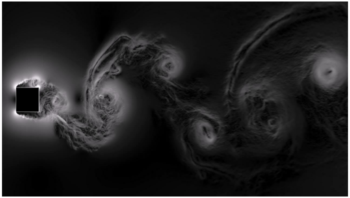
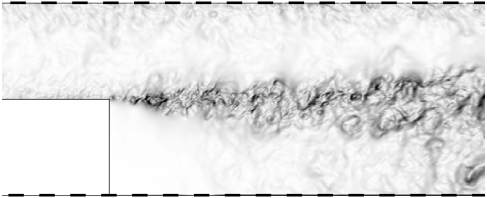
Centre Tecnològic de Transferència de Calor
UNIVERSITAT POLITÈCNICA DE CATALUNYA

Preserving symmetries on unstructured grids

F.Xavier Trias

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





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Preserving symmetries on unstructured grids: paving the way for DNS and LES on complex geometries

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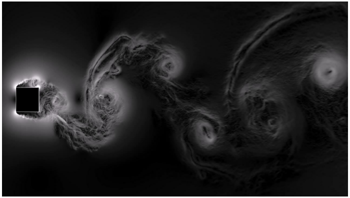

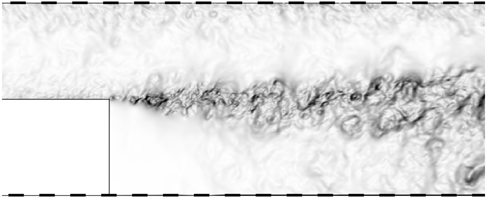

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F.Xavier Trias

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Contents

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 ;-)):

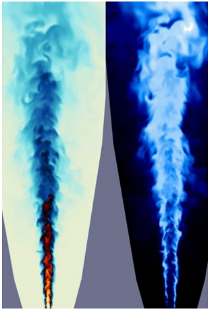
Groningen (2009?)

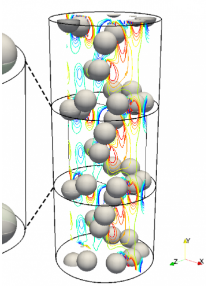
Barcelona (2019)

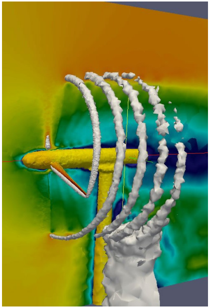
The CTTC research group

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

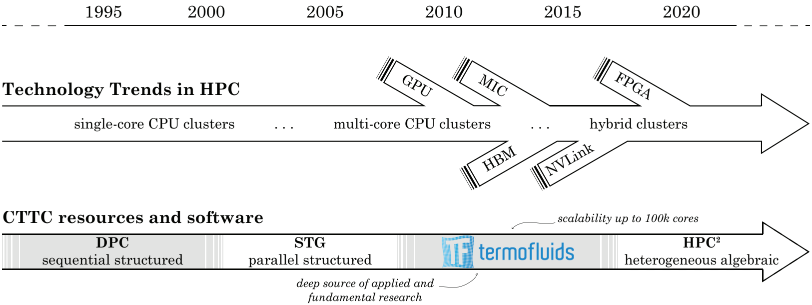
- **Fundamental research** on numerical methods, fluid dynamics and heat and mass transfer phenomena.
- **Applied research** on thermal and fluid dynamic optimization of thermal system and equipment.

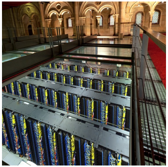


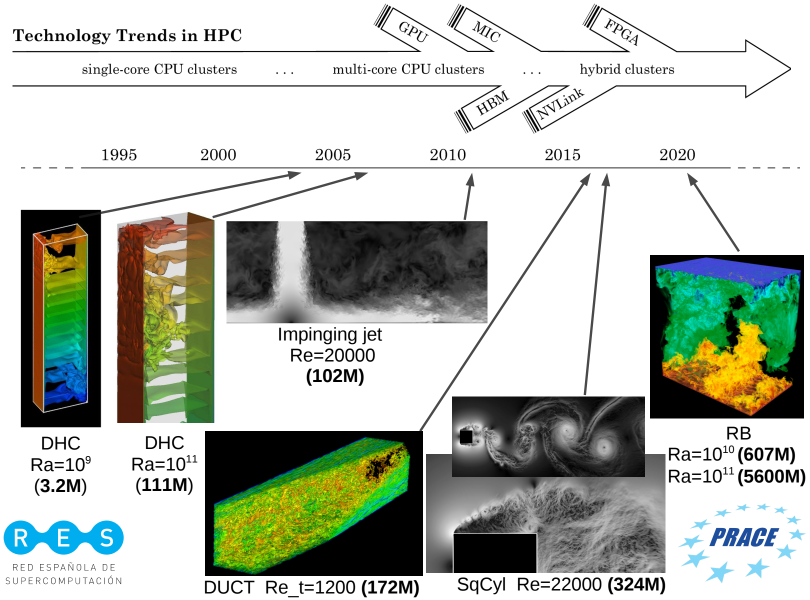




CTTC's historical background in HPC






Technology Trends in HPC
GPU
MIC
FPGA
single-core CPU clusters
. . .
multi-core CPU clusters
. . .
hybrid clusters
HBM
NVLink
1995
2000
2005
2010
2015
2020
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)
RES
RED ESPAÑOLA DE SUPERCOMPUTACIÓN
PRACE

Let's begin with some math...

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

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

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

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

Notation:

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

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)

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

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

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

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!!!

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

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

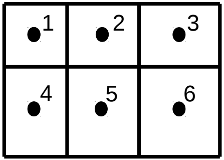
$$\langle C(\vec{u},\phi_1) | \phi_2 \rangle = -\langle C(\vec{u},\phi_2) | \phi_1 \rangle \quad \text{if} \quad \nabla \cdot \vec{u} = 0$$

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

From Calculus to Algebra (C2A)

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

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



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

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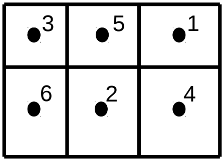

$$a_h = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \\ a_6 \end{pmatrix} \qquad \mathbf{\Omega} = \begin{pmatrix} \Omega_1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \Omega_2 & 0 & 0 & 0 & 0 \\ 0 & 0 & \Omega_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & \Omega_4 & 0 & 0 \\ 0 & 0 & 0 & 0 & \Omega_5 & 0 \\ 0 & 0 & 0 & 0 & 0 & \Omega_6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

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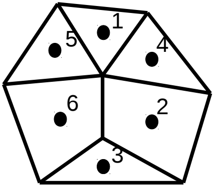

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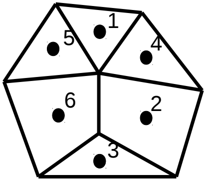
From Calculus to Algebra (C2A)

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

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

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



$$\boldsymbol{\Omega} = \begin{pmatrix} \boldsymbol{\Omega}_u & \\ & \boldsymbol{\Omega}_v \end{pmatrix}$$

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

$$\boldsymbol{\Omega}_u = \boldsymbol{\Omega}_v = \begin{pmatrix} \Omega_1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \Omega_2 & 0 & 0 & 0 & 0 \\ 0 & 0 & \Omega_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & \Omega_4 & 0 & 0 \\ 0 & 0 & 0 & 0 & \Omega_5 & 0 \\ 0 & 0 & 0 & 0 & 0 & \Omega_6 \end{pmatrix}$$

From Calculus to Algebra (C2A)

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

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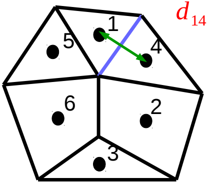


$$d_{14} = \nu A_{14} / \delta_{14}$$

$$\boldsymbol{D} = \begin{pmatrix} \boldsymbol{D}_u & \\ & \boldsymbol{D}_v \end{pmatrix}$$

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

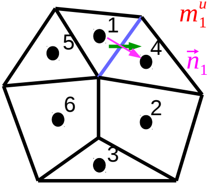
$$\boldsymbol{D}_u = \boldsymbol{D}_v = \begin{pmatrix} d_{11} & 0 & 0 & d_{14} & d_{15} & 0 \\ 0 & d_{22} & d_{23} & d_{24} & 0 & d_{26} \\ 0 & d_{23} & d_{33} & 0 & 0 & d_{36} \\ d_{14} & d_{24} & 0 & d_{44} & 0 & 0 \\ d_{15} & 0 & 0 & 0 & d_{55} & d_{56} \\ 0 & d_{26} & d_{36} & 0 & d_{56} & d_{66}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

From Calculus to Algebra (C2A)

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

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

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



$$m^u_{14} = A_{14} n^x_{14}/2$$

$$\vec{n}_{14} = \begin{pmatrix} n^x_{14} & n^y_{14} \end{pmatrix}$$

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

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

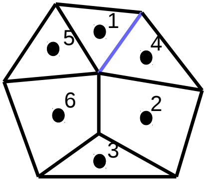
$$\mathbf{M}^u = \begin{pmatrix} 0 & 0 & 0 & m^u_{14} & m^u_{15} & 0 \\ 0 & 0 & m^u_{23} & m^u_{24} & 0 & m^u_{26} \\ 0 & -m^u_{23} & 0 & 0 & 0 & m^u_{36} \\ -m^u_{14} & -m^u_{24} & 0 & 0 & 0 & 0 \\ -m^u_{15} & 0 & 0 & 0 & 0 & m^u_{56} \\ 0 & -m^u_{26} & -m^u_{36} & 0 & -m^u_{56} & 0 \end{pmatrix}$$

From Calculus to Algebra (C2A)

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

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

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



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

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

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

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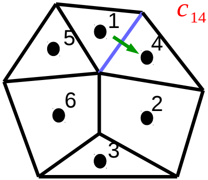
$$\frac{\partial \vec{u}}{\partial t} + (\vec{u}\cdot\nabla)\vec{u} = \nu\nabla^2\vec{u} - \nabla p \qquad \nabla\cdot\vec{u} = 0$$

$$\mathbf{\Omega}\frac{d u_h}{d t} + \mathbf{C}(u_h)u_h = \mathbf{D}u_h - \mathbf{\Omega}\mathbf{G}p_h \qquad \mathbf{M}u_h = 0_h \qquad p_h(t) = \begin{pmatrix} p_1 \\ p_2 \\ p_3 \\ p_4 \\ p_5 \\ p_6 \end{pmatrix} \qquad u_h(t) = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \\ v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \\ v_6 \end{pmatrix}$$



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

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

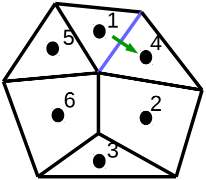
$$\mathbf{T} = \begin{pmatrix} \times & 0 & 0 & \times & \times & 0 \\ 0 & \times & \times & \times & 0 & \times \\ 0 & \times & \times & 0 & 0 & \times \\ \times & \times & 0 & \times & 0 & 0 \\ \times & 0 & 0 & 0 & \times & \times \\ 0 & \times & \times & 0 & \times & \times \end{pmatrix}$$

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

Algebraic operators

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

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



$$\boldsymbol{\Omega} = \begin{pmatrix} \boldsymbol{\Omega}_u & \\ & \boldsymbol{\Omega}_v \end{pmatrix}$$

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

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$$\boldsymbol{C} = \begin{pmatrix} \boldsymbol{C}_u & \\ & \boldsymbol{C}_v \end{pmatrix} \qquad \boldsymbol{D} = \begin{pmatrix} \boldsymbol{D}_u & \\ & \boldsymbol{D}_v \end{pmatrix}$$

Algebraic operators

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

$$\boldsymbol{\Omega}\frac{d u_h}{d t} + \boldsymbol{C}(u_h)u_h = \boldsymbol{D}u_h - \boldsymbol{\Omega}\boldsymbol{G}p_h \qquad \boldsymbol{M}u_h = 0_h \qquad \langle a_h|b_h\rangle := a_h^T\boldsymbol{\Omega}b_h$$

Let's consider the time evolution of $1/2\langle u_h|u_h\rangle$...

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

$$= u_h^T\boldsymbol{D}u_h \leq 0$$

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

REMAINDER!!!

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

Numerical stability!!!

Algebraic operators

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

$$=u_h^T\boldsymbol{D}u_h\leq 0\ ,\quad \text{if}\ \boldsymbol{M}u_h=0_h,\ \forall u_h,p_h$$

$u_h^T\boldsymbol{C}(u_h)u_h=0$	$\longrightarrow$	$\boldsymbol{C}(u_h)=-\boldsymbol{C}^T(u_h)$
$u_h^T\boldsymbol{\Omega}\boldsymbol{G}p_h=0$	$\longrightarrow$	$\boldsymbol{\Omega}\boldsymbol{G}=-\boldsymbol{M}^T$
$u_h^T\boldsymbol{D}u_h\leq 0$	$\longrightarrow$	$\boldsymbol{D}=\boldsymbol{D}^T$ def-

REMAINDER!!!

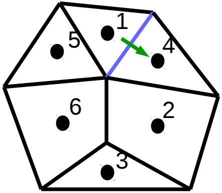
$$\frac{1}{2}\frac{d\langle\vec{u}|\vec{u}\rangle}{dt}=\langle\frac{\partial\vec{u}}{\partial t}|\vec{u}\rangle=-\langle C(\vec{u},\vec{u})|\vec{u}\rangle+\nu\langle\nabla^2\vec{u}|\vec{u}\rangle-\langle\nabla p|\vec{u}\rangle$$
$$=-\nu\langle\nabla\vec{u}|\nabla\vec{u}\rangle=-\nu\|\nabla\vec{u}\|^2\leq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

REMAINDER!!!

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

Algebraic operators

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



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

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

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

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

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

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

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

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

From Calculus to Algebra (C2A)

C2A

$$\frac{\partial \vec{u}}{\partial t} + (\vec{u}\cdot\nabla)\vec{u} = \nu \nabla^2 \vec{u} - \nabla p; \quad \nabla\cdot\vec{u} = 0 \quad \longrightarrow \quad \mathbf{\Omega}\frac{d u_h}{d t} + \mathbf{C}(u_h)u_h = \mathbf{D} u_h - \mathbf{\Omega}\mathbf{G} p_h; \quad \mathbf{M} u_h = 0_h$$

$$\langle a|b\rangle := \int_\Omega ab \, d\Omega \longrightarrow \langle a_h|b_h\rangle := a_h^T \mathbf{\Omega} b_h$$

$$\langle C(\vec{u},\phi_1)|\phi_2\rangle = -\langle C(\vec{u},\phi_2)|\phi_1\rangle \longrightarrow \mathbf{C}(u_h) = -\mathbf{C}^T(u_h)$$

$$\langle \nabla\cdot\vec{a}|\phi\rangle = -\langle \vec{a}|\nabla\phi\rangle \longrightarrow \mathbf{\Omega}\mathbf{G} = -\mathbf{M}^T$$

$$\langle \nabla^2 f|g\rangle = \langle f|\nabla^2 g\rangle \longrightarrow \mathbf{D} = \mathbf{D}^T \ \text{def-}$$

REMAINDER!!!

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

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

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

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

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

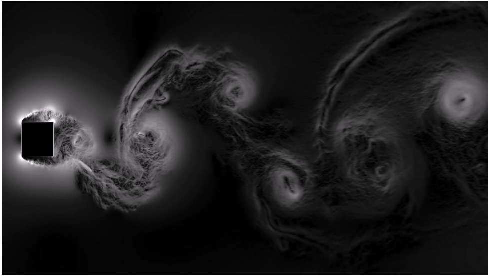
$$u_h^T \mathbf{\Omega}\mathbf{G} p_h = 0 \longrightarrow \mathbf{\Omega}\mathbf{G} = -\mathbf{M}^T$$

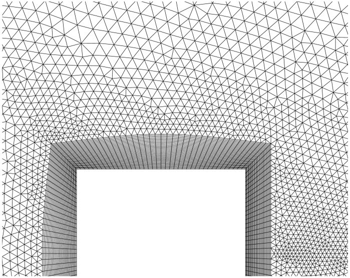
$$u_h^T \mathbf{D} u_h \le 0 \longrightarrow \mathbf{D} = \mathbf{D}^T \ \text{def-}$$

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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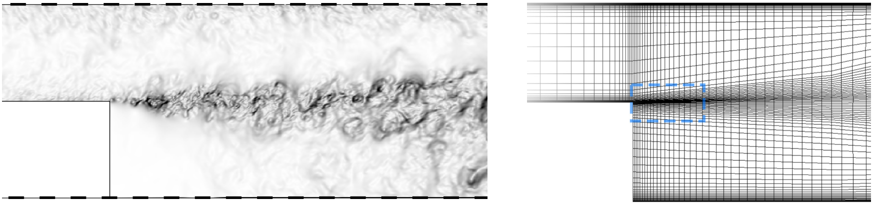


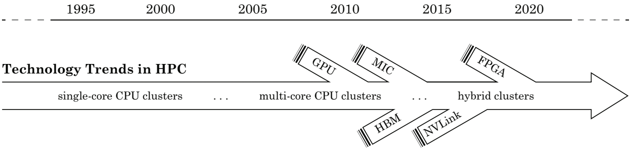
DNS[2] of backward-facing step at $Re_\tau = 395$ and expansion ratio 2

[2] A.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.

Motivation

Research question #2:

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



[3] X.Álvarez, A.Gorobets, F.X.Trias, R.Borrell, and G.Oyarzun. *HPC^2 - a fully portable algebra-dominant framework for heterogeneous computing. Application to CFD*. **Computers & Fluids**, 173:285-292, 2018

[4] X.Álvarez, A.Gorobets, F.X.Trias. *A hierarchical parallel implementation for heterogeneous computing. Application to algebra-based CFD simulations on hybrid supercomputers*. **Computers & Fluids**, 214:104768, 2021.

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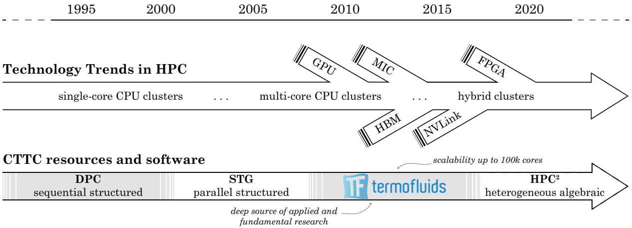

HPC²: portable, algebra-based framework[3] for heterogeneous computing is being developed[4]. Traditional stencil-based data and sweeps are replaced by algebraic structures (sparse matrices and vectors) and kernels. SpMM-based strategies to increase the arithmetic intensity are presented later...

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Motivation

Frequently used general purpose CFD codes:

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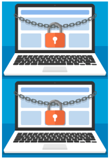


GPL

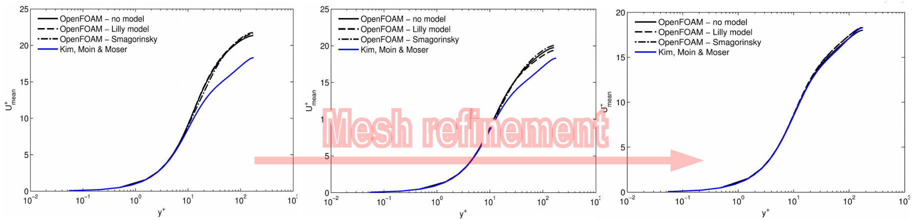
GPLv3 Free Software

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

Open∇FOAM® LES[5] results of a turbulent channel for at $Re_\tau = 180$



$13 \times 76 \times 20$ — $\Delta x^+ = 90, \Delta y^+_{wall} = 0.5, \Delta z^+ = 30$

$19 \times 78 \times 28$ — $\Delta x^+ = 60, \Delta y^+_{wall} = 0.5, \Delta z^+ = 20$

$38 \times 78 \times 57$ — $\Delta x^+ = 30, \Delta y^+_{wall} = 0.5, \Delta z^+ = 10$

[5] E.M.J.Komen, L.H.Camilo, A.Shams, B.J.Geurts, B.Koren. *A quantification method for numerical dissipation in quasi-DNS and under-resolved DNS, and effects of numerical dissipation in quasi-DNS and under-resolved DNS of turbulent channel flows*, **Journal of Computational Physics**, 345, 565-595, 2017.

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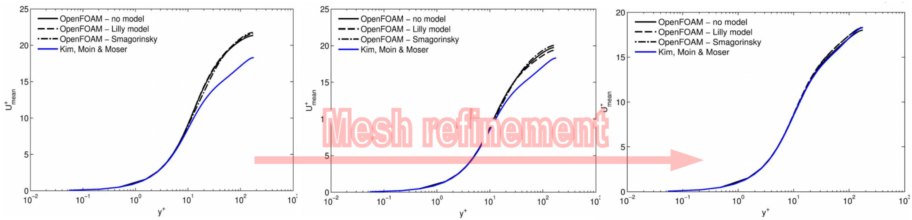

$13\times76\times20$	$19\times78\times28$	$38\times78\times57$
$\Delta x^+=90, \Delta y^+_{wall}=0.5, \Delta z^+=30$	$\Delta x^+=60, \Delta y^+_{wall}=0.5, \Delta z^+=20$	$\Delta x^+=30, \Delta y^+_{wall}=0.5, \Delta z^+=10$

- Are LES results are merit of the SGS model?

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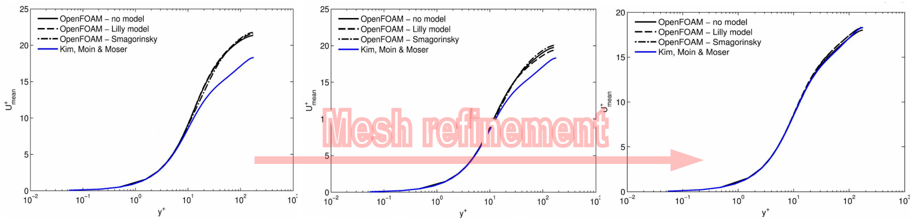

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- Are LES results are merit of the SGS model? Apparently **NOT**!!! ✗

[5] E.M.J.Komen, L.H.Camilo, A.Shams, B.J.Geurts, B.Koren. *A quantification method for numerical dissipation in quasi-DNS and under-resolved DNS, and effects of numerical dissipation in quasi-DNS and under-resolved DNS of turbulent channel flows*, **Journal of Computational Physics**, 345, 565-595, 2017.

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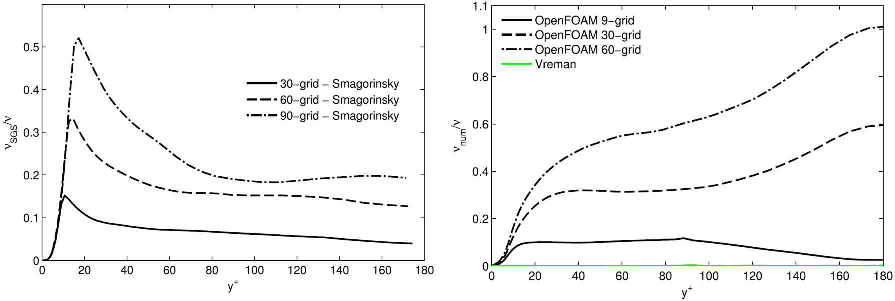

$$\nu_{num} \neq 0$$

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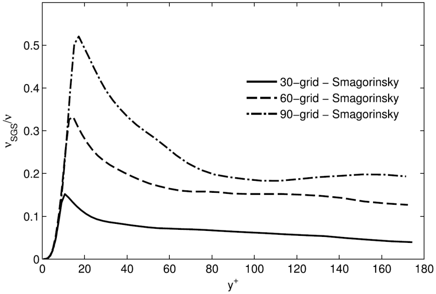

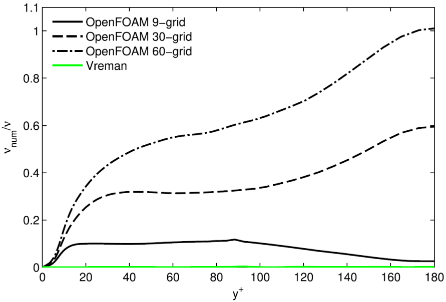

$$\nu_{SGS} < \nu_{num} \neq 0$$

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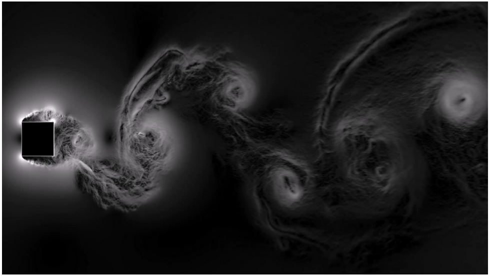

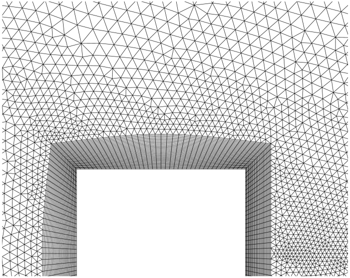

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Symmetry-preserving discretization

Continuous

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

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

Symmetry-preserving discretization

Continuous	Discrete
$\frac{\partial \boldsymbol{u}}{\partial t} + C(\boldsymbol{u}, \boldsymbol{u}) = \nu \nabla^2 \boldsymbol{u} - \nabla p$	$\Omega \frac{d \boldsymbol{u}_h}{dt} + \mathsf{C}(\boldsymbol{u}_h)\, \boldsymbol{u}_h = \mathsf{D} \boldsymbol{u}_h - \mathsf{G} \boldsymbol{p}_h$
$\nabla \cdot \boldsymbol{u} = 0$	$\mathsf{M} \boldsymbol{u}_h = \boldsymbol{0}_h$

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$\langle \boldsymbol{a}, \boldsymbol{b} \rangle = \int_\Omega \boldsymbol{a}\boldsymbol{b}\, d\Omega$	$\langle \boldsymbol{a}_h, \boldsymbol{b}_h \rangle_h = \boldsymbol{a}_h^T \Omega \boldsymbol{b}_h$

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$\langle C(\boldsymbol{u}, \varphi_1), \varphi_2 \rangle = -\langle C(\boldsymbol{u}, \varphi_2), \varphi_1 \rangle$	$\mathsf{C}(\boldsymbol{u}_h) = -\mathsf{C}^T(\boldsymbol{u}_h)$

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$\langle \nabla \cdot \boldsymbol{a}, \varphi \rangle = -\langle \boldsymbol{a}, \nabla \varphi \rangle$	$\Omega \mathsf{G} = -\mathsf{M}^T$

Symmetry-preserving discretization

Continuous	Discrete
$\frac{\partial \boldsymbol{u}}{\partial t} + C(\boldsymbol{u}, \boldsymbol{u}) = \nu \nabla^2 \boldsymbol{u} - \nabla p$	$\Omega \frac{d \boldsymbol{u}_h}{dt} + \mathsf{C}(\boldsymbol{u}_h)\, \boldsymbol{u}_h = \mathsf{D} \boldsymbol{u}_h - \mathsf{G} \boldsymbol{p}_h$
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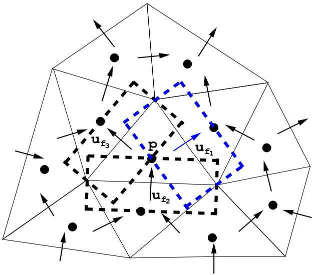
Why collocated arrangements are so popular?

- STAR-CCM+
- ANSYS-FLUENT
- Code-Saturne
- OpenFOAM

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

In staggered meshes

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



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- ANSYS-FLUENT — ANSYS FLUENT
- Code-Saturne — CODE SATURNE, eDF, GPL
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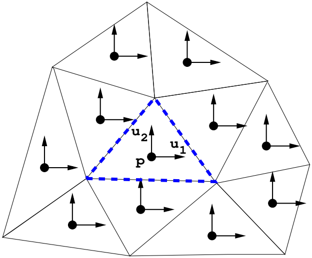
$$\Omega_c \frac{d\boldsymbol{u}_c}{dt} + \mathsf{C}\left(\boldsymbol{u}_s\right)\boldsymbol{u}_c = \mathsf{D}\boldsymbol{u}_c - \mathsf{G}_c\boldsymbol{p}_c; \quad \mathsf{M}_c\boldsymbol{u}_c = \mathbf{0}_c$$

In <u>collocated meshes</u>

- p-$\boldsymbol{u}_c$ coupling is cumbersome ✗
- $\mathsf{C}\left(\boldsymbol{u}_s\right)$ and D easy to discretize ✓
- Cheaper, less memory,... ✓



Why collocated arrangements are so popular?

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

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- OpenFOAM

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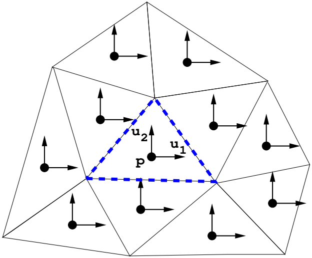

Pressure-velocity coupling on collocated grids

A vicious circle that cannot be broken...

In summary[7]:

- Mass: $\mathsf{M}\Gamma_{c\rightarrow s}\boldsymbol{u}_c = \mathsf{M}\Gamma_{c\rightarrow s}\boldsymbol{u}_c - \mathsf{L}_c\mathsf{L}^{-1}\mathsf{M}\Gamma_{c\rightarrow s}\boldsymbol{u}_c \approx \mathbf{0}_c$ ✗
- Energy: $\boldsymbol{p}_c\left(\mathsf{L} - \mathsf{L}_c\right)\boldsymbol{p}_c \neq 0$ ✗

[7] F.X.Trias, O.Lehmkuhl, A.Oliva, C.D.Pérez-Segarra, R.W.C.P.Verstappen. *Symmetry-preserving discretization of Navier-Stokes equations on collocated unstructured grids*, **Journal of Computational Physics**, 258 (1): 246-267, 2014.

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- Energy: $\boldsymbol{p}_c \boxed{(L - L_c)} \boldsymbol{p}_c \neq 0$ ✗

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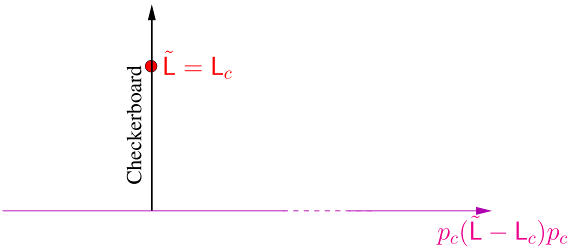

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Pressure-velocity coupling on collocated grids

A vicious circle that cannot be broken...

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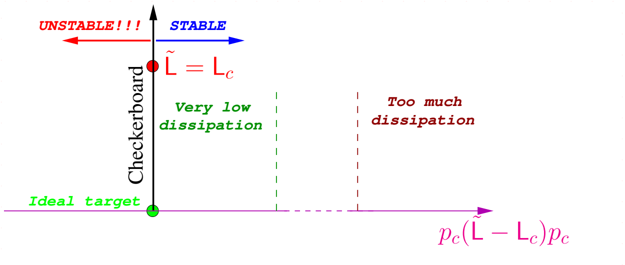

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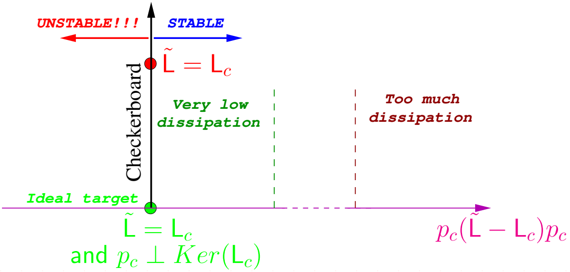

[7] Shashank, J.Larsson, G.Iaccarino. *A co-located incompressible Navier-Stokes solver with exact mass, momentum and kinetic energy conservation in the inviscid limit*, **Journal of Computational Physics**, 229: 4425-4430,2010.

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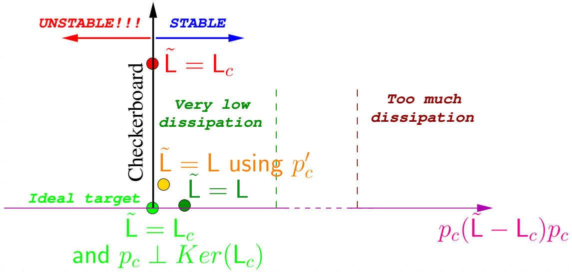

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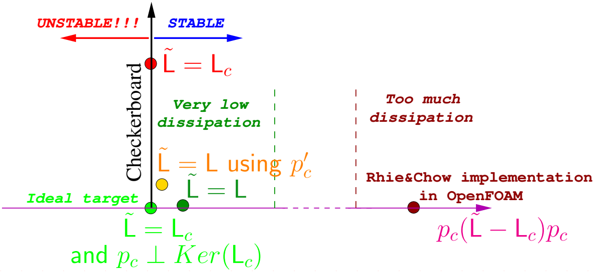

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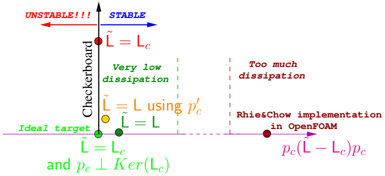

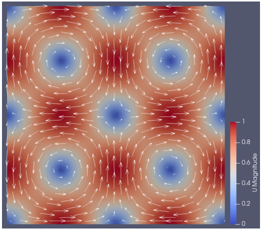

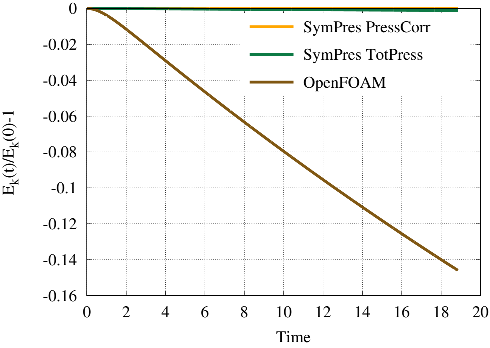

Results for an inviscid Taylor-Green vortex[8]

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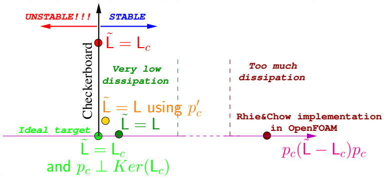

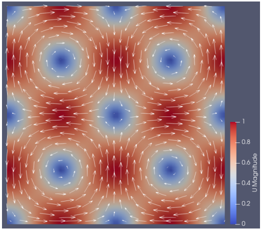

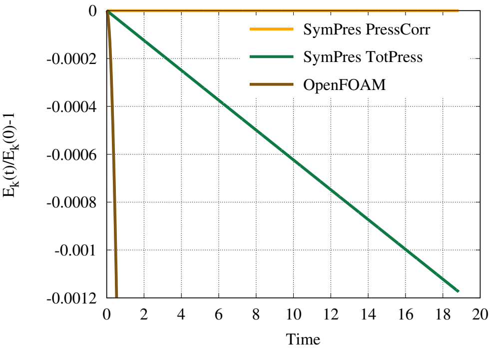

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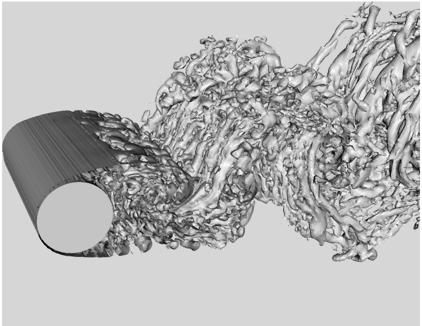
Pressure-velocity coupling on collocated grids

Examples of simulations

Despite these inherent limitations, symmetry-preserving collocated formulation has been successfully used for DNS/LES simulations[9]:



[9] R.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.

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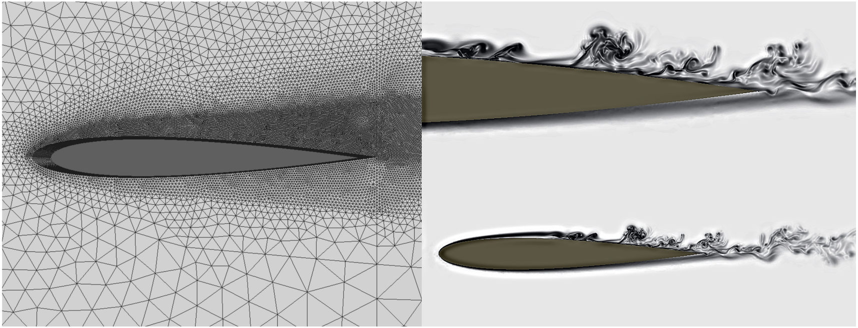
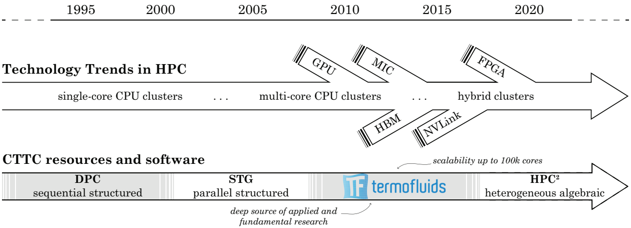


[9] F.X.Trias and O.Lehmkuhl. *A self-adaptive strategy for the time-integration of Navier-Stokes equations.* **Numerical Heat Transfer, part B**, 60(2):116-134, 2011.

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?

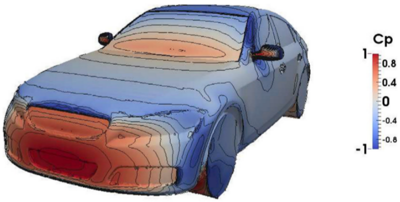


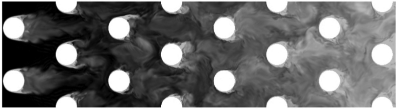
HPC^2: portable, algebra-based framework for heterogeneous computing is being developed. Traditional stencil-based data and sweeps are replaced by algebraic structures (sparse matrices and vectors) and kernels. SpMM-based strategies to increase the arithmetic intensity are presented.

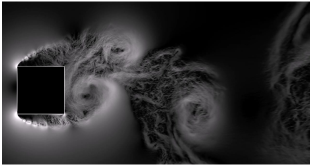
Algebra-based approach naturally leads to portability, to simple and analyzable formulations

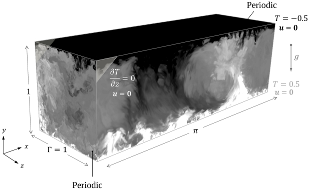
Continuous	Discrete
$\frac{\partial \boldsymbol{u}}{\partial t} + C(\boldsymbol{u}, \boldsymbol{u}) = \nu \nabla^2 \boldsymbol{u} - \nabla p$	$\Omega \frac{d \boldsymbol{u}_h}{dt} + \mathsf{C}(\boldsymbol{u}_h) \boldsymbol{u}_h = \mathsf{D} \boldsymbol{u}_h - \mathsf{G} \boldsymbol{p}_h$
$\nabla \cdot \boldsymbol{u} = 0$	$\mathsf{M} \boldsymbol{u}_h = \boldsymbol{0}_h$
$\langle \boldsymbol{a}, \boldsymbol{b} \rangle = \int_\Omega \boldsymbol{a} \boldsymbol{b} d\Omega$	$\langle \boldsymbol{a}_h, \boldsymbol{b}_h \rangle_h = \boldsymbol{a}_h^T \Omega \boldsymbol{b}_h$
$\langle C(\boldsymbol{u}, \varphi_1), \varphi_2 \rangle = -\langle C(\boldsymbol{u}, \varphi_2), \varphi_1 \rangle$	$\mathsf{C}(\boldsymbol{u}_h) = -\mathsf{C}^T(\boldsymbol{u}_h)$
$\langle \nabla \cdot \boldsymbol{a}, \varphi \rangle = -\langle \boldsymbol{a}, \nabla \varphi \rangle$	$\Omega \mathsf{G} = -\mathsf{M}^T$
$\left\langle \nabla^2 \boldsymbol{a}, \boldsymbol{b} \right\rangle = \left\langle \boldsymbol{a}, \nabla^2 \boldsymbol{b} \right\rangle$	$\mathsf{D} = \mathsf{D}^T \quad def -$

Algebra-based approach naturally leads to portability, to simple and analyzable formulations and opens the door to new strategies[10] to improve its perfomance...









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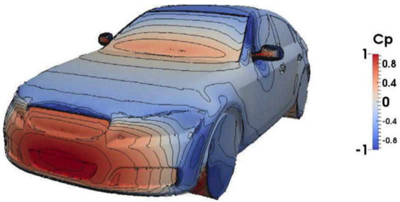
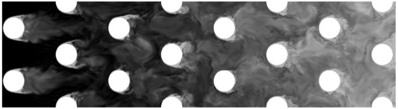
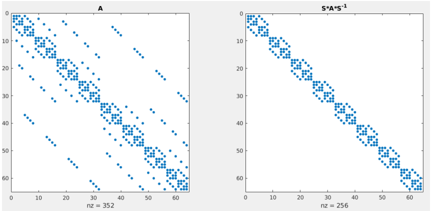




$$\hat{L} = SLS^{-1} = I \otimes L_{inn} + diag(\boldsymbol{d})$$



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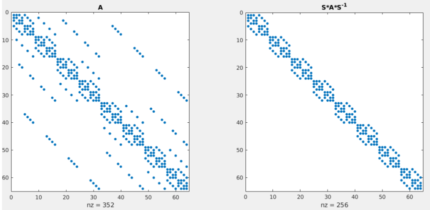

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→ Overall speed-up up to **x2-x3** ✓
→ Memory reduction of ≈**2** ✓

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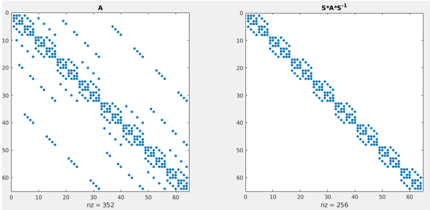

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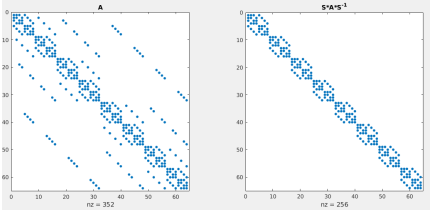
Other SpMM-based strategies to **increase AI** and **reduce memory** footprint:

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

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



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Concluding remarks

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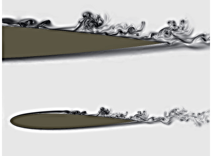

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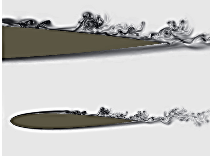

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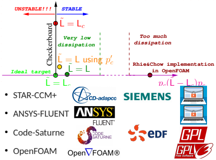

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- Main drawback of **collocated** formulations: you either have **checkerboard** or some (small) amount of **artificial dissipation** due to pressure term.
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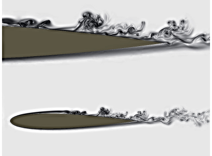
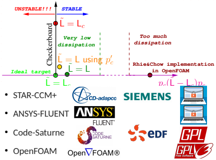
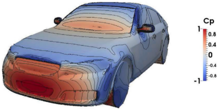
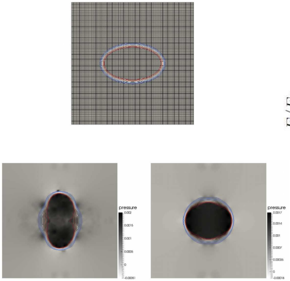


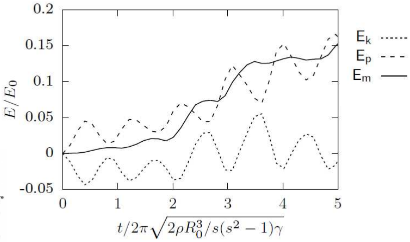




On-going (related) research

- **Rethinking** standard CFD operations (*e.g.* flux limiters[11], 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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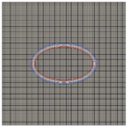

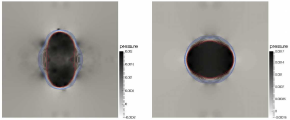

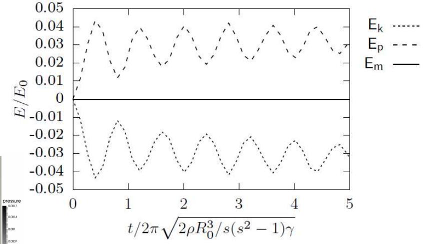

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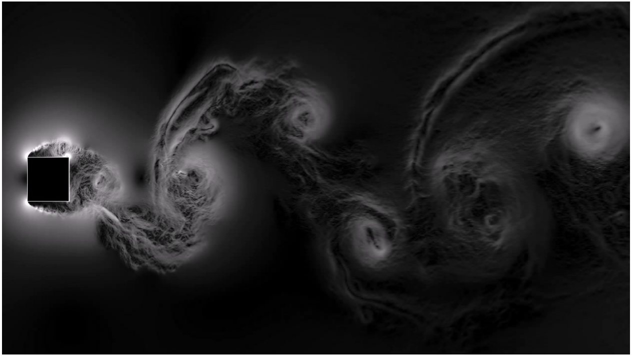
Thank you for your virtual attendance



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?**