



Centre Tecnològic de Transferència de Calor
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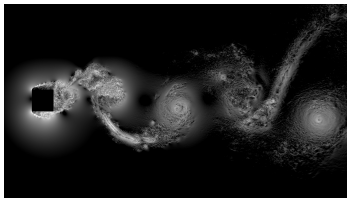
Consistent energy-exchange discretizations

F. Xavier Trias¹, Sara-Medina Šehović¹, Andrey Gorobets², Assensi Oliva¹

¹ Heat and Mass Transfer Technological Center, Technical University of Catalonia (UPC)

² Keldysh Institute of Applied Mathematics of RAS, Russia

WCCM-ECCOMAS 2026, Munich, 19-24 July 2026





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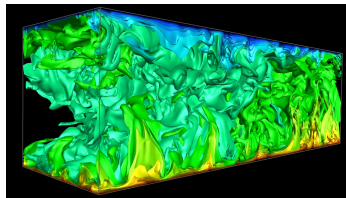
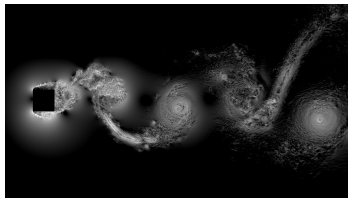
Consistent energy-exchange discretizations for multiphysics flows

F. Xavier Trias¹, Sara-Medina Šehović¹, Andrey Gorobets², Assensi Oliva¹

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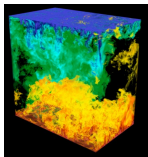


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- 1 Motivation
- 2 Preserving symmetries
- 3 Energy exchange in multiphysics
- 4 A framework for multiphysics
- 5 Results
- 6 Take-away messages

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

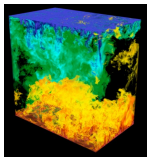
For canonical academic flows...



DNS {

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

For canonical academic flows...



MareNostrum 5-ACC
(Barcelona)



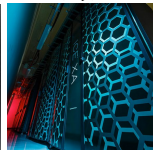
rank #8
1120 nodes with:
2x Intel Shappire Rapids 8460
1x NVIDIA Hopper 64 GB HBM
1x Infiniband NDR200

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

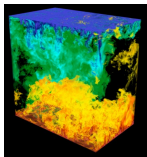


DNS {

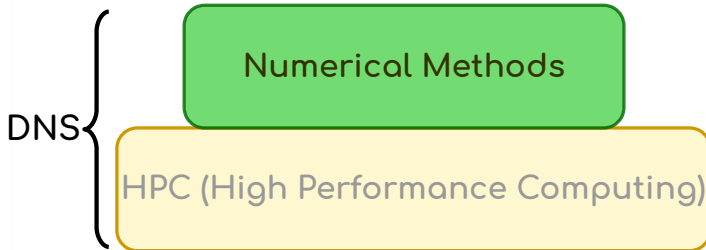
HPC (High Performance Computing)

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

For canonical academic flows...



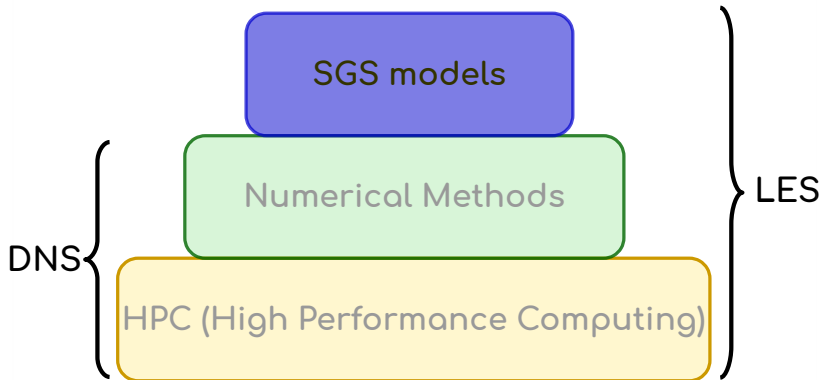
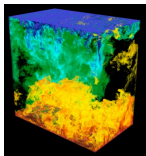
How to properly discretize NS?



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

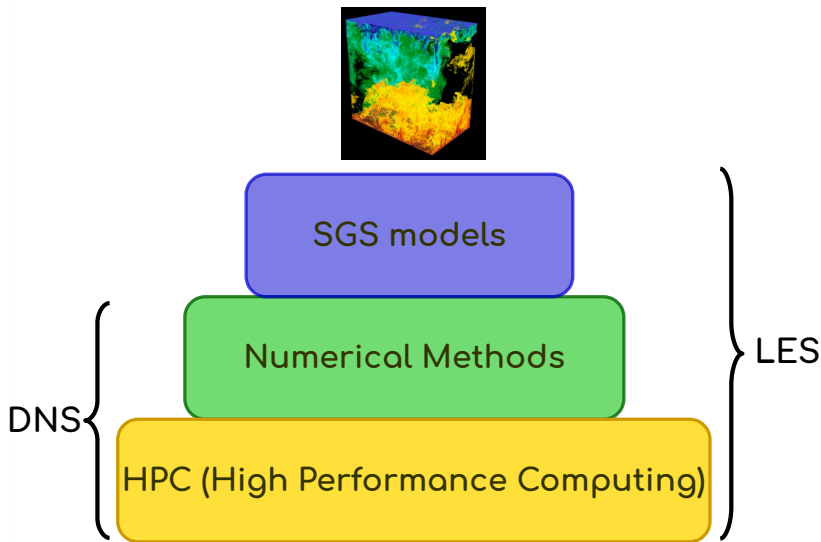
For canonical academic flows...

How to
properly
model SGS?



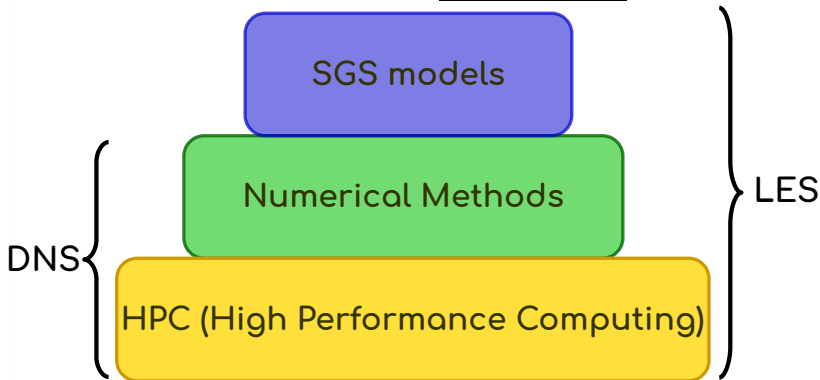
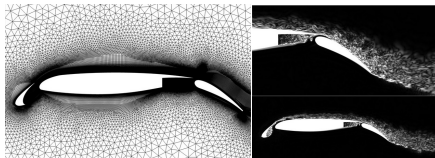
General motivation: (very) large-scale DNS/LES

For canonical academic flows...



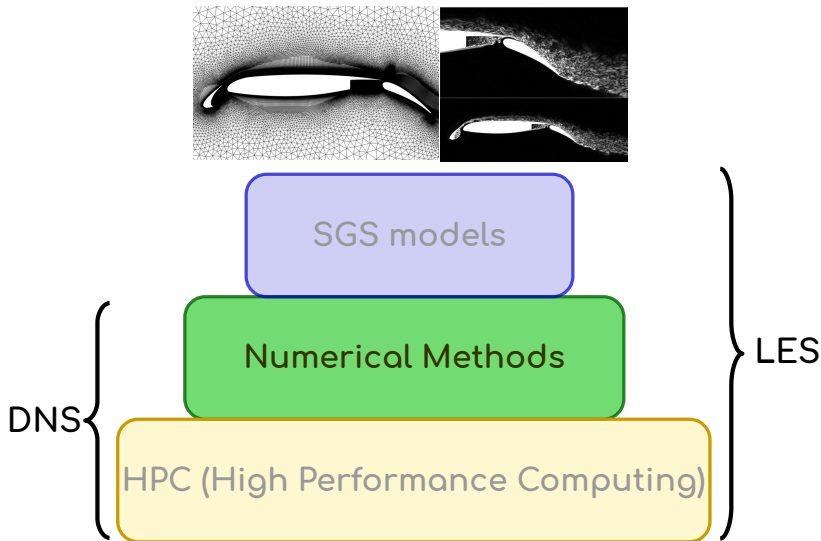
General motivation: (very) large-scale DNS/LES

...but also for industrial applications



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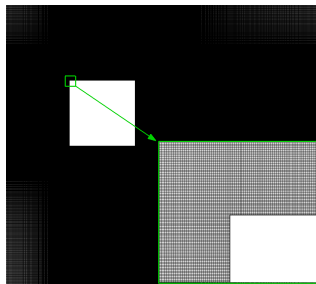
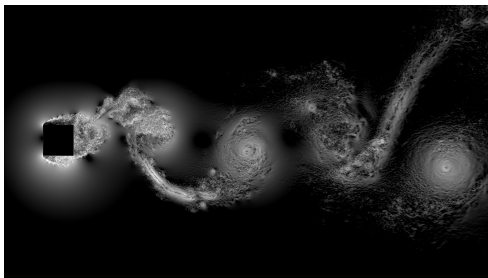
...but also for industrial applications



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?



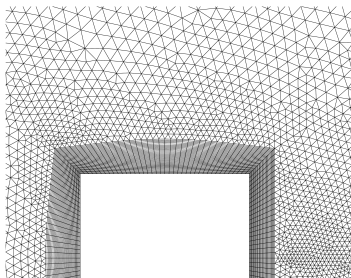
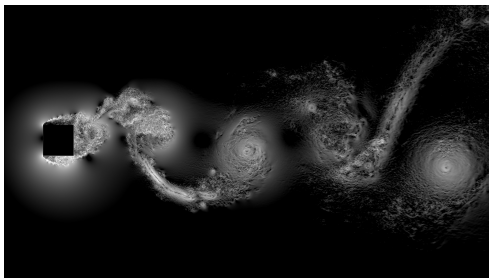
DNS¹ of the flow around a square cylinder at $Re = 55000$ (2.6B grid points)

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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Symmetry-preserving discretization

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

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

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

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

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

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

Symmetry-preserving discretization

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

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Discrete

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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

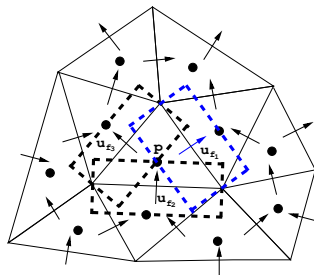
OpenFOAM®



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

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+



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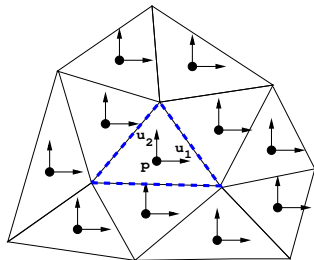
OpenFOAM®



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

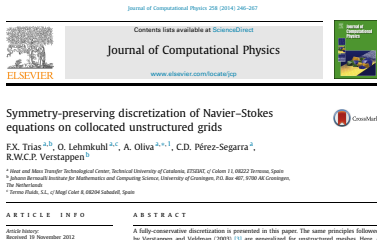
In collocated meshes

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



Why a collocated formulation?

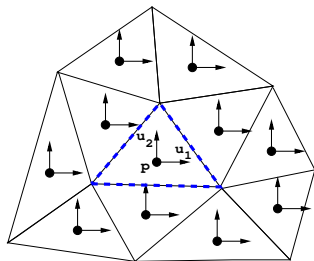
Everything is easy except the pressure-velocity coupling...



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

In collocated meshes

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



Why a collocated formulation?

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



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

^aHeat and Mass Transfer Technological Center, Technical University of Catalonia, ETSEIAT, c/ Colom 11, 08222 Terrassa, Spain
^bJohn von Neumann Institute for Mathematics and Computing Science, University of Göttingen, PO Box 407, 37080 AE Göttingen, The Netherlands
^cTerrassa 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) [1] are generalized for unstructured meshes. Here, a



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

^aResearch and Innovation department, Nuclear Research and consultancy Group NRC, PO Box 25, 2609 PE Petten, The Netherlands
^bHeat and Mass Transfer Technological Center, Technical University of Catalonia, ETSEIAT, c/ Colom 11, Terrassa 08222, Spain
^cRensselaer Institute for Mathematics, Computing Science, and Artificial Intelligence, University of Groningen, PO Box 407, AE Groningen 9700, The Netherlands

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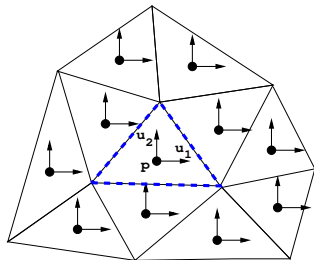
ABSTRACT

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) [1], which is further extended and improved to be more computationally efficient.

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

In collocated meshes

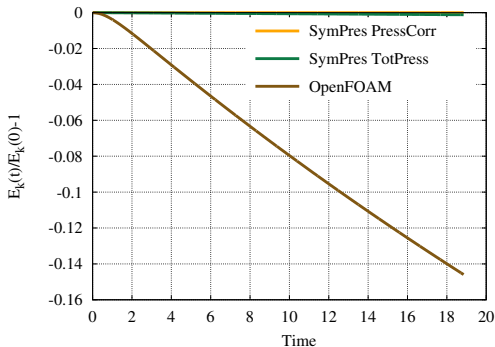
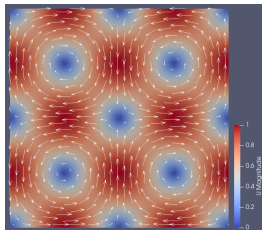
- $p-u_c$ coupling is cumbersome ✗
- $C(u_s)$ and D easy to discretize ✓
- Cheaper, less memory, ... ✓



Pressure-velocity coupling on collocated grids

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

Open▽FOAM

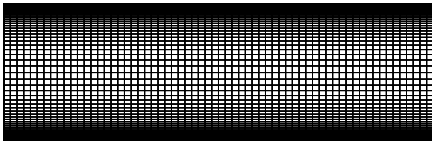


Results for an inviscid Taylor-Green vortex³

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

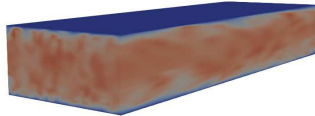
Received 10 May 2024; revised 10 May 2024; accepted 10 May 2024; available online 10 May 2024

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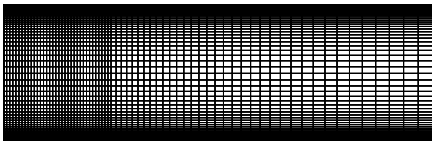
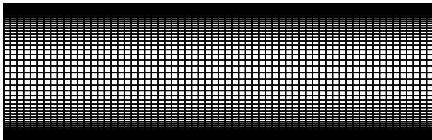
This work establishes the conditions for having a symmetry-preserving unconditionally stable projection method for incompressible flows, such as PISO or Fractional Step Method (FSM), on collocated unstructured grids based on a compact stencil Poisson equation. Its formulation is based on preserving the 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 operator and the geometrical conditions are mathematically verified, even in cases where the mesh is highly distorted. This will be proven both theoretically and numerically. One criterion 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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D. Santos¹, J.A. Hopman, C.D. Pérez-Segarra, F.X. Trias

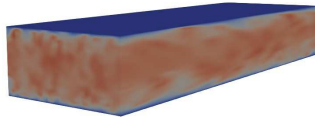
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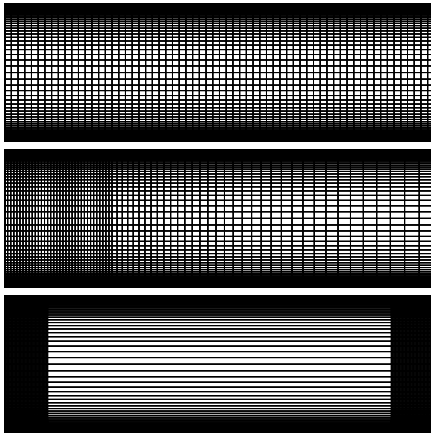
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Journal of Computational Physics 523 (2025) 113631



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

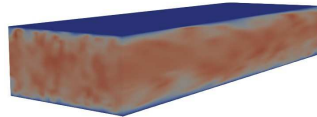
^a Institut de Recerca en Energia del Baix Llobregat (IREB), Departament d'Enginyeria i Ciències de l'Espai, Universitat Politècnica de Catalunya, 08035 Barcelona, Spain

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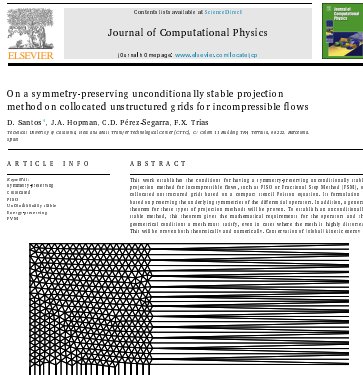
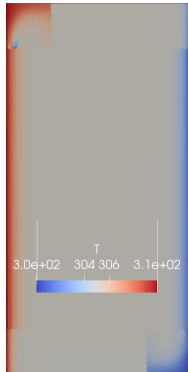
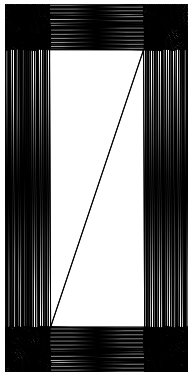
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Pressure-velocity coupling on collocated grids

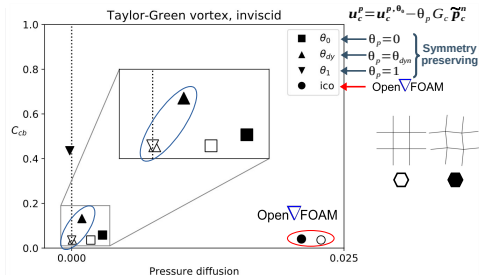
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Pressure-velocity coupling on collocated grids

... 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}, J. Rigola^a, F. X. Trias^a

^a IREC 2018-2021 TALENTS TECHNOLOGICAL CENTER, TECNIO, 16100 L'ESPLEIG DE CAL, C/ COLADA, 11 TERRA, 46120, BURJASSOT, SPAIN

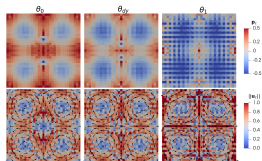
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ABSTRACT

This work presents a comprehensive implementation 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 formulation, 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 dissipation 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



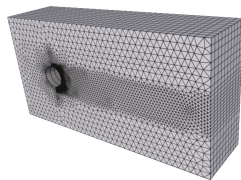
⁵J.A.Hopman, D.Santos, À.Alsaltí, J.Rigola, F.X.Trias. *Quantifying the checkerboard problem to reduce numerical dissipation*, **Journal of Computational Physics**, 521:113537, 2025. [arXiv: 2408.06821](https://arxiv.org/abs/2408.06821)

Pressure-velocity coupling on collocated grids

Summary

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

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

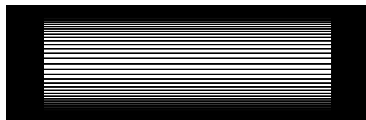


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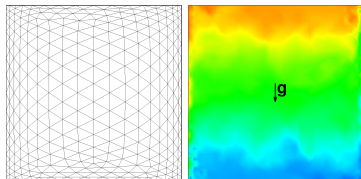


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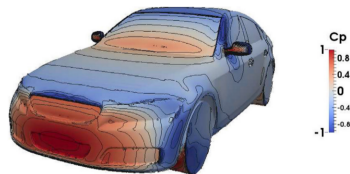
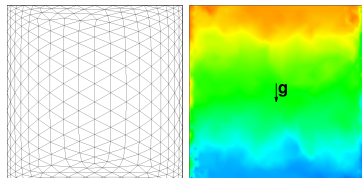


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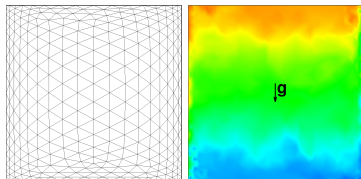


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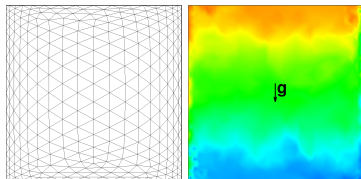


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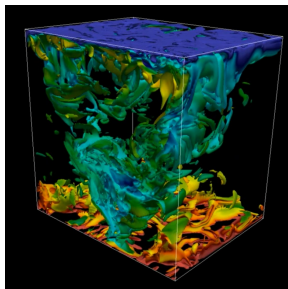


Research question #2:

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

Buoyancy-driven flows

Energy-exchanges



$$E_p$$

$$-(y, T)$$

$$E_k$$

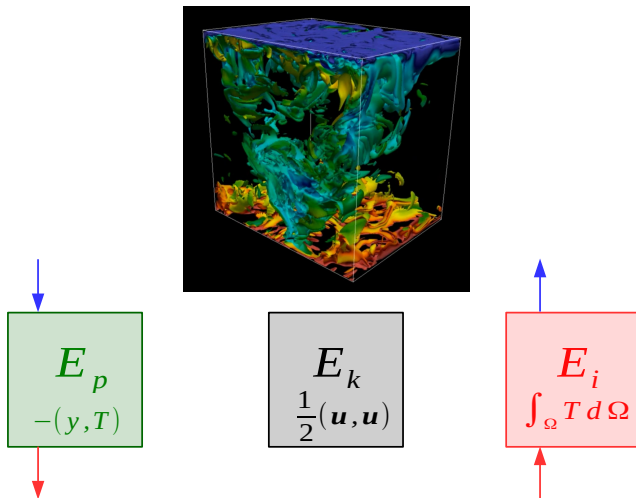
$$\frac{1}{2}(\mathbf{u}, \mathbf{u})$$

$$E_i$$

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

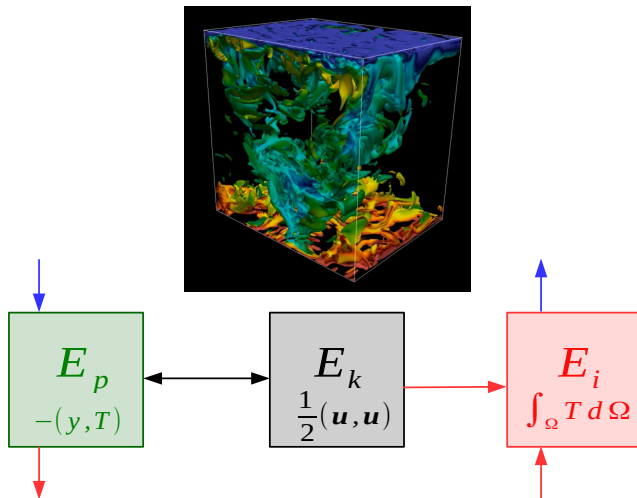
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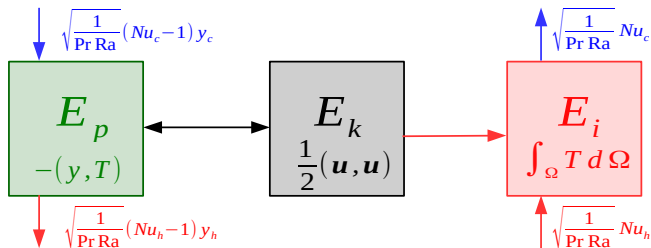
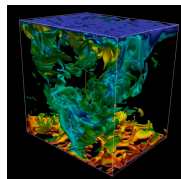


Buoyancy-driven flows

Continuous formulation

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

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



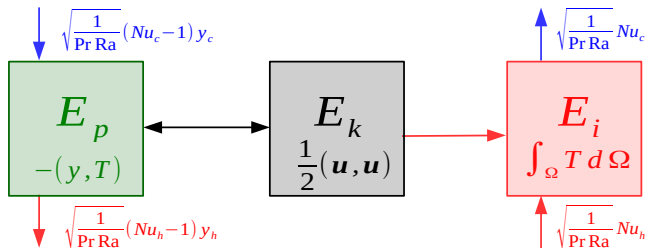
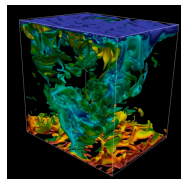
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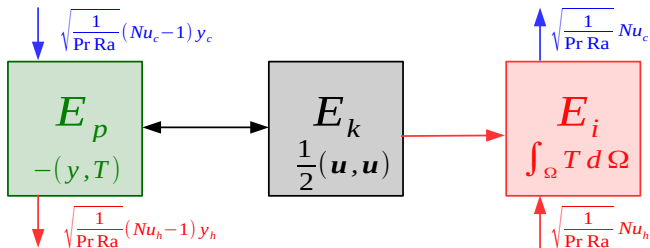
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$$\Phi = \|\nabla \mathbf{u}\|^2 \varepsilon_U = \int_{\Omega} \Phi d\Omega$$

$$(\mathbf{v}, T) = \int_{\Omega} \mathbf{v} T d\Omega$$

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

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



Buoyancy-driven flows

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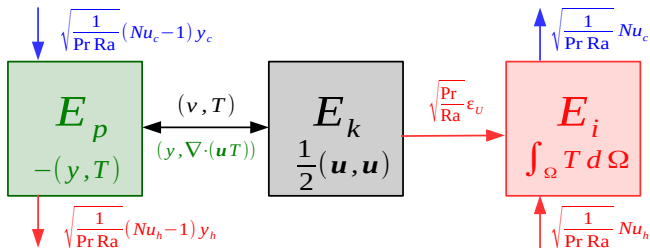
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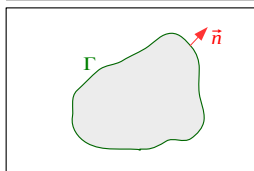
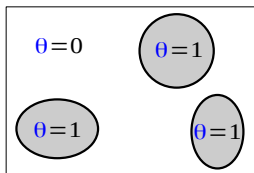
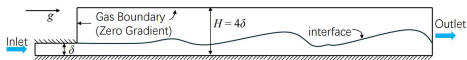
Multiphase flows

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

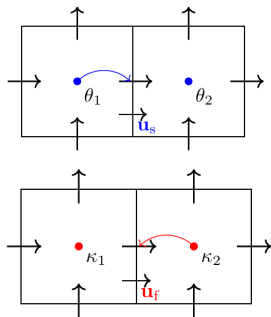
Conservative discrete formulation

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

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Surface tension



An energy-preserving level set method for multiphase flows

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

Heat and Mass Transfer Technological Centre (CTTC), Universitat Politècnica de Catalunya - BarcelonaTech (UPC), ESEMAT, Carrer Colom 11, 08222 Terrassa (Barcelona), Spain

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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

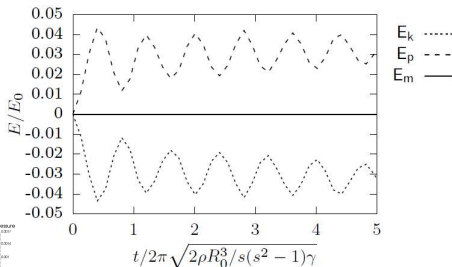
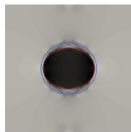
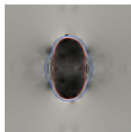
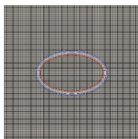
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Mechanical energy (kinetic+potential) is preserved!

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)

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

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Application to buoyancy-driven flows

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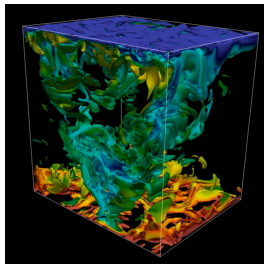
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$$\mathbf{f}^p = -\rho \nabla \mu^p = -\rho g \mathbf{e}_y$$

A new general framework for multiphysics

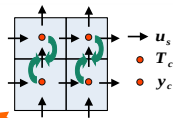
Buoyancy-driven flows on staggered grids

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

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

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

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



Cell-to-face
interpolation

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

$$\mu_c^p = \frac{\delta E^p[\mathbf{p}_c]}{\delta \mathbf{p}_c} = g \mathbf{y}_c$$

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

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A new general framework for multiphysics

Buoyancy-driven flows on staggered grids

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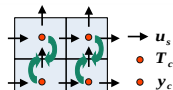
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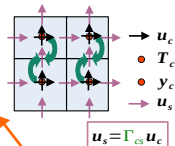
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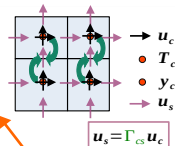
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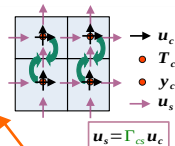
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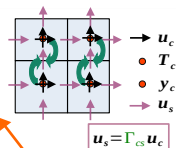
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A new general framework for multiphysics

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

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

Lie derivative

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

Scalar (0-forms)

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

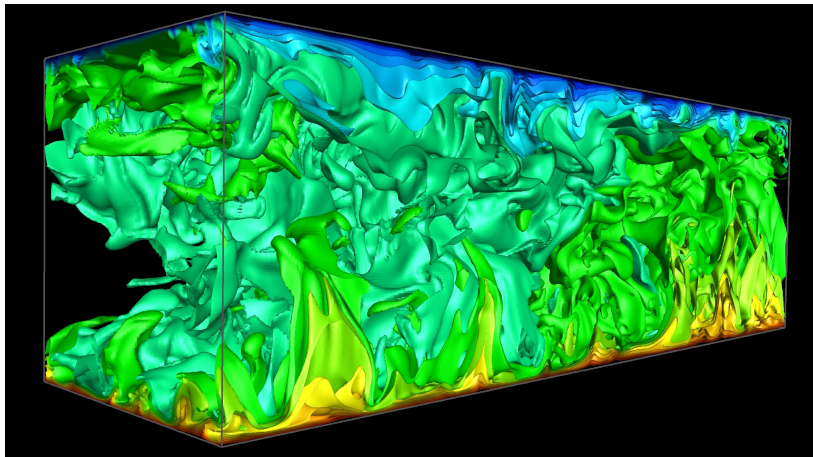
Density-like (3-forms)

$$\left. \begin{array}{ll} E^\phi[\phi] & \text{Associated energy} \\ \mathcal{L}_u & \text{Lie derivative} \end{array} \right\} \Rightarrow \mathbf{f}^\phi$$

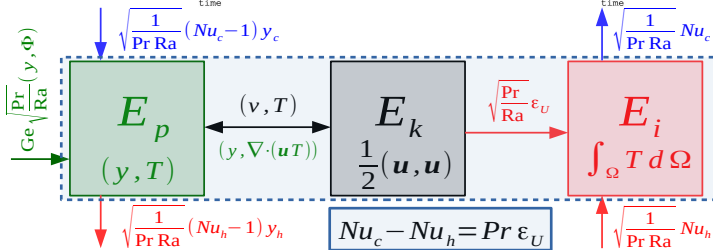
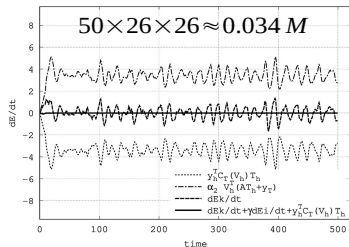
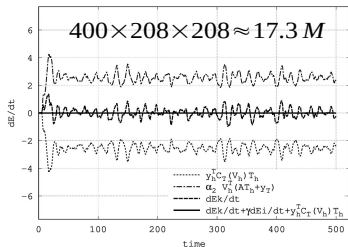
Leitmotiv: transport equation and its associated force
cannot be discretized independently!!!

Buoyancy-driven flows

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

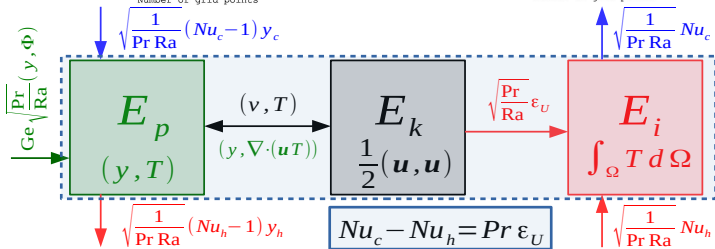
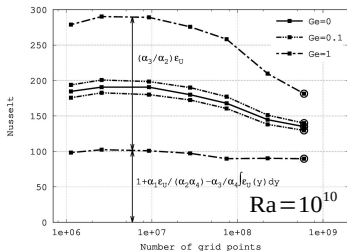
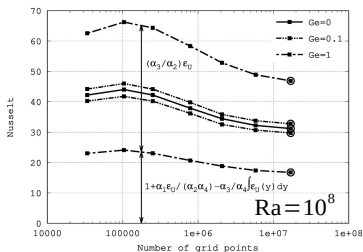


Buoyancy-driven flows⁶



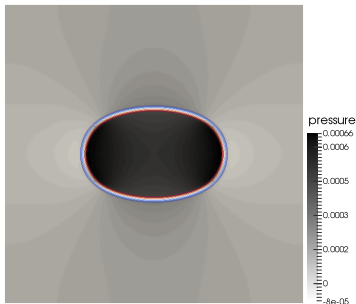
⁶B.Sanderse, F.X.Trias. *Energy-consistent discretization of viscous dissipation with application to natural convection flow*, **Computers & Fluids**, 286:106473, 2025.

Buoyancy-driven flows⁶

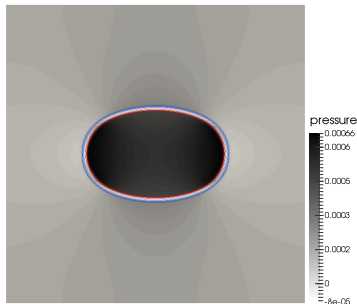


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Multiphase flows⁶



Non-symmetry-preserving!

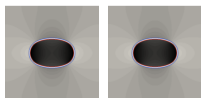
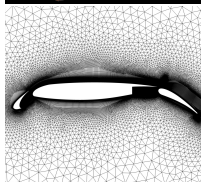
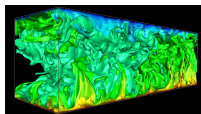


Symmetry-preserving!

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

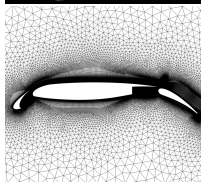
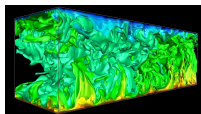
Take-away messages

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



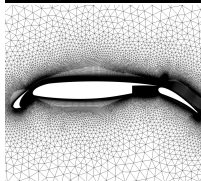
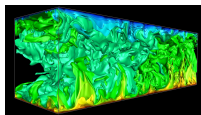
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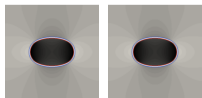
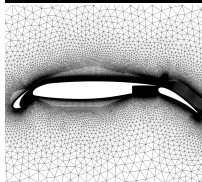
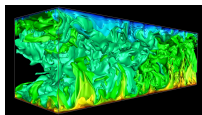


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$$\boxed{\{E^\phi[\phi], \mathcal{L}_u\} \implies \mathbf{f}^\phi}$$

- **Open-source** platforms helps to share and disseminate ideas.
<https://github.com/janneshopman/RKSymFoam>



Open▽FOAM

