$. Remember Bernoulli!

ADDITIONAL REMAINDER!!!

$$\nabla^2 \vec{u} = \nabla(\nabla \cdot \vec{u}) - \nabla \times \nabla \times \vec{u}$$

REMAINDER!!!

$$\langle \nabla \cdot \vec{a} | \phi \rangle = - \langle \vec{a} | \nabla \phi \rangle$$

$$\langle \nabla^2 f | g \rangle = - \langle \nabla f | \nabla g \rangle = \langle f | \nabla^2 g \rangle$$

$$\langle C(\vec{u}, \phi_1) | \phi_2 \rangle = - \langle C(\vec{u}, \phi_2) | \phi_1 \rangle \quad \text{if } \nabla \cdot \vec{u} = 0$$

$$\langle \nabla \times \vec{a} | \vec{b} \rangle = \langle \vec{a} | \nabla \times \vec{b} \rangle$$

From Calculus to Algebra (C2A)

$$\langle a|b \rangle := \int_{\Omega} a b d\Omega \in \mathbb{R}$$

$$\langle a_h|b_h \rangle := a_h^T \mathbf{\Omega} b_h \in \mathbb{R}$$

● ¹	● ²	● ³
● ⁴	● ⁵	● ⁶

$$a_h = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \\ a_6 \end{pmatrix} \quad \mathbf{\Omega} = \begin{pmatrix} \Omega_1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \Omega_2 & 0 & 0 & 0 & 0 \\ 0 & 0 & \Omega_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & \Omega_4 & 0 & 0 \\ 0 & 0 & 0 & 0 & \Omega_5 & 0 \\ 0 & 0 & 0 & 0 & 0 & \Omega_6 \end{pmatrix} \quad b_h = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \\ b_6 \end{pmatrix}$$

From Calculus to Algebra (C2A)

$$\langle a|b \rangle := \int_{\Omega} a b d\Omega \in \mathbb{R}$$

$$\langle a_h|b_h \rangle := a_h^T \Omega b_h \in \mathbb{R}$$

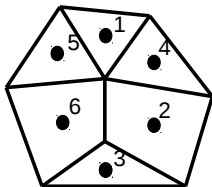
● ³	● ⁵	● ¹
● ⁶	● ²	● ⁴

$$a_h = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \\ a_6 \end{pmatrix} \quad \Omega = \begin{pmatrix} \Omega_1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \Omega_2 & 0 & 0 & 0 & 0 \\ 0 & 0 & \Omega_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & \Omega_4 & 0 & 0 \\ 0 & 0 & 0 & 0 & \Omega_5 & 0 \\ 0 & 0 & 0 & 0 & 0 & \Omega_6 \end{pmatrix} \quad b_h = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \\ b_6 \end{pmatrix}$$

From Calculus to Algebra (C2A)

$$\langle a|b \rangle := \int_{\Omega} ab d\Omega \in \mathbb{R}$$

$$\langle a_h|b_h \rangle := a_h^T \Omega b_h \in \mathbb{R}$$



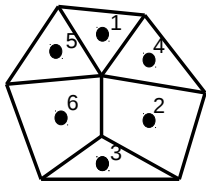
$$a_h = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \\ a_6 \end{pmatrix} \quad \Omega = \begin{pmatrix} \Omega_1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \Omega_2 & 0 & 0 & 0 & 0 \\ 0 & 0 & \Omega_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & \Omega_4 & 0 & 0 \\ 0 & 0 & 0 & 0 & \Omega_5 & 0 \\ 0 & 0 & 0 & 0 & 0 & \Omega_6 \end{pmatrix} \quad b_h = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \\ b_6 \end{pmatrix}$$

From Calculus to Algebra (C2A)

$$\frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla) \vec{u} = \nu \nabla^2 \vec{u} - \nabla p \quad \nabla \cdot \vec{u} = 0$$

$$\Omega \frac{d u_h}{dt} + C(u_h) u_h = D u_h - \Omega G p_h \quad M u_h = 0_h \quad p_h(t) = \begin{pmatrix} p_1 \\ p_2 \\ p_3 \\ p_4 \\ p_5 \\ p_6 \end{pmatrix}$$

$$u_h(t) = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \\ v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \\ v_6 \end{pmatrix}$$



$$T = \begin{pmatrix} \times & 0 & 0 & \times & \times & 0 \\ 0 & \times & \times & \times & 0 & \times \\ 0 & \times & \times & 0 & 0 & \times \\ \times & \times & 0 & \times & 0 & 0 \\ \times & 0 & 0 & 0 & \times & \times \\ 0 & \times & \times & 0 & \times & \times \end{pmatrix}$$

$$\Omega_u = \Omega_v =$$

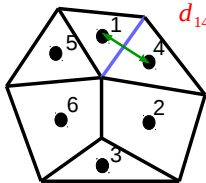
$$\begin{pmatrix} \Omega_1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \Omega_2 & 0 & 0 & 0 & 0 \\ 0 & 0 & \Omega_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & \Omega_4 & 0 & 0 \\ 0 & 0 & 0 & 0 & \Omega_5 & 0 \\ 0 & 0 & 0 & 0 & 0 & \Omega_6 \end{pmatrix}$$

$$\Omega = \begin{pmatrix} \Omega_u & \\ & \Omega_v \end{pmatrix}$$

From Calculus to Algebra (C2A)

$$\frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla) \vec{u} = \nu \nabla^2 \vec{u} - \nabla p \quad \nabla \cdot \vec{u} = 0$$

$$\Omega \frac{d u_h}{d t} + C(u_h) u_h = D u_h - \Omega G p_h \quad M u_h = 0_h \quad p_h(t) = \begin{pmatrix} p_1 \\ p_2 \\ p_3 \\ p_4 \\ p_5 \\ p_6 \end{pmatrix}$$



$$d_{14} = \nu A_{14} / \delta_{14}$$

$$D = \begin{pmatrix} D_u & \\ & D_v \end{pmatrix}$$

$$u_h(t) = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \\ v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \\ v_6 \end{pmatrix}$$

$$r = \begin{pmatrix} \times & 0 & 0 & \times & \times & 0 \\ 0 & \times & \times & \times & 0 & \times \\ 0 & \times & \times & 0 & 0 & \times \\ \times & \times & 0 & \times & 0 & 0 \\ \times & 0 & 0 & 0 & \times & \times \\ 0 & \times & \times & 0 & \times & \times \end{pmatrix}$$

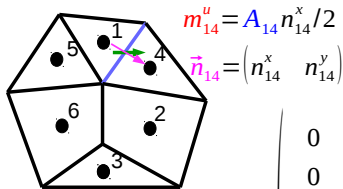
$$D_u = D_v = \begin{pmatrix} d_{11} & 0 & 0 & d_{14} & d_{15} & 0 \\ 0 & d_{22} & d_{23} & d_{24} & 0 & d_{26} \\ 0 & d_{23} & d_{33} & 0 & 0 & d_{36} \\ d_{14} & d_{24} & 0 & d_{44} & 0 & 0 \\ d_{15} & 0 & 0 & 0 & d_{55} & d_{56} \\ 0 & d_{26} & d_{36} & 0 & d_{56} & d_{66} \end{pmatrix}$$

From Calculus to Algebra (C2A)

$$\frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla) \vec{u} = \nu \nabla^2 \vec{u} - \nabla p \quad \nabla \cdot \vec{u} = 0$$

$$\Omega \frac{d u_h}{dt} + C(u_h) u_h = D u_h - \Omega G p_h \quad M u_h = 0_h \quad p_h(t) = \begin{pmatrix} p_1 \\ p_2 \\ p_3 \\ p_4 \\ p_5 \\ p_6 \end{pmatrix}$$

$$u_h(t) = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \\ v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \\ v_6 \end{pmatrix}$$



$$M = (M^u \quad M^v)$$

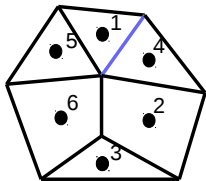
$$r = \begin{pmatrix} \times & 0 & 0 & \times & \times & 0 \\ 0 & \times & \times & \times & 0 & \times \\ 0 & \times & \times & 0 & 0 & \times \\ \times & \times & 0 & \times & 0 & 0 \\ \times & 0 & 0 & 0 & \times & \times \\ 0 & \times & \times & 0 & \times & \times \end{pmatrix} \quad M^u = \begin{pmatrix} 0 & 0 & 0 & m_{14}^u & m_{15}^u & 0 \\ 0 & 0 & m_{23}^u & m_{24}^u & 0 & m_{26}^u \\ 0 & -m_{23}^u & 0 & 0 & 0 & m_{36}^u \\ -m_{14}^u & -m_{24}^u & 0 & 0 & 0 & 0 \\ -m_{15}^u & 0 & 0 & 0 & 0 & m_{56}^u \\ 0 & -m_{26}^u & -m_{36}^u & 0 & -m_{56}^u & 0 \end{pmatrix}$$

From Calculus to Algebra (C2A)

$$\frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla) \vec{u} = \nu \nabla^2 \vec{u} - \nabla p \quad \nabla \cdot \vec{u} = 0$$

$$\Omega \frac{d u_h}{dt} + C(u_h) u_h = D u_h - \Omega G p_h \quad M u_h = 0_h$$

$$p_h(t) = \begin{pmatrix} p_1 \\ p_2 \\ p_3 \\ p_4 \\ p_5 \\ p_6 \end{pmatrix} \quad u_h(t) = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \\ v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \\ v_6 \end{pmatrix}$$



$$T = \begin{pmatrix} \times & 0 & 0 & \times & \times & 0 \\ 0 & \times & \times & \times & 0 & \times \\ 0 & \times & \times & 0 & 0 & \times \\ \times & \times & 0 & \times & 0 & 0 \\ \times & 0 & 0 & 0 & \times & \times \\ 0 & \times & \times & 0 & \times & \times \end{pmatrix}$$

$$G = \begin{pmatrix} G^x \\ G^y \end{pmatrix}$$

$$G^x = \begin{pmatrix} 0 & 0 & 0 & g_{14}^x & g_{15}^x & 0 \\ 0 & 0 & g_{23}^x & g_{24}^x & 0 & g_{26}^x \\ 0 & -g_{23}^x & 0 & 0 & 0 & g_{36}^x \\ -g_{14}^x & -g_{24}^x & 0 & 0 & 0 & 0 \\ -g_{15}^x & 0 & 0 & 0 & 0 & g_{56}^x \\ 0 & -g_{26}^x & -g_{36}^x & 0 & -g_{56}^x & 0 \end{pmatrix}$$

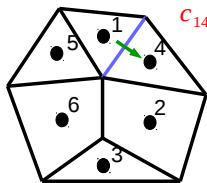
From Calculus to Algebra (C2A)

$$\frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla) \vec{u} = \nu \nabla^2 \vec{u} - \nabla p \quad \nabla \cdot \vec{u} = 0$$

$$\Omega \frac{d u_h}{dt} + \mathbf{C}(u_h) u_h = \mathbf{D} u_h - \Omega \mathbf{G} p_h \quad \mathbf{M} u_h = 0_h$$

$$p_h(t) = \begin{pmatrix} p_1 \\ p_2 \\ p_3 \\ p_4 \\ p_5 \\ p_6 \end{pmatrix}$$

$$u_h(t) = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \\ v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \\ v_6 \end{pmatrix}$$



$$c_{14} = A_{14} U_{14}$$

$$\mathbf{C} = \begin{pmatrix} \mathbf{C}_u & \\ & \mathbf{C}_v \end{pmatrix}$$

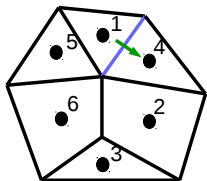
$$r = \begin{pmatrix} \times & 0 & 0 & \times & \times & 0 \\ 0 & \times & \times & \times & 0 & \times \\ 0 & \times & \times & 0 & 0 & \times \\ \times & \times & 0 & \times & 0 & 0 \\ \times & 0 & 0 & 0 & \times & \times \\ 0 & \times & \times & 0 & \times & \times \end{pmatrix}$$

$$\mathbf{C}_u = \mathbf{C}_v = \begin{pmatrix} c_{11} & 0 & 0 & c_{14} & c_{15} & 0 \\ 0 & c_{22} & c_{23} & c_{24} & 0 & c_{26} \\ 0 & c_{32} & c_{33} & 0 & 0 & c_{36} \\ c_{41} & c_{42} & 0 & c_{44} & 0 & 0 \\ c_{51} & 0 & 0 & 0 & c_{55} & c_{56} \\ 0 & c_{62} & c_{63} & 0 & c_{65} & c_{66} \end{pmatrix}$$

Algebraic operators

$$\frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla) \vec{u} = \nu \nabla^2 \vec{u} - \nabla p \quad \nabla \cdot \vec{u} = 0$$

$$\Omega \frac{d \mathbf{u}_h}{dt} + \mathbf{C}(\mathbf{u}_h) \mathbf{u}_h = \mathbf{D} \mathbf{u}_h - \Omega \mathbf{G} p_h \quad \mathbf{M} \mathbf{u}_h = 0_h$$



$$\Omega = \begin{pmatrix} \Omega_u & \\ & \Omega_v \end{pmatrix}$$

$$\mathbf{M} = \begin{pmatrix} M^u & M^v \end{pmatrix}$$

$$\mathbf{G} = \begin{pmatrix} G^x \\ G^y \end{pmatrix}$$

$$\mathbf{r} = \begin{pmatrix} \times & 0 & 0 & \times & \times & 0 \\ 0 & \times & \times & \times & 0 & \times \\ 0 & \times & \times & 0 & 0 & \times \\ \times & \times & 0 & \times & 0 & 0 \\ \times & 0 & 0 & 0 & \times & \times \\ 0 & \times & \times & 0 & \times & \times \end{pmatrix}$$

$$\mathbf{C} = \begin{pmatrix} C_u & \\ & C_v \end{pmatrix}$$

$$\mathbf{D} = \begin{pmatrix} D_u & \\ & D_v \end{pmatrix}$$

Algebraic operators

$$\frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla) \vec{u} = \nu \nabla^2 \vec{u} - \nabla p \quad \nabla \cdot \vec{u} = 0 \quad \langle a|b \rangle := \int_{\Omega} a b d\Omega$$

$$\Omega \frac{d \mathbf{u}_h}{dt} + \mathbf{C}(\mathbf{u}_h) \mathbf{u}_h = \mathbf{D} \mathbf{u}_h - \Omega \mathbf{G} p_h \quad \mathbf{M} \mathbf{u}_h = 0_h \quad \langle a_h|b_h \rangle := a_h^T \Omega b_h$$

Let's consider the time evolution of $1/2 \langle \mathbf{u}_h | \mathbf{u}_h \rangle \dots$

$$\frac{1}{2} \frac{d \langle \mathbf{u}_h | \mathbf{u}_h \rangle}{dt} = \mathbf{u}_h^T \Omega \frac{d \mathbf{u}_h}{dt} = -\mathbf{u}_h^T \mathbf{C}(\mathbf{u}_h) \mathbf{u}_h + \mathbf{u}_h^T \mathbf{D} \mathbf{u}_h - \mathbf{u}_h^T \Omega \mathbf{G} p_h$$

$$= \mathbf{u}_h^T \mathbf{D} \mathbf{u}_h \leq 0$$


...mimicking the properties of continuous NS eqs leads to

REMAINDER!!!

$$\frac{1}{2} \frac{d \langle \vec{u} | \vec{u} \rangle}{dt} = \langle \frac{\partial \vec{u}}{\partial t} | \vec{u} \rangle = -\langle \mathbf{C}(\vec{u}, \vec{u}) | \vec{u} \rangle + \nu \langle \nabla^2 \vec{u} | \vec{u} \rangle - \langle \nabla p | \vec{u} \rangle$$

$$= -\nu \langle \nabla \vec{u} | \nabla \vec{u} \rangle = -\nu \|\nabla \vec{u}\|^2 \leq 0$$

$$= -\nu \langle \nabla \times \nabla \times \vec{u} | \vec{u} \rangle = -\nu \|\omega\|^2 \leq 0$$

 **Numerical stability!!!**

Algebraic operators

$$\begin{aligned} \frac{1}{2} \frac{d\langle u_h | u_h \rangle}{dt} &= u_h^T \Omega \frac{d u_h}{dt} = -u_h^T C(u_h) u_h + u_h^T D u_h - u_h^T \Omega G p_h \\ &= u_h^T D u_h \leq 0, \quad \text{if } M u_h = 0_h, \quad \forall u_h, p_h \end{aligned}$$

$$u_h^T C(u_h) u_h = 0 \quad \longrightarrow \quad C(u_h) = -C^T(u_h)$$

$$u_h^T \Omega G p_h = 0 \quad \longrightarrow \quad \Omega G = -M^T$$

$$u_h^T D u_h \leq 0 \quad \longrightarrow \quad D = D^T \text{ def-}$$

REMAINDER!!!

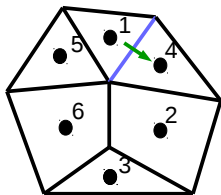
$$\begin{aligned} \frac{1}{2} \frac{d\langle \tilde{u} | \tilde{u} \rangle}{dt} &= \langle \frac{\partial \tilde{u}}{\partial t} | \tilde{u} \rangle = -\langle C(\tilde{u}, \tilde{u}) | \tilde{u} \rangle + \nu \langle \nabla^2 \tilde{u} | \tilde{u} \rangle - \langle \nabla p | \tilde{u} \rangle \\ &= -\nu \langle \nabla \tilde{u} | \nabla \tilde{u} \rangle = -\nu \|\nabla \tilde{u}\|^2 \leq 0 \\ &= -\nu \langle \nabla \times \nabla \times \tilde{u} | \tilde{u} \rangle = -\nu \|\omega\|^2 \leq 0 \end{aligned}$$

REMAINDER!!!

$$\begin{aligned} \langle \nabla \cdot \tilde{a} | \phi \rangle &= -\langle \tilde{a} | \nabla \phi \rangle \\ \langle \nabla^2 f | g \rangle &= -\langle \nabla f | \nabla g \rangle = \langle f | \nabla^2 g \rangle \\ \langle C(\tilde{u}, \phi_1) | \phi_2 \rangle &= -\langle C(\tilde{u}, \phi_2) | \phi_1 \rangle \quad \text{if } \nabla \cdot \tilde{u} = 0 \\ \langle \nabla \times \tilde{a} | b \rangle &= \langle \tilde{a} | \nabla \times b \rangle \end{aligned}$$

Algebraic operators

$$\Omega \frac{d u_h}{d t} + C(u_h) u_h = D u_h - \Omega G p_h \quad M u_h = 0_h$$



$$T = \begin{pmatrix} \times & 0 & 0 & \times & \times & 0 \\ 0 & \times & \times & \times & 0 & \times \\ 0 & \times & \times & 0 & 0 & \times \\ \times & \times & 0 & \times & 0 & 0 \\ \times & 0 & 0 & 0 & \times & \times \\ 0 & \times & \times & 0 & \times & \times \end{pmatrix}$$

$$\Omega = \begin{pmatrix} \Omega_u & \\ & \Omega_v \end{pmatrix}$$

$$M = \begin{pmatrix} M^u & M^v \end{pmatrix}$$

$$\Omega G = -M^T$$

$$G = \begin{pmatrix} G^x \\ G^y \end{pmatrix}$$

$$D_u = D_v = M G = -M \Omega^{-1} M^T$$

$$C = \begin{pmatrix} C_u & \\ & C_v \end{pmatrix}$$

$$D = \begin{pmatrix} D_u & \\ & D_v \end{pmatrix}$$

From Calculus to Algebra (C2A)

$$\frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla) \vec{u} = \nu \nabla^2 \vec{u} - \nabla p; \quad \nabla \cdot \vec{u} = 0$$

$$\langle a | b \rangle := \int_{\Omega} a b d\Omega$$

$$\langle C(\vec{u}, \phi_1) | \phi_2 \rangle = -\langle C(\vec{u}, \phi_2) | \phi_1 \rangle$$

$$\langle \nabla \cdot \vec{a} | \phi \rangle = -\langle \vec{a} | \nabla \phi \rangle$$

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$$\langle \nabla \times \vec{a} | \vec{b} \rangle = \langle \vec{a} | \nabla \times \vec{b} \rangle$$

C2A

$$\Omega \frac{d u_h}{dt} + C(u_h) u_h = D u_h - \Omega G p_h; \quad M u_h = 0_h$$

$$\longrightarrow \langle a_h | b_h \rangle := a_h^T \Omega b_h$$

$$\longrightarrow C(u_h) = -C^T(u_h)$$

$$\longrightarrow \Omega G = -M^T$$

$$\longrightarrow D = D^T \text{ def-}$$

$$u_h^T C(u_h) u_h = 0 \longrightarrow C(u_h) = -C^T(u_h)$$

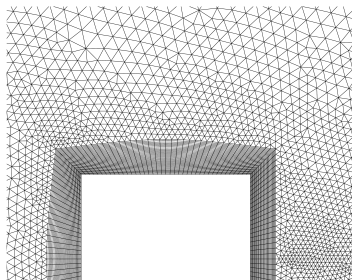
$$u_h^T \Omega G p_h = 0 \longrightarrow \Omega G = -M^T$$

$$u_h^T D u_h \leq 0 \longrightarrow D = D^T \text{ def-}$$

Motivation

Research question #1:

- Can we construct numerical discretizations of the Navier-Stokes equations suitable for **complex geometries**, such that the **symmetry properties** are exactly preserved?



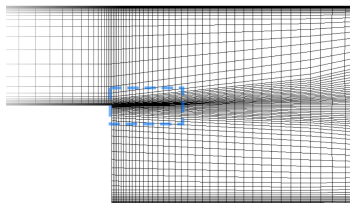
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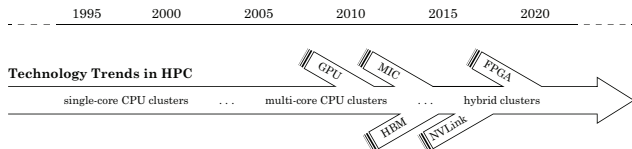
DNS² of backward-facing step at $Re_\tau = 395$ and expansion ratio 2

²A.Pont-Vílchez, F.X.Trias, A.Gorobets, A.Oliva. *DNS of Backward-Facing Step flow at $Re_\tau = 395$ and expansion ratio 2*. **Journal of Fluid Mechanics**, 863:341-363, 2019.

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- How can we develop **portable** and **efficient** CFD codes for large-scale simulations on modern supercomputers?



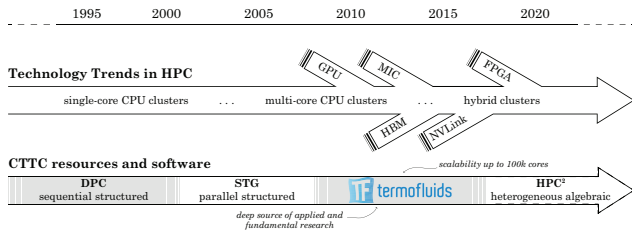
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HPC²: portable, algebra-based framework³ for heterogeneous computing is being developed⁴. Traditional stencil-based data and sweeps are replaced by algebraic structures (sparse matrices and vectors) and kernels. SpMM-based strategies to increase the arithmetic intensity are presented later...

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Motivation

Frequently used general purpose CFD codes:

- STAR-CCM+



SIEMENS



- ANSYS-FLUENT



- Code-Saturne



- OpenFOAM

Open  FOAM®



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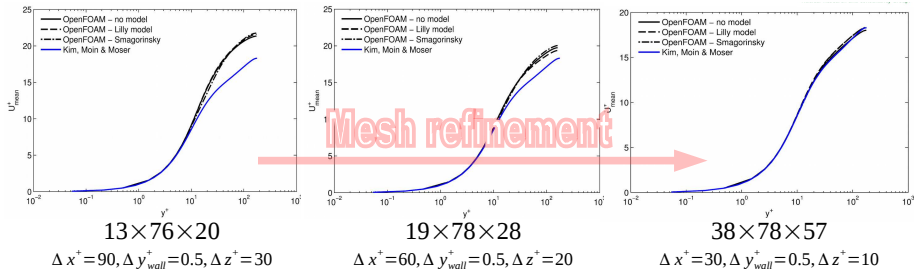


Main common characteristics of LES in such codes:

- **Unstructured finite volume** method, **collocated** grid
- Second-order spatial and temporal discretisation
- Eddy-viscosity type LES models

Motivation

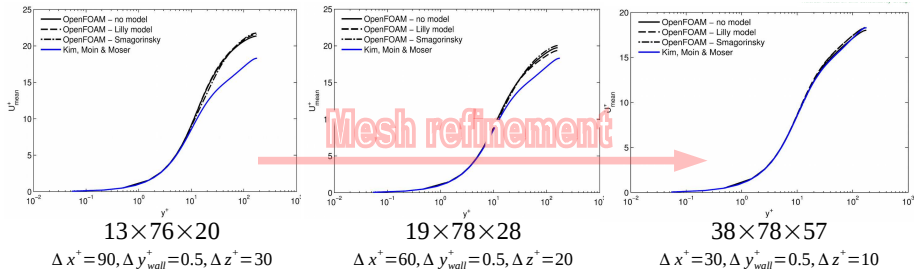
OpenFOAM® LES⁵ results of a turbulent channel for at $Re_\tau = 180$



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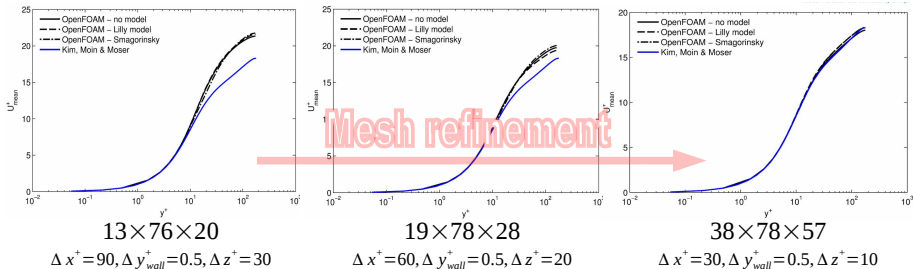


- Are LES results are merit of the SGS model?

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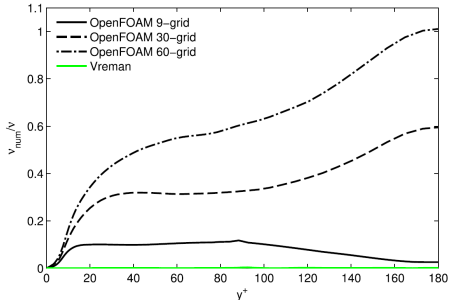
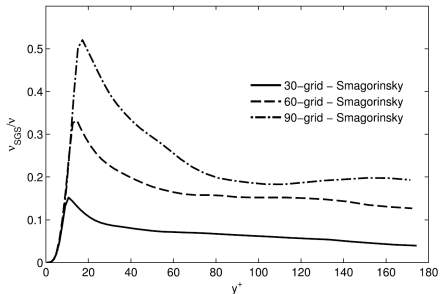


- Are LES results are merit of the SGS model? Apparently **NOT!!!** ❌

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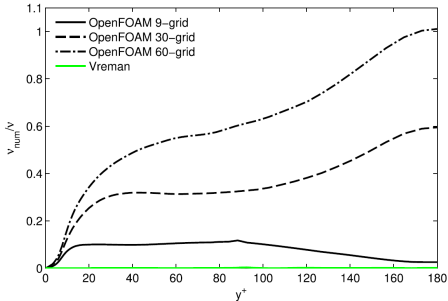
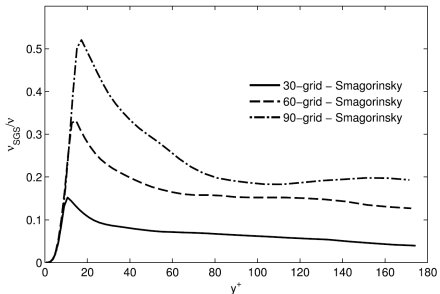


$$\nu_{num} \neq 0$$

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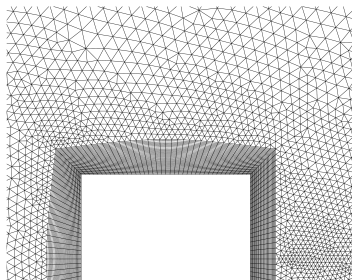
$$\nu_{SGS} < \nu_{num} \neq 0$$

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Symmetry-preserving discretization

Continuous

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{C}(\mathbf{u}, \mathbf{u}) = \nu \nabla^2 \mathbf{u} - \nabla p$$

$$\nabla \cdot \mathbf{u} = 0$$

Symmetry-preserving discretization

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Discrete

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Why collocated arrangements are so popular?

- STAR-CCM+



SIEMENS



- ANSYS-FLUENT



- Code-Saturne



- OpenFOAM

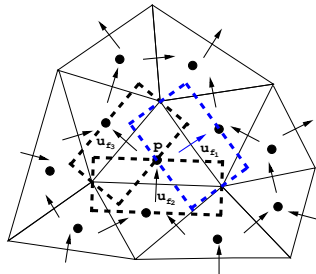
OpenFOAM®



$$\Omega_s \frac{d\mathbf{u}_s}{dt} + \mathbf{C}(\mathbf{u}_s) \mathbf{u}_s = \mathbf{D} \mathbf{u}_s - \mathbf{G} p_c; \quad \mathbf{M} \mathbf{u}_s = \mathbf{0}_c$$

In staggered meshes

- p - \mathbf{u}_s coupling is naturally solved ✓
- $\mathbf{C}(\mathbf{u}_s)$ and \mathbf{D} difficult to discretize ✗



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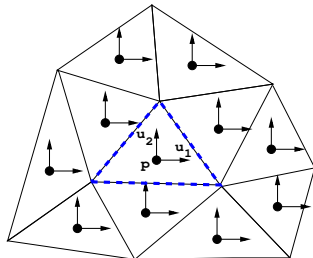
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In collocated meshes

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- Cheaper, less memory, ... **✓**



Why collocated arrangements are so popular?

Everything is easy except the pressure-velocity coupling...

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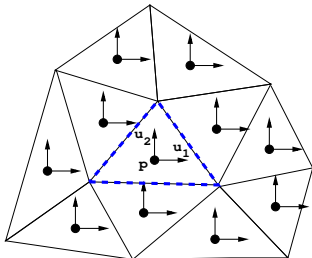
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Pressure-velocity coupling on collocated grids

A vicious circle that cannot be broken...

In summary⁷:

- Mass: $M\Gamma_{c \rightarrow s} \mathbf{u}_c = M\Gamma_{c \rightarrow s} \mathbf{u}_c - L_c L_c^{-1} M\Gamma_{c \rightarrow s} \mathbf{u}_c \approx \mathbf{0}_c \quad \mathbf{X}$
- Energy: $\mathbf{p}_c (L - L_c) \mathbf{p}_c \neq 0 \quad \mathbf{X}$

⁷F.X.Trias, O.Lehmkuhl, A.Oliva, C.D.Pérez-Segarra, R.W.C.P.Verstappen.
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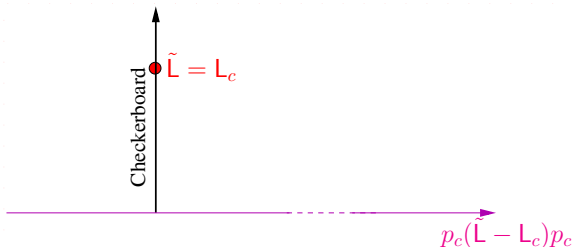
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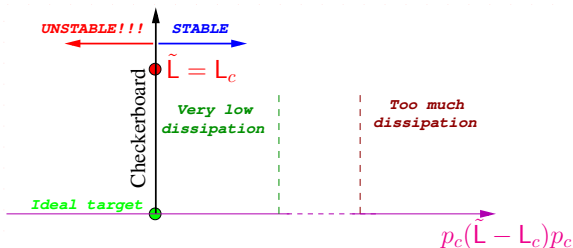
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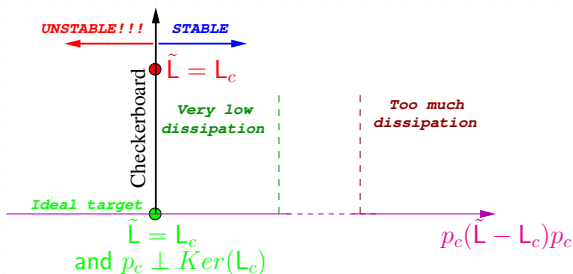
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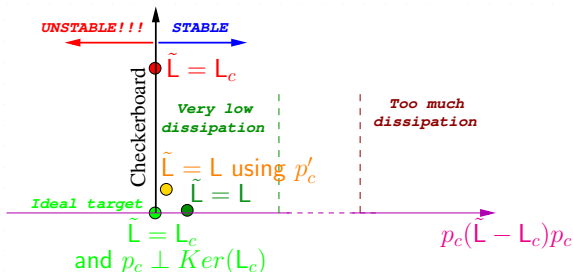
⁷Shashank, J.Larsson, G.laccarino. A co-located incompressible Navier-Stokes solver with exact mass, momentum and kinetic energy conservation in the inviscid limit, *Journal of Computational Physics*, 229: 4425-4430,2010.

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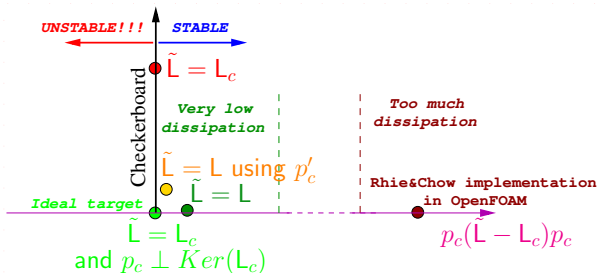
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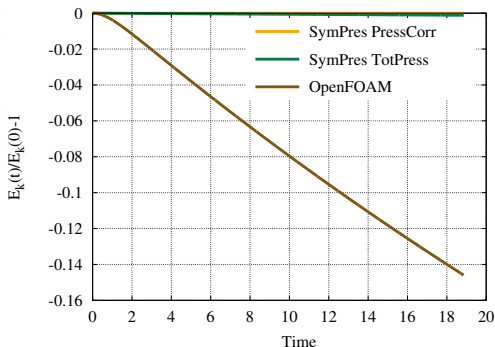
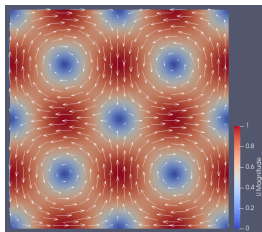
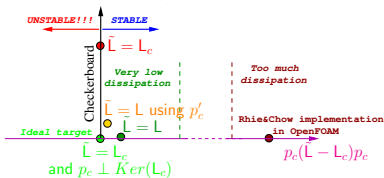
- Mass: $M\Gamma_{c \rightarrow s} u_c = M\Gamma_{c \rightarrow s} u_c - L_c L^{-1} M\Gamma_{c \rightarrow s} u_c \approx 0_c \times$
- Energy: $p_c (L - L_c) p_c \neq 0 \times$



⁷E.Komen, J.A.Hopman, E.M.A.Frederix, F.X.Trias, R.W.C.P.Verstappen. "A symmetry-preserving second-order time-accurate PISO-based method". **Computers & Fluids**, 225:104979, 2021.

Pressure-velocity coupling on collocated grids

A vicious circle that ~~cannot be broken~~ can almost be broken...

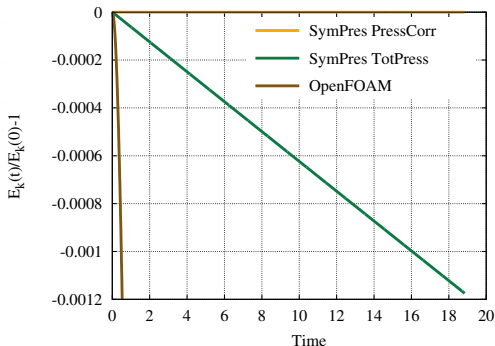
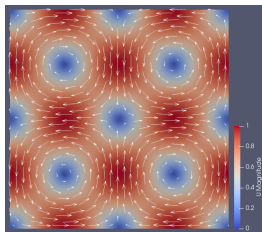
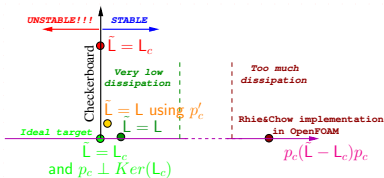


Results for an inviscid Taylor-Green vortex⁸

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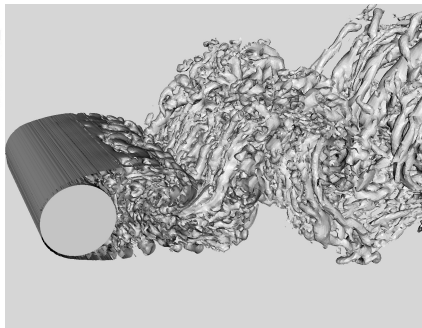
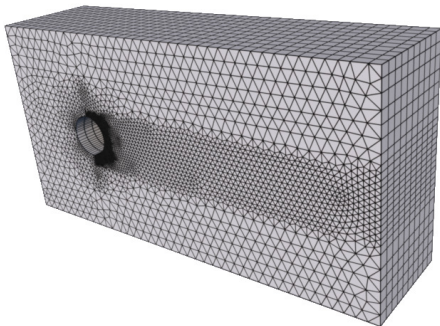
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Pressure-velocity coupling on collocated grids

Examples of simulations

Despite these inherent limitations, symmetry-preserving collocated formulation has been successfully used for DNS/LES simulations⁹:

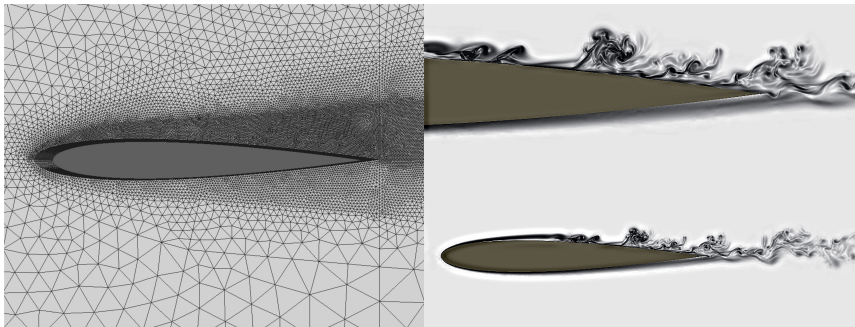


⁹R.Borrell, O.Lehmkuhl, F.X.Trias, A.Oliva. *Parallel Direct Poisson solver for discretizations with one Fourier diagonalizable direction*. **Journal of Computational Physics**, 230:4723-4741, 2011.

Pressure-velocity coupling on collocated grids

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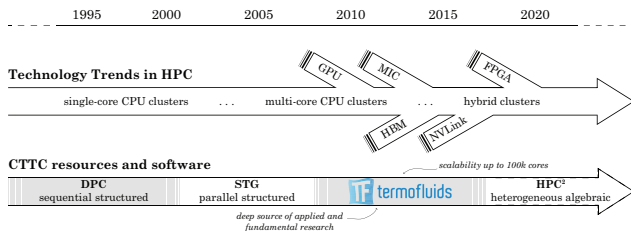


⁹F.X.Trias and O.Lehmkuhl. *A self-adaptive strategy for the time-integration of Navier-Stokes equations*. **Numerical Heat Transfer, part B**, 60(2):116-134, 2011.

Algebra-based approach naturally leads to portability

Research question #2:

- How can we develop **portable** and **efficient** CFD codes for large-scale simulations on modern supercomputers?



HPC²: portable, algebra-based framework for heterogeneous computing is being developed. Traditional stencil-based data and sweeps are replaced by algebraic structures (sparse matrices and vectors) and kernels. SpMM-based strategies to increase the arithmetic intensity are presented.

Algebra-based approach naturally leads to portability, to simple and analyzable formulations

Continuous

Discrete

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{C}(\mathbf{u}, \mathbf{u}) = \nu \nabla^2 \mathbf{u} - \nabla p$$

$$\nabla \cdot \mathbf{u} = 0$$

$$\langle \mathbf{a}, \mathbf{b} \rangle = \int_{\Omega} \mathbf{a} \mathbf{b} d\Omega$$

$$\langle \mathbf{C}(\mathbf{u}, \varphi_1), \varphi_2 \rangle = - \langle \mathbf{C}(\mathbf{u}, \varphi_2), \varphi_1 \rangle$$

$$\langle \nabla \cdot \mathbf{a}, \varphi \rangle = - \langle \mathbf{a}, \nabla \varphi \rangle$$

$$\langle \nabla^2 \mathbf{a}, \mathbf{b} \rangle = \langle \mathbf{a}, \nabla^2 \mathbf{b} \rangle$$

$$\Omega \frac{d\mathbf{u}_h}{dt} + \mathbf{C}(\mathbf{u}_h) \mathbf{u}_h = \mathbf{D} \mathbf{u}_h - \mathbf{G} \mathbf{p}_h$$

$$\mathbf{M} \mathbf{u}_h = \mathbf{0}_h$$

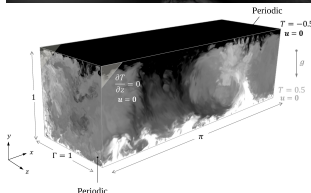
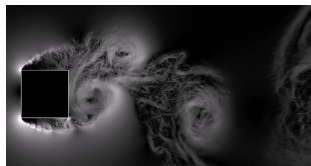
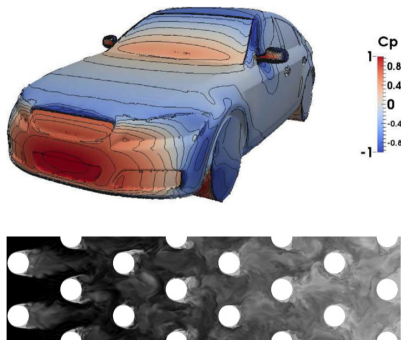
$$\langle \mathbf{a}_h, \mathbf{b}_h \rangle_h = \mathbf{a}_h^T \Omega \mathbf{b}_h$$

$$\mathbf{C}(\mathbf{u}_h) = -\mathbf{C}^T(\mathbf{u}_h)$$

$$\Omega \mathbf{G} = -\mathbf{M}^T$$

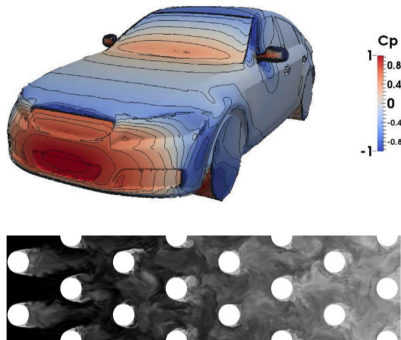
$$\mathbf{D} = \mathbf{D}^T \quad \text{def -}$$

Algebra-based approach naturally leads to portability, to simple and analyzable formulations and opens the door to new strategies¹⁰ to improve its performance...

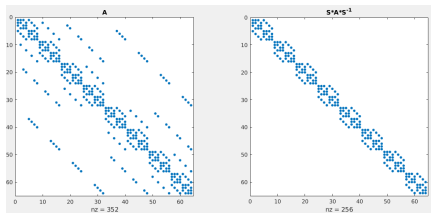


¹⁰ A. Alsalti-Baldellou, X. Álvarez-Farré, A. Oliva, F.X. Trias. *Profiting spatial symmetries on solving the Poisson equation.* *Journal of Computational Physics* (submitted)

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$$\hat{L} = SLS^{-1} = I \otimes L_{inn} + \text{diag}(\mathbf{d})$$



SpMM can be used \implies **higher AI**

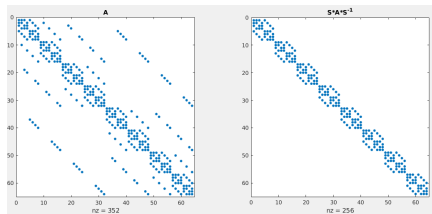
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Benefits for Poisson solver are 3-fold:

- Higher arithmetic intensity (AI)
- Reduction of memory footprint
- Reduction in the number of iterations

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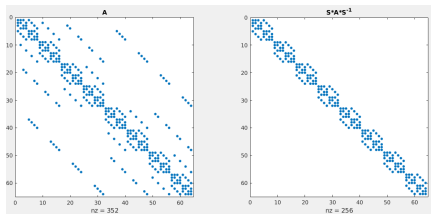
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→ Overall speed-up up to **x2-x3** ✓

→ Memory reduction of ≈ 2 ✓

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SpMM can be used \implies **higher AI**

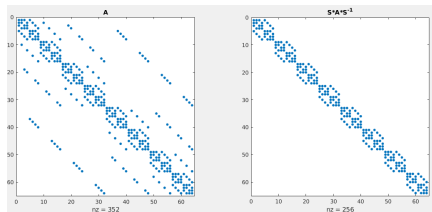
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Other SpMM-based strategies to **increase AI** and **reduce memory footprint**:

- Multiple transport equations
- Parametric studies
- Parallel-in-time simulations
- Go to higher-order?

$$\hat{L} = SLS^{-1} = I \otimes L_{inn} + \text{diag}(\mathbf{d})$$

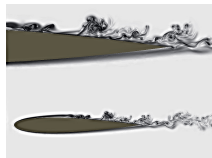


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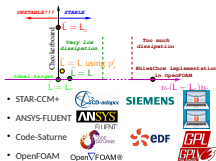
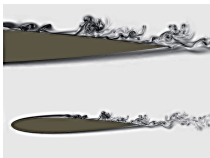
Concluding remarks

- **Preserving symmetries** either using staggered or collocated formulations is the key point for **reliable LES/DNS** simulations.



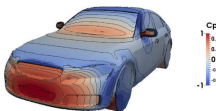
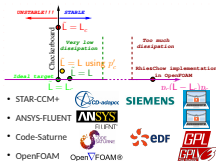
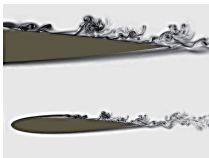
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- Main drawback of **collocated** formulations: you either have **checkerboard** or some (small) amount of **artificial dissipation** due to pressure term.



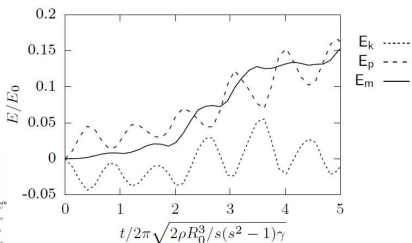
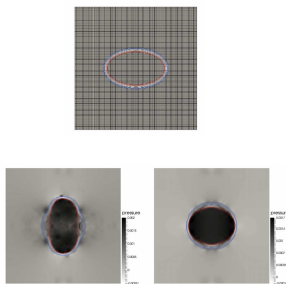
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- Main drawback of **collocated** formulations: you either have **checkerboard** or some (small) amount of **artificial dissipation** due to pressure term.
- Algebra-based approach naturally leads to **portability**, to simple and **analyzable** formulations and opens the door to **new strategies to improve its performance**.



On-going (related) research

- **Rethinking** standard CFD operations (e.g. flux limiters¹¹, CFL,...) to adapt them into an algebraic framework (Motivation: maintaining a minimal number of basic kernels is crucial for portability!!!)
- Symmetry-preserving formulations for **staggered unstructured** grids
- Symmetry-preserving formulations for **multiphase flows**¹²



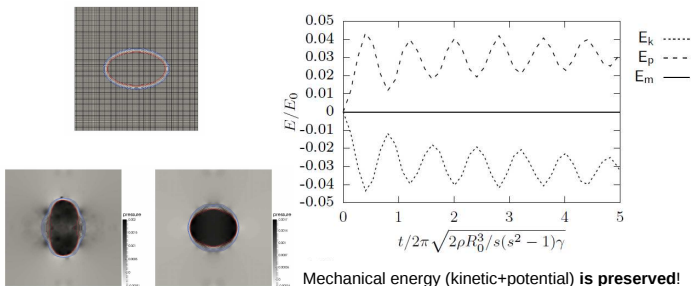
Mechanical energy (kinetic+potential) is not preserved!

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Thank you for your virtual
attendance

Open questions and ideas for roundtable discussion

- I. **Discrete conservation and turbulence modeling**
Reconciling numerics with subgrid-scale modeling, ILES, LES, DES, ...
- II. **Are we satisfied with the existing SGS models for LES?**
Do we need better models? Is eddy-viscosity/eddy-diffusivity assumption good enough?
- III. **What is (if it is) preventing LES/WMLES/Hybrid RANS-LES techniques to be routinely used in industrial applications?**
Robustness, computational cost, proper mesh generation, grey-area (or similar) issues,...
- IV. **We can preserve (kinetic) energy. What about other inviscid invariants such as enstrophy (in 2D) or helicity?**
- V. **What about time-integration methods?**
We tend to ignore their effect. Shall we use symplectic time-integration methods?
- VI. **Is it possible to preserve linear momentum in multiphase flows?**

