Paving the way for DNS and LES on unstructured grids

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Paving the (right?) way for DNS and LES on unstructured grids

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Paving the (right?) way for DNS and LES on unstructured grids: fully conservative collocated/staggered discretizations

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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?

DNS\(^1\) of the turbulent flow around a square cylinder at \(Re = 22000\)

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?

DNS$^2$ of backward-facing step at $Re_τ = 395$ and expansion ratio 2

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Motivation

Research question #2:

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

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5. X. Álvarez, A. Gorobets, F. X. Trias, A. Oliva. NUMA-aware strategies for the efficient execution of CFD simulations on CPU supercomputers *ParCFD2021*. Don’t miss it!
Motivation

**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$^3$ for heterogeneous computing is being developed$^4$. Traditional stencil-based data and sweeps are replaced by algebraic structures (sparse matrices and vectors) and kernels. NUMA-aware execution strategies for CFD are presented in this conference$^5$.

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$^5$X.Álvarez, A.Gorobets, F.X.Trias, A.Oliva. NUMA-aware strategies for the efficient execution of CFD simulations on CPU supercomputers ParCFD2021. Don’t miss it!
Motivation

Frequently used general purpose CFD codes:

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

Frequently used general purpose CFD codes:

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

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® LES results of a turbulent channel for at $Re_T = 180$

![Graphs showing flow behavior](image)

$13 \times 76 \times 20$
\[ \Delta x^+ = 90, \Delta y_{wall}^+ = 0.5, \Delta z^+ = 30 \]

$19 \times 78 \times 28$
\[ \Delta x^+ = 60, \Delta y_{wall}^+ = 0.5, \Delta z^+ = 20 \]

$38 \times 78 \times 57$
\[ \Delta x^+ = 30, \Delta y_{wall}^+ = 0.5, \Delta z^+ = 10 \]

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OpenFOAM® LES results of a turbulent channel flow for at $Re_T = 180$

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

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**Motivation**

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

\[ \nu_{num} \neq 0 \]

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Does all this really matter?

Effect of (artificial) numerical dissipation in real-world applications

LES results of a turbulent channel flow. Provided by Artificial numerical dissipation, \( \nu_{\text{num}} \), is bigger than the dissipation of the subgrid scale (SGS) model, \( \nu_{\text{SGS}} \):

\[
\nu_{\text{SGS}} < \nu_{\text{num}} \neq 0
\]

---

Symmetry-preserving discretization

Continuous

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

\[ \nabla \cdot u = 0 \]
Symmetry-preserving discretization

Continuous
\[
\frac{\partial u}{\partial t} + C(u, u) = \nu \nabla^2 u - \nabla p \\
\nabla \cdot u = 0
\]

Discrete
\[
\Omega \frac{du_h}{dt} + C(u_h) u_h = Du_h - Gp_h \\
M u_h = 0_h
\]
Symmetry-preserving discretization

**Continuous**

\[
\frac{\partial u}{\partial t} + C(u, u) = \nu \nabla^2 u - \nabla p \\
\nabla \cdot u = 0
\]

\[
\langle a, b \rangle = \int_{\Omega} ab d\Omega
\]

**Discrete**

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

\[
\langle a_h, b_h \rangle_h = a_h^T \Omega b_h
\]
Symmetry-preserving discretization

**Continuous**

\[
\frac{\partial u}{\partial t} + C(u, u) = \nu \nabla^2 u - \nabla p \\
\nabla \cdot u = 0
\]

\[\langle a, b \rangle = \int_\Omega ab \, d\Omega\]

\[\langle C(u, \varphi_1), \varphi_2 \rangle = -\langle C(u, \varphi_2), \varphi_1 \rangle\]

**Discrete**

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

\[\langle a_h, b_h \rangle_h = a_h^T \Omega b_h\]

\[C(u_h) = -C^T(u_h)\]
Symmetry-preserving discretization

**Continuous**

\[
\frac{\partial u}{\partial t} + C(u, u) = \nu \nabla^2 u - \nabla p \\
\nabla \cdot u = 0
\]

\[\langle a, b \rangle = \int_{\Omega} ab \, d\Omega\]

\[\langle C(u, \varphi_1), \varphi_2 \rangle = -\langle C(u, \varphi_2), \varphi_1 \rangle\]

\[\langle \nabla \cdot a, \varphi \rangle = -\langle a, \nabla \varphi \rangle\]

**Discrete**

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

\[\langle a_h, b_h \rangle_h = a_h^T \Omega b_h\]

\[C(u_h) = -C^T(u_h)\]

\[\Omega G = -M^T\]
Symmetry-preserving discretization

### Continuous

\[
\frac{\partial u}{\partial t} + C(u, u) = \nu \nabla^2 u - \nabla p \\
\nabla \cdot u = 0
\]

\[
\langle a, b \rangle = \int_\Omega ab d\Omega
\]

\[
\langle C(u, \varphi_1), \varphi_2 \rangle = -\langle C(u, \varphi_2), \varphi_1 \rangle \\
\langle \nabla \cdot a, \varphi \rangle = -\langle a, \nabla \varphi \rangle \\
\langle \nabla^2 a, b \rangle = \langle a, \nabla^2 b \rangle
\]

### Discrete

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

\[
\langle a_h, b_h \rangle_h = a_h^T \Omega b_h
\]

\[
C(u_h) = -C^T(u_h) \\
\Omega G = -M^T \\
D = D^T \quad \text{def}
\]
Collocated vs staggered
Collocated vs staggered
Collocated vs staggered

Collocated
Collocated vs staggered
Collocated vs staggered
Collocated vs staggered
Why staggered?

\[ \Omega_s \frac{d\mathbf{u}_s}{dt} + \mathbf{C}(\mathbf{u}_s) \mathbf{u}_s = \mathbf{D}\mathbf{u}_s - \mathbf{G}\rho_c; \quad \mathbf{M}\mathbf{u}_s = \mathbf{0}_c \]
Why staggered?

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

Let’s consider we have \( \mathbf{u}_s \) such as

\[
\mathbf{M}\mathbf{u}_s \neq 0_c
\]
Why staggered?

Let’s consider we have \( \mathbf{u}_s \) such as

\[
M \mathbf{u}_s \neq 0_c
\]

then, we can easily project \( \mathbf{u}_s \)

\[
\mathbf{u}_s = \mathbf{u}_s - G \rho_c
\]
Why staggered?

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

Let’s consider we have \(\mathbf{u}_s\) such as

\[
\mathbf{M}\mathbf{u}_s \neq \mathbf{0}_c
\]

then, we can easily project \(\mathbf{u}_s\)

\[
\mathbf{M}\mathbf{u}_s = \mathbf{M}(\mathbf{u}_s - \mathbf{G}\mathbf{p}_c) = \mathbf{0}_c
\]
Why staggered?

\[
\Omega_s \frac{du_s}{dt} + C(u_s)u_s = Du_s - Gp_c; \quad Mu_s = 0_c
\]

Let’s consider we have \(u_s\) such as

\[Mu_s \neq 0_c\]

then, we can easily project \(u_s\)

\[Mu_s = M(u_s - Gp_c) = 0_c\]

Finally, this leads to a Poisson eq.

\[MGp_c = Mu_s\]
Motivation
Preserving symmetries: collocated vs staggered

Why staggered?

Let’s consider we have \( u_s \) such as

\[
M u_s \neq 0_c
\]

then, we can easily project \( u_s \)

\[
M u_s = M(u_s - Gp_c) = 0_c
\]

Finally, this leads to a Poisson eq.

\[
MGp_c = Mu_s
\]

If \( \Omega_s G = -M^T \)

\[
\langle \nabla \cdot a, \varphi \rangle = -\langle a, \nabla \varphi \rangle
\]
**Why staggered? Everything seems to be in the right place!**

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

Let’s consider we have \( \mathbf{u}_s \) such as

\[
\mathbf{M}\mathbf{u}_s \neq \mathbf{0}_c
\]

then, we can easily project \( \mathbf{u}_s \)

\[
\mathbf{M}\mathbf{u}_s = \mathbf{M}(\mathbf{u}_s - \mathbf{G}\mathbf{p}_c) = \mathbf{0}_c
\]

Finally, this leads to a Poisson eq.

\[
\mathbf{M}\mathbf{G}\mathbf{p}_c = \mathbf{M}\mathbf{u}_s
\]

If \( \Omega_s \mathbf{G} = -\mathbf{M}^T \implies \langle \mathbf{u}_s, \mathbf{G}\mathbf{p}_c \rangle_h = \langle \mathbf{u}_s, \Omega_s \mathbf{G}\mathbf{p}_c \rangle_h = -(\mathbf{M}\mathbf{u}_s)^T \mathbf{p}_c = 0
\]

\[
\langle \nabla \cdot \mathbf{a}, \mathbf{\varphi} \rangle = -\langle \mathbf{a}, \nabla \mathbf{\varphi} \rangle \implies \langle \mathbf{u}, \nabla \mathbf{p} \rangle = -\langle \nabla \cdot \mathbf{u}, \mathbf{p} \rangle = 0
\]
But is this discrete Laplacian accurate?

\[ \nabla^2 \varphi = f(x, y) \quad \text{with} \quad f(x, y) = \nabla^2 (k^{-2} \sin(kx) \sin(ky)) \quad \text{and} \quad k = 25\pi \]
But is this discrete Laplacian accurate?

Without stretching

With stretching

\[ \nabla^2 \varphi = f(x, y) \quad \text{with} \quad f(x, y) = \nabla^2 (k^{-2} \sin(kx) \sin(ky)) \quad \text{and} \quad k = 25\pi \]
But is this discrete Laplacian accurate?
Yes, even for distorted unstructured meshes! And symmetries are preserved!

\[ \nabla^2 \varphi = f(x, y) \quad \text{with} \quad f(x, y) = \nabla^2(k^{-2} \sin(kx) \sin(ky)) \quad \text{and} \quad k = 25\pi \]
Then, why collocated arrangements are so popular?

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

\[ \Omega_s \frac{du_s}{dt} + C(u_s) u_s = Du_s - Gp_c; \quad Mu_s = 0_c \]

In staggered meshes
- \( p-u_s \) coupling is naturally solved \( \checkmark \)
- \( C(u_s) \) and \( D \) difficult to discretize \( \times \)
Then, why collocated arrangements are so popular?

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

\[ \Omega_c \frac{du_c}{dt} + C\left(u_s\right) u_c = Du_c - G_c p_c; \quad M_c u_c = 0_c \]

In collocated meshes

- \( p-u_c \) coupling is cumbersome \( \times \)
- \( C\left(u_s\right) \) and \( D \) easy to discretize \( \checkmark \)
- Cheaper, less memory,... \( \checkmark \)
Then, why collocated arrangements are so popular?

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

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

In collocated meshes
- $p-u_c$ coupling is cumbersome $\times$
- $C(u_s)$ and $D$ easy to discretize $\checkmark$
- Cheaper, less memory, ... $\checkmark$
Pressure-velocity coupling on staggered grids

Works perfectly!
Pressure-velocity coupling on staggered grids

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Pressure-velocity coupling on staggered grids
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Pressure-velocity coupling on staggered grids

Works perfectly!

\[-\Omega_{s}^{-1} p_{s} - GL^{-1} M u_{s} \]

\[M u_{s} \neq 0_{c}\]
Pressure-velocity coupling on staggered grids

Works perfectly!

\[ \mathbf{u}_s = \mathbf{u}_s - \mathbf{G} L^{-1} \mathbf{M} \mathbf{u}_s \]
Pressure-velocity coupling on staggered grids

Works perfectly!

\[ \mathbf{u}_s = \mathbf{u}_s - \mathbf{G} \mathbf{L}^{-1} \mathbf{M} \mathbf{u}_s = (I - \Omega_s^{-1} \mathbf{P}_s) \mathbf{u}_s = \mathbf{F}_s \mathbf{u}_s \]
Pressure-velocity coupling on staggered grids

Works perfectly!

\[ \mathbf{u}_s = \mathbf{u}_s - G L^{-1} \mathbf{M} \mathbf{u}_s = \left( I - \Omega_s^{-1} P_s \right) \mathbf{u}_s = \mathbf{F}_s \mathbf{u}_s \]

\[ \mathbf{M} \mathbf{u}_s = \mathbf{M} \mathbf{u}_s - MG L^{-1} \mathbf{M} \mathbf{u}_s = \mathbf{0}_c \]
Pressure-velocity coupling on collocated grids

A vicious circle that cannot be broken...

\[ u \quad u_c \]

\[ -\Omega_s^{-1} p_s \]

\[ M \]

\[ L^{-1} \]

\[ G \]

\[ -G p_c \]

\[ u_s \quad M u_s \neq 0_c \]

\[ u_c \]

\[ M \Gamma_c \]
Pressure-velocity coupling on collocated grids
A vicious circle that cannot be broken...

\[ \Gamma_{c \rightarrow s} u_c \]
Pressure-velocity coupling on collocated grids

A vicious circle that cannot be broken...

\[ \text{GL}^{-1} \text{M} \Gamma_{c \rightarrow s} \text{u}_c \]
Pressure-velocity coupling on collocated grids
A vicious circle that cannot be broken...

\[-\Omega_s^{-1} p_s \begin{pmatrix} -G \\ \Gamma_{s \to c} \end{pmatrix} \Gamma_{c \to s} \Omega^{-1} M \Gamma_{c \to s} u_c \]
Pressure-velocity coupling on collocated grids

A vicious circle that cannot be broken...

\[ u_c = u_c - \Gamma_{s\rightarrow c} G L^{-1} M \Gamma_{c\rightarrow s} u_c \]
Pressure-velocity coupling on collocated grids

A vicious circle that cannot be broken...

\[ u_c = u_c - \Gamma_{s \rightarrow c} G L^{-1} M \Gamma_{c \rightarrow s} u_c = F_c u_c \]
Pressure-velocity coupling on collocated grids

A vicious circle that cannot be broken...

\[ u_c = u_c - \Gamma_{s\rightarrow c} G L^{-1} M \Gamma_{c\rightarrow s} u_c = F_c u_c \]

To preserve symmetry we impose \( \Gamma_{s\rightarrow c} = \Omega_c^{-1} \Gamma_{c\rightarrow s}^T \Omega_s \). This leads to

\[ M \Gamma_{c\rightarrow s} u_c = M \Gamma_{c\rightarrow s} u_c - L_c L^{-1} M \Gamma_{c\rightarrow s} u_c \approx 0_c X \]

where \( L_c = -M \Gamma_{c\rightarrow s} \Omega_c^{-1} \Gamma_{c\rightarrow s}^T M \) (wide-stencil discrete Laplacian).
Pressure-velocity coupling on collocated grids

A vicious circle that cannot be broken...

To preserve symmetry we impose $\Gamma_{s\rightarrow c} = \Omega_c^{-1} \Gamma_{c\rightarrow s}^T \Omega_s$. This leads to

$$M \Gamma_{c\rightarrow s} u_c = M \Gamma_{c\rightarrow s} u_c - L_c L^{-1} M \Gamma_{c\rightarrow s} u_c \approx 0_c \mathbf{X}$$

where $L_c = -M \Gamma_{c\rightarrow s} \Omega_c^{-1} \Gamma_{c\rightarrow s}^T M$ (wide-stencil discrete Laplacian).

Moreover, contribution to kinetic energy: $p_c (L - L_c) p_c \neq 0 \mathbf{X}$
Pressure-velocity coupling on collocated grids

A vicious circle that cannot be broken...

In summary\(^8\):

- **Mass**: \(M \Gamma_{c \rightarrow s} u_c = M \Gamma_{c \rightarrow s} u_c - L_c L^{-1} M \Gamma_{c \rightarrow s} u_c \approx 0_c X\)

- **Energy**: \(p_c (L - L_c) p_c \neq 0 X\)

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Pressure-velocity coupling on collocated grids

A vicious circle that cannot be broken...

In summary\(^8\):

- Mass: \(M\Gamma_{c\to s} u_c = M\Gamma_{c\to s} u_c - (L_c L^{-1}) M\Gamma_{c\to s} u_c \approx 0_c \times\)

- Energy: \(p_c (L - L_c) p_c \neq 0 \times\)

---

Pressure-velocity coupling on collocated grids

A vicious circle that cannot be broken...

In summary\(^8\):

- **Mass**: \( M\Gamma_{c\rightarrow s} \mathbf{u}_c = M\Gamma_{c\rightarrow s} \mathbf{u}_c - \left( L_c L^{-1} \right) M\Gamma_{c\rightarrow s} \mathbf{u}_c \approx 0_c \mathbf{x} \)

- **Energy**: \( p_c(L - L_c) p_c \neq 0 \mathbf{x} \)

---

Pressure-velocity coupling on collocated grids

A vicious circle that cannot be broken...

In summary\(^8\):

- Mass: \( M_{\Gamma_{c\rightarrow s}} \mathbf{u}_c = M_{\Gamma_{c\rightarrow s}} \mathbf{u}_c - \mathbf{L}_c \mathbf{L}^{-1} M_{\Gamma_{c\rightarrow s}} \mathbf{u}_c \approx 0_c \times \)

- Energy: \( p_c (\mathbf{L} - \mathbf{L}_c) p_c \neq 0 \times \)

Pressure-velocity coupling on collocated grids

A vicious circle that cannot be broken...

In summary\(^8\):

- **Mass:** \( \mathbf{M}_{\Gamma_c \rightarrow s} \mathbf{u}_c = \mathbf{M}_{\Gamma_c \rightarrow s} \mathbf{u}_c - \mathbf{L}_c \mathbf{L}^{-1} \mathbf{M}_{\Gamma_c \rightarrow s} \mathbf{u}_c \approx \mathbf{0}_c \times \)

- **Energy:** \( \mathbf{p}_c \left( \mathbf{L} - \mathbf{L}_c \right) \mathbf{p}_c \neq 0 \times \)

Pressure-velocity coupling on collocated grids

A vicious circle that cannot be broken...

In summary\(^8\):

- **Mass**: \( M\Gamma_{c\to s}u_c = M\Gamma_{c\to s}u_c - L_c L^{-1} M\Gamma_{c\to s}u_c \approx 0_c X \)

- **Energy**: \( p_c (L - L_c) p_c \neq 0 X \)

\[^8\text{F.X.Trias, O.Lehmkuhl, A.Oliva, C.D.Pérez-Segarra, R.W.C.P.Verstappen.} \]

Pressure-velocity coupling on collocated grids
A vicious circle that cannot be broken...

In summary\(^8\):

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

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Pressure-velocity coupling on collocated grids
A vicious circle that cannot be broken can almost be broken...

Results for an inviscid Taylor-Green vortex

Preserving symmetries: collocated vs staggered

Pressure-velocity coupling on collocated grids
A vicious circle that cannot be broken can almost be broken...

\[ \tilde{L} = L \text{ using } p'_c \]
\[ \tilde{L} = L_c \]
\[ p_c \perp \text{Ker}(L_c) \]

\[ \tilde{L} = L \]
\[ L = L_c \]
\[ pc(\tilde{L} - L_c)p_c \]

Results for an inviscid Taylor-Green vortex

\[ E_k(t)/E_k(0)-1 \]

Time

\[ \text{SymPres PressCorr} \]
\[ \text{SymPres TotPress} \]
\[ \text{OpenFOAM} \]

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\textsuperscript{10}:

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\textsuperscript{10}:

Are staggered and collocated so different at the end?

Collocated:  \[ \mathbf{u}_c^{n+1} = \left( \mathbf{I}_c - \Gamma_{s\rightarrow c} \Omega_{s}^{-1} \mathbf{P}_s \Gamma_{c\rightarrow s} \right) \left( \mathbf{I}_c + \mathbf{\tilde{d}}_t \right) \mathbf{u}_c^n = \mathbf{F}_c \mathbf{T}_c \mathbf{u}_c^n \]
Are staggered and collocated so different at the end?

Collocated: \[ \mathbf{u}_c^{n+1} = \left( I_c - \Gamma_{s \rightarrow c} \Omega_{s}^{-1} P_s \Gamma_{c \rightarrow s} \right) \mathbf{u}_c^n + \left[ \mathbf{F}_c \mathbf{T}_c \right] \mathbf{u}_c^n \]

Naïve collocated: \[ \mathbf{u}_c^{n+1} = \left( \Gamma_{s \rightarrow c} \mathbf{F}_s \mathbf{T}_c \right) \mathbf{u}_c^n \]
Are staggered and collocated so different at the end?

Collocated:

\[ u_c^{n+1} = \left( I_c - \Gamma_{s\rightarrow c} \Omega_s^{-1} P_s \Gamma_{c\rightarrow s} \right) \left[ I_c + \partial_t^c \right] u_c^n = \underbrace{F_c \; T_c \; u_c^n}_{\text{NS}_c} \]

Naïve collocated:

\[ u_c^{n+1} = \Gamma_{s\rightarrow c} F_s \Gamma_{c\rightarrow s} T_c \; u_c^n \]

Naïve staggered:

\[ u_s^{n+1} = F_s \Gamma_{c\rightarrow s} T_c \Gamma_{s\rightarrow c} u_s^n \]
Motivation

Preserving symmetries: collocated vs staggered

Building a staggered formulation

Portability and beyond

Conclusions

Are staggered and collocated so different at the end?

Collocated:

\[
\begin{align*}
\mathbf{u}_c^{n+1} &= \left( \mathbf{I}_c - \Gamma_{s\rightarrow c} \mathbf{\Omega}_s^{-1} \mathbf{P}_s \Gamma_{c\rightarrow s} \right) \left[ \mathbf{I}_c + \partial_t \mathbf{T}_c \right] \mathbf{u}_c^n = \mathbf{F}_c \mathbf{T}_c \mathbf{u}_c^n \\
\end{align*}
\]

Naïve collocated:

\[
\begin{align*}
\mathbf{u}_c^{n+1} &= \Gamma_{s\rightarrow c} \mathbf{F}_s \mathbf{T}_c \mathbf{u}_c^n \\
\end{align*}
\]

Naïve staggered:

\[
\begin{align*}
\mathbf{u}_s^{n+1} &= \mathbf{F}_s \mathbf{T}_c \Gamma_{s\rightarrow c} \mathbf{u}_s^n \\
\end{align*}
\]

\[
\Gamma_{s\rightarrow c} (\mathbf{\tilde{N}S}_s)^n = (\mathbf{\tilde{N}S}_c)^n \Gamma_{c\rightarrow s}
\]
Are staggered and collocated so different at the end?

Collocated:  \[ u_c^{n+1} = \left( I_c - \Gamma_s \rightarrow c \Omega_s^{-1} P_s \Gamma_c \rightarrow s \right) \left( I_c + \partial_t^c \right) u_c^n = F_c T_c u_c^n \]

Staggered:  \[ u_s^{n+1} = \left( I_s - \Omega_s^{-1} P_s \right) \left( I_s + \Gamma_s \rightarrow c \partial_t^c \Gamma_s \rightarrow c \right) u_s \]
Can we have a staggered formulation based only on collocated operators?

Then, it could be easily implemented in existing collocated codes such as OpenFOAM.

Staggered: \( \mathbf{u}_s^{n+1} = (I_s - \Omega_s^{-1}\mathbf{P}_s) \left[ I_s + \Gamma_{c \rightarrow s} \partial_t \Gamma_{s \rightarrow c} \right] \mathbf{u}_s \)

Similar approaches have been proposed in the literature before\(^{11,12,13,14,15} \).

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**References**


Can we have a staggered formulation based only on collocated operators?

Then, it could be easily implemented in existing collocated codes such as OpenFOAM.

Staggered: $\mathbf{u}_s^{n+1} = \left( I_s - \Omega_s^{-1} P_s \right) \left[ I_s + \Gamma_{c\rightarrow s} \partial_t c \Gamma_{s\rightarrow c} \right] \mathbf{u}_s$

Similar approaches have been proposed in the literature before $^{11,12,13,14,15}$.

Research question: then, why at the end collocated approach seems to be the winner?

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Results for a turbulent channel flow at $Re_T = 180$

Staggered $C_0$: $u_s^{n+1} = (I_s - \Omega_s^{-1}P_s) [I_s + \Gamma_{c\rightarrow s} \partial_t \Gamma_{s\rightarrow c}] u_s$

![Graph showing DNS (KMM) results with y+ on the y-axis and y+ on the x-axis.](image)
Results for a turbulent channel flow at $Re_T = 180$

Staggered $C^0_s$:

$u_{s}^{n+1} = \left( I_s - \Omega_s^{-1} P_s \right) \left[ I_s + \Gamma_{c \rightarrow s} \partial_t \Gamma_{s \rightarrow c} \right] u_s$

$$
\begin{align*}
\text{DNS (KMM)} \\
\text{16x16x8}
\end{align*}
$$
Results for a turbulent channel flow at $Re_T = 180$

Staggered $C_s^0$: \[ u_{s}^{n+1} = (I_s - \Omega_s^{-1} P_s) \left[ I_s + \Gamma_{c \to s} \partial_t \Gamma_{s \to c} \right] u_s \]

\begin{figure}
\centering
\includegraphics[width=\textwidth]{channel_flow_results}
\caption{Comparison of DNS (KMM) with different grid resolutions.}
\end{figure}
Results for a turbulent channel flow at $Re_T = 180$

Staggered $C^0_s$: $u^{n+1}_s = (I_s - \Omega^{-1}_s P_s) \left[ I_s + \Gamma_{c\rightarrow s} \frac{\partial c}{\partial \tau} \Gamma_{s\rightarrow c} \right] u_s$
Results for a turbulent channel flow at $Re_T = 180$

Staggered $C_s^0$: $u_{s}^{n+1} = (I_s - \Omega_s^{-1}P_s)\left[ I_s + \Gamma_{c\rightarrow s} \partial_t \Gamma_{s\rightarrow c} \right] u_s$
Results for a turbulent channel flow at $Re_T = 180$

Staggered $C_s^0$:

$$u_{s}^{n+1} = (I_s - \Omega_s^{-1} P_s) \left[ F_s + \Gamma_{c\rightarrow s} \frac{\partial}{\partial t} \Gamma_{s\rightarrow c} \right] u_s$$

![Graph showing DNS results for different grid resolutions](image-url)
Dispersion errors analysis

Staggered $C_s^0$:

$$u_s^{n+1} = (l_s - \Omega_s^{-1} P_s) \left[ l_s + \Gamma_c \partial_t \Gamma_s \right] u_s$$

$F_s$ and $T_s$
Dispersion errors analysis

Staggered $C_s^0$: 

$$u_s^{n+1} = \left( I_s - \Omega_s^{-1} P_s \right) \left[ I_s + \left\{ \Gamma_{c\rightarrow s} \partial_t \Gamma_{s\rightarrow c} \right\} u_s \right]$$

\[ F_s \]

\[ T_s \]
Dispersion errors analysis

Staggered $C_s^1$: $u_{s}^{n+1} = (I_s - \Omega_s^{-1}P_s) \left( I_s + F_{s} \Gamma_{c\rightarrow s} \partial_t \Gamma_{s\rightarrow c} \bar{F} \right) u_s$

Filter: $\bar{F} = \Gamma_{s\rightarrow c} \Gamma_{c\rightarrow s}$ ($\bar{F} = \bar{F}^T$ and positive semi-definite)
Dispersion errors analysis

Staggered $C_s^2$: $u_s^{n+1} = (I_s - \Omega_s^{-1} P_s) \left[ I_s + \tilde{F} \tilde{F} \Gamma_{c \rightarrow s} \partial_t \Gamma_{s \rightarrow c} \tilde{F} \tilde{F} \right] u_s$

Filter: $\tilde{F} = \Gamma_{s \rightarrow c} \Gamma_{c \rightarrow s}$ ($\tilde{F} = \tilde{F}^T$ and positive semi-definite)
Results for a turbulent channel flow at $Re_τ = 180$

Staggered $C_s^2$: \[
\mathbf{u}^{n+1}_s = (I_s - \Omega_s^{-1} P_s) \left[ I_s + \mathcal{F} \mathcal{F} \Gamma_{c \rightarrow s} \partial_t \mathcal{G}_{s \rightarrow c} \mathcal{F} \mathcal{F} \right] \mathbf{u}_s
\]

![Graph showing DNS (KMM) results](image-url)
Results for a turbulent channel flow at $Re_T = 180$

Staggered $C_s^2$: \[ u_s^{n+1} = (I_s - \Omega_s^{-1} P_s) \left[ I_s + \sum_{c \to s} \Gamma_c \partial_t^{c} \Gamma_{s \to c} \sum_{T_s} \right] u_s \]
Results for a turbulent channel flow at $Re_T = 180$

Staggered $C_s^2$: $u_{s}^{n+1} = (I_s - \Omega_s^{-1}P_s) \left[ I_s + \int_{\Gamma_{s \rightarrow c}} \partial_t \Gamma_{s \rightarrow c} \right] u_s$

Graph showing DNS (KMM) results for different grid resolutions: $32 \times 32 \times 16$, $16 \times 16 \times 8$.
Results for a turbulent channel flow at $Re_T = 180$

Staggered $C_s^2$:

$$u_s^{n+1} = (I_s - \Omega_s^{-1}P_s)\left(\sum_{s \to c} \Gamma \partial_t \Gamma_{s \to c} \bar{F} \Gamma_c \nabla_{s} \Gamma_{c \to s} \bar{F} \right) u_s$$

![Graph showing DNS (KMM) results with different grid resolutions: 64x64x32, 32x32x16, 16x16x8.](attachment:graph.png)
Results for a turbulent channel flow at $Re_T = 180$

Staggered $C_s^2$: $u_{s}^{n+1} = (I_s - \Omega_s^{-1}P_s) \left[ I_s + \tilde{F} \tilde{F} \Gamma_{c \rightarrow s} \partial_{t} \Gamma_{s \rightarrow c} \tilde{F} \tilde{F} \right] u_s$

![Graph showing DNS results for different resolutions](image-url)
Results for a turbulent channel flow at $Re_T = 180$

Staggered $C_s^2$: $u_{s}^{n+1} = \left( I_s - \Omega_{s}^{-1} P_s \right) \left[ I_s + \tilde{F} \tilde{F} \Gamma_{c \rightarrow s} \partial_t \Gamma_{s \rightarrow c} \tilde{F} \tilde{F} \right] u_s$

![Graph showing DNS results for various resolutions]

- DNS (KMM)
- 160x160x80
- 128x128x64
- 64x64x32
- 32x32x16
- 16x16x8
Results for a turbulent channel flow at $Re_\tau = 180$

Staggered $C_s^2$: 

$$u_s^{n+1} = (I_s - \Omega_s^{-1} P_s) \left[ I_s + \tilde{F}_s \Gamma_{c \rightarrow s} \partial_t \Gamma_{s \rightarrow c} \tilde{F}_s \right] u_s$$
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. NUMA-aware execution strategies for CFD are presented in this conference\(^\text{16}\).

\(^\text{16}\) X. Álvarez, A. Gorobets, F.X. Trias, A. Oliva. *NUMA-aware strategies for the efficient execution of CFD simulations on CPU supercomputers* ParCFD2021. Don’t miss it!
Algebra-based approach naturally leads to portability, to simple and analyzable formulations.

**Collocated:**

\[ u_c^{n+1} = (I_c - \Gamma_{s\to c} \Omega_{s}^{-1} P_s \Gamma_{c\to s}) \left( I_c + \partial_t^c \right) u_c^n = F_c T_c u_c^n \]

**Staggered:**

\[ u_s^{n+1} = (I_s - \Omega_s^{-1} P_s) \left( I_s + \Gamma_{c\to s} \partial_t^c \Gamma_{s\to c} \right) u_s = F_s T_s u_s \]
Algebra-based approach naturally leads to portability, to simple and analyzable formulations and opens the door to new strategies\textsuperscript{17} to improve its performance...

\textsuperscript{17} A.Alsalti, X.Álvarez, F.X.Trias, A.Gorobets, A.Oliva. A highly portable heterogeneous implementation of a Poisson solver for flows with one periodic direction ParCFD2021. Don’t miss it!
Algebra-based approach naturally leads to portability, to simple and analyzable formulations and opens the door to new strategies\textsuperscript{17} to improve its performance...

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

SpMMV can be used $\implies$ higher AI

\footnote{A.Alsalti, X.Álvarez, F.X.Trias, A.Gorobets, A.Oliva. A highly portable heterogeneous implementation of a Poisson solver for flows with one periodic direction ParCFD2021. Don’t miss it!}
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.
Concluding remarks

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

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

- Despite this, the CFD community have generally adopted collocated formulations due to the inherent difficulties to formulate a simple and robust staggered discretization of momentum.

  ➔ A potential solution has been presented here...
Concluding remarks

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

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On-going research:

- Complete the analysis for higher $Re_{\tau}$

- Test for complex geometries using unstructured meshes
Thank you for your virtual attendance