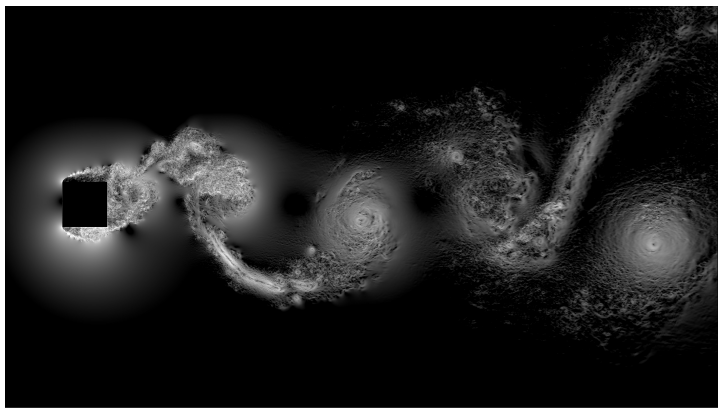
Centre Tecnològic de Transferència de Calor
UNIVERSITAT POLITÈCNICA DE CATALUNYA

Consistent energy-exchange discretizations

F. Xavier Trias[1], Sara-Medina Šehović[1], Andrey Gorobets[2], Assensi Oliva[1]

[1] Heat and Mass Transfer Technological Center, Technical University of Catalonia (UPC)
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WCCM-ECCOMAS 2026, Munich, 19-24 July 2026



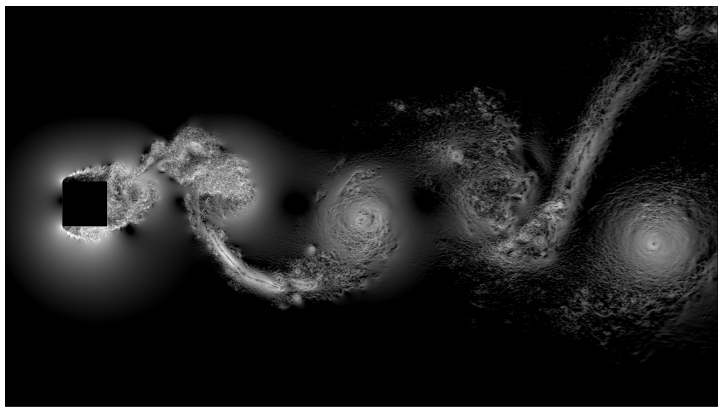
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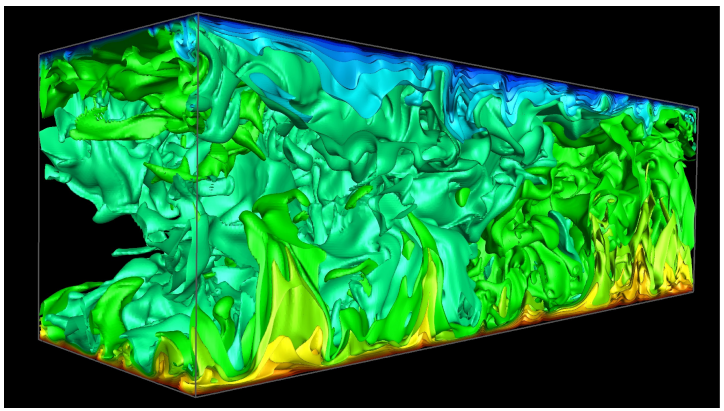
Consistent energy-exchange discretizations for multiphysics flows

F. Xavier Trias[1], Sara-Medina Šehović[1], Andrey Gorobets[2], Assensi Oliva[1]

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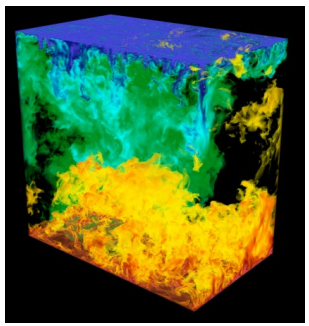


Contents

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

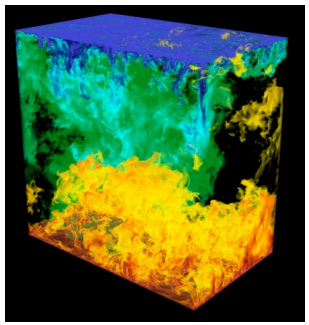
For canonical **academic** flows...



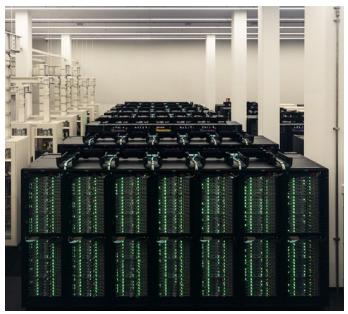
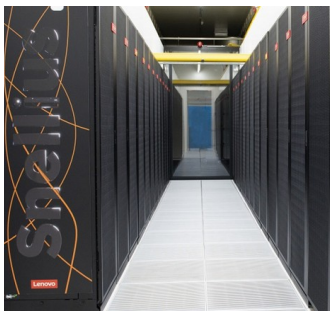
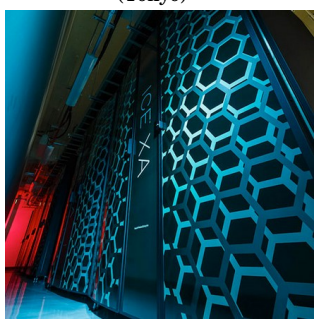
DNS

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

For canonical **academic** flows...



DNS

MareNostrum 5-ACC (Barcelona)	Snellius (Amsterdam)	TSUBAME4.0 (Tokyo)
		
rank #8 1120 nodes with: 2× Intel Shappire Rapids 8460 1× NVIDIA Hopper 64 GB HBM 1× Infiniband NDR200	rank #165 714 nodes with: 2× AMD EPYC 9654 96C 1× Infiniband NDR200	rank #31 240 nodes with: 2× AMD EPYC 9654 96-Core 4× NVIDIA H100 SXM5 1× Infiniband NDR200

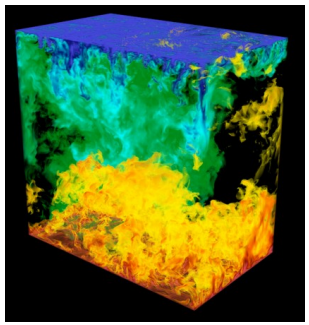




HPC (High Performance Computing)

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

For canonical **academic** flows...



How to properly discretize NS?

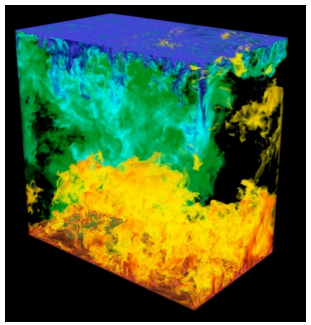
DNS

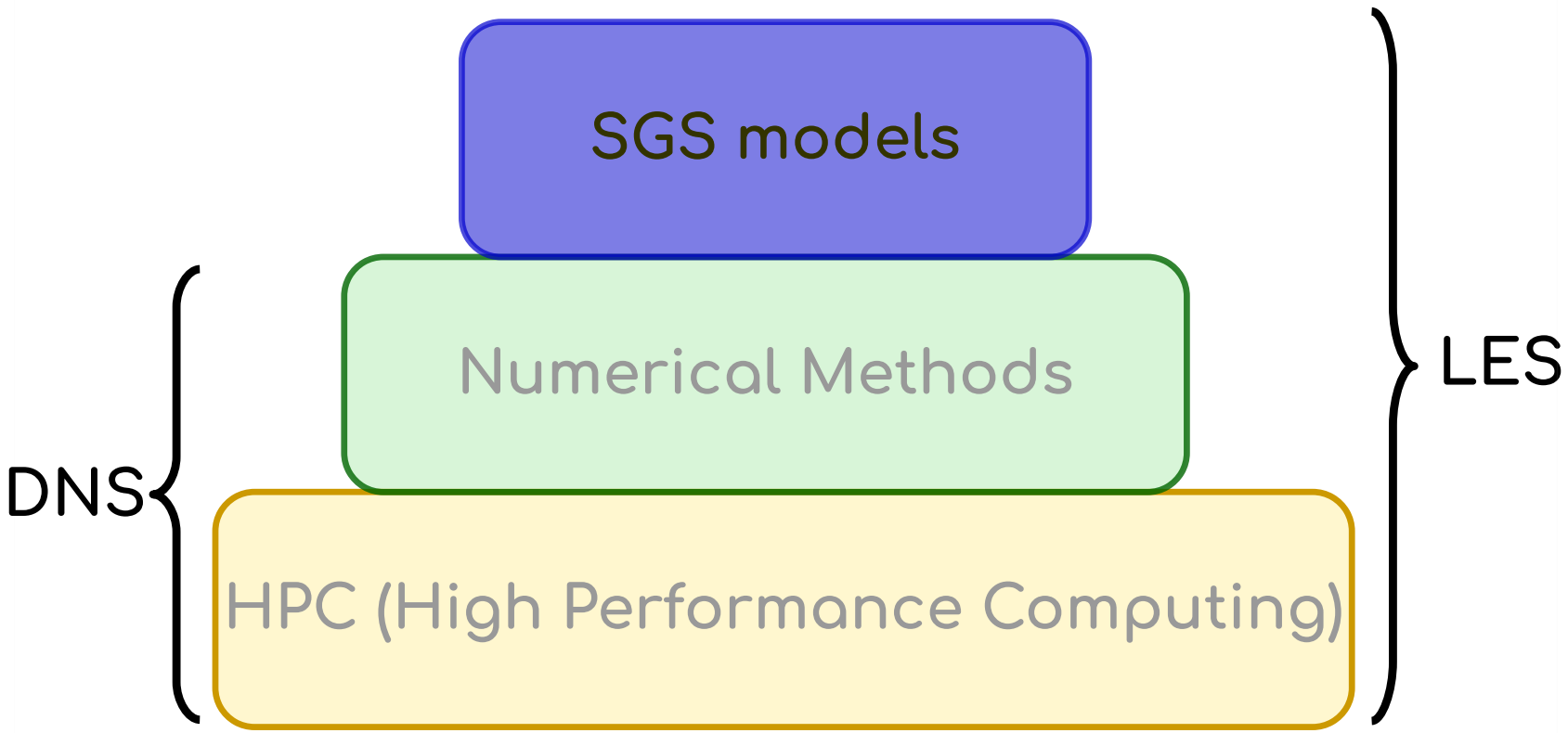
- Numerical Methods
- HPC (High Performance Computing)

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

For canonical **academic** flows...

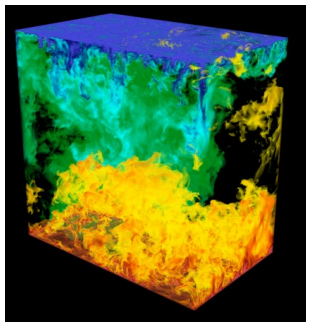
How to properly model SGS?

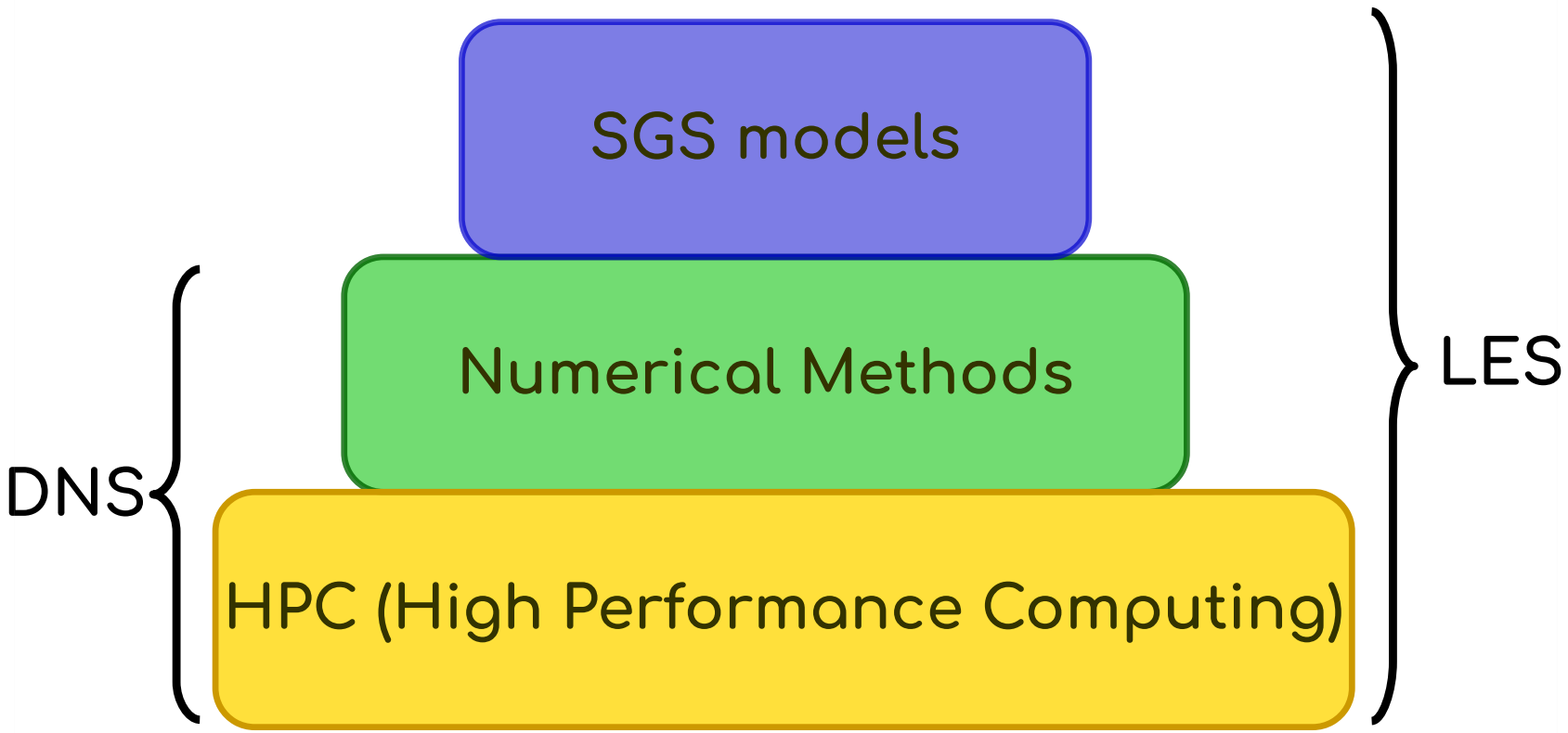




General motivation: (very) large-scale DNS/LES

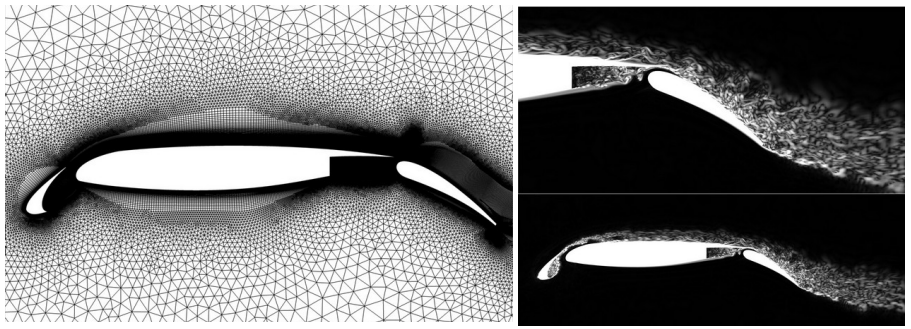
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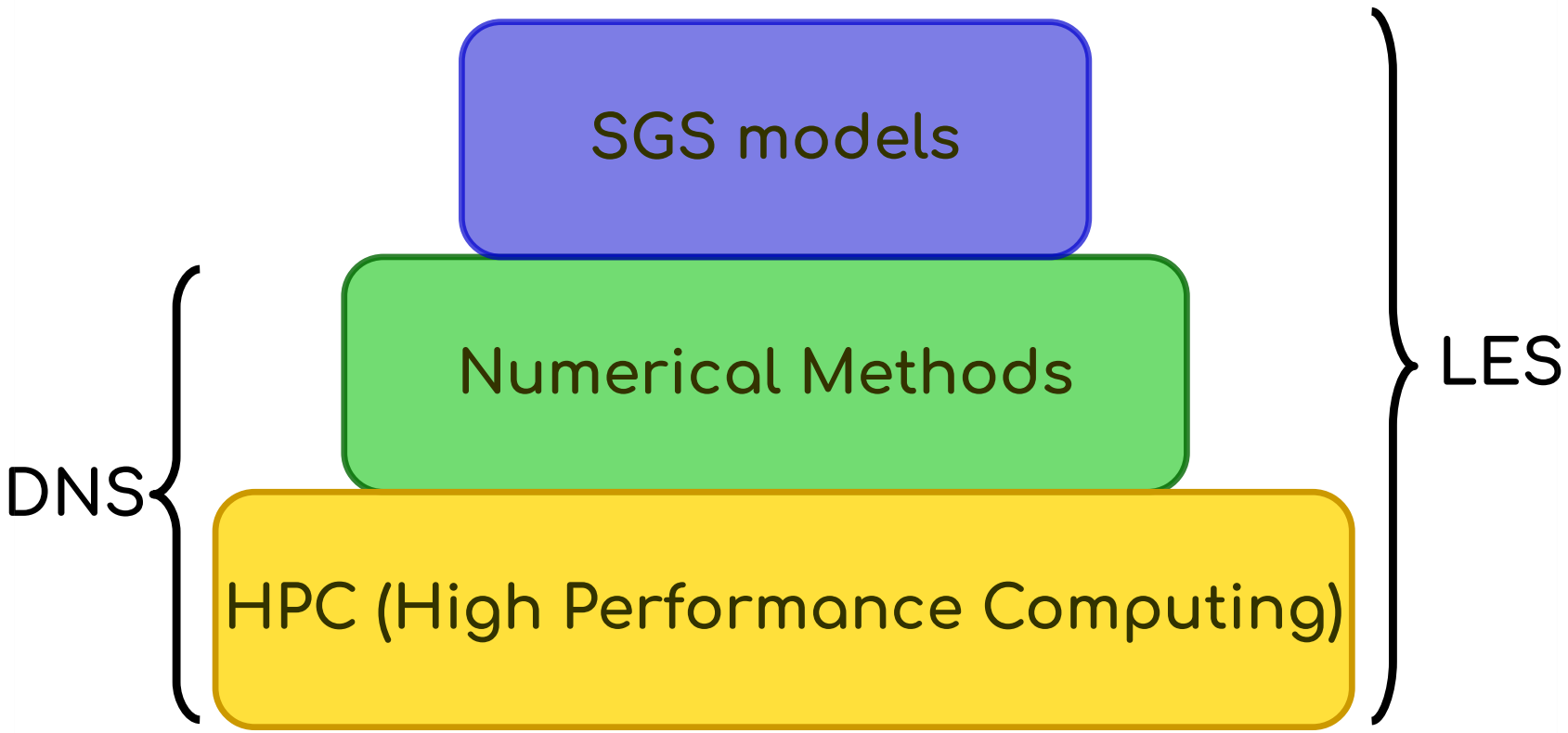




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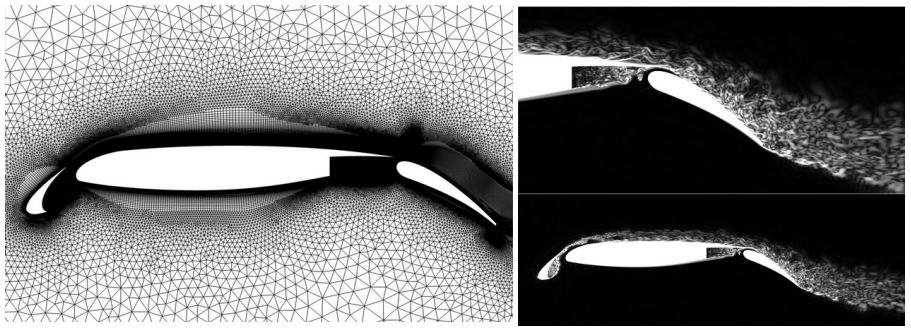
...but also for **industrial** applications

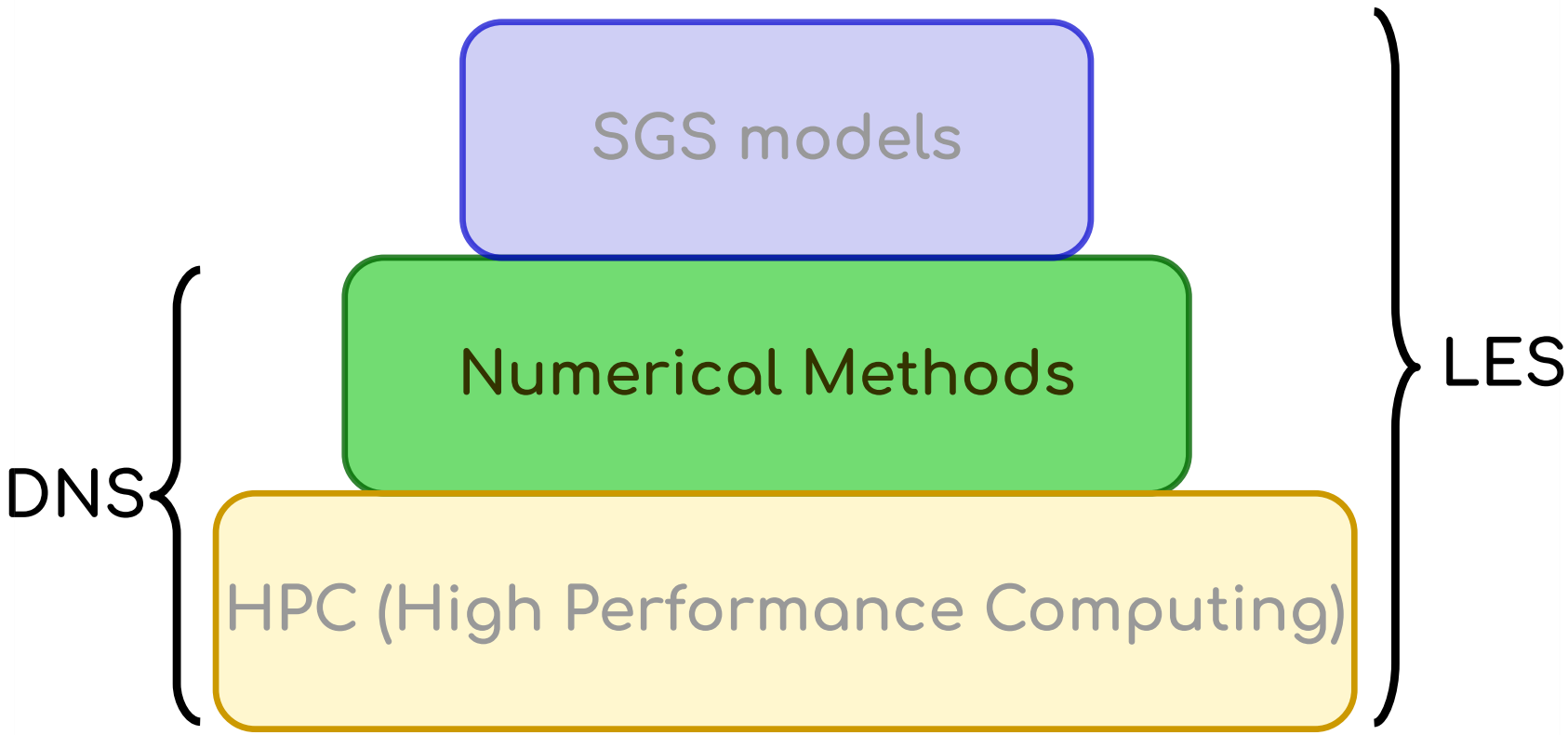




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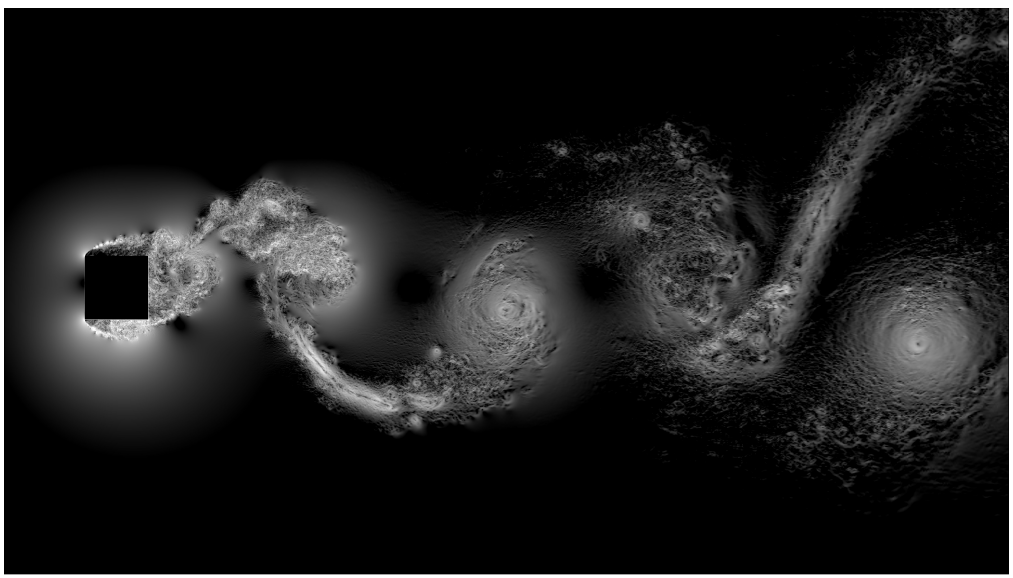


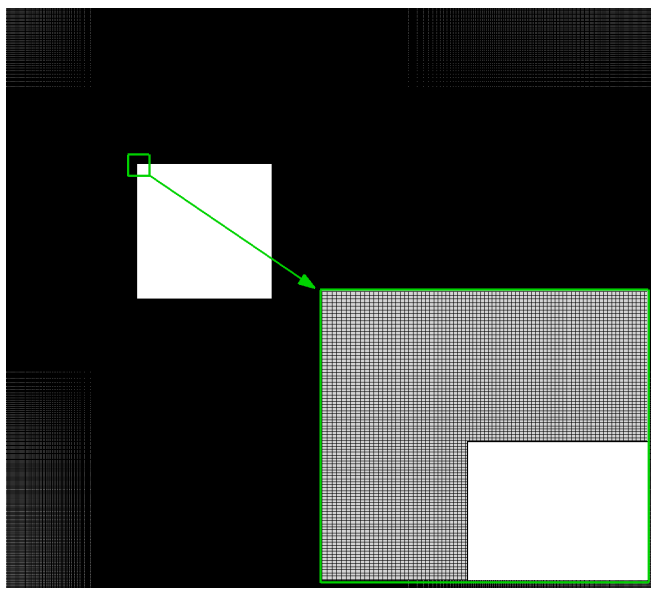


Numerical methods for DNS/LES

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?





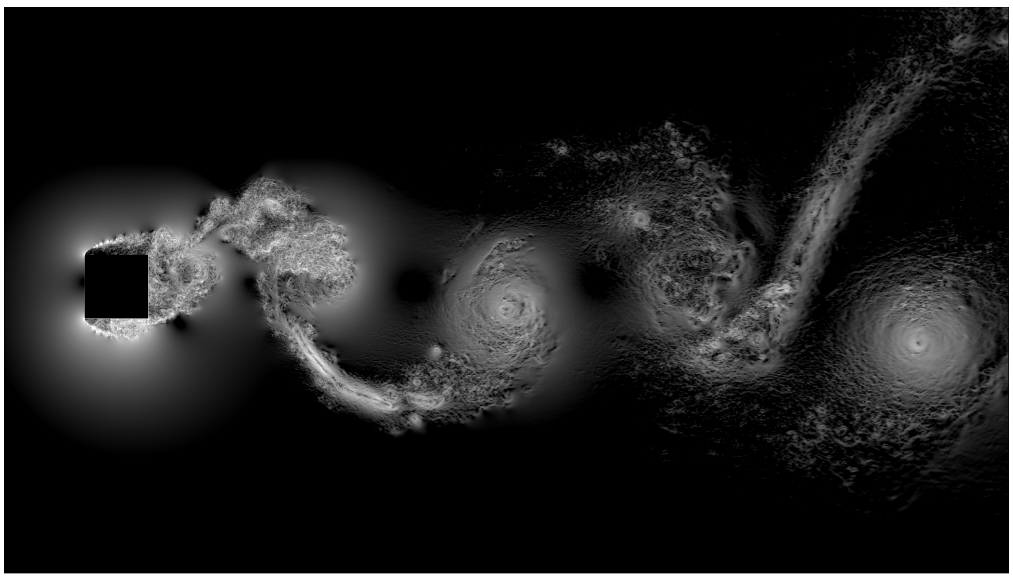
DNS[1] of the flow around a square cylinder at $Re = 55000$ (2.6B grid points)

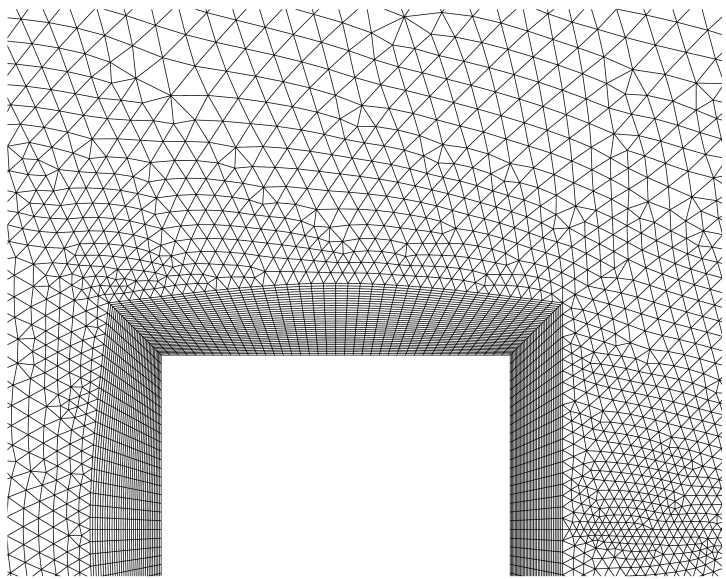
[1] F.X.Trias, À.Alsalti-Baldellou, A.Oliva. *On the Reynolds-number scaling of Poisson solver complexity*, **Physics of Fluids**, 38 (4):045157, 2026.

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Symmetry-preserving discretization

Continuous

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

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

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

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Discrete

$$\Omega \frac{d\boldsymbol{u}_h}{dt} + \mathrm{C}\left(\boldsymbol{u}_h\right) \boldsymbol{u}_h = \mathrm{D}\boldsymbol{u}_h - \mathrm{G}\boldsymbol{p}_h$$

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

Symmetry-preserving discretization

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

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$\langle \boldsymbol{a}, \boldsymbol{b} \rangle = \int_\Omega \boldsymbol{a}\boldsymbol{b} d\Omega$	$\langle \boldsymbol{a}_h, \boldsymbol{b}_h \rangle_h = \boldsymbol{a}_h^T \Omega \boldsymbol{b}_h$
$\langle C(\boldsymbol{u}, \varphi_1), \varphi_2 \rangle = -\langle C(\boldsymbol{u}, \varphi_2), \varphi_1 \rangle$	$\mathrm{C}(\boldsymbol{u}_h) = -\mathrm{C}^T(\boldsymbol{u}_h)$

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$\frac{\partial \boldsymbol{u}}{\partial t} + C(\boldsymbol{u}, \boldsymbol{u}) = \nu \nabla^2 \boldsymbol{u} - \nabla p$	$\Omega \frac{d\boldsymbol{u}_h}{dt} + \mathrm{C}(\boldsymbol{u}_h)\,\boldsymbol{u}_h = \mathrm{D}\boldsymbol{u}_h - \mathrm{G}\boldsymbol{p}_h$
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$\langle \nabla \cdot \boldsymbol{a}, \varphi \rangle = -\langle \boldsymbol{a}, \nabla \varphi \rangle$	$\Omega \mathrm{G} = -\mathrm{M}^T$

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$$\mathrm{C}\left(\boldsymbol{u}_h\right) = -\mathrm{C}^T\left(\boldsymbol{u}_h\right)$$

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

$$\mathrm{D} = \mathrm{D}^T \qquad def -$$

Why a collocated formulation?

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

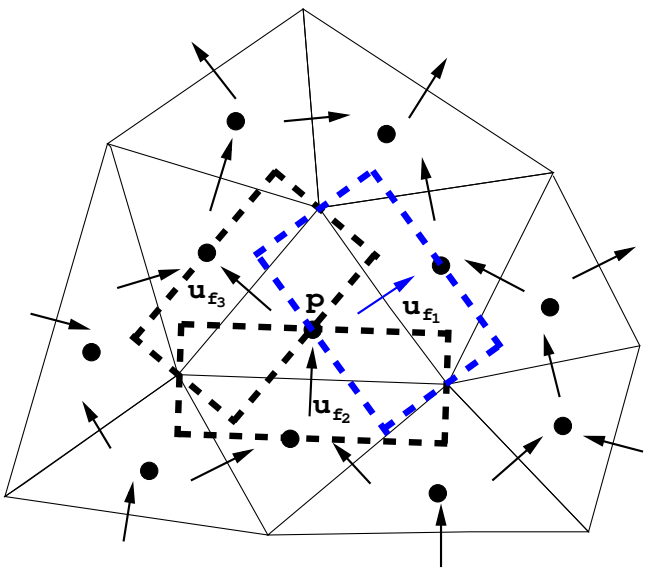




$$\Omega_s \frac{d\boldsymbol{u}_s}{dt} + \mathrm{C}(\boldsymbol{u}_s)\,\boldsymbol{u}_s = \mathrm{D}\boldsymbol{u}_s - \mathrm{G}\boldsymbol{p}_c; \quad \mathrm{M}\boldsymbol{u}_s = \mathbf{0}_c$$

In staggered meshes

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



Why a collocated formulation?

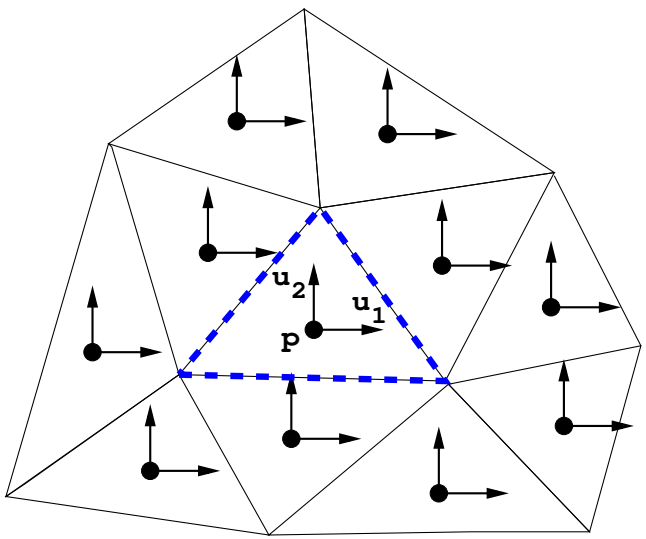
- STAR-CCM+
- ANSYS-FLUENT
- Code-Saturne
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$$\Omega_c \frac{d\boldsymbol{u}_c}{dt} + \mathrm{C}(\boldsymbol{u}_s)\,\boldsymbol{u}_c = \mathrm{D}\boldsymbol{u}_c - \mathrm{G}_c\boldsymbol{p}_c; \quad \mathrm{M}_c\boldsymbol{u}_c = \mathbf{0}_c$$

In collocated meshes

- p-$\boldsymbol{u}_c$ coupling is cumbersome ✗
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- Cheaper, less memory,... ✓



Why a collocated formulation?

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

Journal of Computational Physics 258 (2014) 246–267

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

F.X. Trias [a,b], O. Lehmkuhl [a,c], A. Oliva [a,*,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 AK Groningen, The Netherlands
[c] Termo Fluids, S.L., c/ Magí Colet 8, 08204 Sabadell, Spain

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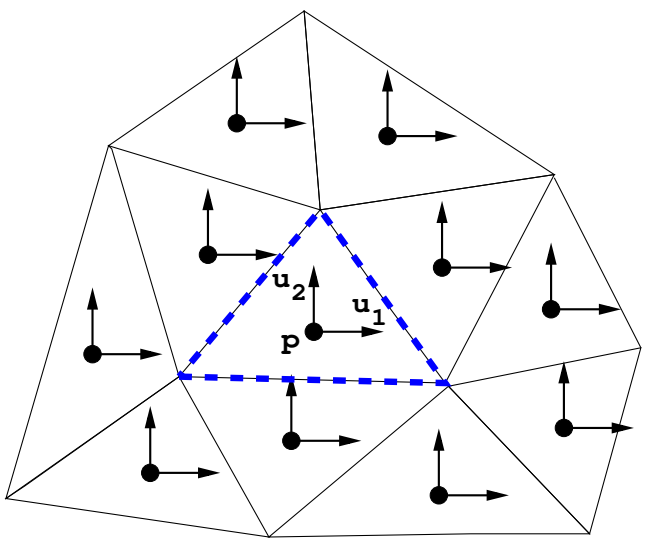
ABSTRACT

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

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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 NRG, P.O. Box 25, ZG Petten 1755, The Netherlands
[b] Heat and Mass Transfer Technological Center, Technical University of Catalonia, ESEIAAT, c/ Colom 11, Terrassa 08222, Spain
[c] Bernoulli Institute for Mathematics, Computing Science, and Artificial Intelligence, University of Groningen, P.O. Box 407, AK Groningen 9700, The Netherlands

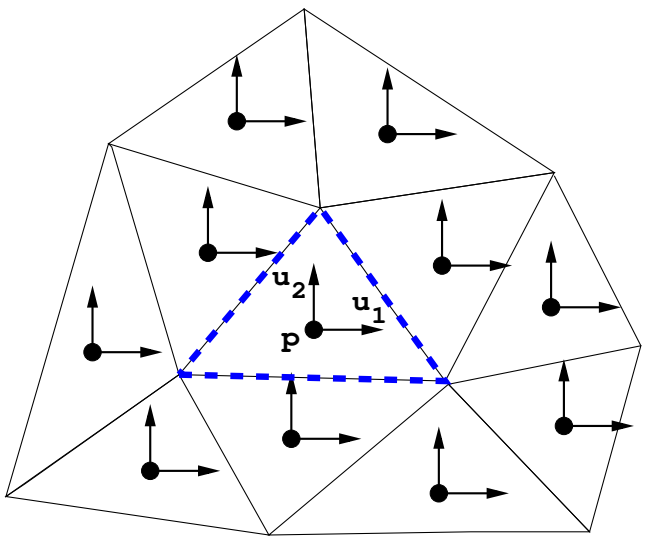
ARTICLE INFO

Article history:
Received 27 November 2020
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Available online 27 April 2021

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

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



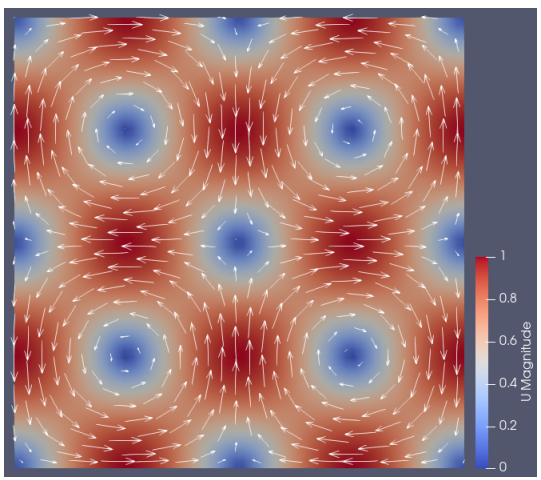
In collocated meshes

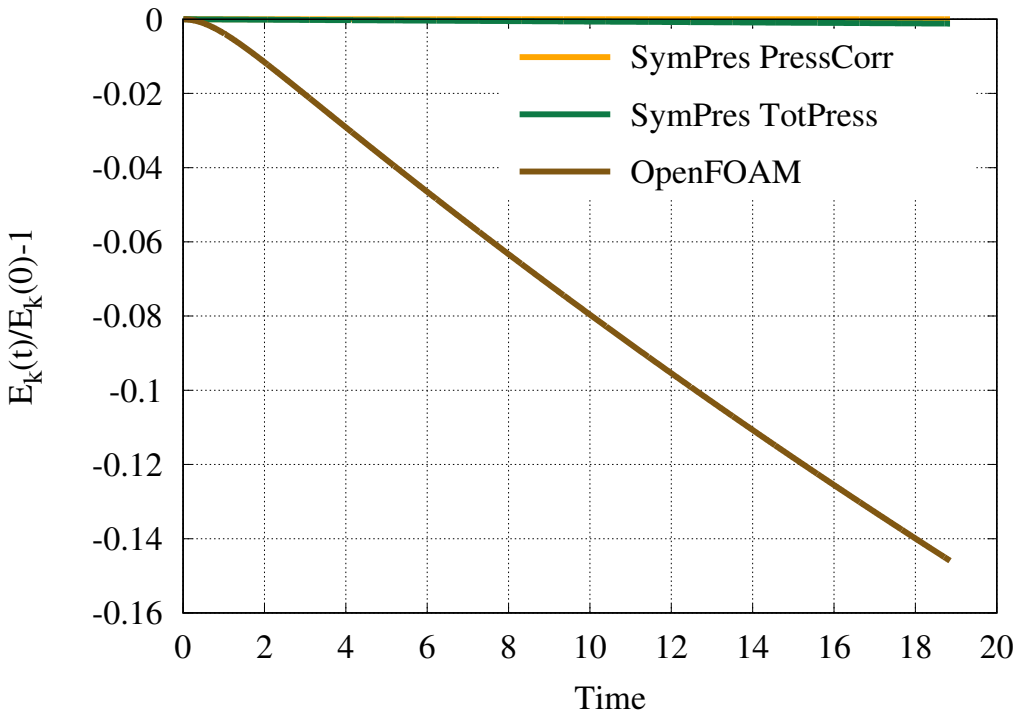
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Pressure-velocity coupling on collocated grids

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

OpenFOAM



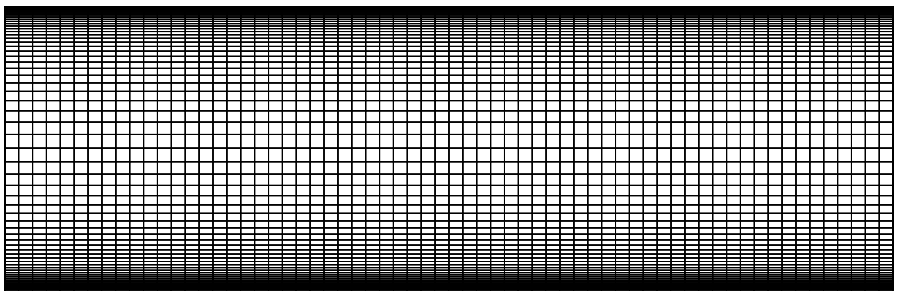


Results for an inviscid Taylor-Green vortex[3]

[3] E.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!



Journal of Computational Physics 523 (2025) 113631

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

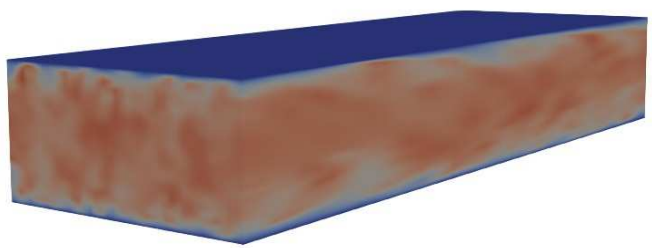
Technical University of Catalonia, Heat and Mass Transfer Technological Center (CTTC), C/ Colom 11 Building TR4, Terrassa, 08222, Barcelona, Spain

ARTICLE INFO

Keywords:
Symmetry-preserving
Collocated
PISO
Unconditionally stable
Energy-preserving
FVM

ABSTRACT

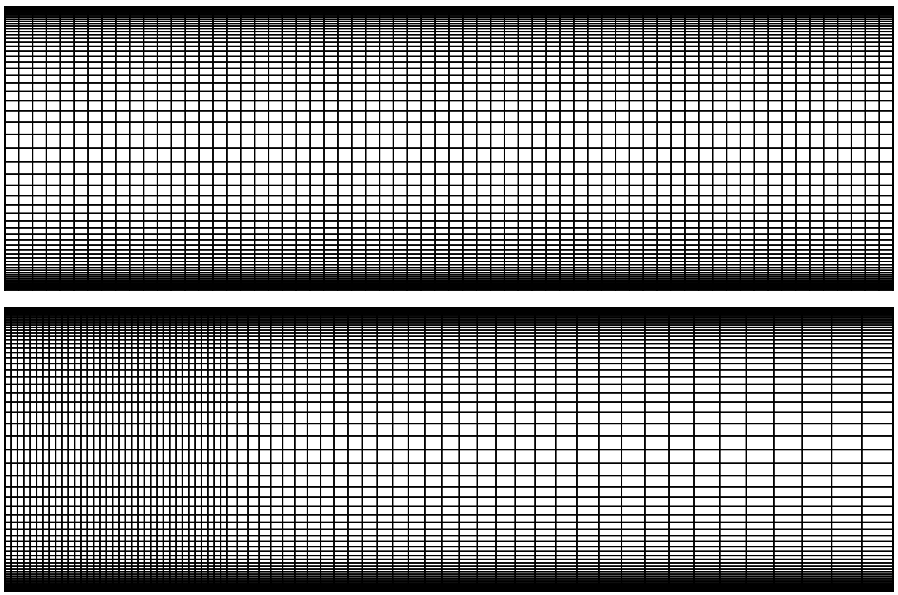
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[4] D.Santos, J.A.Hopman, C.D.Pérez-Segarra, F.X.Trias. *On a symmetry-preserving unconditionally stable projection method on collocated unstructured grids for incompressible flows*, **Journal of Computational Physics**, 523:113631, 2025.

Pressure-velocity coupling on collocated grids

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



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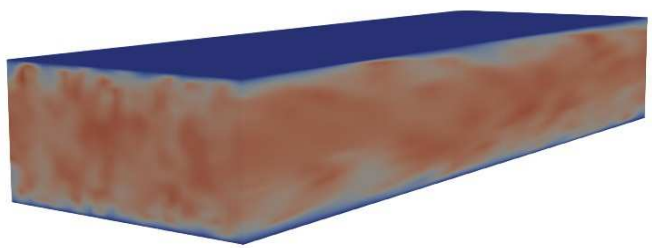
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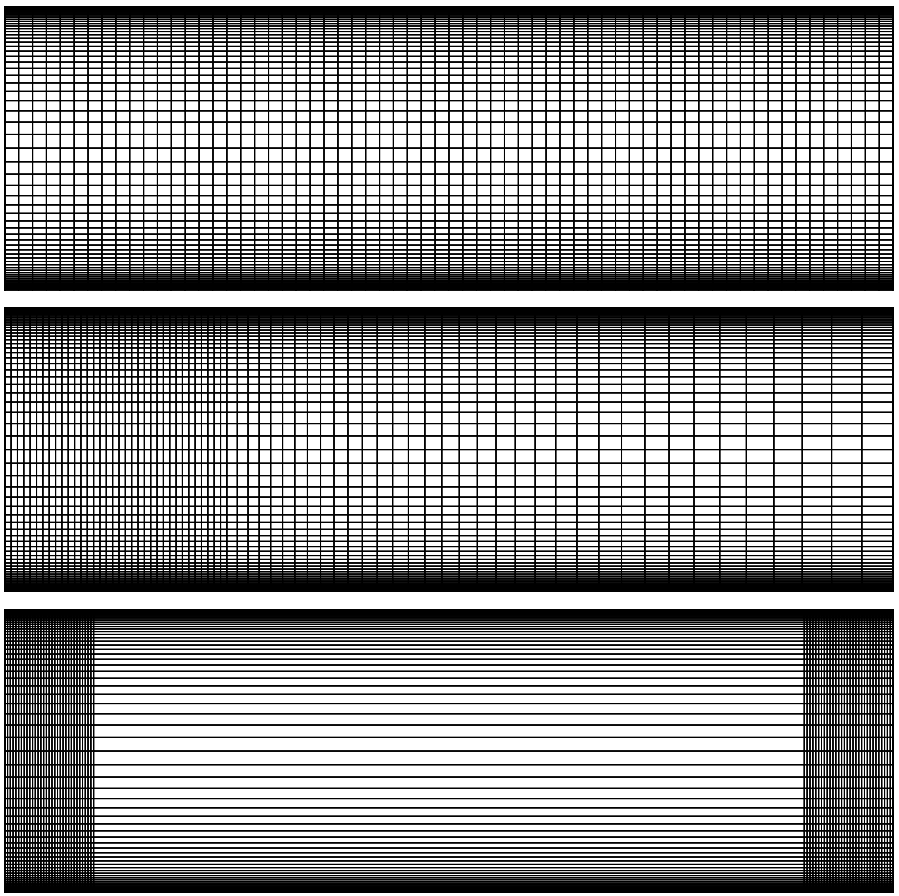
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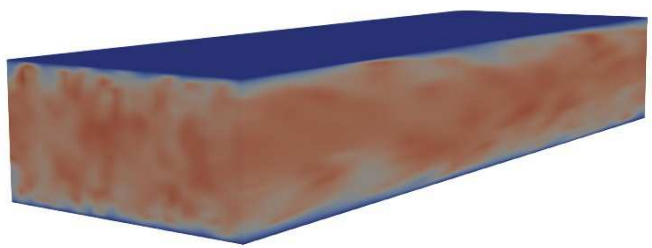
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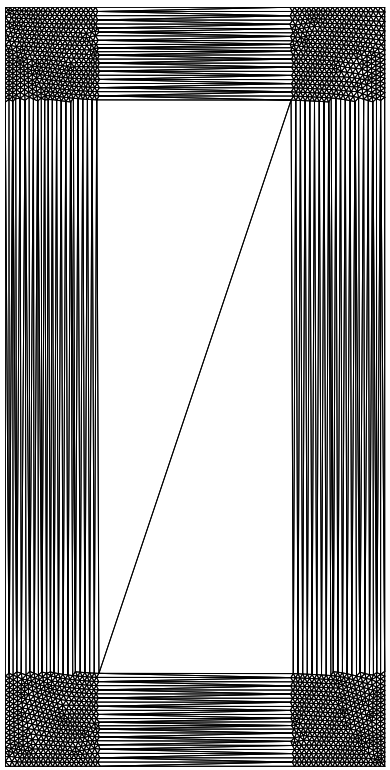
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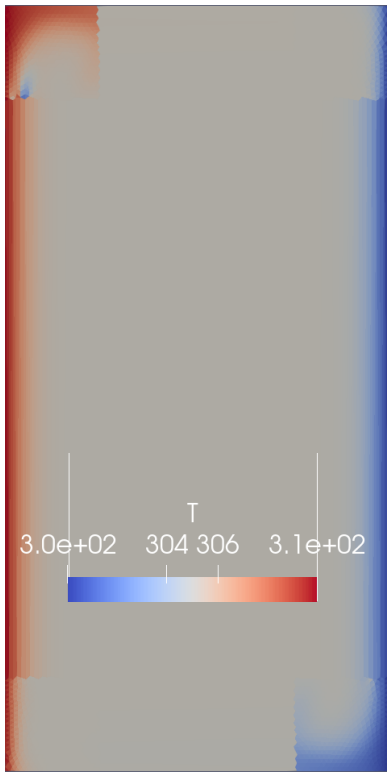


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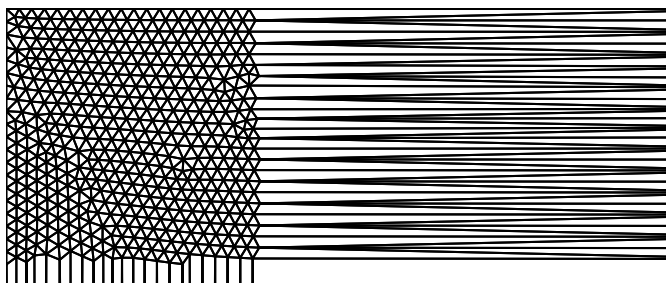
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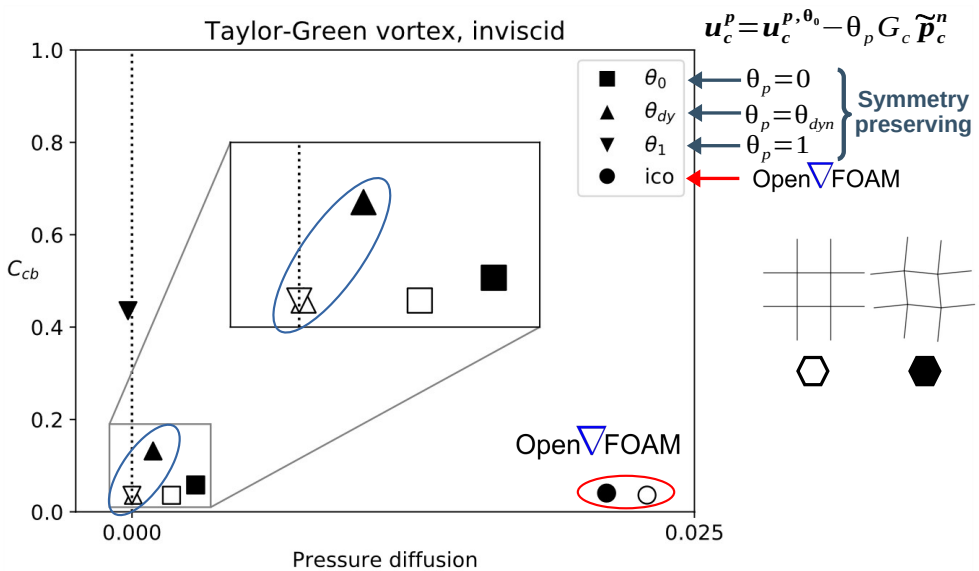
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Pressure-velocity coupling on collocated grids

... and minimize the **checkerboard**[5] problem with a minimal artificial dissipation!



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Quantifying the checkerboard problem to reduce numerical dissipation

J.A. Hopman [a,*], D. Santos [a], À. Alsalti-Baldellou [a,b], J. Rigola [a], F.X. Trias [a]

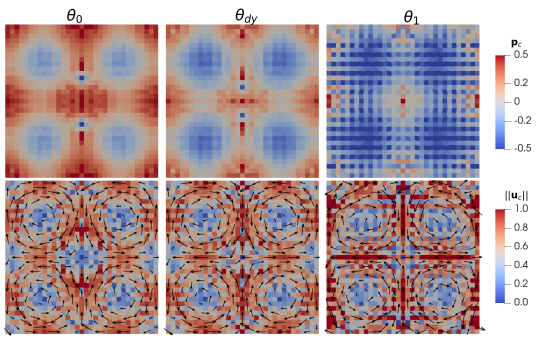
[a] Heat and Mass Transfer Technological Center, Technical University of Catalonia, ESEIAAT, c/Colom 11, Terrassa, 08222, Barcelona, Spain
[b] Termo Fluids SL, c/Magí Colet 8, Sabadell, 08204, Barcelona, Spain

ARTICLE INFO

Keywords:
Checkerboarding
Collocated grids
Conservative discretisation

ABSTRACT

This work provides a comprehensive exploration of various methods in 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 derivation and implementation of discrete operators while also addressing the associated numerical errors. The lack of a proper definition for the checkerboard problem is addressed by proposing a physics-based coefficient. This coefficient, rooted in the disparity between the compact- and wide-stencil Laplacian operators, is able to quantify oscillatory solution fields with a physics-based, global, normalised, non-dimensional value. The influence of mesh and time-step



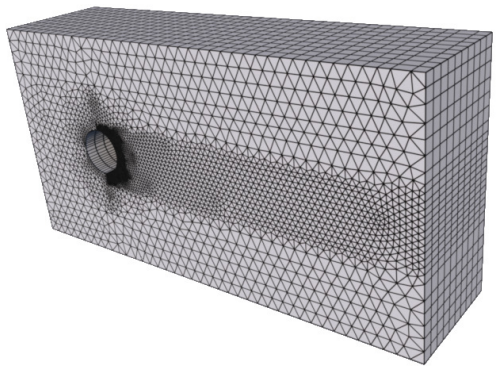
[5] J.A.Hopman, D.Santos, À.Alsalti, J.Rigola, F.X.Trias. *Quantifying the checkerboard problem to reduce numerical dissipation*, **Journal of Computational Physics**, 521:113537, 2025. arXiv: 2408.06821

Pressure-velocity coupling on collocated grids

Summary

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

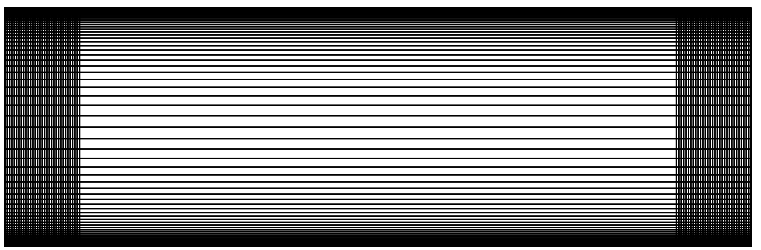
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- Suitable for **unstructured** grids



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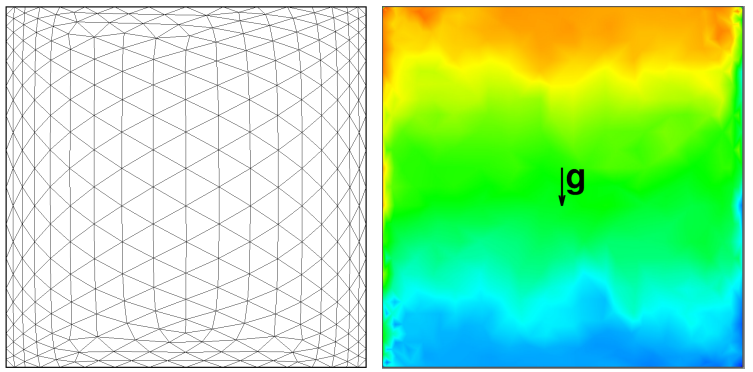
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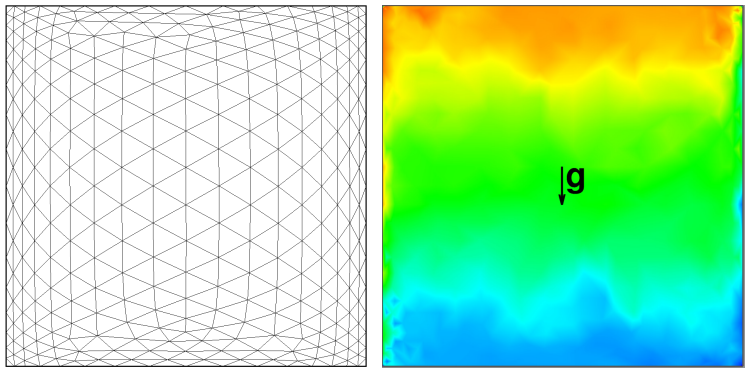


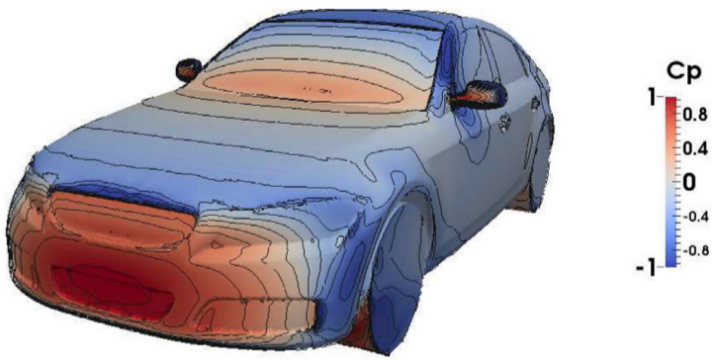
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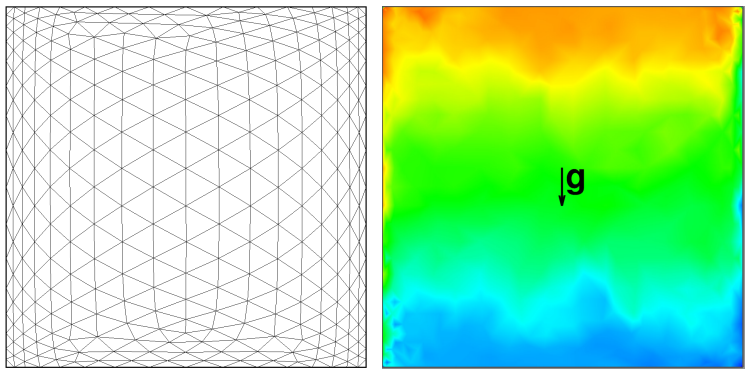


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- Suitable for **industrial** applications
- Also available in **OpenFOAM**

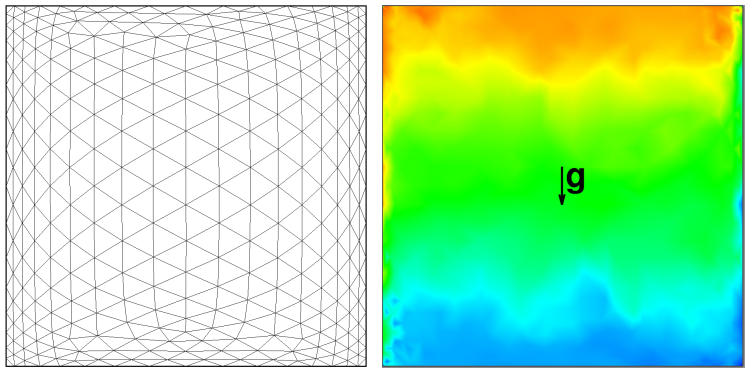


OpenFOAM

Pressure-velocity coupling on collocated grids

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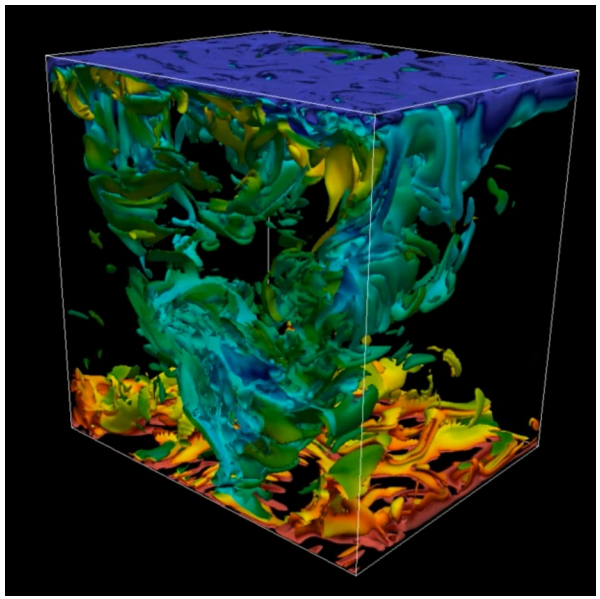
OpenFOAM

Research question #2:

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

Buoyancy-driven flows

Energy-exchanges



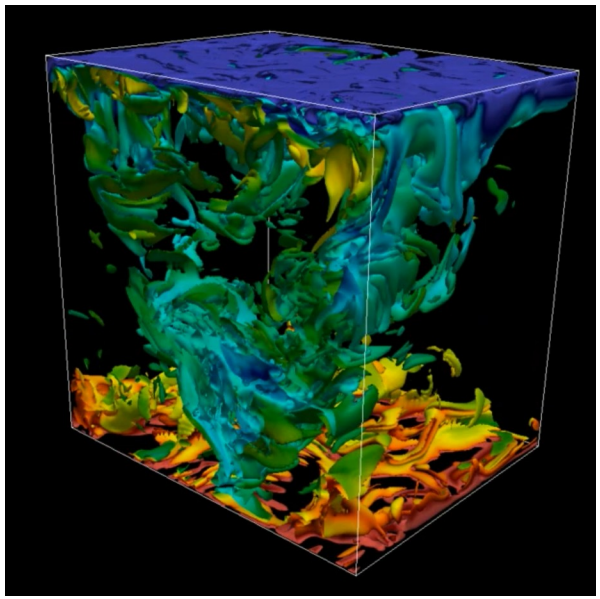
E_p
$-(y,T)$

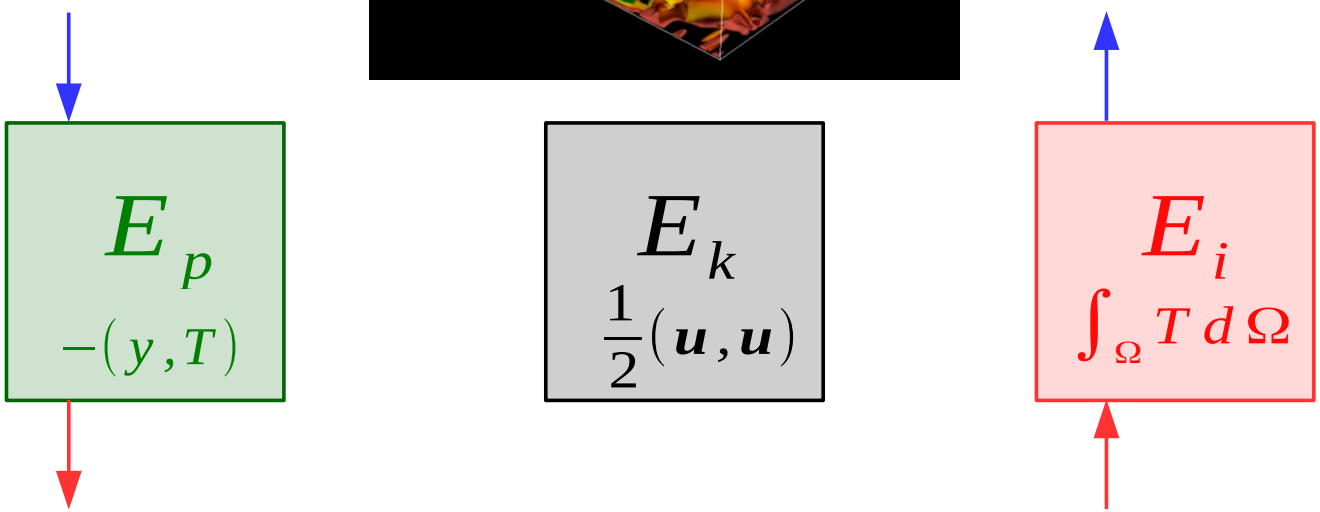
E_k
$\frac{1}{2}(\boldsymbol{u},\boldsymbol{u})$

E_i
$\int_\Omega T\, d\,\Omega$

Buoyancy-driven flows

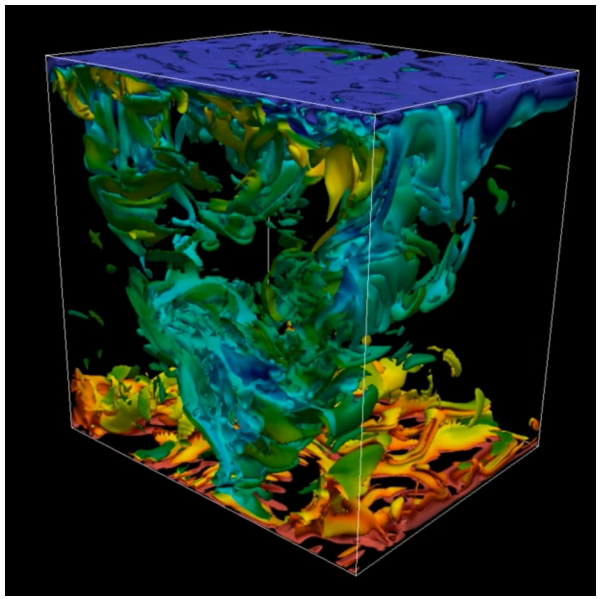
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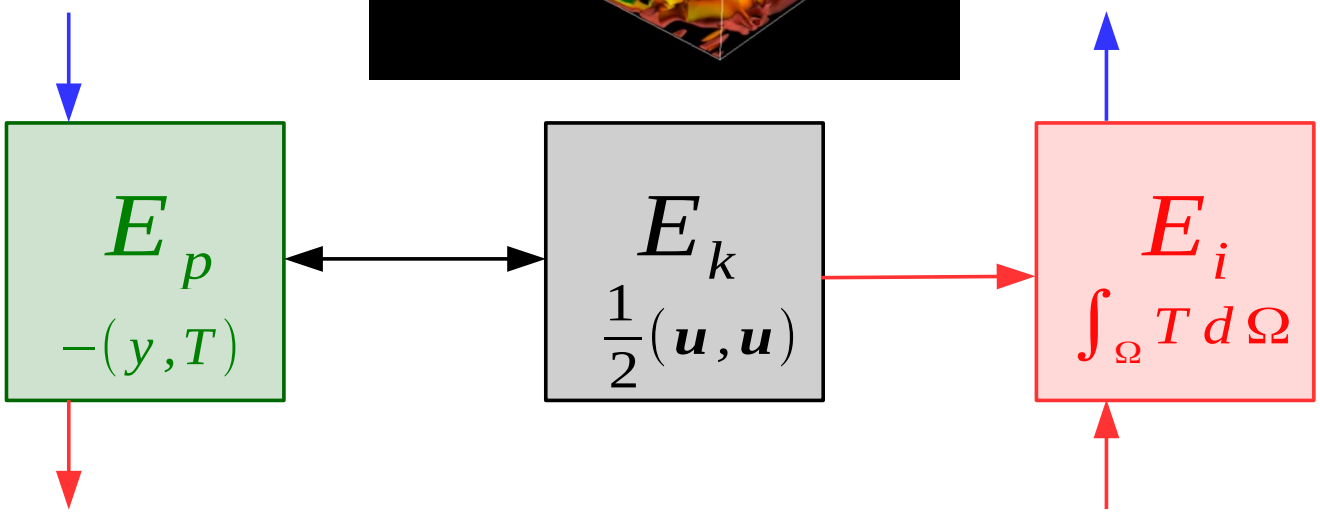




Buoyancy-driven flows

Energy-exchanges





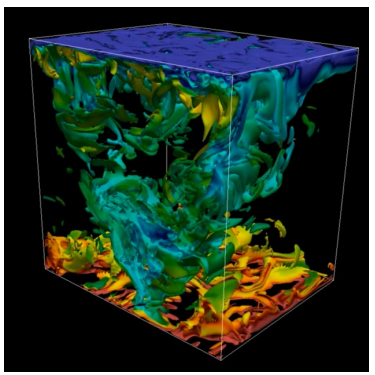
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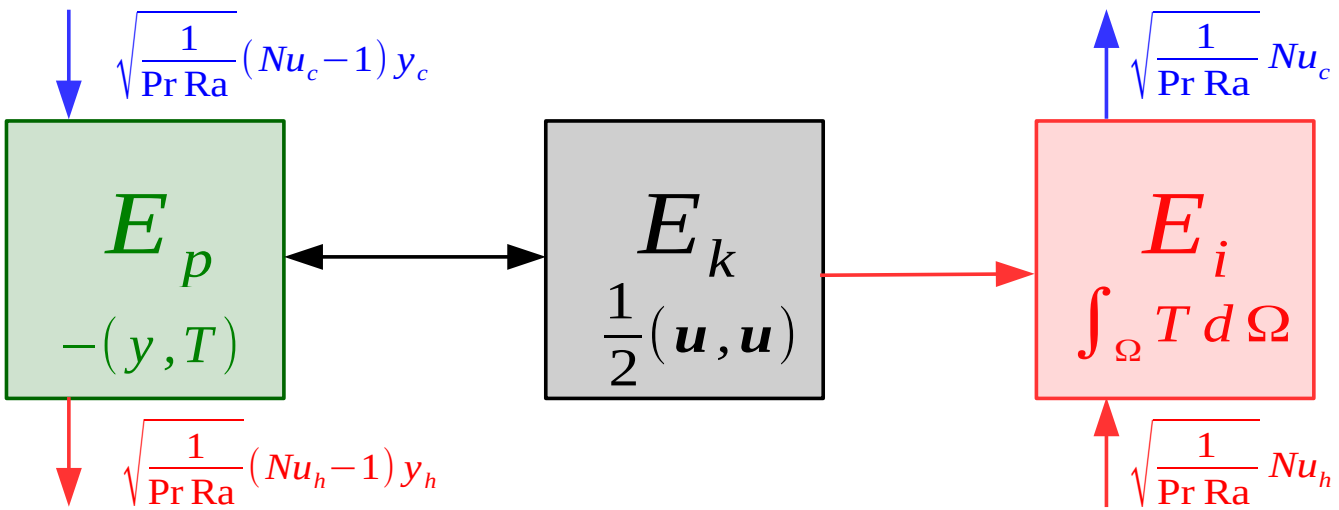
Continuous formulation

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u} = \sqrt{\frac{\mathrm{Pr}}{\mathrm{Ra}}}\nabla^2\boldsymbol{u} - \nabla p + T\,\boldsymbol{e}_y \qquad \text{Boussinesq}$$

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

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





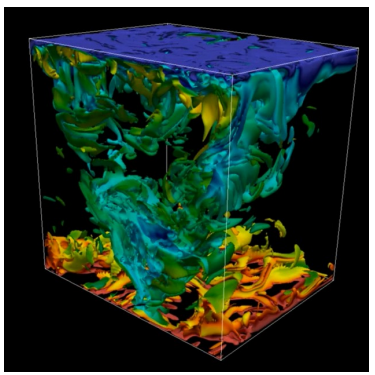
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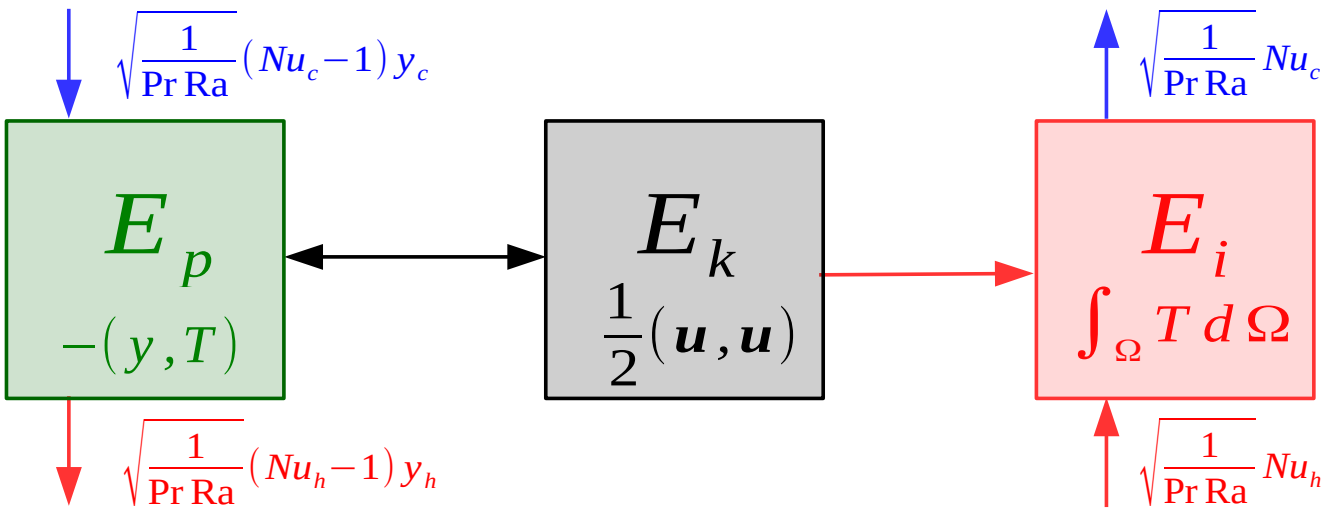
$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u} = \sqrt{\frac{\mathrm{Pr}}{\mathrm{Ra}}}\nabla^2\boldsymbol{u} - \nabla p + T\,\boldsymbol{e}_y \qquad \text{Boussinesq}$$

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

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



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



Buoyancy-driven flows

Continuous formulation

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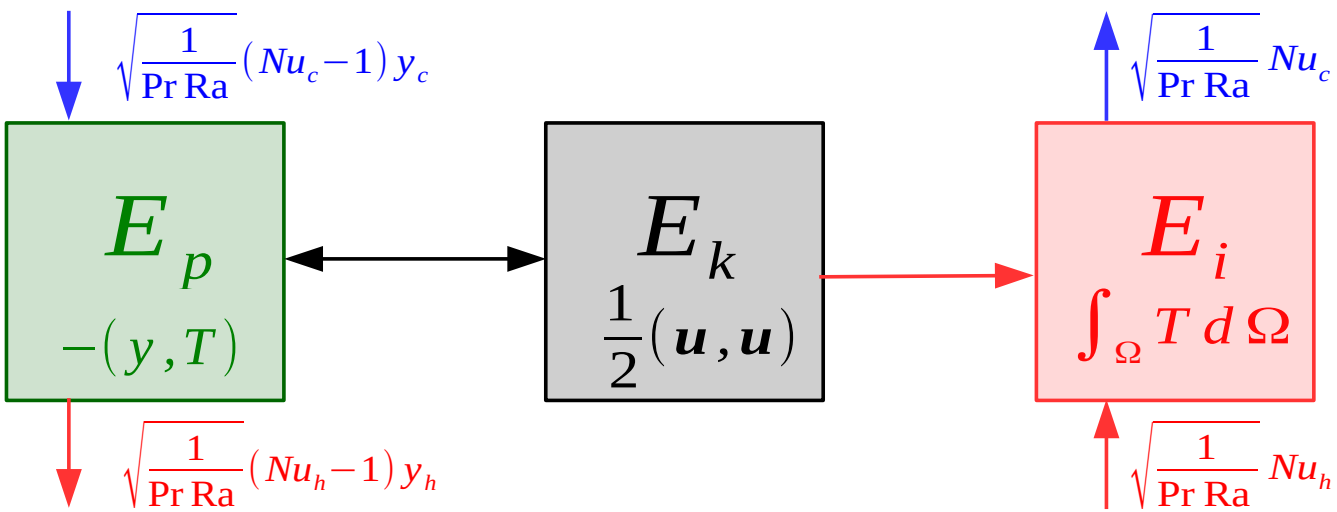
$$\frac{\partial T}{\partial t}+(\boldsymbol{u}\cdot\nabla)T=\sqrt{\frac{1}{\mathrm{Pr}\,\mathrm{Ra}}}\nabla^2 T$$

$$\Phi=\|\nabla\boldsymbol{u}\|^2 \quad \varepsilon_U=\int_\Omega \Phi\, d\Omega$$

$$(v,T)=\int_\Omega vT\, d\Omega$$

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

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



Buoyancy-driven flows

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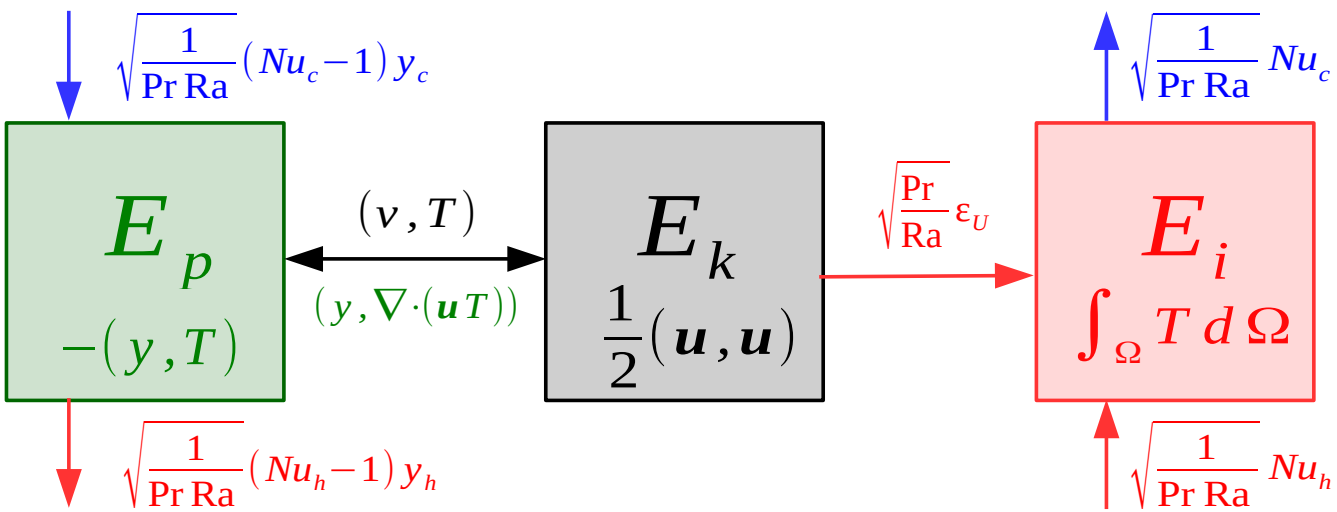
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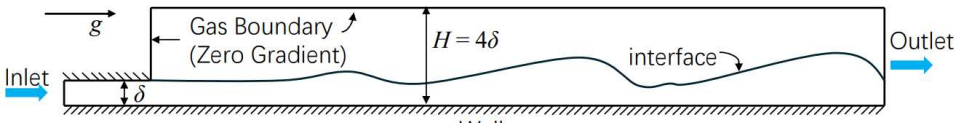
Multiphase flows

Continuous formulation

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

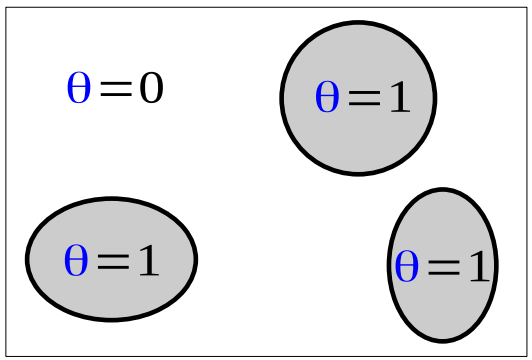
$$\frac{\partial\theta}{\partial t}+(\vec{u}\cdot\nabla)\theta=0$$

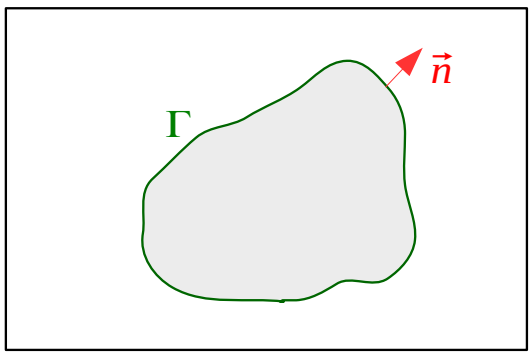
$$\kappa=-\nabla\cdot\vec{n}\quad\text{where}\quad\vec{n}=\frac{\nabla\theta}{|\nabla\theta|}$$











Multiphase flows

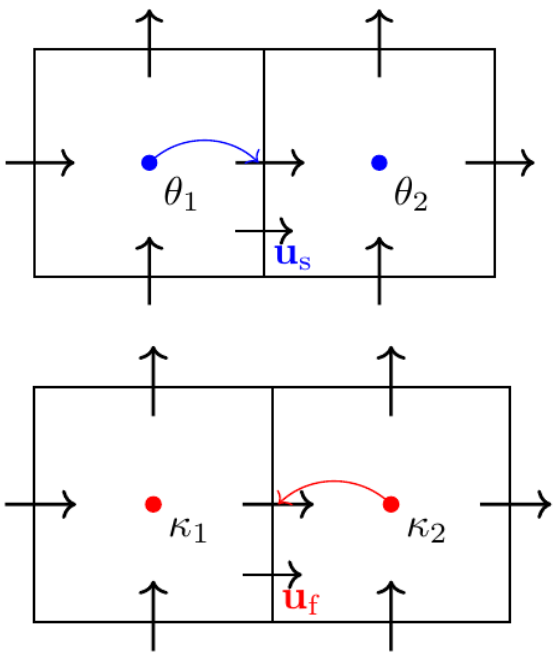
Conservative discrete formulation

Surface tension

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

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

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



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An energy-preserving level set method for multiphase flows

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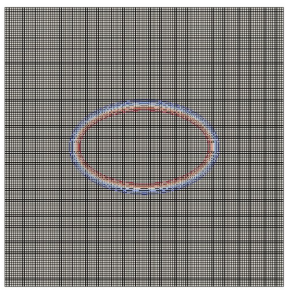
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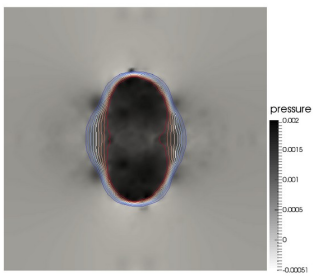
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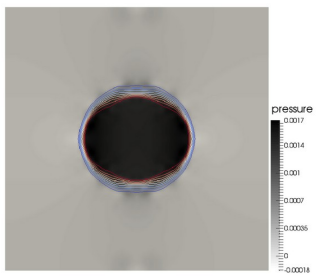
$$\rho\frac{\partial\vec{u}}{\partial t}+\rho(\vec{u}\cdot\nabla)\vec{u}=\nabla\cdot(2\mu\,S(\vec{u}))-\nabla p+\gamma\,\kappa\cdot\vec{n} \qquad \nabla\cdot\vec{u}=0$$

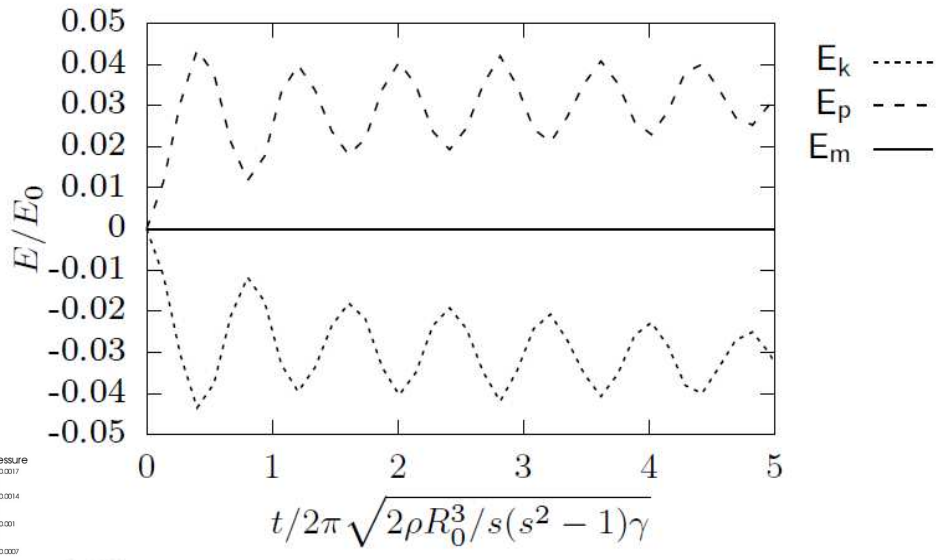
$$\frac{\partial\theta}{\partial t}+(\vec{u}\cdot\nabla)\theta=0$$

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Mechanical energy (kinetic+potential) **is preserved**!

A new general framework for multiphysics

Variational formulation

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

Associated force

$$\frac{\partial \phi}{\partial t} + \mathscr{L}_{\boldsymbol{u}}\phi = 0$$

Lie derivative

$$\mathscr{L}_{\boldsymbol{u}}\phi = (\boldsymbol{u}\cdot\nabla)\phi$$

Scalar (0-forms)

$$\mathscr{L}_{\boldsymbol{u}}\phi = \nabla\cdot(\boldsymbol{u}\phi)$$

Density-like (3-forms)

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

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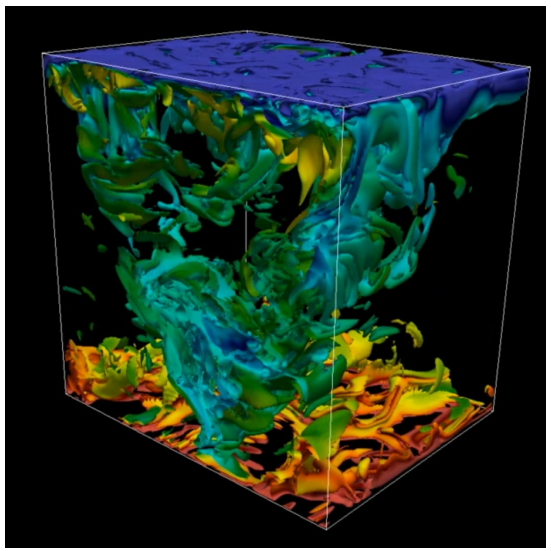
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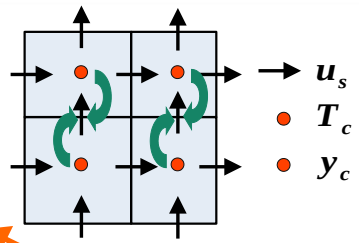
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Cell-to-face interpolation

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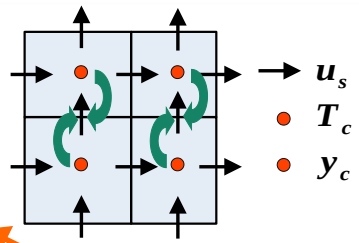
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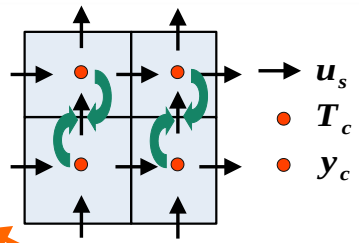
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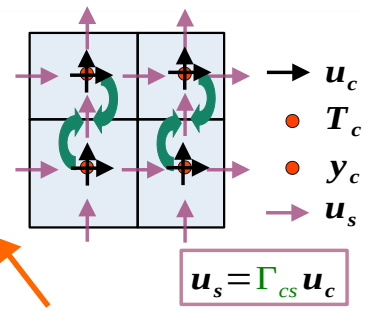
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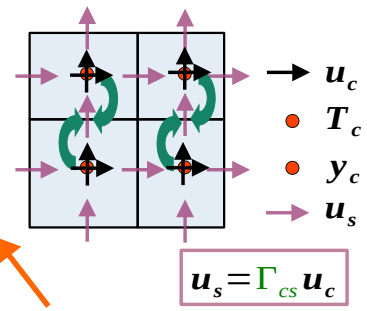
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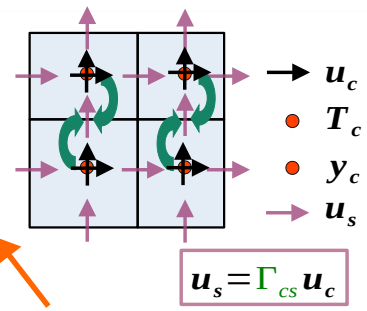
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$$= -\langle \nabla \mu^{\rho}, \boldsymbol{u}\rho \rangle$$
$$= -\langle \rho \nabla \mu^{\rho}, \boldsymbol{u} \rangle$$

$$M = -(\Omega_s G)^T \qquad \Gamma_{sc} = \Omega^{-1} \Gamma_{cs}^T \Omega_s$$

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

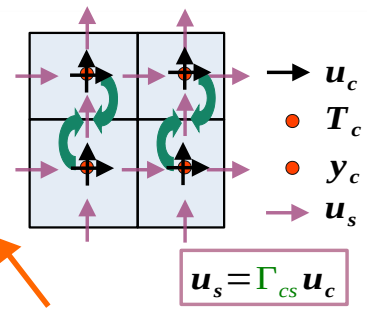
A new general framework for multiphysics

Buoyancy-driven flows on collocated grids

$$\Omega \frac{d\boldsymbol{u}_c}{dt} + C(\boldsymbol{u}_s)\boldsymbol{u}_c = D\boldsymbol{u}_c - \Omega G_c \boldsymbol{p}_c + \Omega \boldsymbol{f}_c^{\rho}$$

$$\Omega_c \frac{d\boldsymbol{\rho}_c}{dt} + C_c(\boldsymbol{u}_s)\boldsymbol{\rho}_c = \boldsymbol{0}_c \qquad C_c(\boldsymbol{u}_s) := M U_s \Pi_{cs}$$

$$U_s = diag(\boldsymbol{u}_s)$$



Cell-to-face interpolation

$$E_h^{\rho}[\boldsymbol{\rho}_c] := g\boldsymbol{\rho}_c \cdot \Omega_c \boldsymbol{y}_c \qquad E^{\rho}[\rho] = \int_{\Omega} \rho g y \, d\Omega$$

$$\boldsymbol{\mu}_c^{\rho} = \frac{\delta E^{\rho}[\boldsymbol{\rho}_c]}{\delta \boldsymbol{\rho}_c} = g\boldsymbol{y}_c \qquad \mu^{\rho} = \frac{\delta E^{\rho}[\rho]}{\delta \rho} = gy$$

$$\boldsymbol{\mu}_c^{\rho} \cdot C_c(\boldsymbol{u}_s)\rho_c = \boldsymbol{\mu}_c^{\rho} \cdot M U_s \Pi_{cs} \boldsymbol{\rho}_c \qquad \langle \mu^{\rho}, \mathscr{L}_{\boldsymbol{u}} \rho \rangle = \langle \mu^{\rho}, \nabla \cdot (\boldsymbol{u}\rho) \rangle$$

$$= -(G\boldsymbol{\mu}_c^{\rho}) \cdot \Omega_s U_s \Pi_{cs} \boldsymbol{\rho}_c \qquad = -\langle \nabla \mu^{\rho}, \boldsymbol{u}\rho \rangle$$

$$= -((\Pi_{cs}\boldsymbol{\rho}_c) \odot (G\boldsymbol{\mu}_c^{\rho})) \cdot \Gamma_{sc}^T \Omega \boldsymbol{u}_c \qquad = -\langle \rho \nabla \mu^{\rho}, \boldsymbol{u} \rangle$$

$$\boldsymbol{f}_c^{\rho} = -\Gamma_{sc}((\Pi_{cs}\boldsymbol{\rho}_c) \odot (G\boldsymbol{\mu}_c^{\rho})) = -(\Gamma_{sc}\Pi_{cs}\boldsymbol{\rho}_c) g E_y \qquad \boldsymbol{f}^{\rho} = -\rho \nabla \mu^{\rho} = -\rho g \boldsymbol{e}_y$$

A new general framework for multiphysics

Summary

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

Associated force

$$\frac{\partial \phi}{\partial t} + \mathscr{L}_{\boldsymbol{u}}\phi = 0$$

Lie derivative

$$\mathscr{L}_{\boldsymbol{u}}\phi = (\boldsymbol{u}\cdot\nabla)\phi$$ Scalar (0-forms)

$$\mathscr{L}_{\boldsymbol{u}}\phi = \nabla\cdot(\boldsymbol{u}\phi)$$ Density-like (3-forms)

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

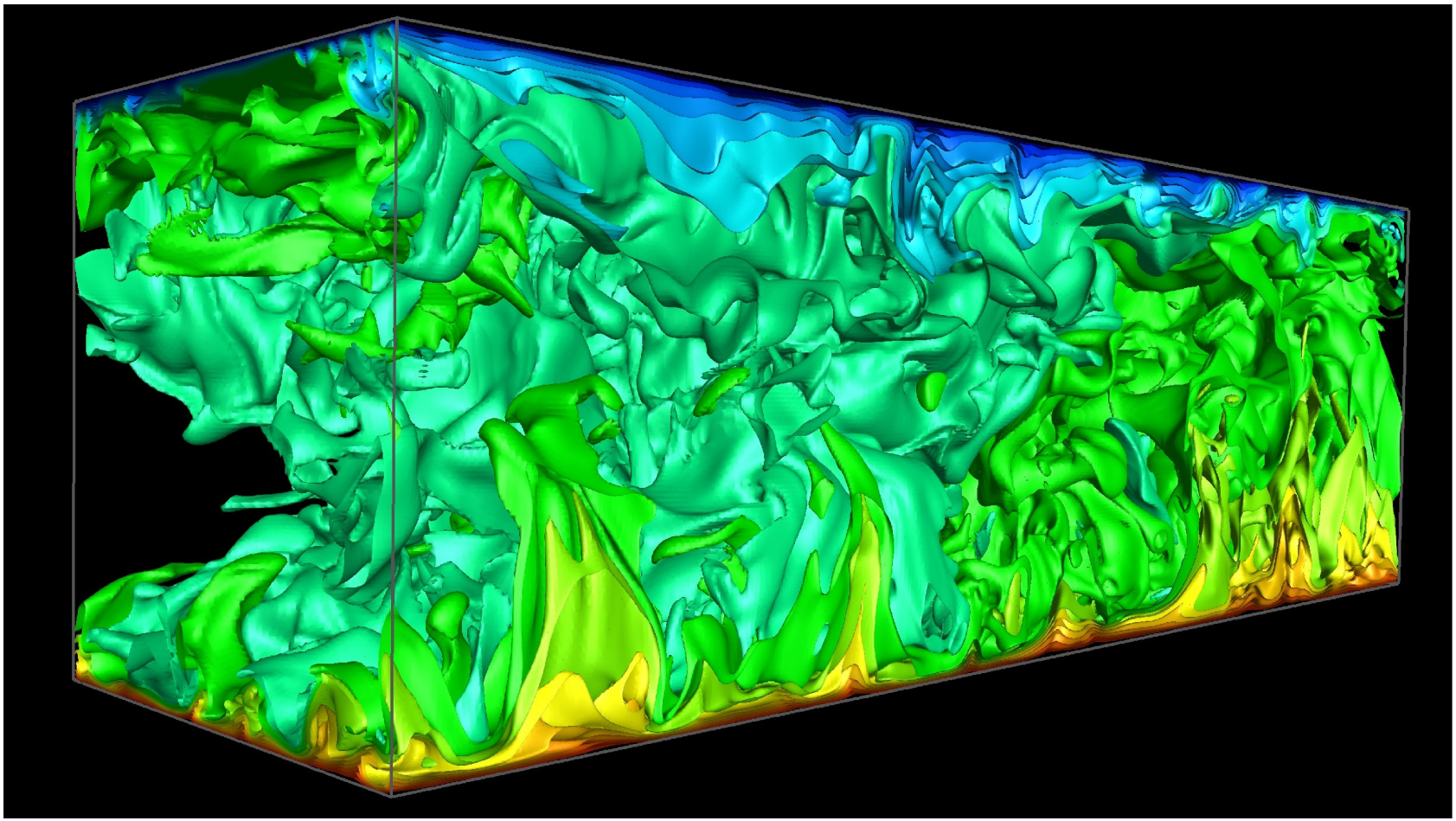
$\mathscr{L}_{\boldsymbol{u}}$ Lie derivative

$\Rightarrow \quad \boldsymbol{f}^{\phi}$

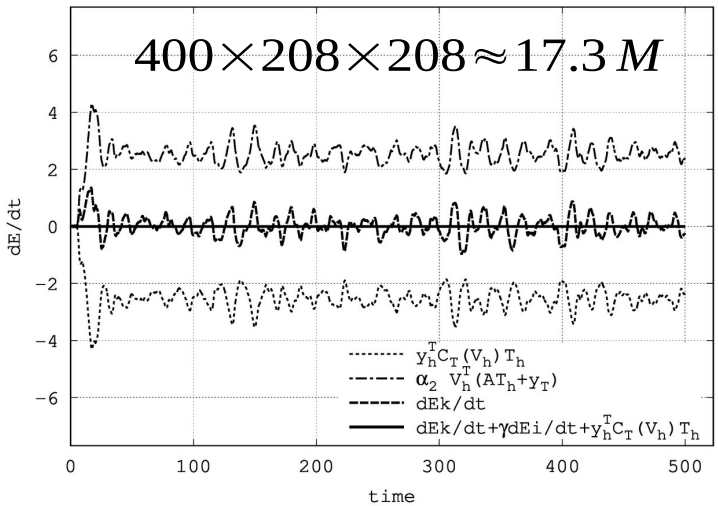
Leitmotiv: transport equation and its associated force **cannot** be discretized independently!!!

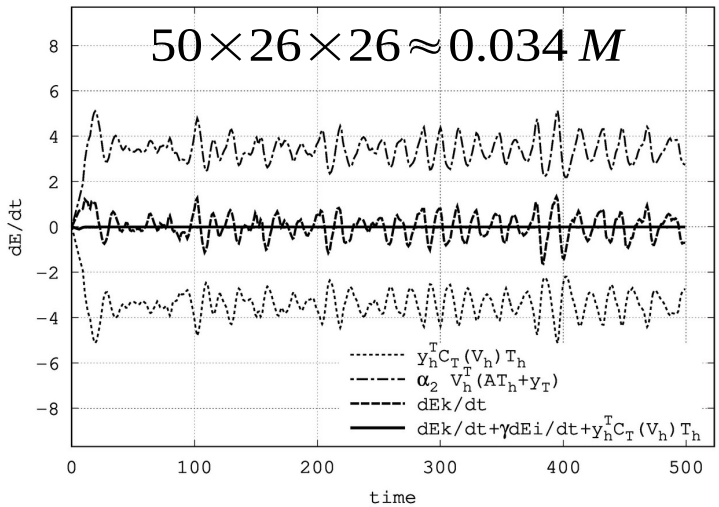
Buoyancy-driven flows

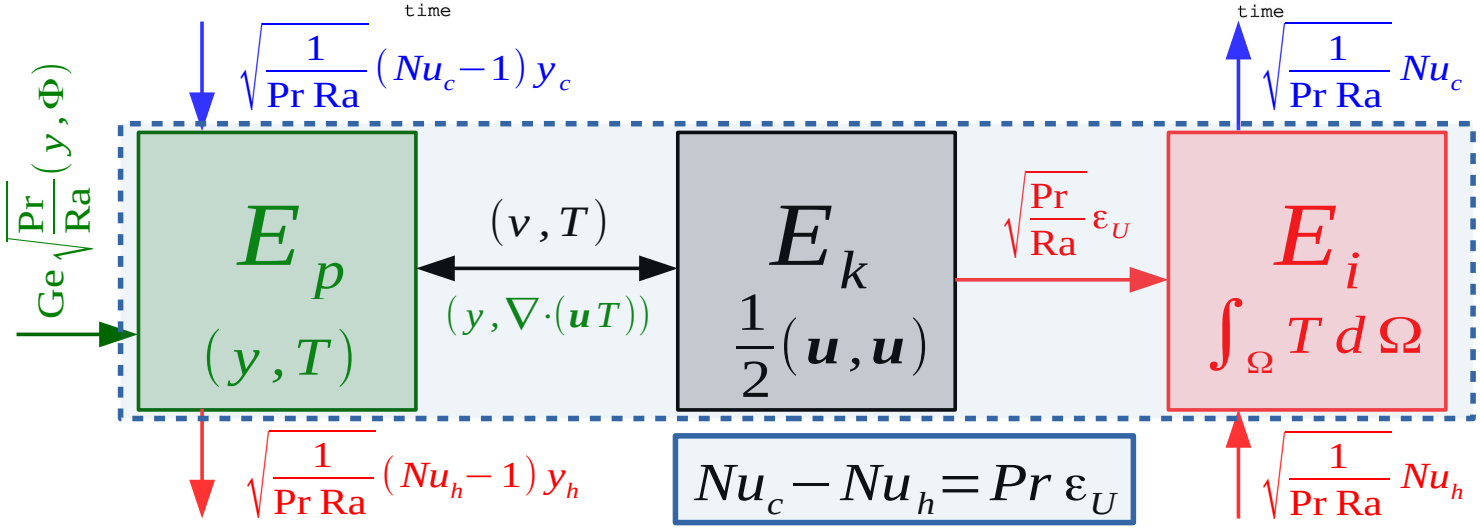
Turbulent Rayleigh–Bénard convection at $Ra = 10^8$



Buoyancy-driven flows[6]

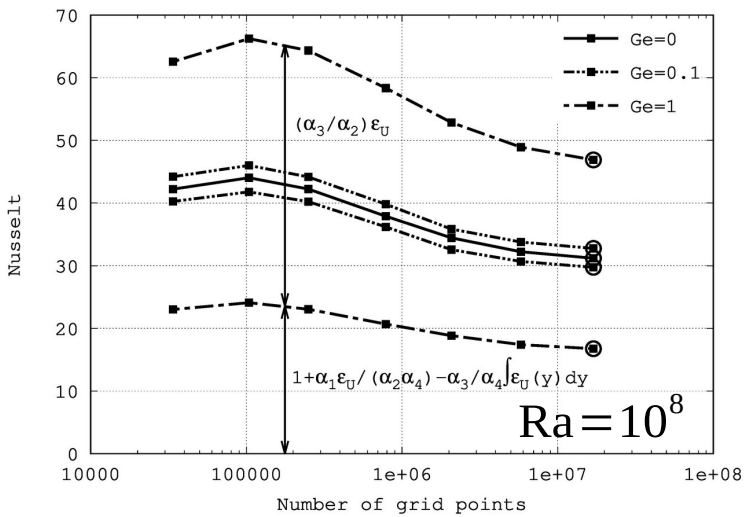


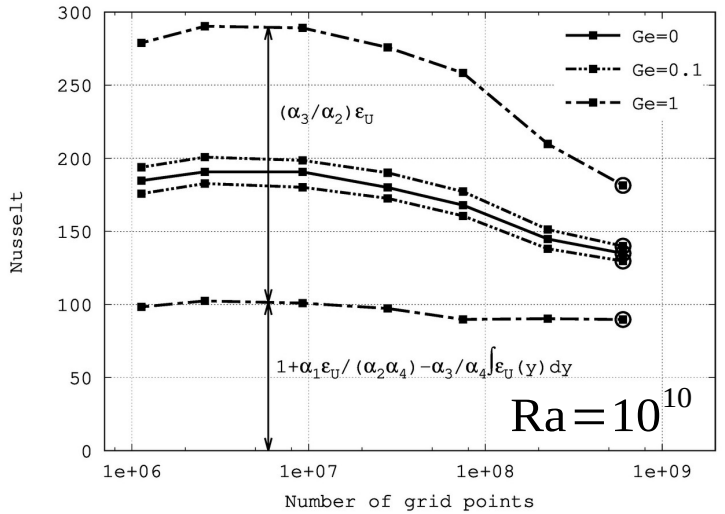


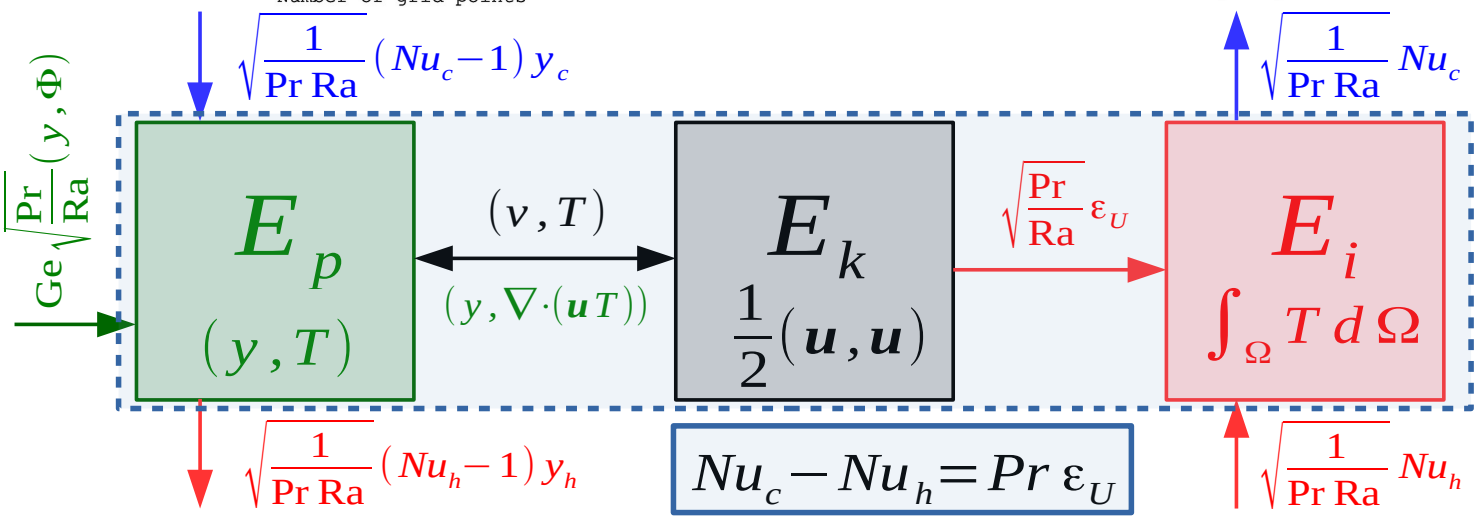


[6] B.Sanderse, F.X.Trias. *Energy-consistent discretization of viscous dissipation with application to natural convection flow*, **Computers & Fluids**, 286:106473, 2025.

Buoyancy-driven flows[6]

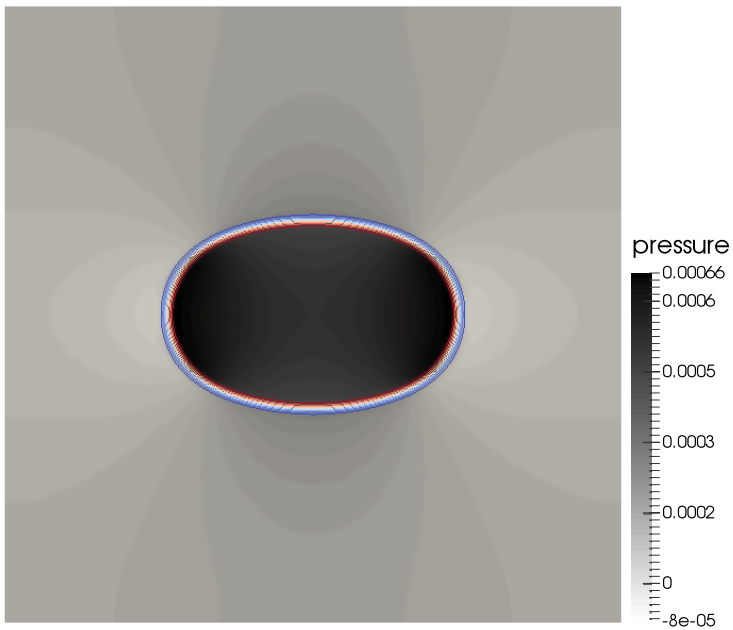




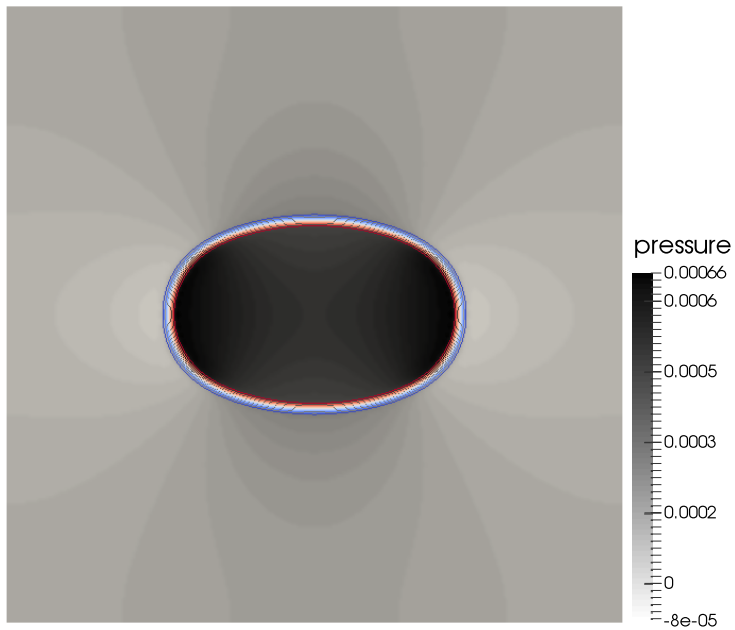


[6] B.Sanderse, F.X.Trias. *Energy-consistent discretization of viscous dissipation with application to natural convection flow*, **Computers & Fluids**, 286:106473, 2025.

Multiphase flows[6]



Non-symmetry-preserving!

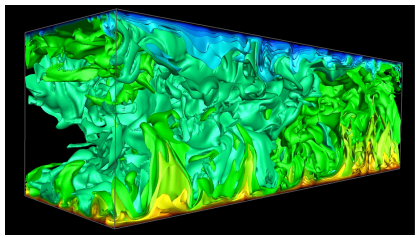


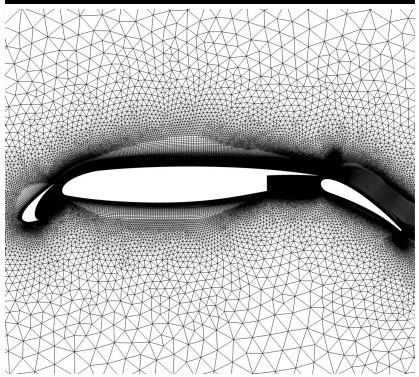
Symmetry-preserving!

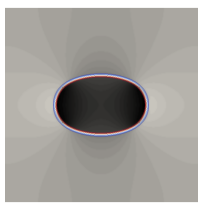
[6] N.Valle, F.X.Trias, and J.Castro. *An energy-preserving level set method for multiphase flows*. **Journal of Computational Physics**, 400(1):108991, 2020

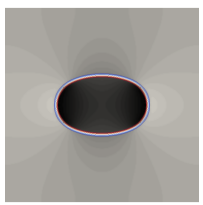
Take-away messages

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



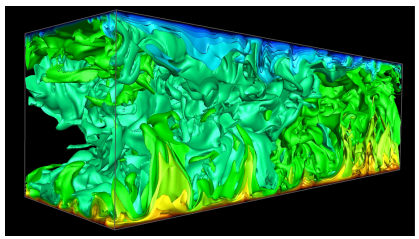


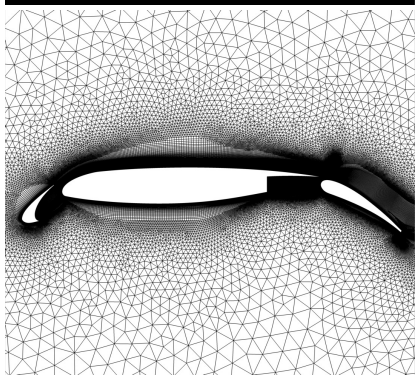


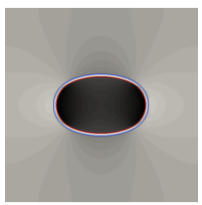


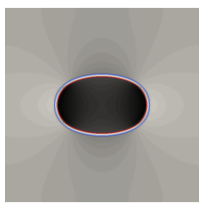
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- **Preserving symmetries** is the key point for **reliable LES/DNS** simulations also for industrial problems.
- We usually focus on quadratic invariants (kinetic energy) but **energy exchanges** are also crucial.



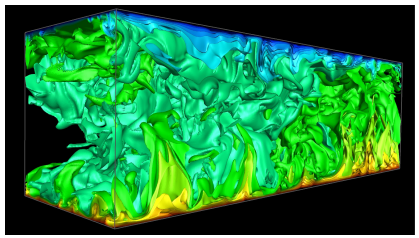


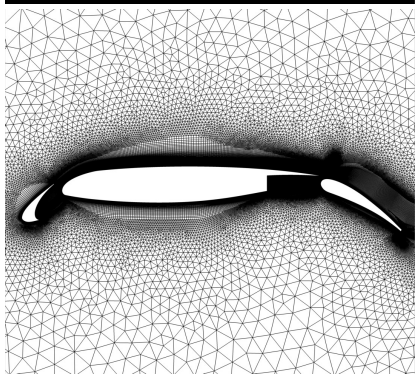


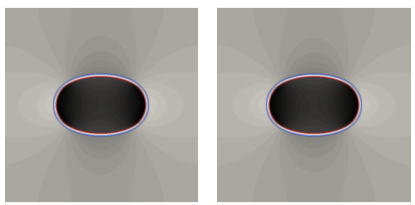


Take-away messages

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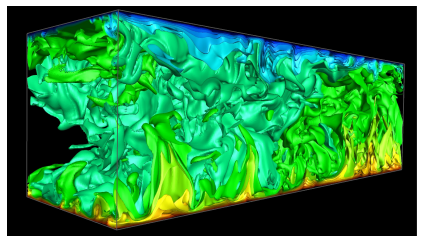


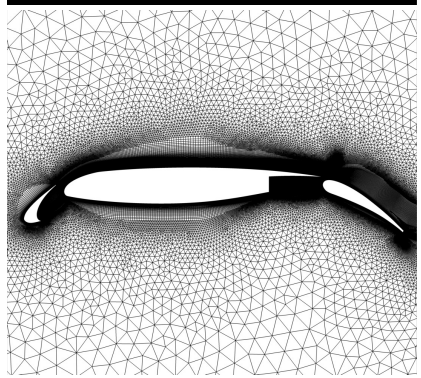
Take-away messages

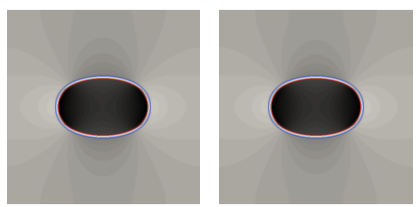
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- Transport equations and their associated forces **cannot be discretized independently**.

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

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







OpenFOAM