



Centre Tecnològic de Transferència de Calor
UNIVERSITAT POLITÈCNICA DE CATALUNYA

Rethinking CFD for modern HPC systems

F.Xavier Trias

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



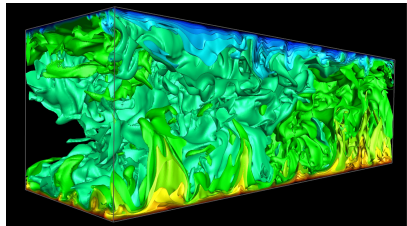
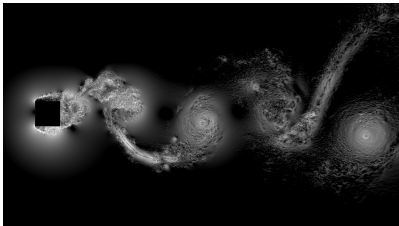


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This talk builds on joint work with...

HPC & solvers

À. Alsalti-Baldellou, X. Álvarez-Farré,
G. Colomer, A. Gorobets,
M. Mosqueda-Otero

Numerical methods

J.A. Hopman, M. Mosqueda-Otero,
J. Plana-Riu, D. Santos, S.-M. Šehović,
N. Valle

Turbulence modelling

F. Dabbagh, D. Folch, J. Ruano



A subset of the team at ECCOMAS 2026,
Munich

Contents

- 1 Background
- 2 Preserving symmetries
- 3 Energy exchange in multiphysics
- 4 Portability and beyond
- 5 Take-away messages

The CTTC research group

Heat and Mass Transfer Technological Center (Catalan: *Centre Tecnològic de Transferència de Calor*) has more than 30 years experience in CFD.

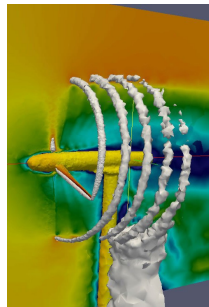
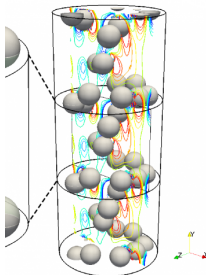
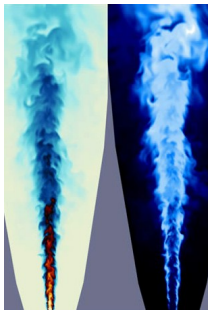
- Research center at Universitat Politècnica de Catalunya (UPC)
- Staff:
 - 4 full professors, 3 associate professors, 3 lecturers and 1 emeritus
 - 7 senior researchers/postdocs
 - 15 PhD students
 - 3 technical and IT staff



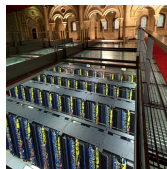
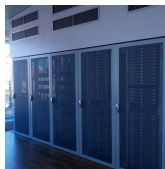
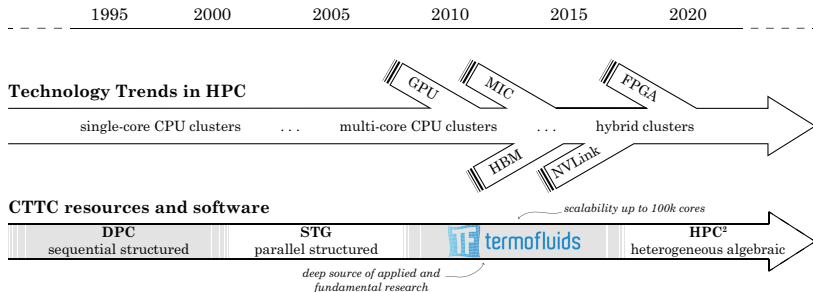
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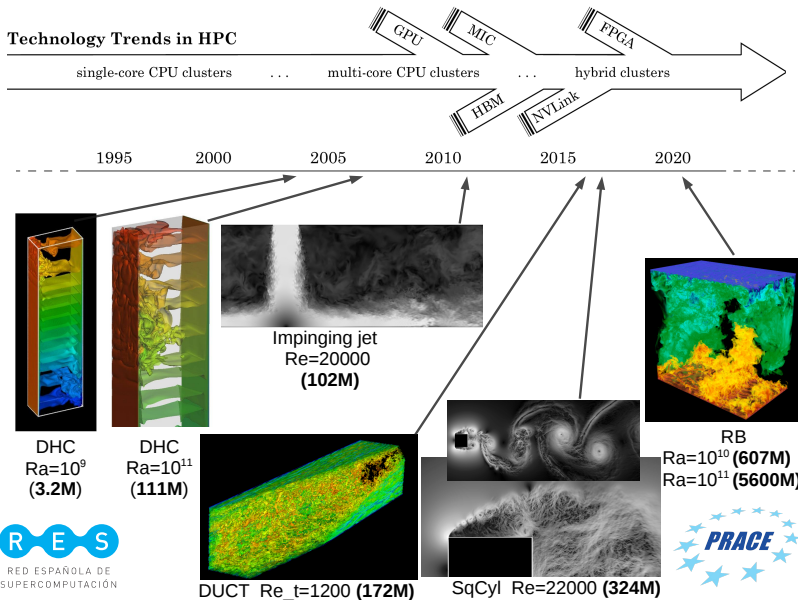
- **Fundamental research** on numerical methods, fluid dynamics and heat and mass transfer phenomena.
- **Applied research** on thermal and fluid dynamic optimization of thermal system and equipment.



CTTC's historical background in HPC

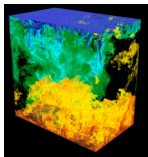


Technology Trends in HPC



General motivation: (very) large-scale DNS/LES

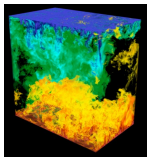
For canonical academic flows...



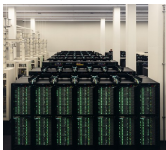
DNS {

General motivation: (very) large-scale DNS/LES

For canonical academic flows...



MareNostrum 5-ACC
(Barcelona)



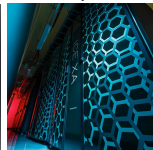
rank #8
1120 nodes with:
2x Intel Shappire Rapids 8460
1x NVIDIA Hopper 64 GB HBM
1x Infiniband NDR200

Snellius
(Amsterdam)



rank #165
714 nodes with:
2x AMD EPYC 9654 96C
1x Infiniband NDR200

TSUBAME4.0
(Tokyo)



rank #31
240 nodes with:
2x AMD EPYC 9654 96-Core
4x NVIDIA H100 SXM5
1x Infiniband NDR200

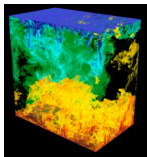


DNS {

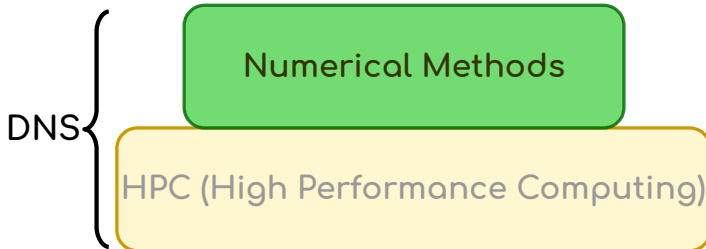
HPC (High Performance Computing)

General motivation: (very) large-scale DNS/LES

For canonical academic flows...



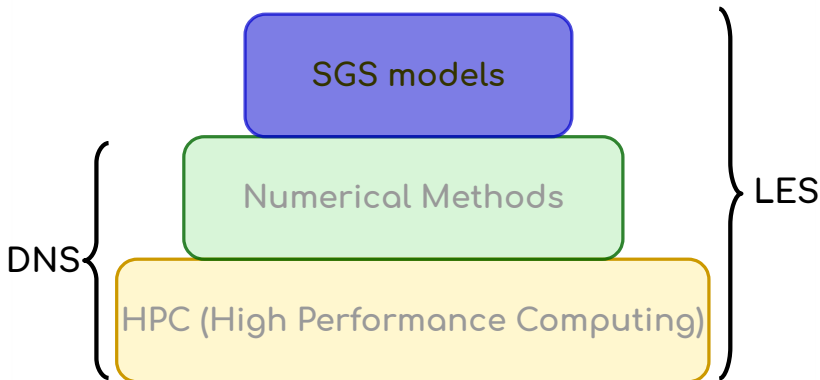
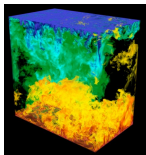
How to properly discretize NS?



General motivation: (very) large-scale DNS/LES

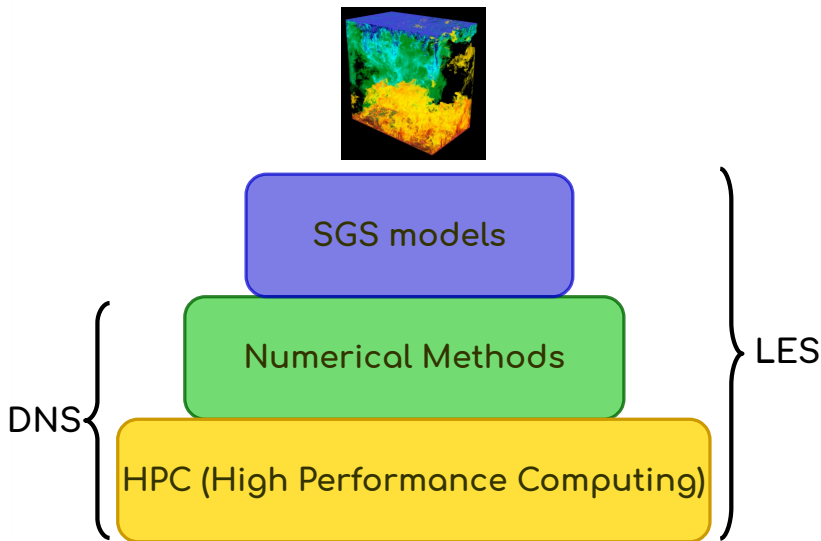
For canonical academic flows...

How to
properly
model SGS?



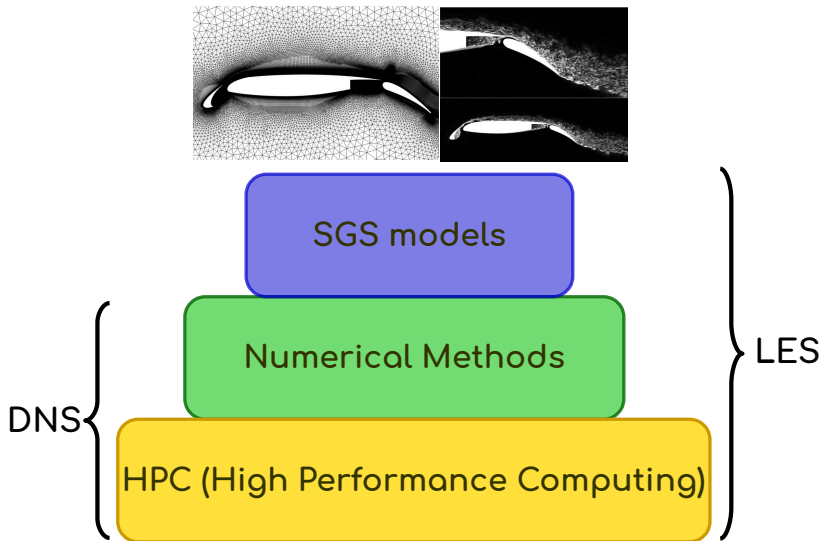
General motivation: (very) large-scale DNS/LES

For canonical academic flows...



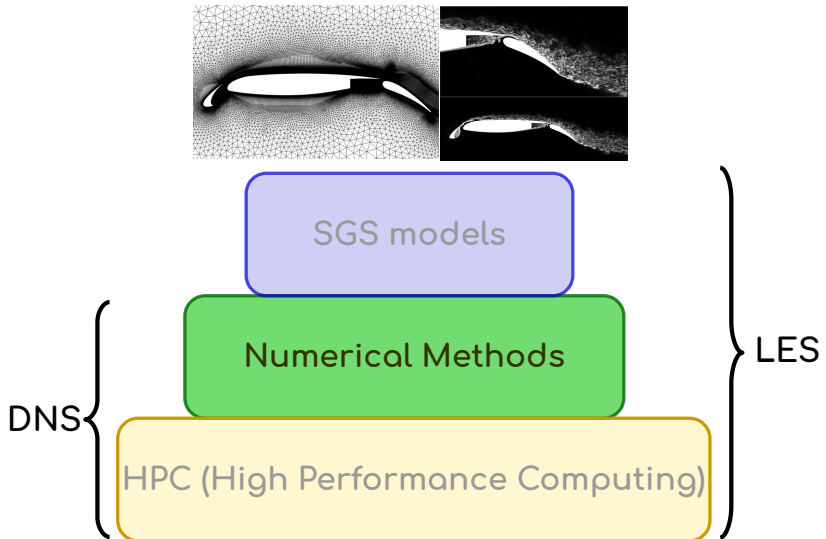
General motivation: (very) large-scale DNS/LES

...but also for industrial applications



General motivation: (very) large-scale DNS/LES

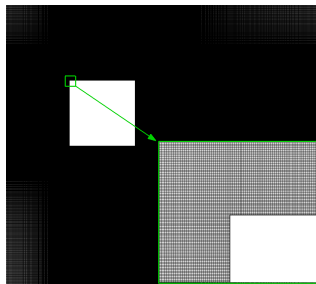
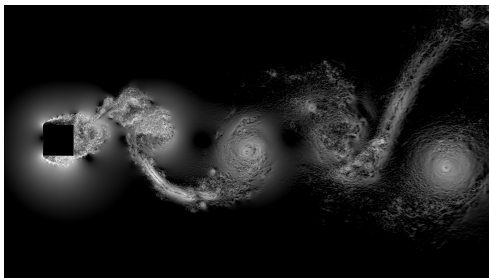
...but also for industrial applications



Numerical methods for DNS/LES

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?



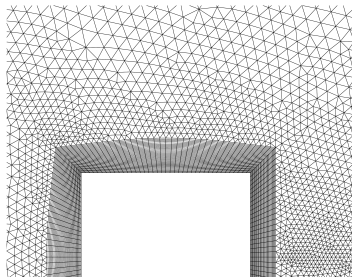
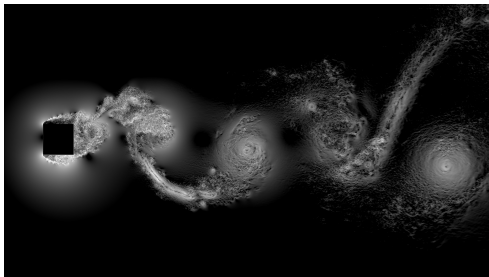
DNS¹ of the flow around a square cylinder at $Re = 55000$ (2.6B grid points)

¹F.X.Trias, À.Alsaltí-Baldellou, A.Oliva. *On the Reynolds-number scaling of Poisson solver complexity*, **Physics of Fluids**, 38 (4):045157, 2026.

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Symmetry-preserving discretization

Continuous

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

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

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Discrete

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

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

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

Symmetry-preserving discretization

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

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

Discrete

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Symmetry-preserving discretization

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Symmetry-preserving discretization

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

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

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

Why a collocated formulation?

- STAR-CCM+



SIEMENS

- ANSYS-FLUENT



- Code-Saturne



- OpenFOAM

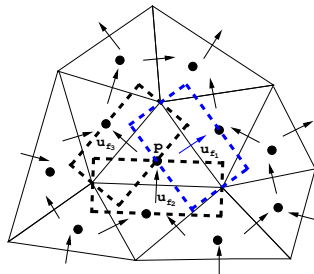
OpenFOAM®



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

In staggered meshes

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



Why a collocated formulation?

- STAR-CCM+

**SIEMENS**

- ANSYS-FLUENT



- Code-Saturne



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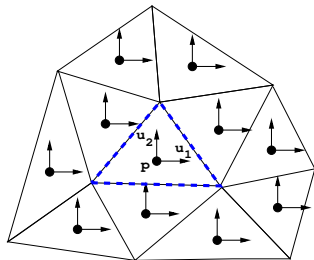
OpenFOAM®



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

In collocated meshes

- $\mathbf{p}-\mathbf{u}_c$ coupling is cumbersome $\times$
- $\mathbf{C}(\mathbf{u}_s)$ and $\mathbf{D}$ easy to discretize $\checkmark$
- Cheaper, less memory, ... $\checkmark$



Why a collocated formulation?

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

Journal of Computational Physics 258 (2014) 240–267

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Journal of Computational Physics

www.elsevier.com/locate/jcp

Symmetry-preserving discretization of Navier–Stokes equations on collocated unstructured grids

F.X. Trias^{a,b}, O. Lehmkuhl^{a,c}, A. Oliva^{a,c,1}, C.D. Pérez-Segarra^a, R.W.C.P. Verstappen^b

^a Heat and Mass Transfer Technological Center, Technical University of Catalonia, ETSEIAT, c/ Colom 11, 08222 Terrassa, Spain
^b Johann Bernoulli Institute for Mathematics and Computing Science, University of Groningen, P.O. Box 407, 9700 AR Groningen, The Netherlands
^c Tercero Fluids, S.L., c/ Magi Cebal 8, 08204 Sabadell, Spain

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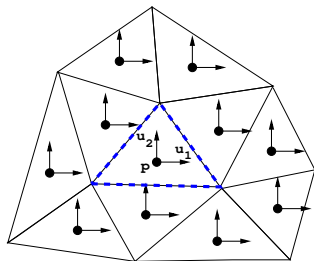
ABSTRACT

A fully-conservative discretization is presented in this paper. The same principles followed by Verstappen and Veldman (2003) [3] are generalized for unstructured meshes. Here, a

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

In collocated meshes

- $\mathbf{p}-\mathbf{u}_c$ coupling is cumbersome ✗
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Computers and Fluids 225 (2013) 104679



Contents lists available at ScienceDirect

Computers and Fluids

journal homepage: www.elsevier.com/locate/comfluid



A symmetry-preserving second-order time-accurate PISO-based method

E.M.J. Komen^{a,*}, J.A. Hopman^a, E.M.A. Frederix^a, F.X. Trias^b, R.W.C.P. Verstappen^c

^a Research and Innovation department, Nuclear Research and consultancy Group NRC, P.O. Box 25, 26 Petten T35, The Netherlands
^b Heat and Mass Transfer Technological Center, Technical University of Catalonia, ETSEIAT, c/ Colom 11, Terrassa 08222, Spain
^c Bernoulli Institute for Mathematics, Computing Science, and Artificial Intelligence, University of Groningen, P.O. Box 407, AR Groningen 9700, The Netherlands



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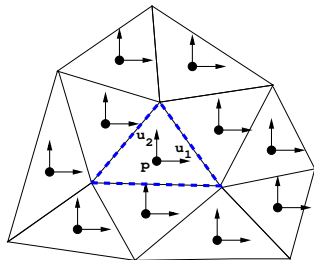
ABSTRACT

A new conservative symmetry-preserving second-order time-accurate PISO-based pressure-velocity coupling for solving the incompressible Navier–Stokes equations on unstructured collocated grids is presented in this paper. This new method for implicit time stepping is an extension of the conservative symmetry-preserving incremental-pressure projection method for explicit time stepping and unstructured collocated meshes of Trias et al. (1993). It enables the pressure and velocity fields, respectively, to be discretized on the same

$$\Omega_c \frac{du_c}{dt} + C(u_s) u_c = D u_c - G_c p_c; \quad M_c u_c = 0_c$$

In collocated meshes

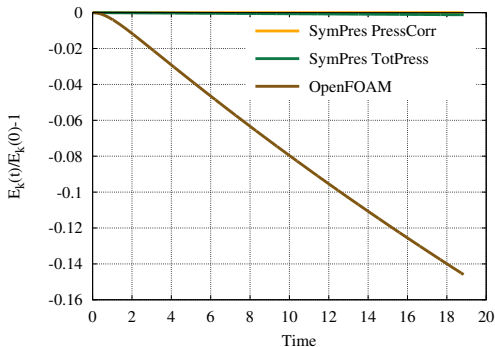
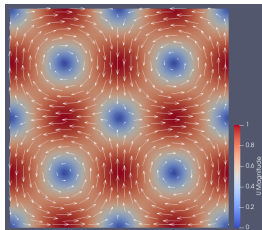
- p - u_c coupling is cumbersome ✗
- $C(u_s)$ and D easy to discretize ✓
- Cheaper, less memory, ... ✓



Pressure-velocity coupling on collocated grids

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

Open▽FOAM

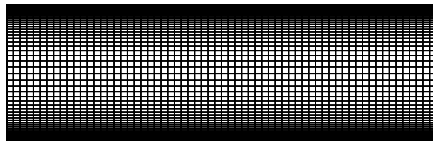


Results for an inviscid Taylor-Green vortex³

³E.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

... and make it **unconditionally stable**⁴ even on extremely bad meshes!



On a symmetry-preserving unconditionally stable projection method on collocated unstructured grids for incompressible flows

D. Santos¹, J.A. Hopman, C.D. Pérez-Segarra, F.X. Trias

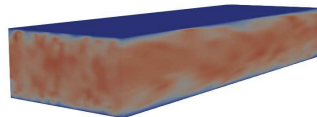
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Projection method
PISO
Unconditionally stable
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PISO

ABSTRACT

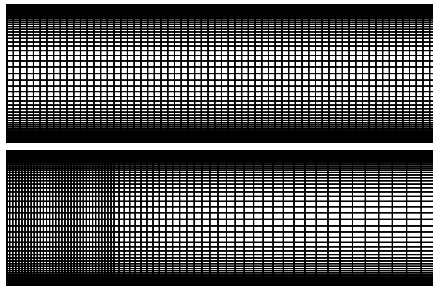
This work establishes the conditions for having a symmetry-preserving unconditionally stable projection method for incompressible flows, such as PISO or Fractional Step Method (FSM), on collocated unstructured grids based on a compact stencil Poisson equation. Its formulation is based on preserving the underlying symmetries of the differential operators. In addition, a general theorem for these types of projection methods will be proven. To establish an unconditionally stable method, the chosen grid, the mathematical requirements for the operators and the generalization establish a method more easily, even in cases where the mesh is highly distorted. This will be proven both theoretically and numerically. One outcome of robust kinetic energy is



⁴D.Santos, J.A.Hopman, C.D.Pérez-Segarra, F.X.Trias. *On a symmetry-preserving unconditionally stable projection method on collocated unstructured grids for incompressible flows*, **Journal of Computational Physics**, 523:113631, 2025.

Pressure-velocity coupling on collocated grids

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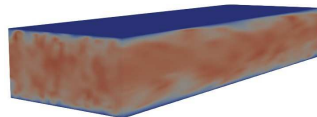
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ABSTRACT

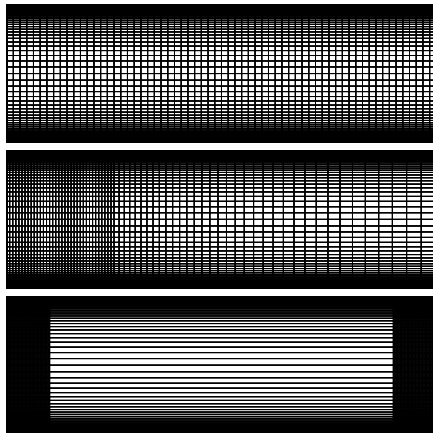
This work establishes the conditions for having a symmetry-preserving unconditionally stable projection method for incompressible flows, such as PISO or Fractional Step Method (FSM), on collocated unstructured grids based on a compact stencil Poisson equation. Its formulation is based on preserving the underlying symmetries of the differential operators. In addition, a general theorem for these types of projection methods will be proven. To establish an unconditionally stable method, the theorem gives the mathematical requirements for the operator and the projection equation a matrix must satisfy, even in cases where the mesh is highly distorted. This will be proven both theoretically and numerically. One formulation of incompressible Navier-Stokes



⁴D.Santos, J.A.Hopman, C.D.Pérez-Segarra, F.X.Trias. *On a symmetry-preserving unconditionally stable projection method on collocated unstructured grids for incompressible flows*, **Journal of Computational Physics**, 523:111631, 2025.

Pressure-velocity coupling on collocated grids

... and make it **unconditionally stable**⁴ even on extremely bad meshes!



Journal of Computational Physics 523 (2025) 113631



Contents lists available at ScienceDirect
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On a symmetry-preserving unconditionally stable projection method on collocated unstructured grids for incompressible flows

D. Santos^a, J.A. Hopman, C.D. Pérez-Segarra, F.X. Trias

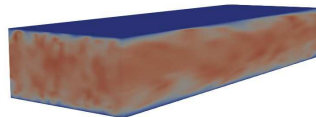
^a Institut de Recerca en Energia del Baix Llobregat (IREB), CSIC, Universitat Politècnica de Catalunya, 08860 Sabadell, Spain

ARTICLE INFO

Keywords:
Symmetry-preserving
Projection method
PISO
Unconditionally stable
Symmetry-preserving
PISO

ABSTRACT

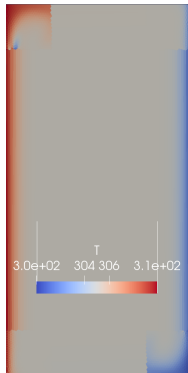
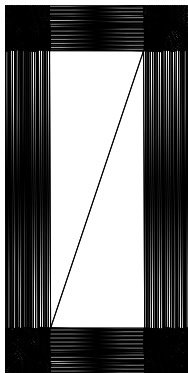
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⁴D.Santos, J.A.Hopman, C.D.Pérez-Segarra, F.X.Trias. *On a symmetry-preserving unconditionally stable projection method on collocated unstructured grids for incompressible flows*, **Journal of Computational Physics**, 523:113631, 2025.

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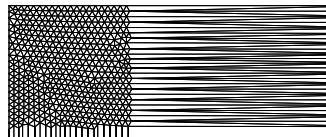
^a Institut de Recerca en Energia Industrial (IREN), Departament d'Enginyeria i Ciència dels Materials (ECM), Universitat de València, 46100 Burjassot, València, Spain

ARTICLE INFO

Keywords:
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Projection
PISO
Unconditionally stable
Energy-preserving
PVM

ABSTRACT

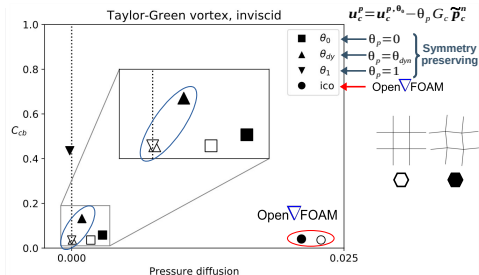
This work establishes the conditions for having a symmetry-preserving unconditionally stable projection method for incompressible flows, such as PISO or Fractional Step Method (FSM), on collocated unstructured grids based on a compact stencil Poisson equation. Its formulation is based on projecting the unphysical components of the differential operators. In addition, a general theorem for these types of projection methods will be proven. The viability as an unconditionally stable method, the theorem gives the mathematical requirements for the operators and the geometrical conditions a mesh must satisfy, even in cases where the mesh is highly distorted. This will be proven both theoretically and numerically. Characteristics of robust kinetic energy



⁴D.Santos, J.A.Hopman, C.D.Pérez-Segarra, F.X.Trias. *On a symmetry-preserving unconditionally stable projection method on collocated unstructured grids for incompressible flows*, **Journal of Computational Physics**, 523:113631, 2025.

Pressure-velocity coupling on collocated grids

... and minimize the checkerboard⁵ problem with a minimal artificial dissipation!



Quantifying the checkerboard problem to reduce numerical dissipation

J. A. Hopman^{1,a}, D. Santos^a, À. Alsaltí-Baldellou^{1,a,2}, J. Rigola^a, F. X. Trias¹

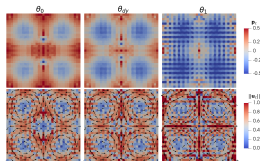
¹ IREC 2018-2021 TITELUP-TECHNOLOGICAL CENTER, UNIVERSITAT DE CATALUNYA, BARCELONA, SPAIN; ² TITELUP-TECHNOLOGICAL CENTER, UNIVERSITAT DE CATALUNYA, BARCELONA, SPAIN

ARTICLE INFO

Keywords:
checkerboard
dissipation
numerical error

ABSTRACT

This work presents a comprehensive exploration of various methods to solving incompressible flows using a projection method, and their relation to the occurrence and management of checkerboard oscillations. It employs an algebraic symmetry-preserving framework, clarifying the detection and implementation of its own operation while also addressing the numerical error. The lack of a proper definition for the checkerboard problem is addressed by preparing a ghost-based coefficient. This coefficient, mixed in the dissipative between the compact and wide-stencil Laplacian operators, while in a case of oscillatory behavior with a checkerboard, global, normalized, non-dimensional value. The influence of mesh and time-step



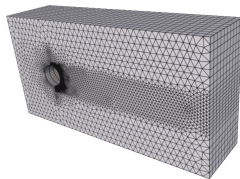
⁵J.A.Hopman, D.Santos, À.Alsaltí, J.Rigola, F.X.Trias. *Quantifying the checkerboard problem to reduce numerical dissipation*, **Journal of Computational Physics**, 521:113537, 2025. [arXiv: 2408.06821](https://arxiv.org/abs/2408.06821)

Pressure-velocity coupling on collocated grids

Summary

A robust and reliable symmetry-preserving collocated formulation...

- Virtually **artificial-dissipation-free**
- Suitable for **unstructured** grids

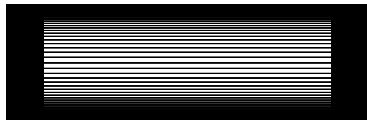


Pressure-velocity coupling on collocated grids

Summary

A robust and reliable symmetry-preserving collocated formulation...

- Virtually **artificial-dissipation-free**
- Suitable for **unstructured** grids
- **Unconditionally stable** even on:
 - Very low quality grids

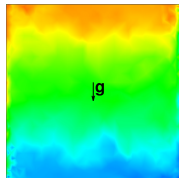
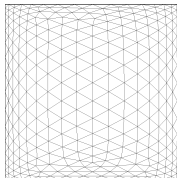


Pressure-velocity coupling on collocated grids

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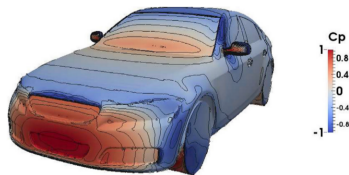
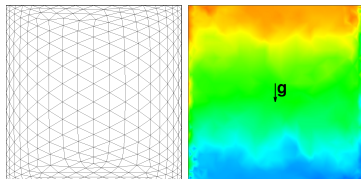


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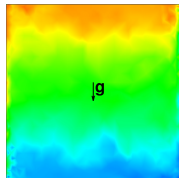
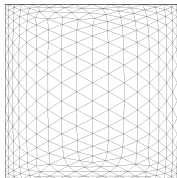


Pressure-velocity coupling on collocated grids

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 - Very coarse grids
- Suitable for **industrial** applications
- Also available in **OpenFOAM**



Open▽FOAM

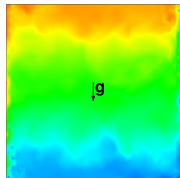
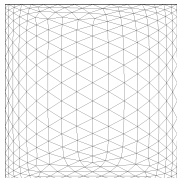


Pressure-velocity coupling on collocated grids

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Open  FOAM

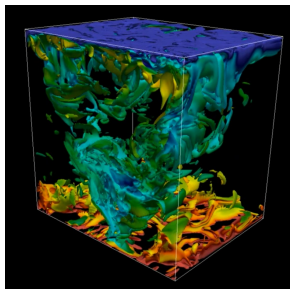


Research question #2:

- What happens to the **other forms of energy** and their **exchanges**?

Buoyancy-driven flows

Energy-exchanges



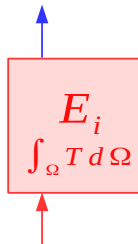
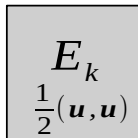
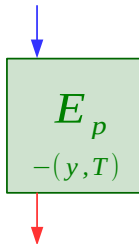
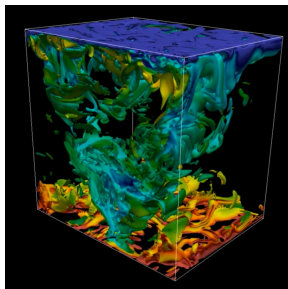
$$E_p$$
$$-(y, T)$$

$$E_k$$
$$\frac{1}{2}(\mathbf{u}, \mathbf{u})$$

$$E_i$$
$$\int_{\Omega} T d\Omega$$

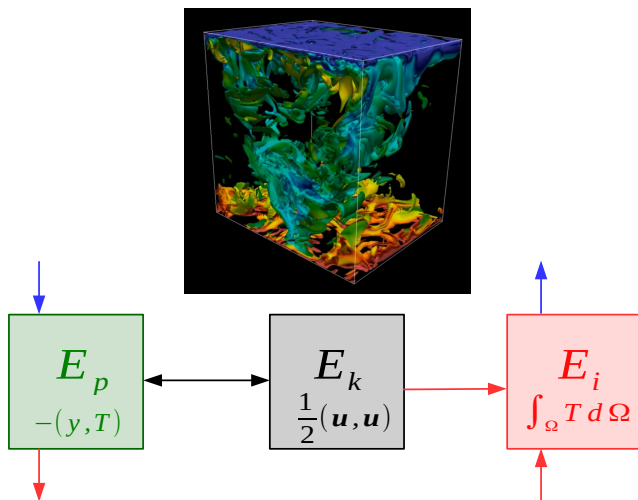
Buoyancy-driven flows

Energy-exchanges



Buoyancy-driven flows

Energy-exchanges

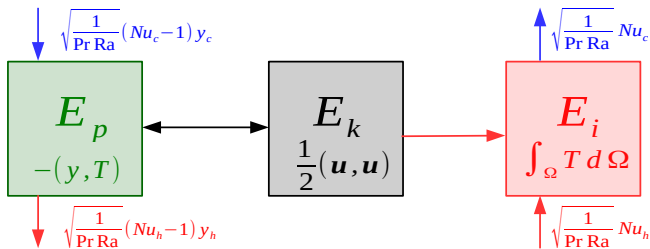
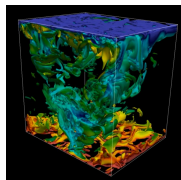


Buoyancy-driven flows

Continuous formulation

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = \sqrt{\frac{\text{Pr}}{\text{Ra}}} \nabla^2 \mathbf{u} - \nabla p + \underbrace{T \mathbf{e}_y}_{\text{Boussinesq}} \quad \nabla \cdot \mathbf{u} = 0$$

$$\frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla) T = \sqrt{\frac{1}{\text{Pr Ra}}} \nabla^2 T$$



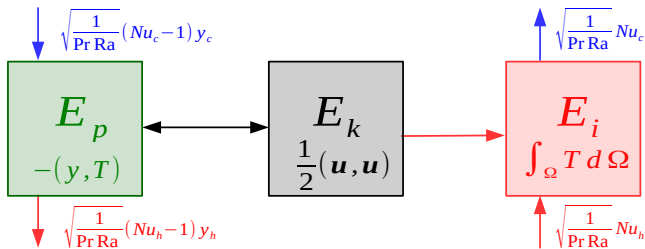
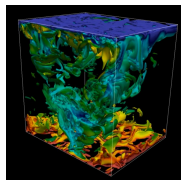
Buoyancy-driven flows

Continuous formulation

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = \sqrt{\frac{\text{Pr}}{\text{Ra}}} \nabla^2 \mathbf{u} - \nabla p + T \mathbf{e}_y \quad \text{Boussinesq} \quad \nabla \cdot \mathbf{u} = 0$$

$$\frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla) T = \sqrt{\frac{1}{\text{Pr Ra}}} \nabla^2 T$$

$$\frac{dE_p}{dt} = (y, \nabla \cdot (\mathbf{u} T)) - \sqrt{\frac{1}{\text{Pr Ra}}} (y, \nabla^2 T)$$



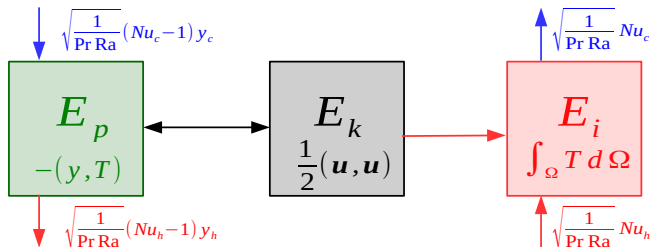
Buoyancy-driven flows

Continuous formulation

$$\begin{aligned} \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} &= \sqrt{\frac{\text{Pr}}{\text{Ra}}} \nabla^2 \mathbf{u} - \nabla p + \underbrace{T \mathbf{e}_y}_{\text{Boussinesq}} & \nabla \cdot \mathbf{u} &= 0 \\ \frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla) T &= \sqrt{\frac{1}{\text{Pr Ra}}} \nabla^2 T & \Phi &= \|\nabla \mathbf{u}\|^2 \varepsilon_U = \int_{\Omega} \Phi d\Omega \\ & & (v, T) &= \int_{\Omega} v T d\Omega \end{aligned}$$

$$\frac{dE_p}{dt} = (y, \nabla \cdot (\mathbf{u} T)) - \sqrt{\frac{1}{\text{Pr Ra}}} (y, \nabla^2 T)$$

$$\frac{dE_k}{dt} = -\sqrt{\frac{\text{Pr}}{\text{Ra}}} \varepsilon_U + (v, T)$$



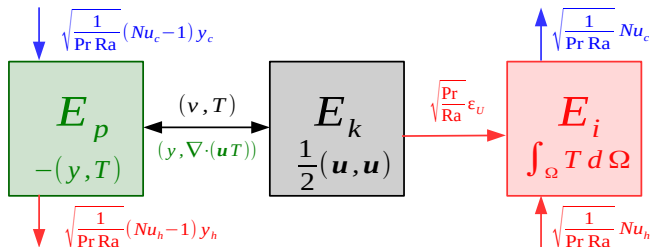
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$$\frac{dE_k}{dt} = -\sqrt{\frac{\text{Pr}}{\text{Ra}}} \varepsilon_U + (v, T)$$



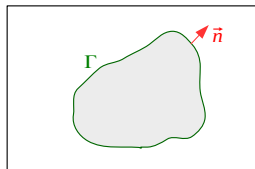
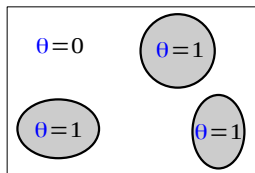
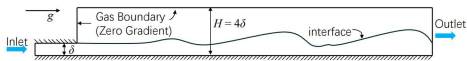
Multiphase flows

Continuous formulation

$$\rho \frac{\partial \vec{u}}{\partial t} + \rho (\vec{u} \cdot \nabla) \vec{u} = \nabla \cdot (2\mu S(\vec{u})) - \nabla p + \gamma \kappa \vec{n} \quad \nabla \cdot \vec{u} = 0$$

$$\frac{\partial \theta}{\partial t} + (\vec{u} \cdot \nabla) \theta = 0$$

$$\kappa = -\nabla \cdot \vec{n} \quad \text{where} \quad \vec{n} = \frac{\nabla \theta}{|\nabla \theta|}$$



Multiphase flows

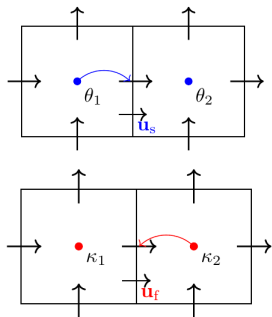
Conservative discrete formulation

$$\rho \frac{\partial \vec{u}}{\partial t} + \rho (\vec{u} \cdot \nabla) \vec{u} = \nabla \cdot (2\mu S(\vec{u})) - \nabla p + \gamma \kappa \cdot \vec{n} \quad \nabla \cdot \vec{u} = 0$$

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$$\kappa = -\nabla \cdot \vec{n} \quad \text{where} \quad \vec{n} = \frac{\nabla \theta}{|\nabla \theta|}$$

Surface tension



Journal of Computational Physics 400 (2020) 108991



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An energy-preserving level set method for multiphase flows

N. Valle, F.X. Trias, J. Castro*

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ABSTRACT

The computation of multiphase flows presents a subtle energetic equilibrium between potential (i.e., surface) and kinetic energies. The use of traditional interface-capturing schemes provides no control over such a dynamic balance. In the spirit of the well-known symmetry-preserving and mimetic schemes, whose physics-compatible discretizations rely upon preserving the underlying mathematical structures of the space, we identify the corresponding structure and propose a new discretization strategy for curvature. The new scheme ensures conservation of mechanical energy (i.e., surface plus kinetic) up to temporal integration. Inviscid numerical simulations are performed to show the robustness of such a method.

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Multiphase flows

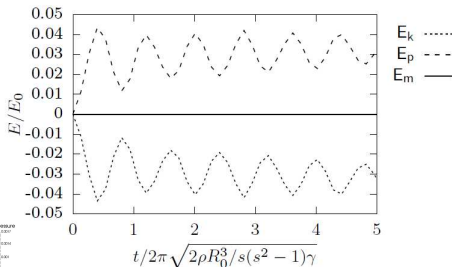
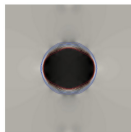
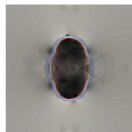
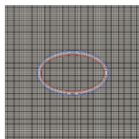
Conservative discrete formulation

$$\rho \frac{\partial \vec{u}}{\partial t} + \rho (\vec{u} \cdot \nabla) \vec{u} = \nabla \cdot (2\mu S(\vec{u})) - \nabla p + \gamma \kappa \vec{n} \quad \nabla \cdot \vec{u} = 0$$

Surface tension

$$\frac{\partial \theta}{\partial t} + (\vec{u} \cdot \nabla) \theta = 0$$

$$\kappa = -\nabla \cdot \vec{n} \quad \text{where} \quad \vec{n} = \frac{\nabla \theta}{|\nabla \theta|}$$



Mechanical energy (kinetic+potential) is preserved!

A new general framework for multiphysics

Variational formulation

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = \nu \nabla^2 \mathbf{u} - \nabla p + \mathbf{f}^\phi$$

Associated force

$$\frac{\partial \phi}{\partial t} + \mathcal{L}_u \phi = 0$$

Lie derivative

$$\mathcal{L}_u \phi = (\mathbf{u} \cdot \nabla) \phi$$

Scalar (0-forms)

$$\mathcal{L}_u \phi = \nabla \cdot (\mathbf{u} \phi)$$

Density-like (3-forms)

$$\langle \mathbf{a}, \mathbf{b} \rangle := \int_{\Omega} \mathbf{a} \cdot \mathbf{b} \, d\Omega \quad \langle \mathbf{a}, \nabla \phi \rangle = -\langle \nabla \cdot \mathbf{a}, \phi \rangle$$

A new general framework for multiphysics

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$$\mathcal{L}_u \phi = \nabla \cdot (\mathbf{u} \phi)$$

Density-like (3-forms)

$$E^\phi[\phi]$$

Associated energy

$$\mu^\phi = \frac{\delta E^\phi[\phi]}{\delta \phi}$$

Variational derivative

$$\langle \mathbf{a}, \mathbf{b} \rangle := \int_{\Omega} \mathbf{a} \cdot \mathbf{b} \, d\Omega \quad \langle \mathbf{a}, \nabla \phi \rangle = -\langle \nabla \cdot \mathbf{a}, \phi \rangle$$

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$$E^\phi[\phi] \quad \text{Associated energy}$$

$$\mu^\phi = \frac{\delta E^\phi[\phi]}{\delta \phi} \quad \text{Variational derivative}$$

$$\frac{d E^\phi}{dt} = \langle \mu^\phi, \partial_t \phi \rangle = - \langle \mu^\phi, \mathcal{L}_u \phi \rangle$$

$$\langle \mathbf{u}, \mathbf{f}^\phi \rangle = \langle \mu^\phi, \mathcal{L}_u \phi \rangle \quad \text{Energy balance}$$

$$\langle \mathbf{a}, \mathbf{b} \rangle := \int_{\Omega} \mathbf{a} \cdot \mathbf{b} \, d\Omega \quad \langle \mathbf{a}, \nabla \phi \rangle = - \langle \nabla \cdot \mathbf{a}, \phi \rangle$$

A new general framework for multiphysics

Application to buoyancy-driven flows

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

Associated force

$$\frac{\partial \rho}{\partial t} + \mathcal{L}_u \rho = 0$$

Lie derivative

$$\mathcal{L}_u \phi = (\mathbf{u} \cdot \nabla) \phi$$

Scalar (0-forms)

$$\mathcal{L}_u \rho = \nabla \cdot (\mathbf{u} \rho)$$

Density-like (3-forms)

$$E^\phi[\phi]$$

Associated energy

$$\mu^\phi = \frac{\delta E^\phi[\phi]}{\delta \phi}$$

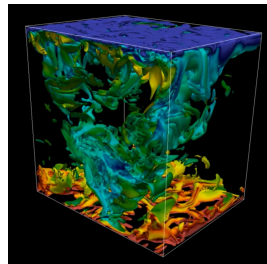
Variational derivative

$$\frac{d E^\phi}{dt} = \langle \mu^\phi, \partial_t \phi \rangle = - \langle \mu^\phi, \mathcal{L}_u \phi \rangle$$

$$\langle \mathbf{u}, \mathbf{f}^p \rangle = \langle \mu^\phi, \mathcal{L}_u \phi \rangle$$

Energy balance

$$\langle a, b \rangle := \int_{\Omega} ab \, d\Omega \quad \langle \mathbf{a}, \nabla \phi \rangle = - \langle \nabla \cdot \mathbf{a}, \phi \rangle$$



A new general framework for multiphysics

Application to buoyancy-driven flows

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

Associated force

$$\frac{\partial \rho}{\partial t} + \mathcal{L}_u \rho = 0$$

Lie derivative

$$\mathcal{L}_u \phi = (\mathbf{u} \cdot \nabla) \phi$$

Scalar (0-forms)

$$\mathcal{L}_u \rho = \nabla \cdot (\mathbf{u} \rho)$$

Density-like (3-forms)

$$E^\phi[\phi]$$

Associated energy

$$E^p[\rho] = \int_{\Omega} \rho g y d\Omega$$

$$\mu^\phi = \frac{\delta E^\phi[\phi]}{\delta \phi}$$

Variational derivative

$$\mu^p = \frac{\delta E^p[\rho]}{\delta \rho} = gy$$

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Energy balance

$$\langle \mathbf{a}, \mathbf{b} \rangle := \int_{\Omega} \mathbf{a} \cdot \mathbf{b} d\Omega \quad \langle \mathbf{a}, \nabla \phi \rangle = - \langle \nabla \cdot \mathbf{a}, \phi \rangle$$

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Energy balance

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A new general framework for multiphysics

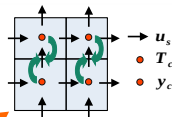
Buoyancy-driven flows on staggered grids

$$\Omega_s \frac{d\mathbf{u}_s}{dt} + C(\mathbf{u}_s) \mathbf{u}_s = D \mathbf{u}_s - \Omega_s \mathbf{p}_c + \Omega_s \mathbf{f}_s^p$$

$$\Omega_c \frac{d\mathbf{p}_c}{dt} + C_c(\mathbf{u}_s) \mathbf{p}_c = \mathbf{0}_c$$

$$C_c(\mathbf{u}_s) := M U_s \Pi_{cs}$$

$$U_s = \text{diag}(\mathbf{u}_s)$$



Cell-to-face
interpolation

$$E_h^p[\mathbf{p}_c] := g \mathbf{p}_c \cdot \Omega_c \mathbf{y}_c$$

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A new general framework for multiphysics

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Cell-to-face interpolation

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A new general framework for multiphysics

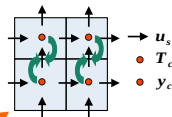
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A new general framework for multiphysics

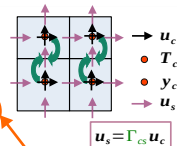
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A new general framework for multiphysics

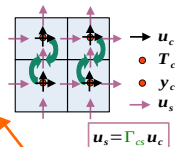
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A new general framework for multiphysics

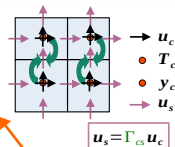
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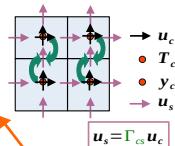
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$$\mathbf{f}^p = -\rho \nabla \mu^p = -\rho g \mathbf{e}_y$$

A new general framework for multiphysics

Summary

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = \nu \nabla^2 \mathbf{u} - \nabla p + \mathbf{f}^\phi$$

Associated force

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$$\mathcal{L}_u \phi = (\mathbf{u} \cdot \nabla) \phi$$

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Associated energy

$$\mathcal{L}_u$$

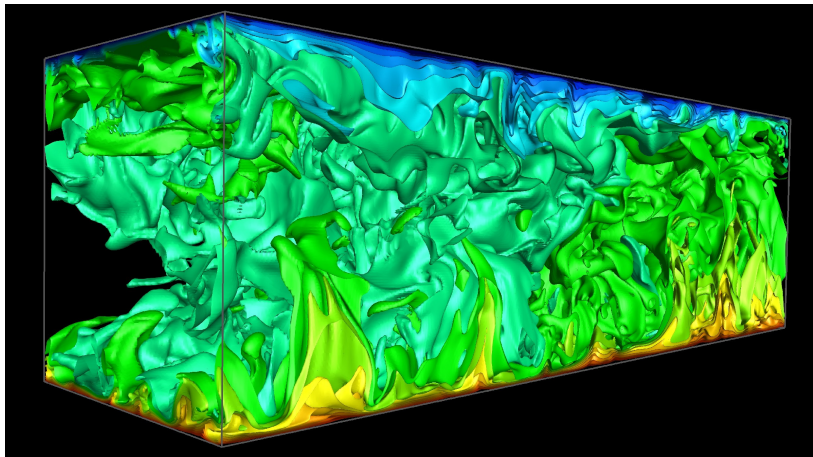
Lie derivative

$$\left. \begin{array}{l} E^\phi[\phi] \\ \mathcal{L}_u \end{array} \right\} \Rightarrow \mathbf{f}^\phi$$

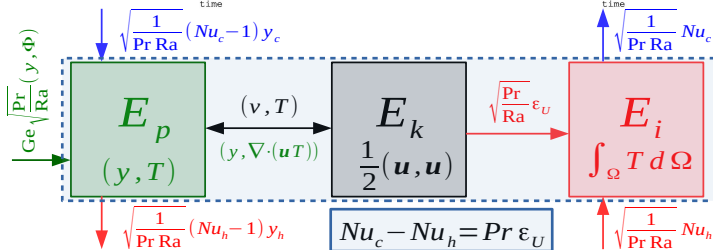
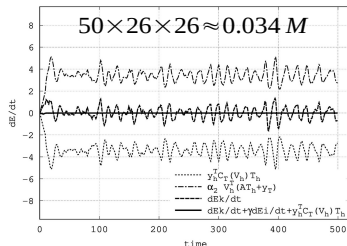
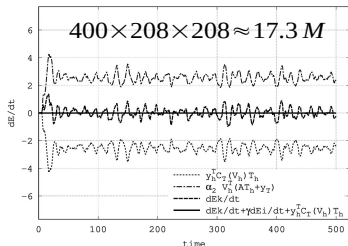
Leitmotiv: transport equation and its associated force
cannot be discretized independently!!!

Buoyancy-driven flows

Turbulent Rayleigh–Bénard convection at $Ra = 10^8$

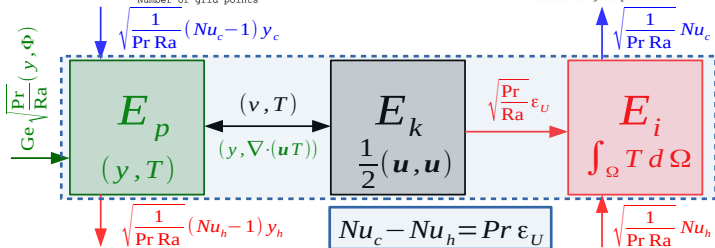
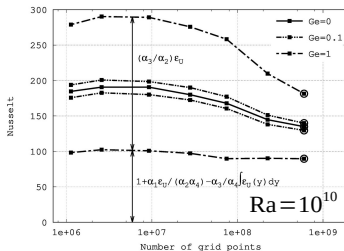
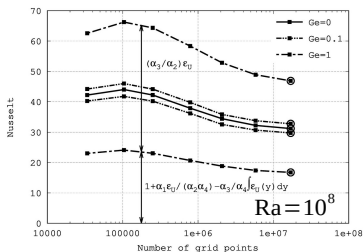


Buoyancy-driven flows⁶



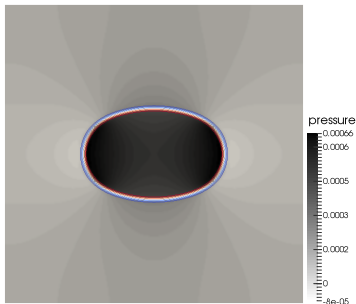
⁶B.Sanderse, F.X.Trias. *Energy-consistent discretization of viscous dissipation with application to natural convection flow*, **Computers & Fluids**, 286:106473, 2025.

Buoyancy-driven flows⁶

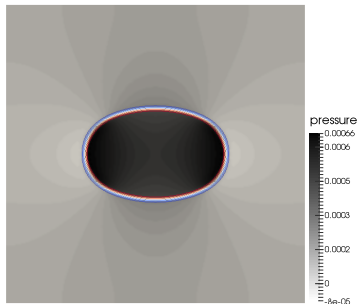


⁶B.Sanderse, F.X.Trias. *Energy-consistent discretization of viscous dissipation with application to natural convection flow*, **Computers & Fluids**, 286:106473, 2025.

Multiphase flows⁶



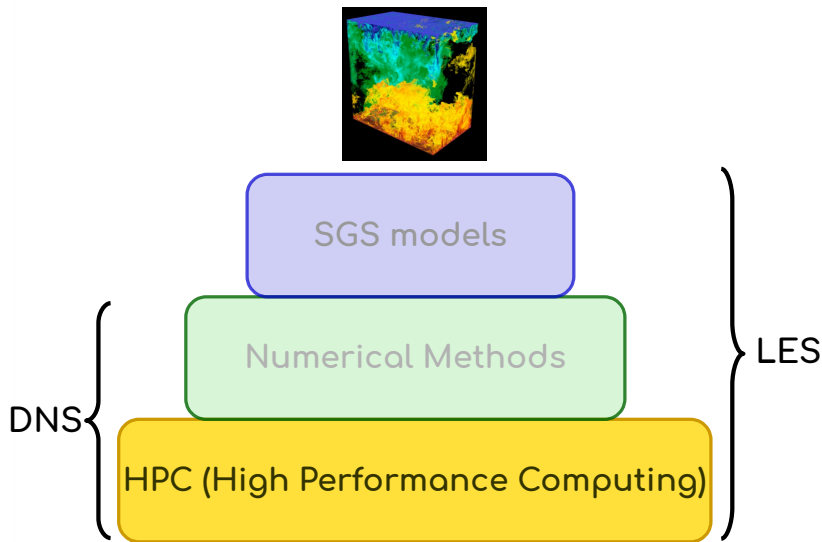
Non-symmetry-preserving!



Symmetry-preserving!

⁶N.Valle, F.X.Trias, and J.Castro. *An energy-preserving level set method for multiphase flows*. **Journal of Computational Physics**, 400(1):108991, 2020

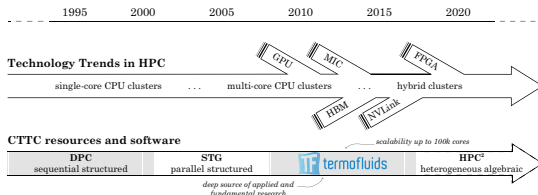
HPC on modern supercomputers



HPC on modern supercomputers

Research question #3:

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



⁷ X.Álvarez, A.Gorobets, F.X.Trias, R.Borrell, and G.Oyarzun. *HPC² - a fully portable algebra-dominant framework for heterogeneous computing. Application to CFD*. **Computers & Fluids**, 173:285-292, 2018

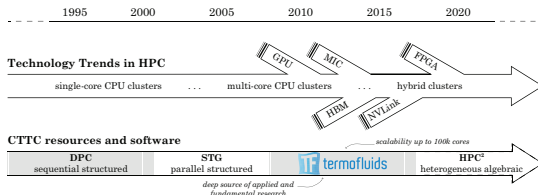
⁸ À.Alsalti-Baldellou, X.Álvarez-Farré, F.X.Trias, A.Oliva. *Exploiting spatial symmetries for solving Poisson's equation*. **Journal of Computational Physics** 486:112133, 2023.

⁹ J.Plana-Riu, F.X.Trias, À.Alsalti-Baldellou, X.Álvarez-Farré, G.Colomer, A.Oliva. *Exploiting repeated matrix block structures for more efficient CFD on modern supercomputers*, **Computer Physics Communications**, 326:110232, 2026.

HPC on modern supercomputers

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HPC²: portable, algebra-based framework for heterogeneous computing is developed⁷. 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 developed^{8,9}.

⁷ X.Álvarez, A.Gorobets, F.X.Trias, R.Borrell, and G.Oyarzun. *HPC² - a fully portable algebra-dominant framework for heterogeneous computing. Application to CFD*. **Computers & Fluids**, 173:285-292, 2018

⁸ À.Alsalti-Baldellou, X.Álvarez-Farré, F.X.Trias, A.Oliva. *Exploiting spatial symmetries for solving Poisson's equation*. **Journal of Computational Physics** 486:112133, 2023.

⁹ J.Plana-Riu, F.X.Trias, À.Alsalti-Baldellou, X.Álvarez-Farré, G.Colomer, A.Oliva. *Exploiting repeated matrix block structures for more efficient CFD on modern supercomputers*, **Computer Physics Communications**, 326:110232, 2026.

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

Continuous

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

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

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

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

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

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

Discrete

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

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

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

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

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

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

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Minimal set of kernels:

$$\text{SpMV} : \quad \mathbf{y} \leftarrow \mathbf{A} \mathbf{x}$$

$$\text{axpy} : \quad \mathbf{z} \leftarrow \mathbf{a} \mathbf{x} + \mathbf{b} \mathbf{y}$$

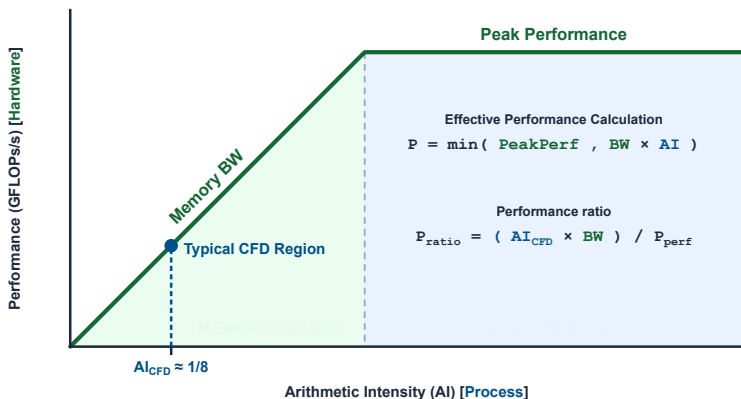
$$\text{dot} : \quad r \leftarrow \mathbf{x} \cdot \mathbf{y}$$

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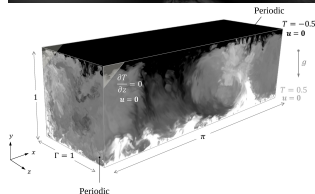
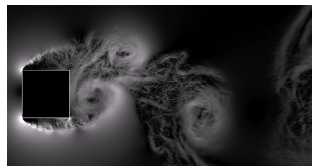
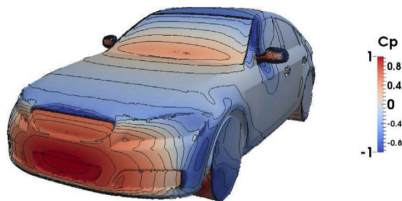
SpMV : $y \leftarrow Ax$

axpy : $z \leftarrow ax + by$

dot : $r \leftarrow x \cdot y$

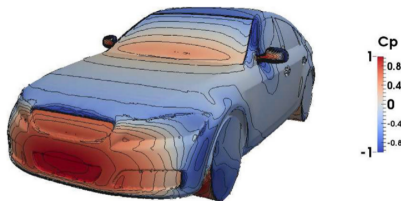


Algebra-based approach naturally leads to portability, to simple and analyzable formulations and opens the door to new strategies^{10,11} to improve its performance...

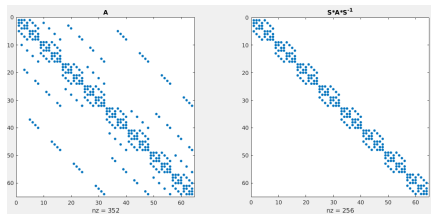


¹⁰À. Alsalti-Baldellou, X. Álvarez-Farré, F.X. Trias, A. Oliva. *Exploiting spatial symmetries for solving Poisson's equation.* *Journal of Computational Physics* 486:112133, 2023.

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



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

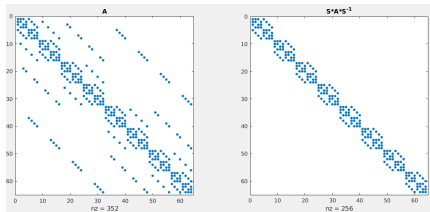
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- Higher arithmetic intensity (AI)
- Reduction of memory footprint
- Reduction in the number of iterations

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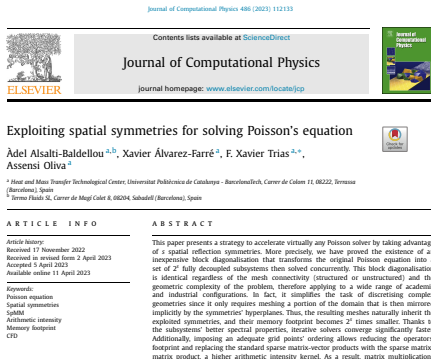
Benefits for Poisson solver are 3-fold:

- Higher arithmetic intensity (AI)
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→ Overall speed-up up to **x2-x3** ✓

→ Memory reduction of **≈2** ✓

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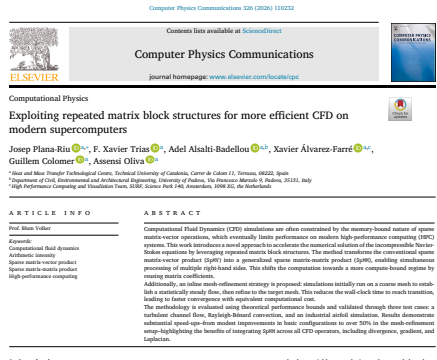
Algebra-based approach naturally leads to portability, to simple and analyzable formulations and opens the door to new strategies^{10,11} to improve its performance...

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

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

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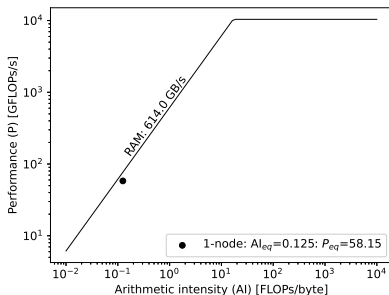
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Performance analysis

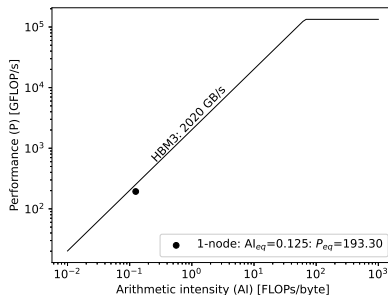
Roofline

MareNostrum 5-GPP



- 2 × Intel Xeon Platinum 8480+ (Sapphire Rapids)
- DP peak: **7.17 Tflop/s/node**
- Theoretical memory BW: **614 GB/s/node**
- Roofline ridge point: ≈ 11.7 flop/byte

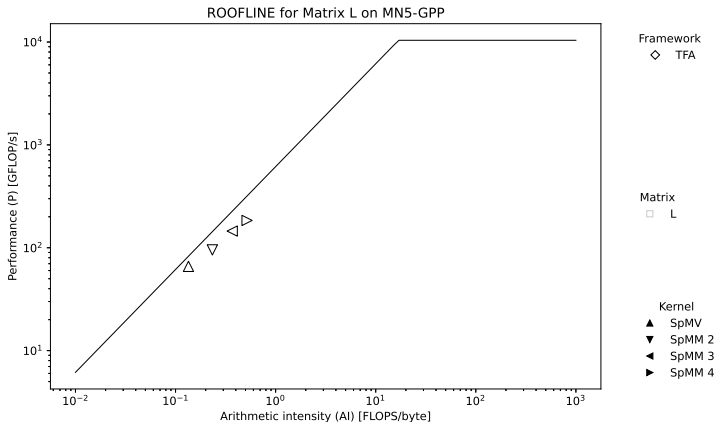
MareNostrum 5-ACC



- 4 × NVIDIA H100 64 GB per node
- FP64 peak: ≈ 27 Tflop/s/GPU
- HBM bandwidth: ≈ 2.02 TB/s/GPU
- Roofline ridge point: ≈ 13.4 flop/byte

Performance analysis

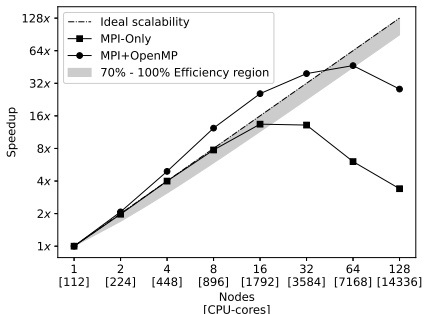
Roofline: SpMV versus SpMM



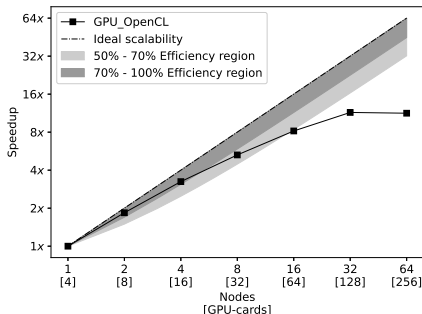
Performance analysis

Strong scaling

MareNostrum 5-GPP



MareNostrum 5-ACC



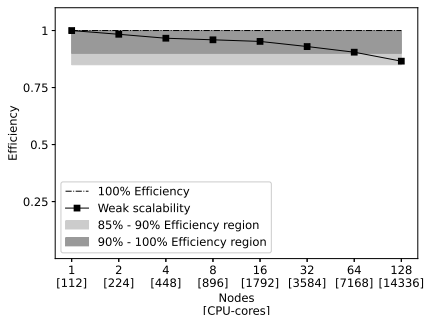
- $350 \times 480 \times 350 \approx 58.8M$ CVs
- 525k CVs (1 node) $\rightarrow$ 4100 CV (128 nodes) per core

- $500 \times 1000 \times 340 \approx 170M$ CVs
- 42.5M CVs (1 node) $\rightarrow$ 664k (64 nodes) per GPU

Performance analysis

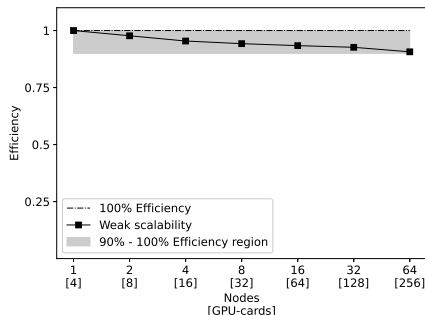
Weak scaling

MareNostrum 5-GPP



- 350 × 480 × 350 ≈ 58.8M CVs per node
- 58.8M CVs (1 node) → 7.52B CVs (128 nodes)

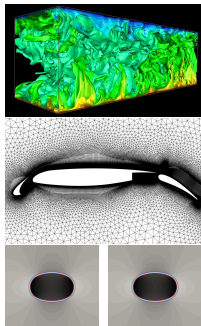
MareNostrum 5-ACC



- 500 × 1000 × 340 ≈ 170M CVs per node
- 170M CVs (1 node) → 10.88B (64 nodes) per GPU

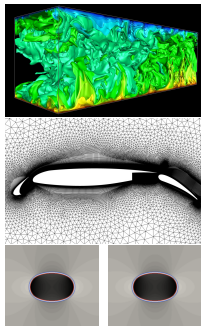
Take-away messages

- **Preserving symmetries** is the key point for **reliable LES/DNS** simulations also for industrial problems.



Take-away messages

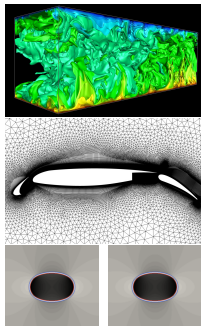
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$$\boxed{\{E^\phi[\phi], \mathcal{L}_u\} \implies \mathbf{f}^\phi}$$

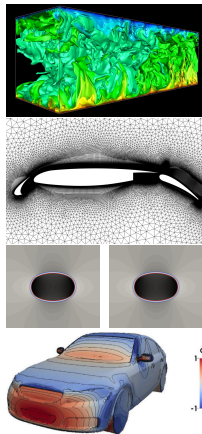


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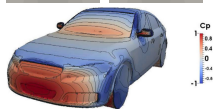
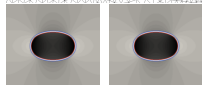
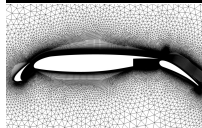
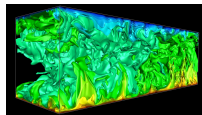
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- **Open-source** platforms help to share and disseminate ideas.

<https://github.com/janneshopman/RKSymFoam>



OpenFOAM



Thank you for your attention

