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)

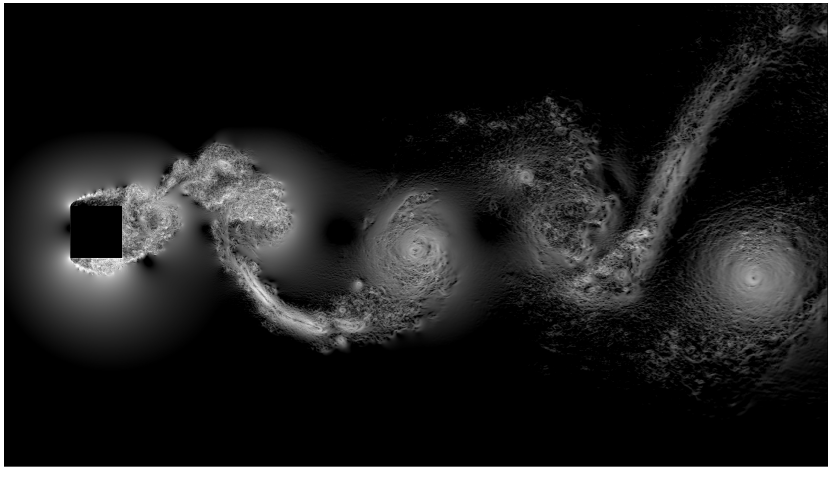


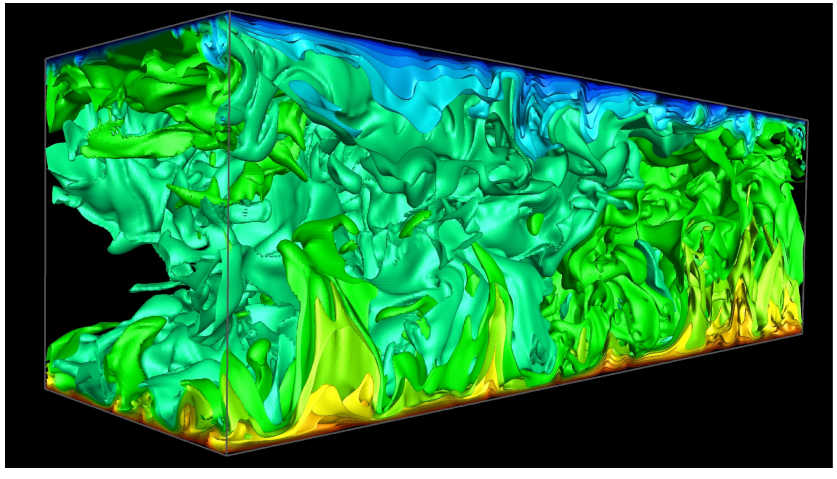
Centre Tecnològic de Transferència de Calor
UNIVERSITAT POLITÈCNICA DE CATALUNYA

Rethinking CFD for modern HPC systems

F.Xavier Trias

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





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)



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)





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

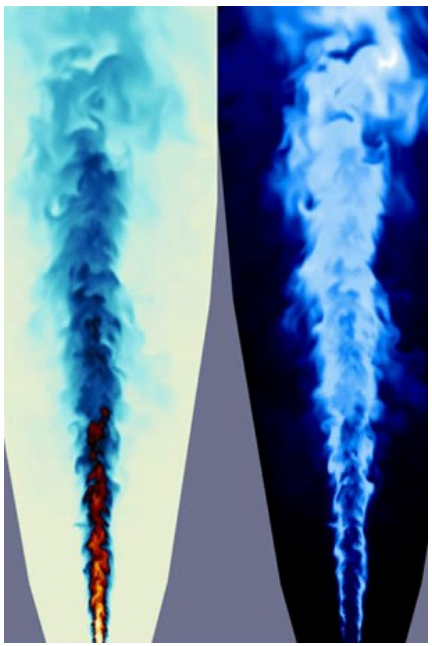


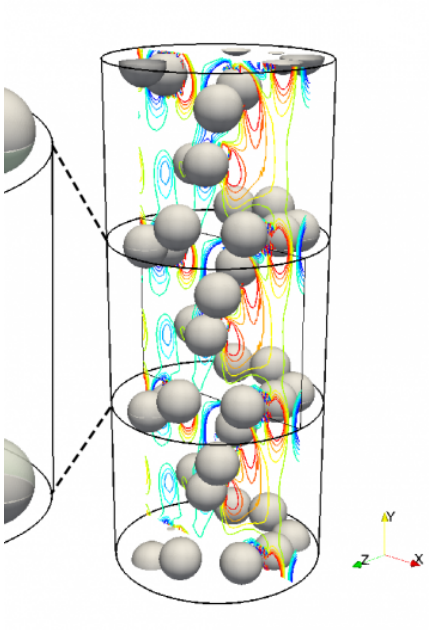


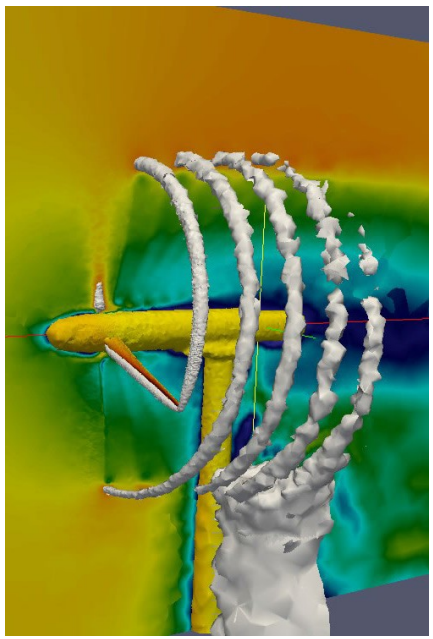
The CTTC research group

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

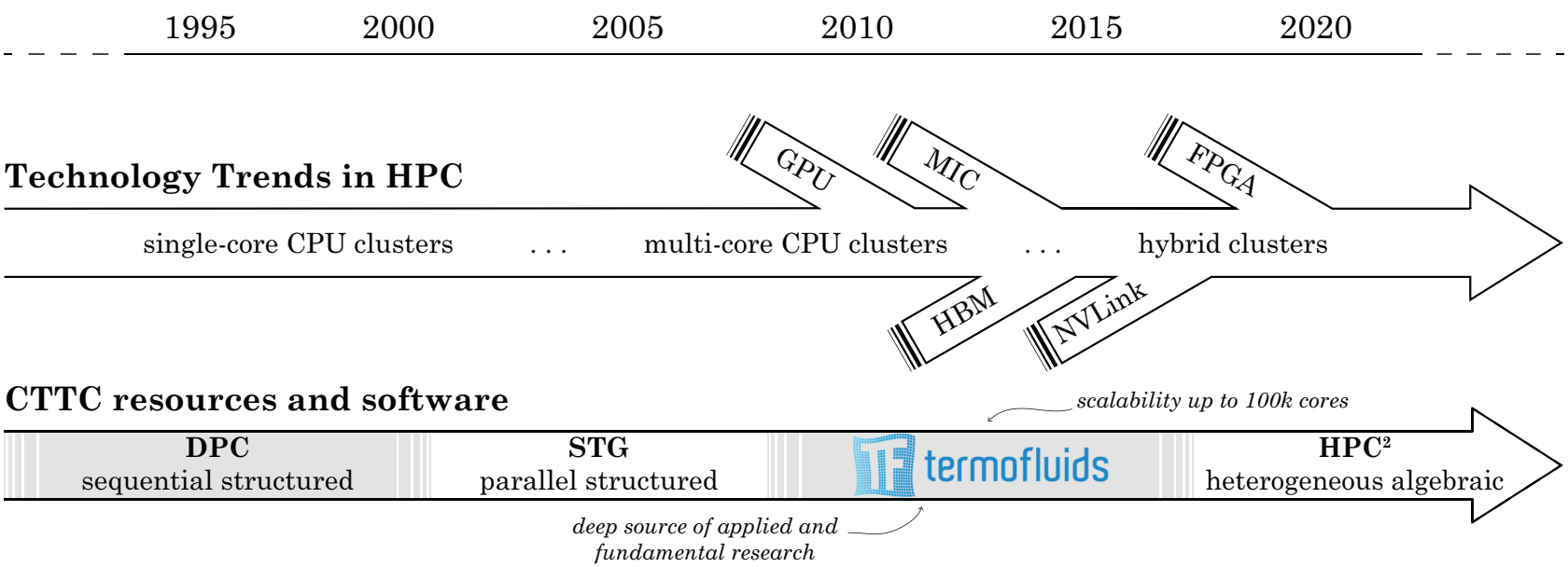
- **Fundamental research** on numerical methods, fluid dynamics and heat and mass transfer phenomena.
- **Applied research** on thermal and fluid dynamic optimization of thermal system and equipment.





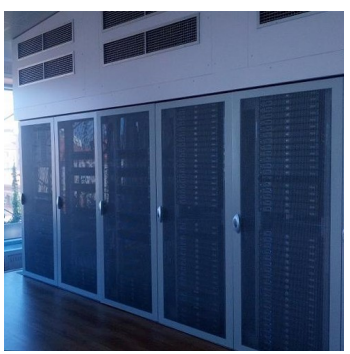


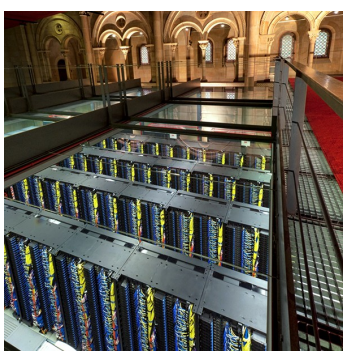
CTTC's historical background in HPC

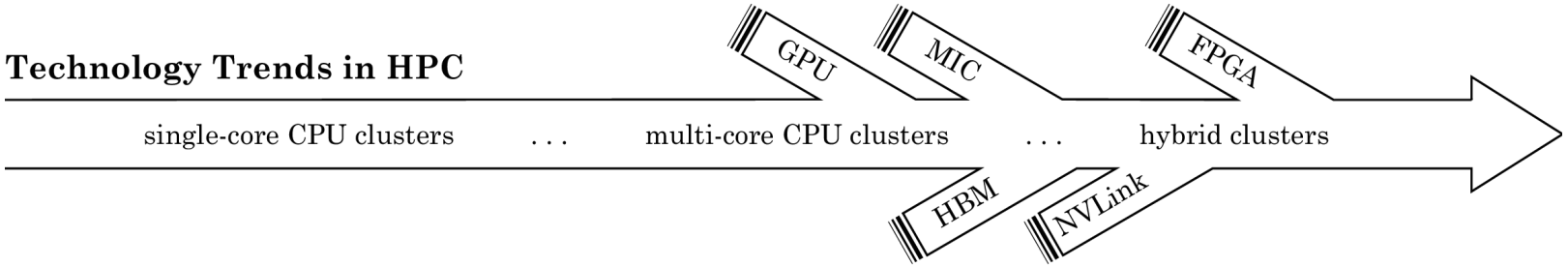






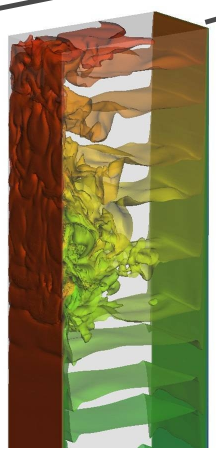




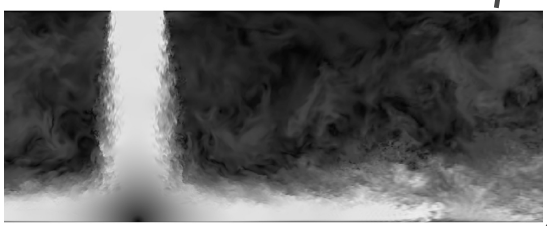




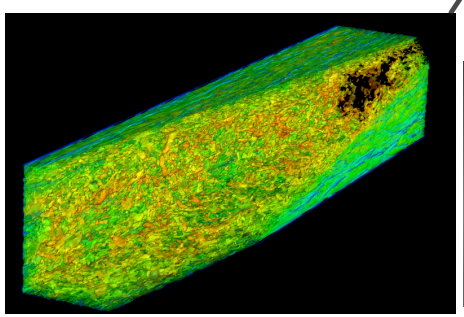
DHC
$Ra=10^9$
(3.2M)



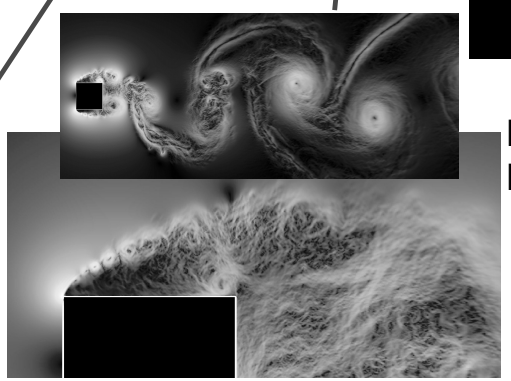
DHC
$Ra=10^{11}$
(111M)



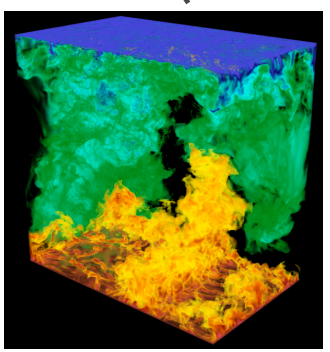
Impinging jet
Re=20000
(102M)



DUCT Re_t=1200 **(172M)**



SqCyl Re=22000 **(324M)**



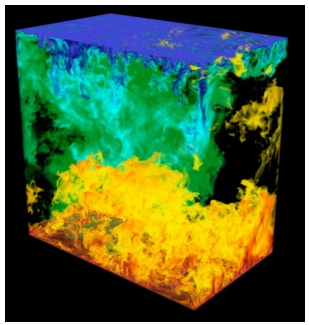
RB
$Ra=10^{10}$ **(607M)**
$Ra=10^{11}$ **(5600M)**

RED ESPAÑOLA DE SUPERCOMPUTACIÓN

PRACE

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

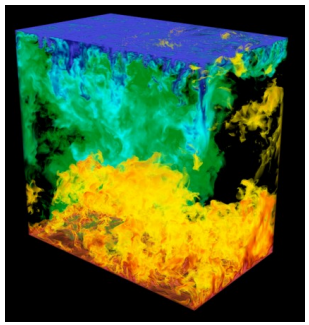
For canonical **academic** flows...



DNS

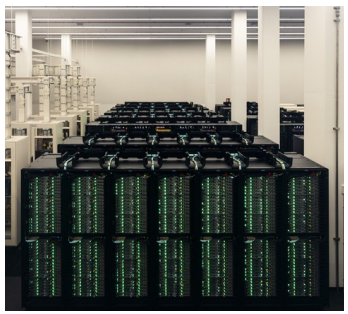
General motivation: (very) large-scale DNS/LES

For canonical **academic** flows...



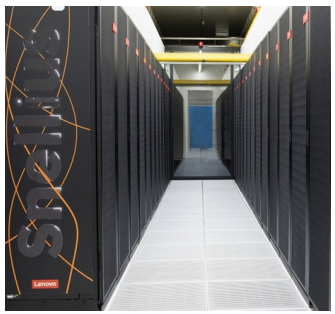
DNS

MareNostrum 5-ACC
(Barcelona)



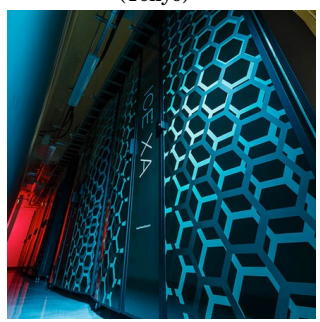
rank #8
1120 nodes with:
- 2× Intel Shappire Rapids 8460
- 1× NVIDIA Hopper 64 GB HBM
- 1× Infiniband NDR200

Snellius
(Amsterdam)



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

TSUBAME4.0
(Tokyo)



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

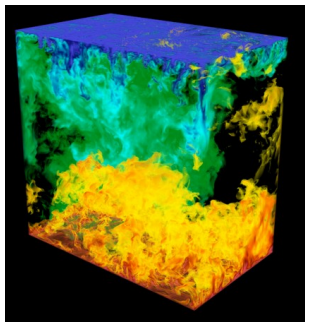




HPC (High Performance Computing)

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

For canonical **academic** flows...



How to properly discretize NS?

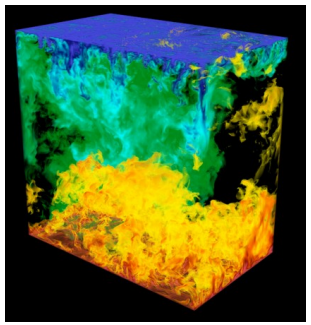
DNS

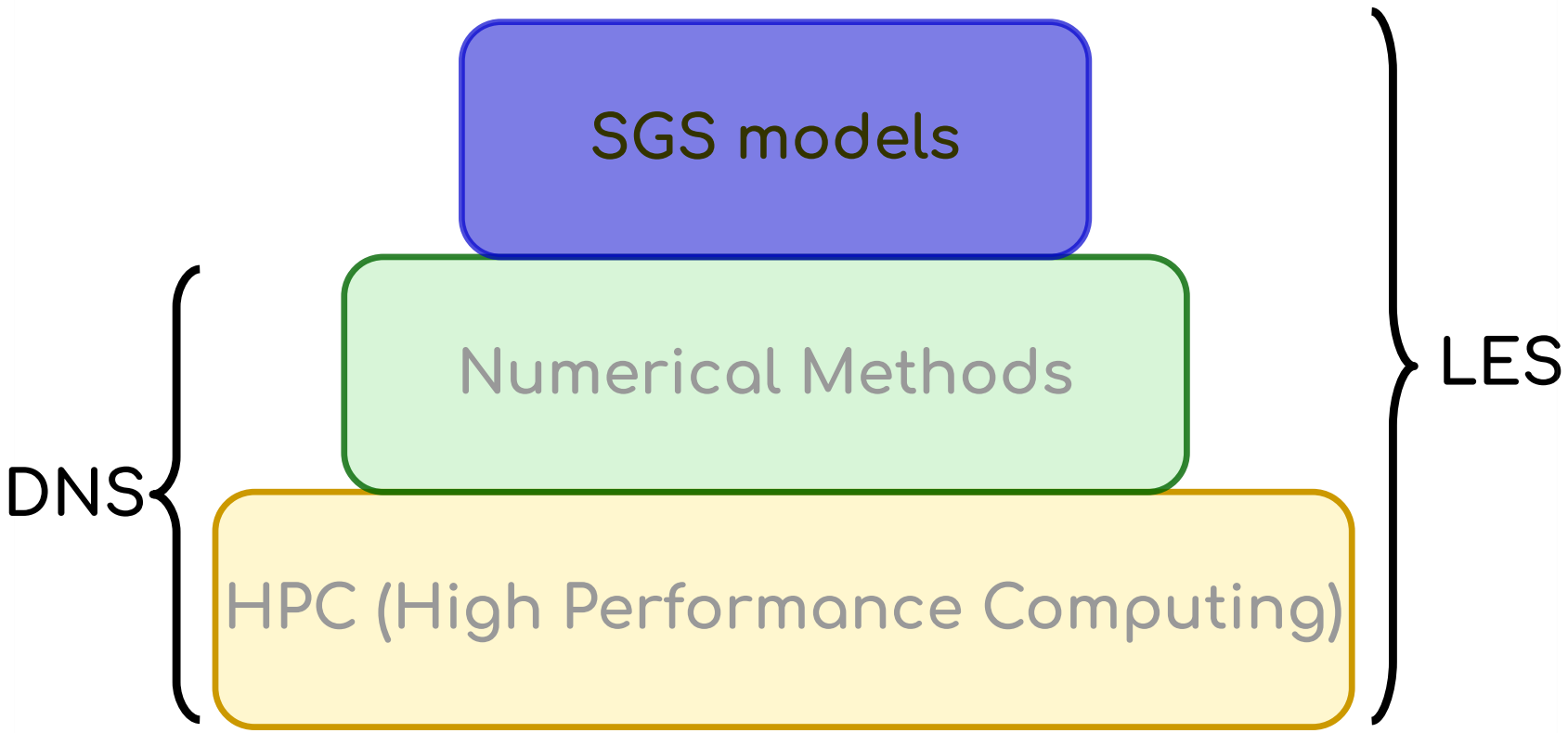
- Numerical Methods
- HPC (High Performance Computing)

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

For canonical **academic** flows...

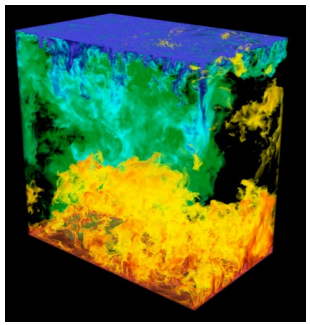
How to properly model SGS?

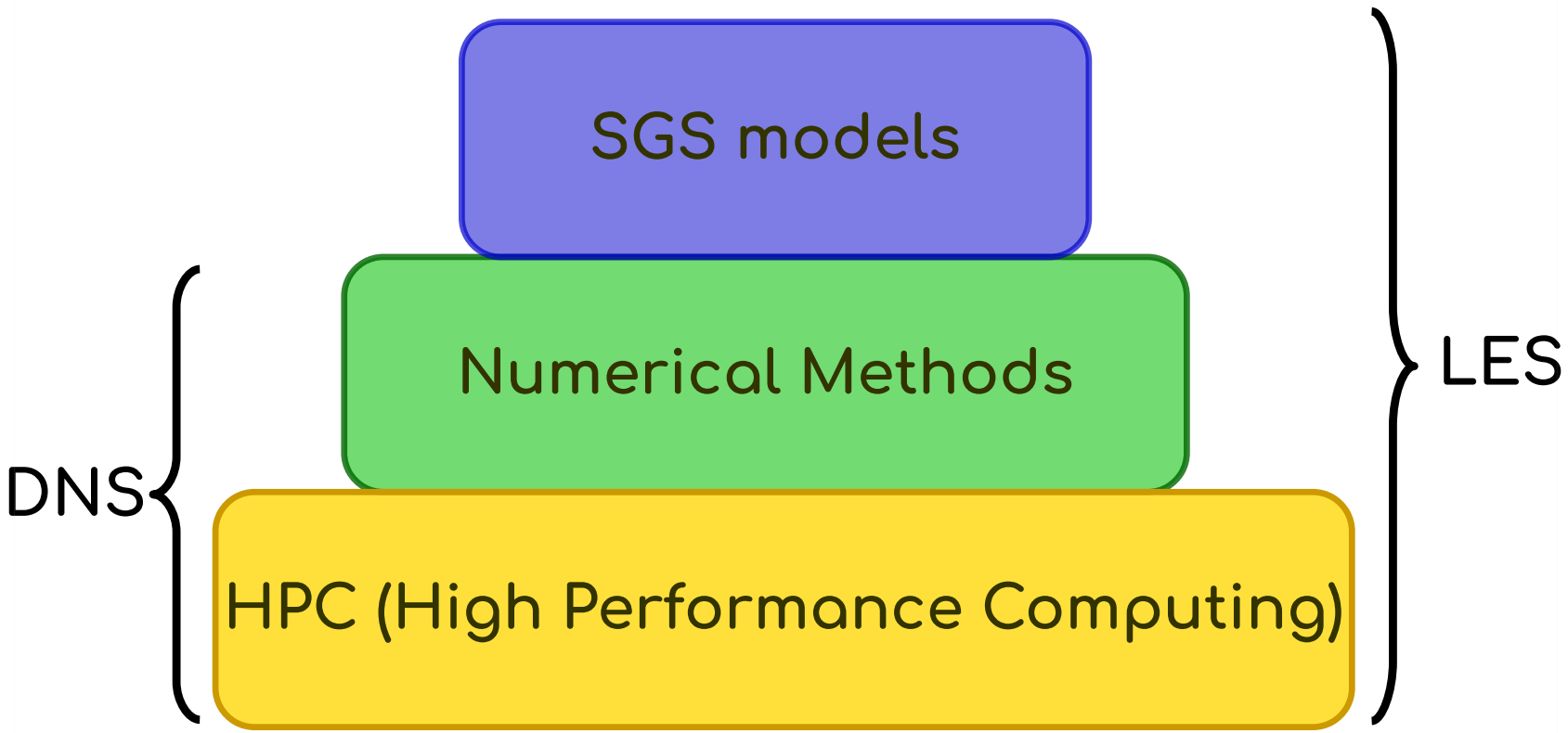




General motivation: (very) large-scale DNS/LES

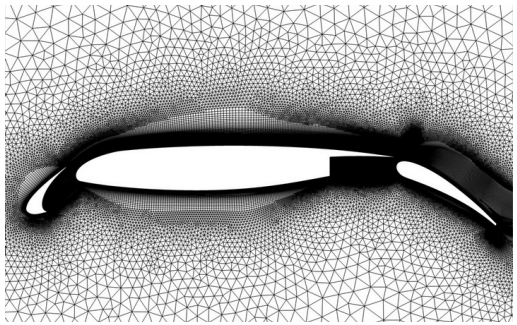
For canonical **academic** flows...

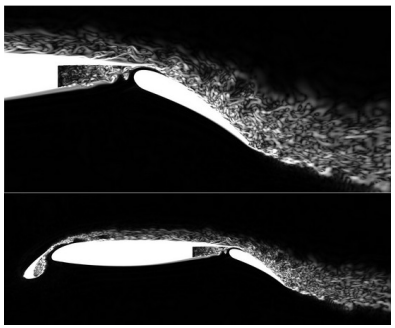


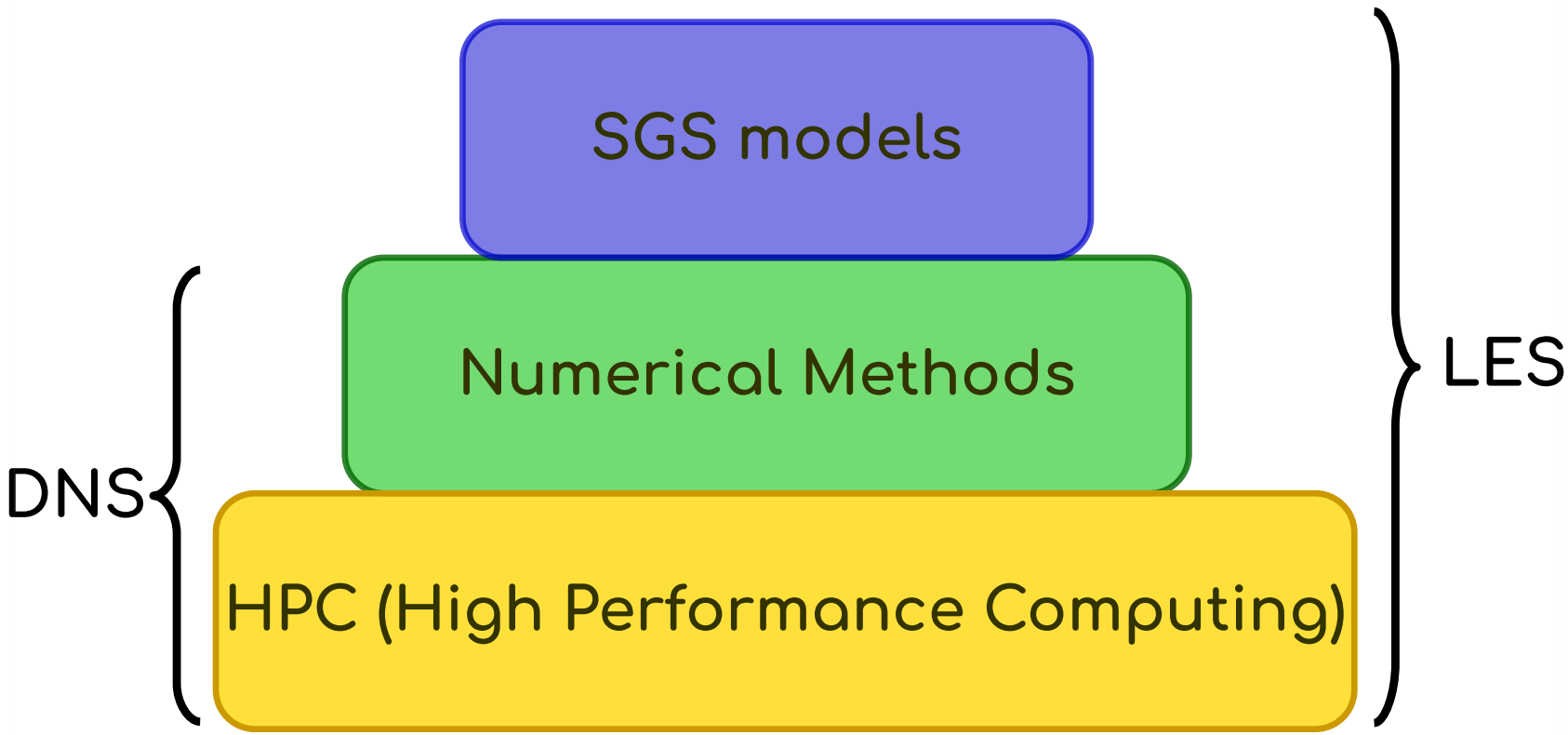


General motivation: (very) large-scale DNS/LES

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

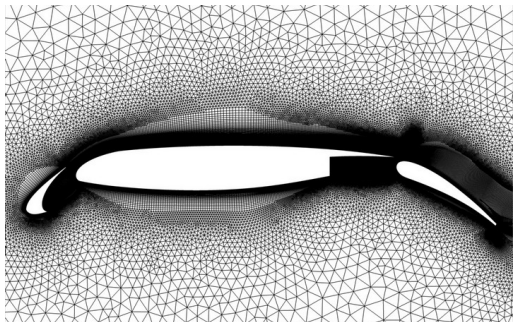


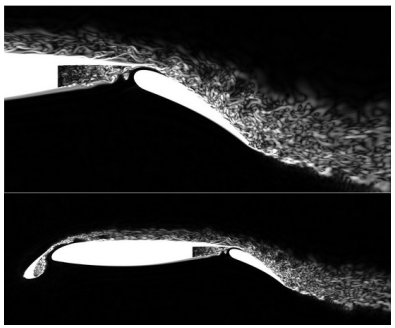


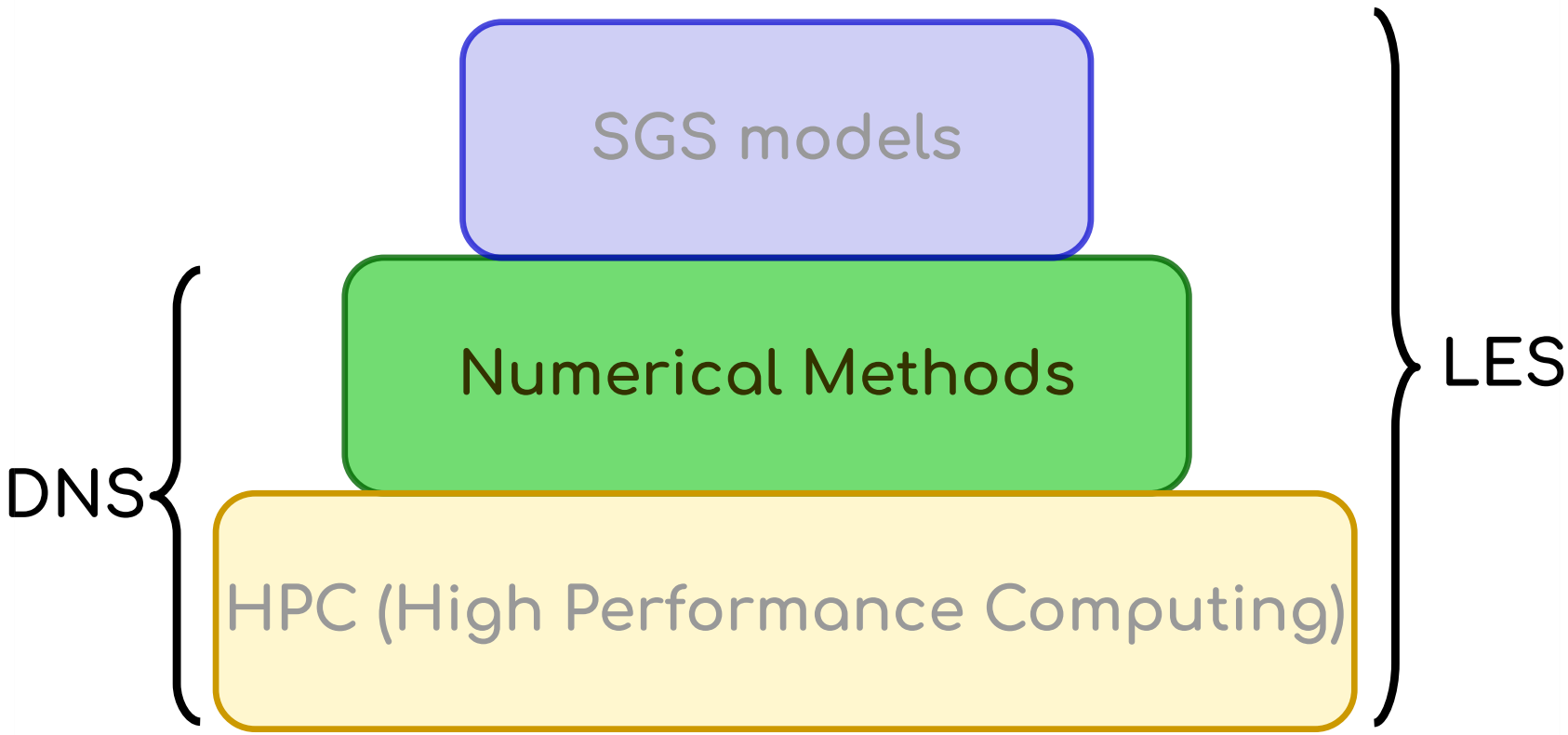


General motivation: (very) large-scale DNS/LES

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



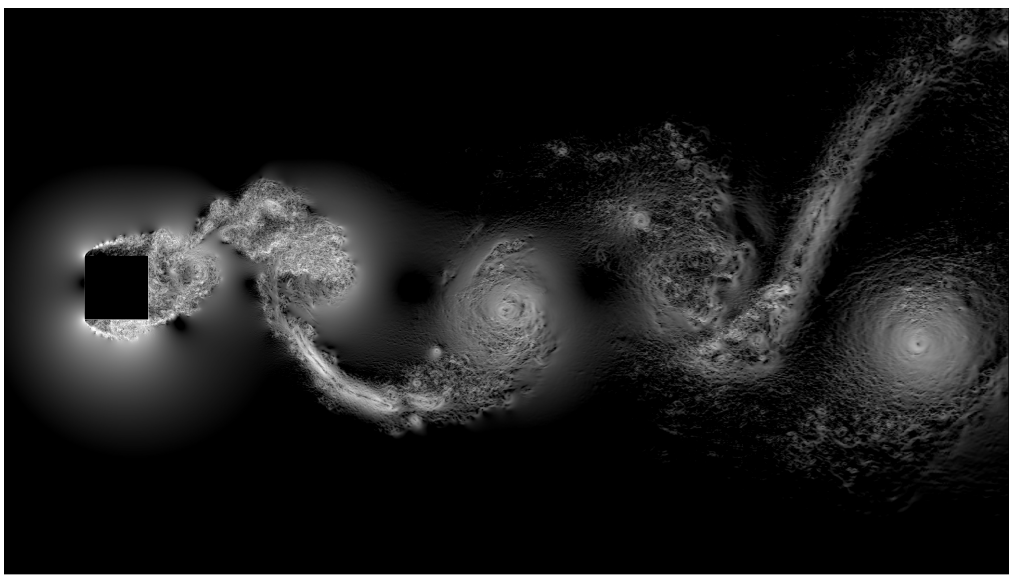


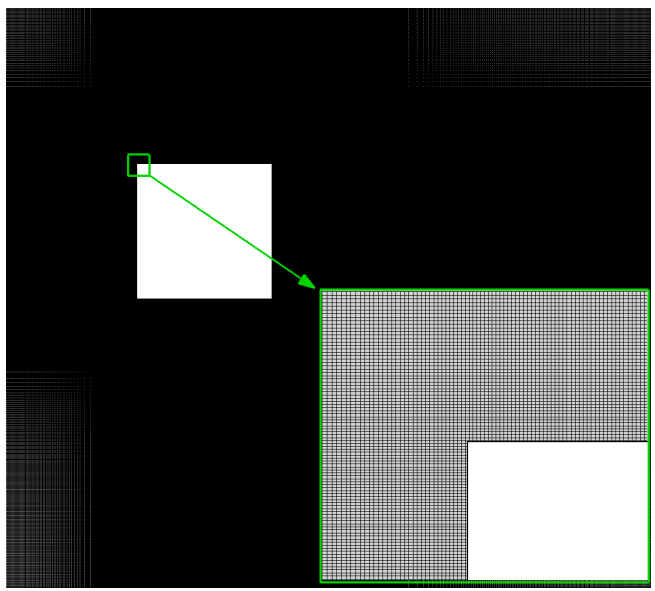


Numerical methods for DNS/LES

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?





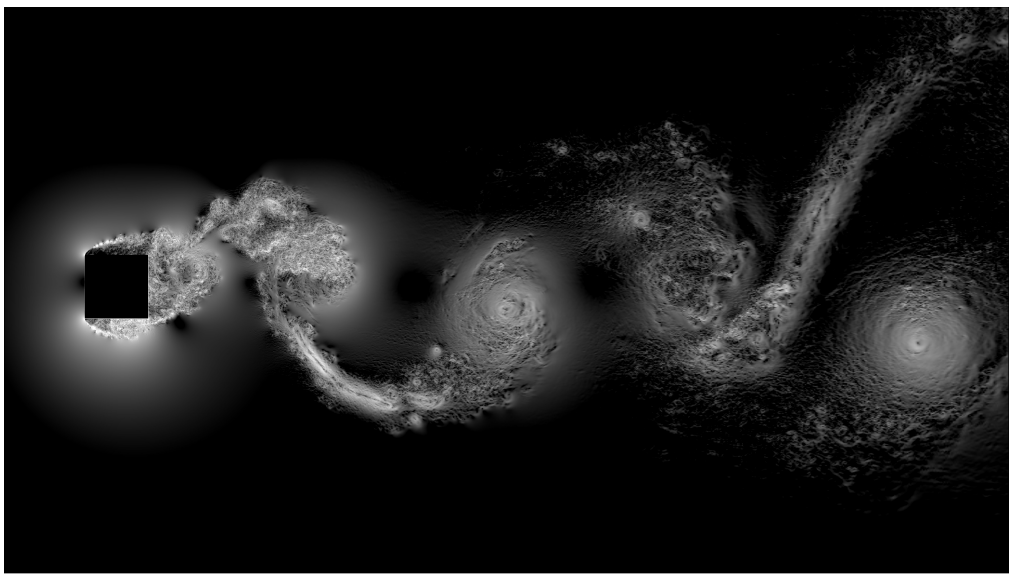
DNS[1] of the flow around a square cylinder at $Re = 55000$ (2.6B grid points)

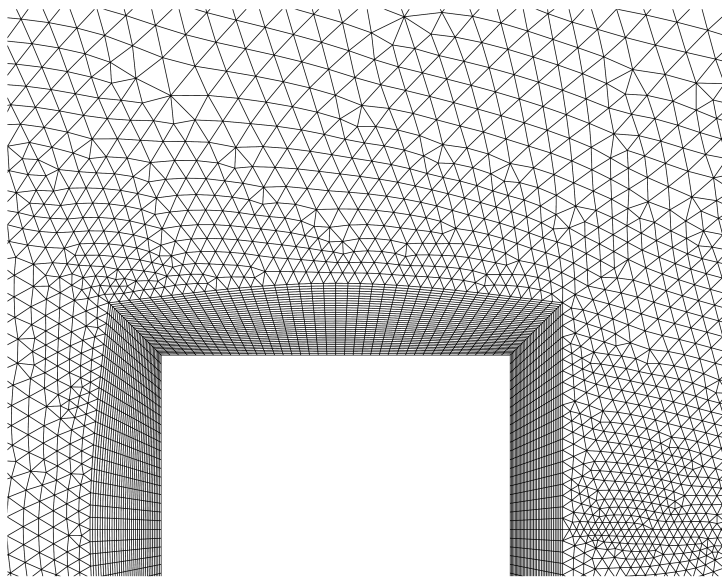
[1] F.X.Trias, À.Alsalti-Baldellou, A.Oliva. *On the Reynolds-number scaling of Poisson solver complexity*, **Physics of Fluids**, 38 (4):045157, 2026.

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.

Symmetry-preserving discretization

Continuous

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

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

Symmetry-preserving discretization

Continuous

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

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

Discrete

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

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

Symmetry-preserving discretization

Continuous

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

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

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

Discrete

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

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

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

Symmetry-preserving discretization

Continuous

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

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

$$\left\langle \boldsymbol{a}, \boldsymbol{b} \right\rangle = \int_\Omega \boldsymbol{a}\boldsymbol{b} d\Omega$$

$$\left\langle C\left(\boldsymbol{u}, \varphi_1\right), \varphi_2 \right\rangle = -\left\langle C\left(\boldsymbol{u}, \varphi_2\right), \varphi_1 \right\rangle$$

Discrete

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

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

$$\left\langle \boldsymbol{a}_h, \boldsymbol{b}_h \right\rangle_h = \boldsymbol{a}_h^T \Omega \boldsymbol{b}_h$$

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

Symmetry-preserving discretization

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

Symmetry-preserving discretization

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

Why a collocated formulation?

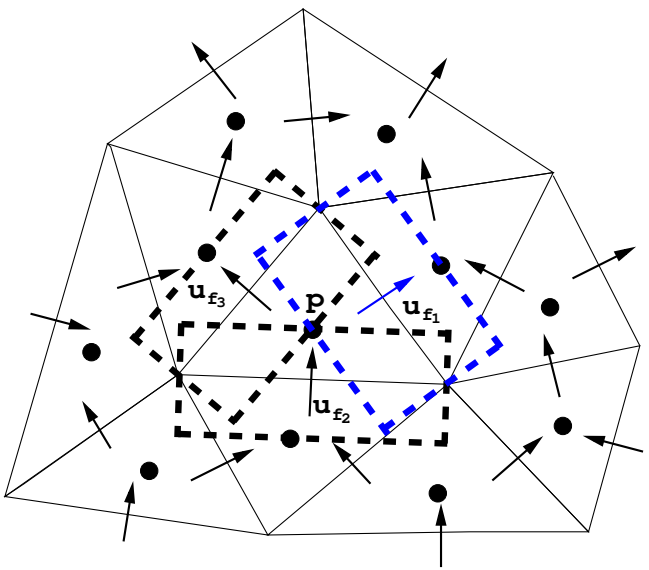
- STAR-CCM+
- ANSYS-FLUENT
- Code-Saturne
- OpenFOAM



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

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?

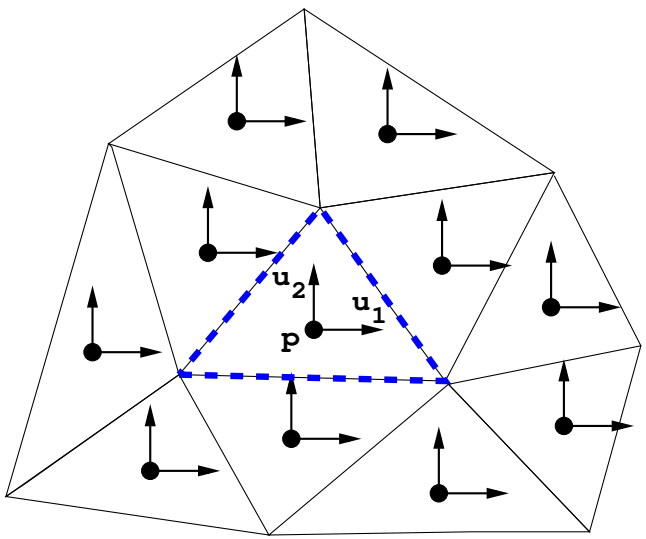
- STAR-CCM+
- ANSYS-FLUENT
- Code-Saturne
- OpenFOAM



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

In collocated meshes

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



Why a collocated formulation?

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

Journal of Computational Physics 258 (2014) 246–267

Contents lists available at ScienceDirect

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,*,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

ARTICLE INFO

Article history:
Received 19 November 2012

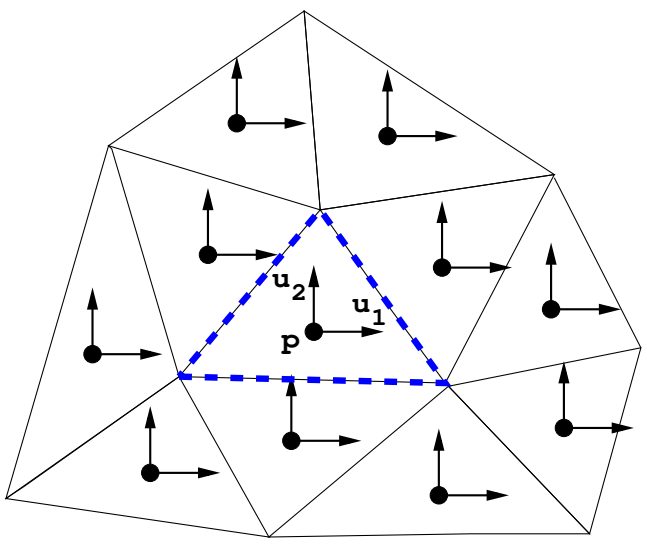
ABSTRACT

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

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

In collocated meshes

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



Why a collocated formulation?

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

Journal of Computational Physics 258 (2014) 246–267

Contents lists available at ScienceDirect

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,*,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

ARTICLE INFO

Article history:
Received 19 November 2012

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

Computers and Fluids 225 (2021) 104979

Contents lists available at ScienceDirect

Computers and Fluids

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

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
Revised 22 March 2021
Accepted 23 April 2021
Available online 27 April 2021

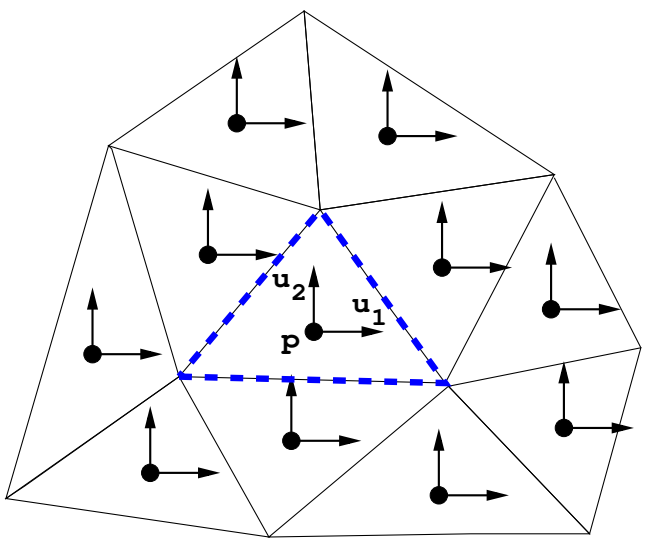
ABSTRACT

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

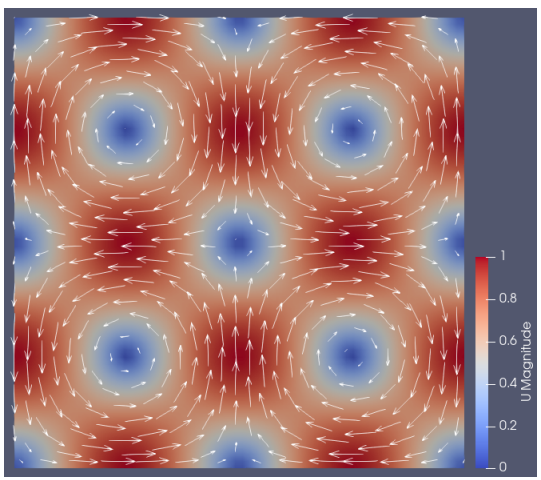
- p-$\boldsymbol{u}_c$ coupling is cumbersome ✗
- $\mathrm{C}(\boldsymbol{u}_s)$ and D easy to discretize ✓
- Cheaper, less memory,... ✓

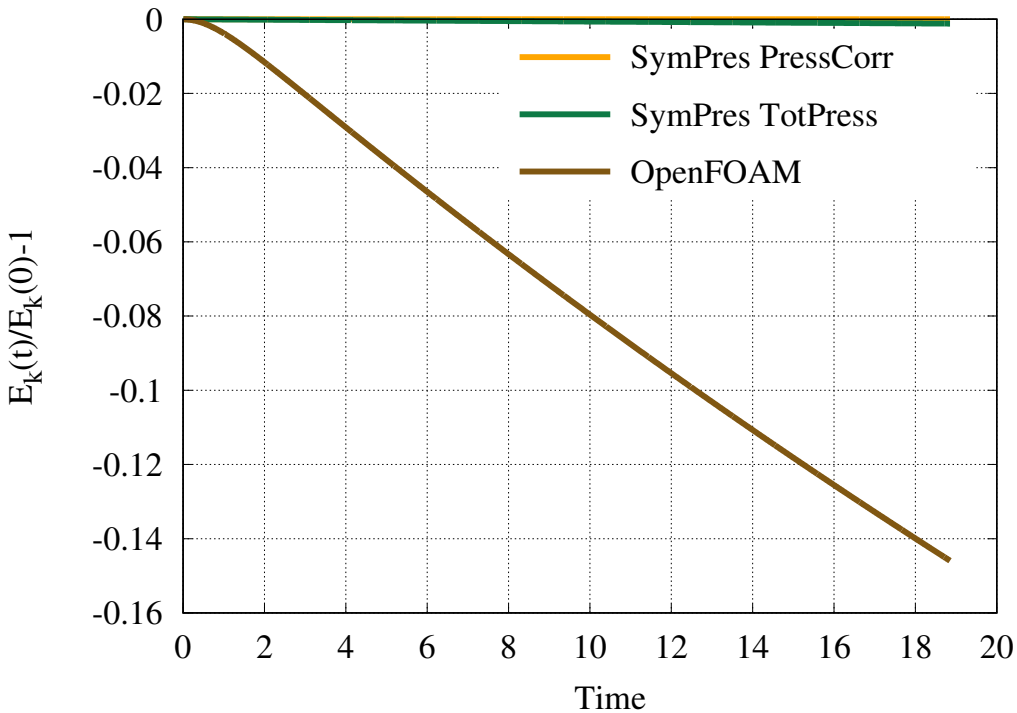


Pressure-velocity coupling on collocated grids

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

OpenFOAM



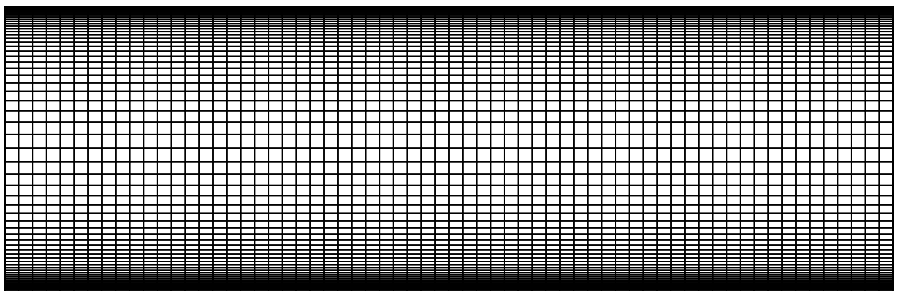


Results for an inviscid Taylor-Green vortex[3]

[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

Contents lists available at ScienceDirect

Journal of Computational Physics

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

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

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

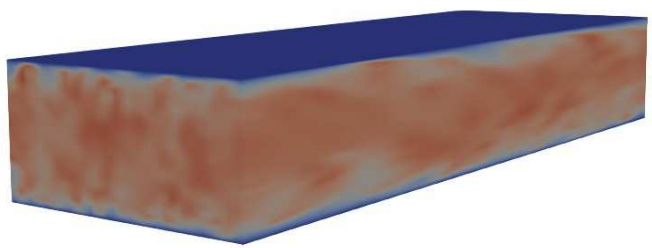
Technical University of Catalonia, Heat and Mass Transfer Technological Center (CTTC), C/ Colom 11 Building TR4, Terrassa, 08222, Barcelona, Spain

ARTICLE INFO

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

ABSTRACT

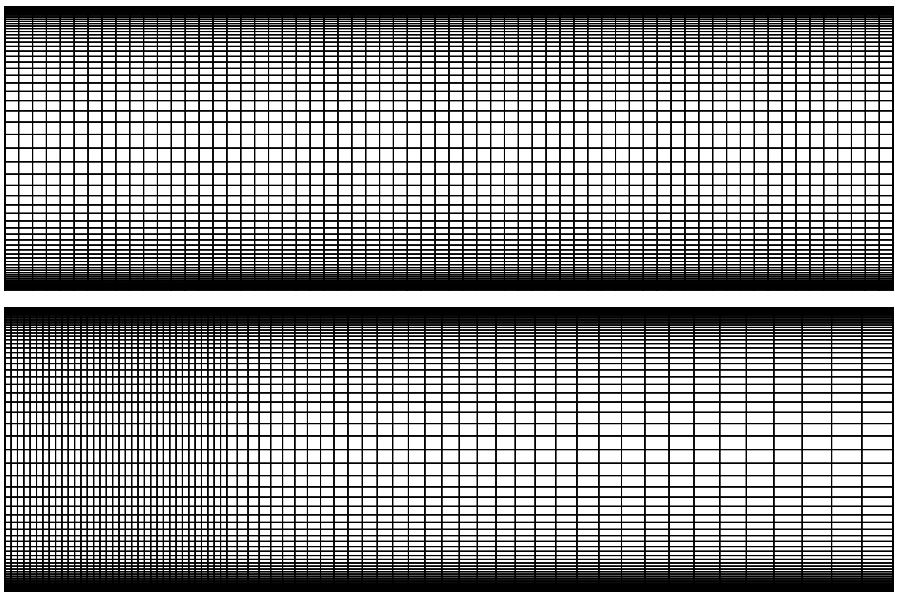
This work establishes the conditions for having a symmetry-preserving unconditionally stable projection method for incompressible flows, such as PISO or Fractional Step Method (FSM), on collocated unstructured grids based on a compact stencil Poisson equation. Its formulation is based on preserving the 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, this 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. Conservation of (global) kinetic energy is



[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!



Journal of Computational Physics 523 (2025) 113631

Contents lists available at ScienceDirect

Journal of Computational Physics

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

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

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

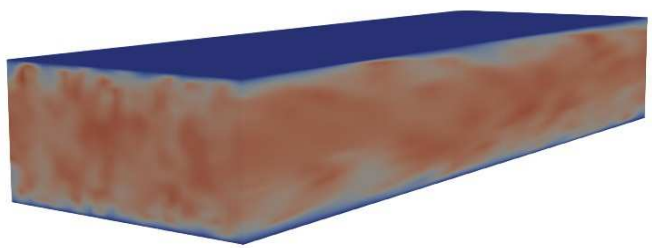
Technical University of Catalonia, Heat and Mass Transfer Technological Center (CTTC), C/ Colom 11 Building TR4, Terrassa, 08222, Barcelona, Spain

ARTICLE INFO

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

ABSTRACT

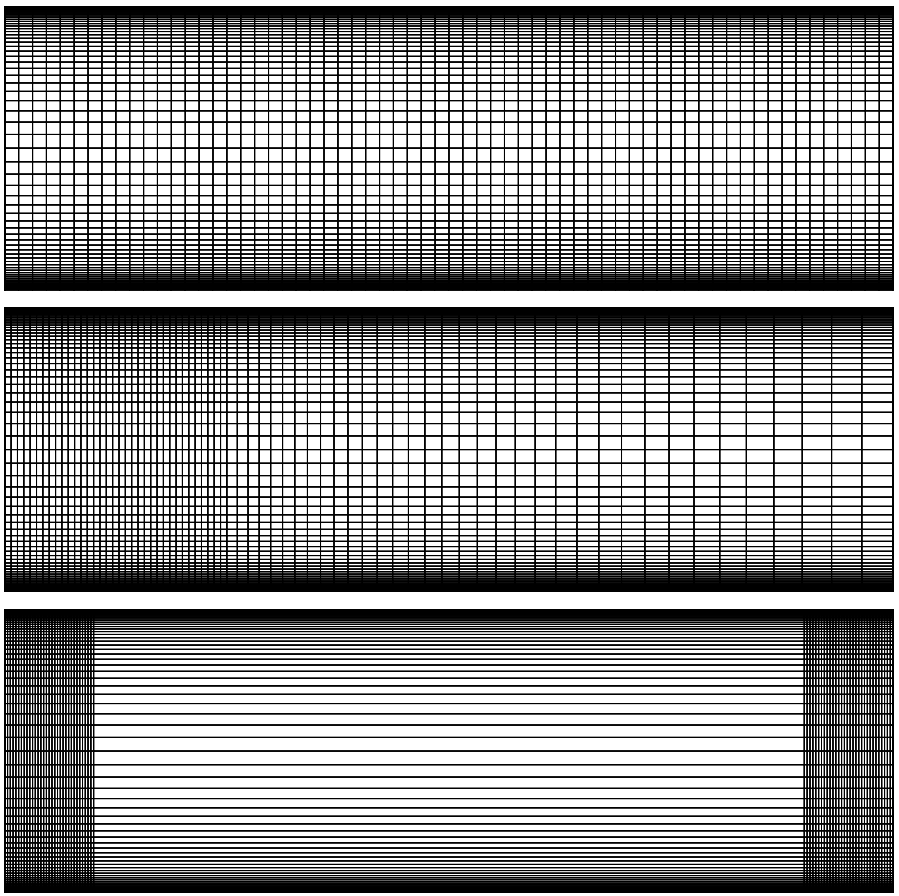
This work establishes the conditions for having a symmetry-preserving unconditionally stable projection method for incompressible flows, such as PISO or Fractional Step Method (FSM), on collocated unstructured grids based on a compact stencil Poisson equation. Its formulation is based on preserving the 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, this 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. Conservation of (global) kinetic energy is



[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!



Journal of Computational Physics 523 (2025) 113631

Contents lists available at ScienceDirect

Journal of Computational Physics

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

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

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

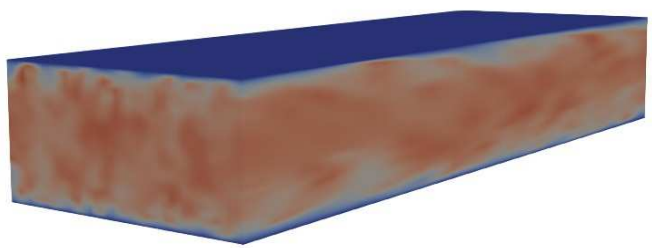
Technical University of Catalonia, Heat and Mass Transfer Technological Center (CTTC), C/ Colom 11 Building TR4, Terrassa, 08222, Barcelona, Spain

ARTICLE INFO

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

ABSTRACT

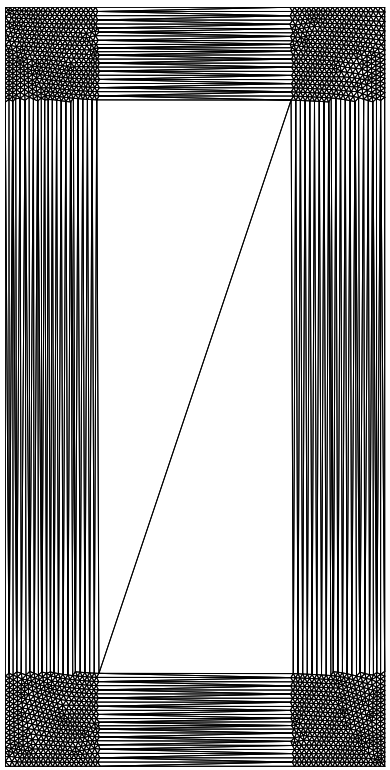
This work establishes the conditions for having a symmetry-preserving unconditionally stable projection method for incompressible flows, such as PISO or Fractional Step Method (FSM), on collocated unstructured grids based on a compact stencil Poisson equation. Its formulation is based on preserving the 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, this 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. Conservation of (global) kinetic energy is

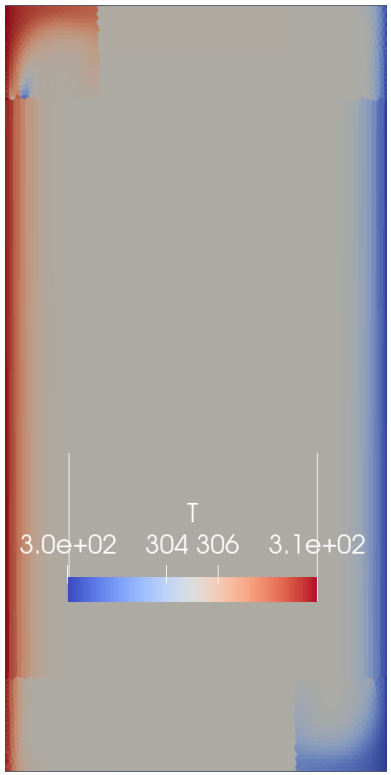


[4] D.Santos, J.A.Hopman, C.D.Pérez-Segarra, F.X.Trias. *On a symmetry-preserving unconditionally stable projection method on collocated unstructured grids for incompressible flows*, **Journal of Computational Physics**, 523:113631, 2025.

Pressure-velocity coupling on collocated grids

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





Journal of Computational Physics 523 (2025) 113631

Contents lists available at ScienceDirect

Journal of Computational Physics

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

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

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

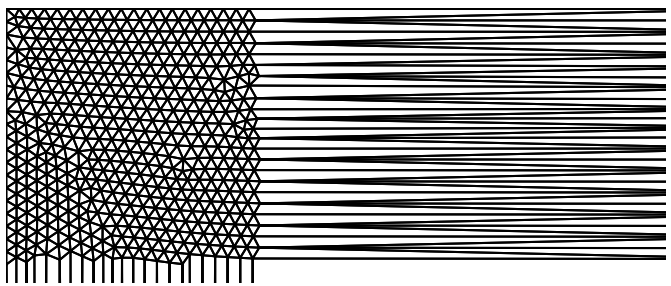
Technical University of Catalonia, Heat and Mass Transfer Technological Center (CTTC), C/ Colom 11 Building TR4, Terrassa, 08222, Barcelona, Spain

ARTICLE INFO

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

ABSTRACT

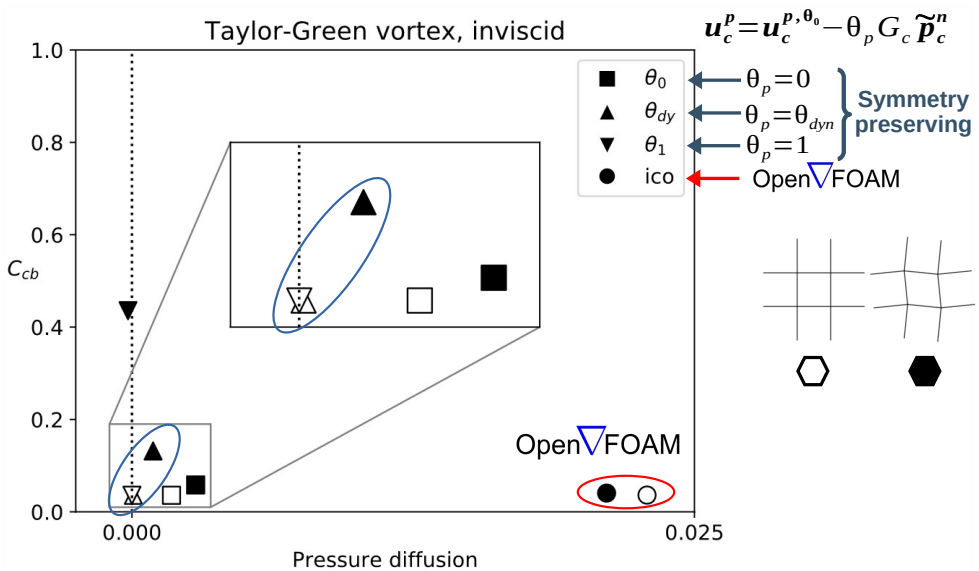
This work establishes the conditions for having a symmetry-preserving unconditionally stable projection method for incompressible flows, such as PISO or Fractional Step Method (FSM), on collocated unstructured grids based on a compact stencil Poisson equation. Its formulation is based on preserving the 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, this 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. Conservation of (global) kinetic energy is



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



Journal of Computational Physics 521 (2025) 113537

Contents lists available at ScienceDirect

Journal of Computational Physics

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

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]

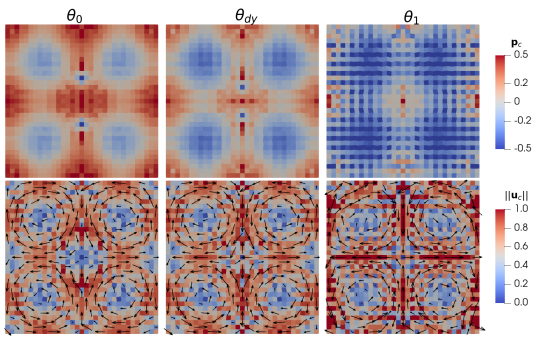
[a] Heat and Mass Transfer Technological Center, Technical University of Catalonia, ESEIAAT, c/Colom 11, Terrassa, 08222, Barcelona, Spain
[b] Termo Fluids SL, c/Magí Colet 8, Sabadell, 08204, Barcelona, Spain

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



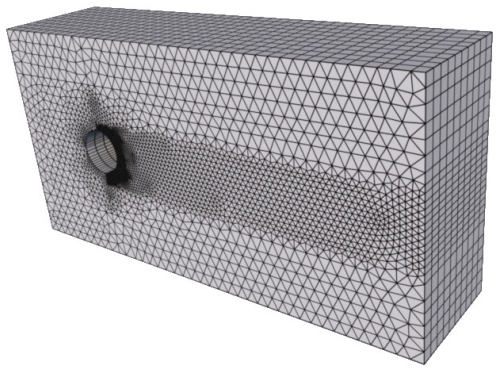
[5] J.A.Hopman, D.Santos, À.Alsalti, J.Rigola, F.X.Trias. *Quantifying the checkerboard problem to reduce numerical dissipation*, **Journal of Computational Physics**, 521:113537, 2025. arXiv: 2408.06821

Pressure-velocity coupling on collocated grids

Summary

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

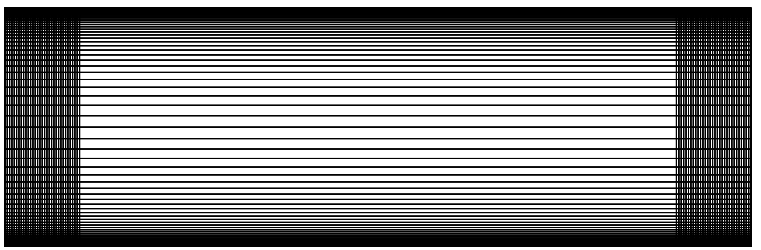
- Virtually **artificial-dissipation-free**
- Suitable for **unstructured** grids



Pressure-velocity coupling on collocated grids

Summary

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

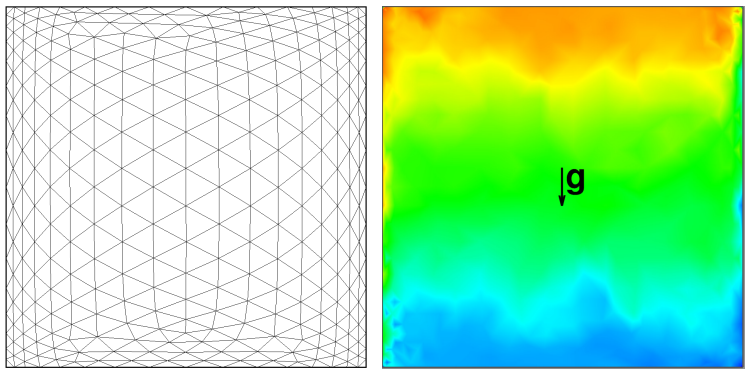


- Virtually **artificial-dissipation-free**
- Suitable for **unstructured** grids
- **Unconditionally stable** even on:
  - Very low quality grids

Pressure-velocity coupling on collocated grids

Summary

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



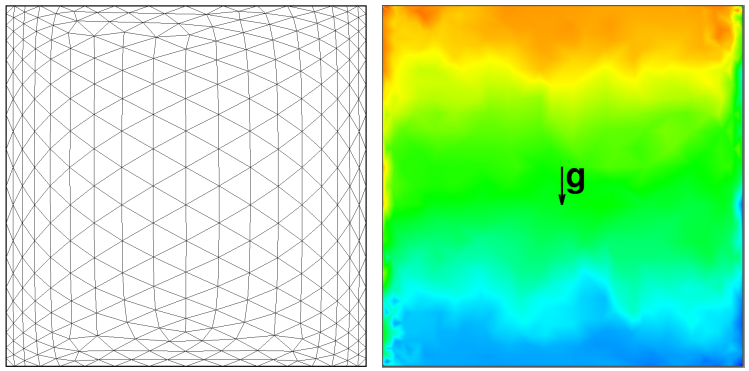
- Virtually **artificial-dissipation-free**
- Suitable for **unstructured** grids
- **Unconditionally stable** even on:
  - Very low quality grids
  - Very coarse grids

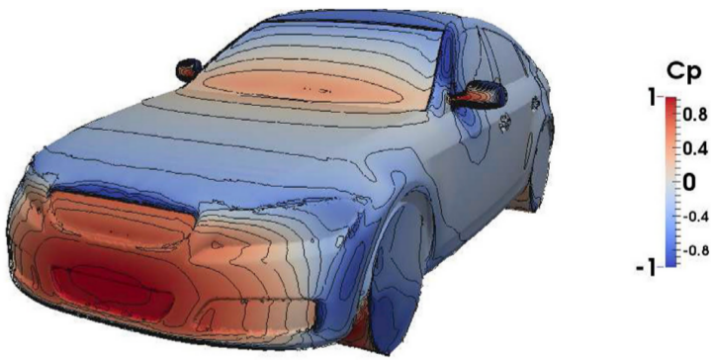
Pressure-velocity coupling on collocated grids

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
  - Very coarse grids
- Suitable for **industrial** applications



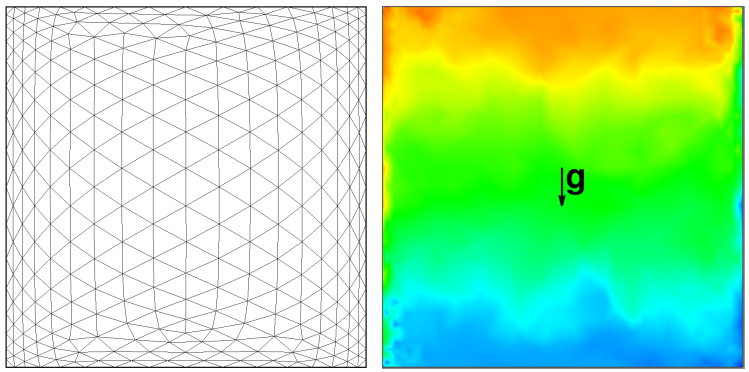


Pressure-velocity coupling on collocated grids

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

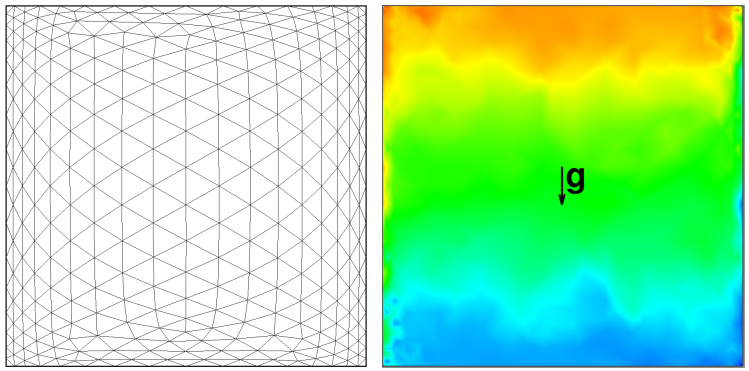


OpenFOAM

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

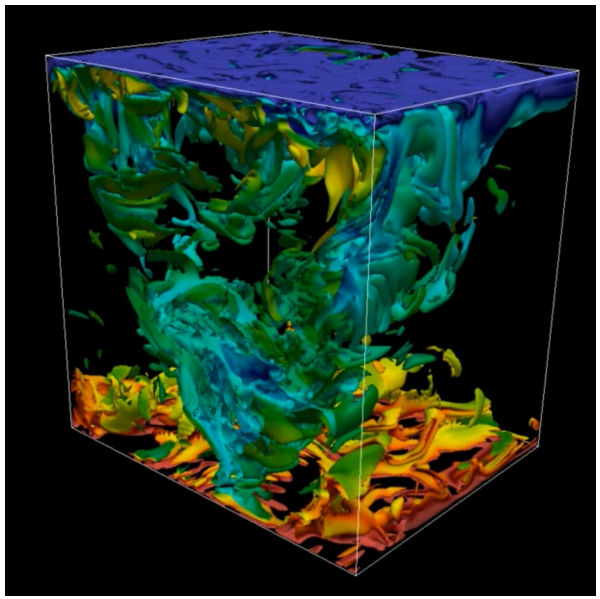
OpenFOAM

Research question #2:

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

Buoyancy-driven flows

Energy-exchanges



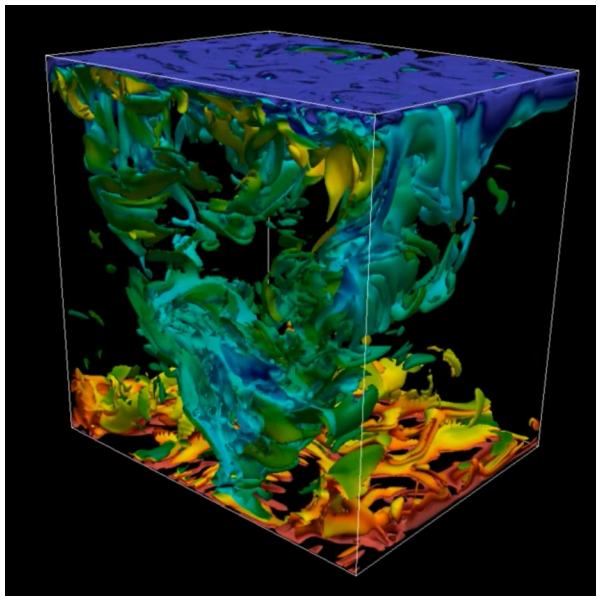
E_p
$-(y,T)$

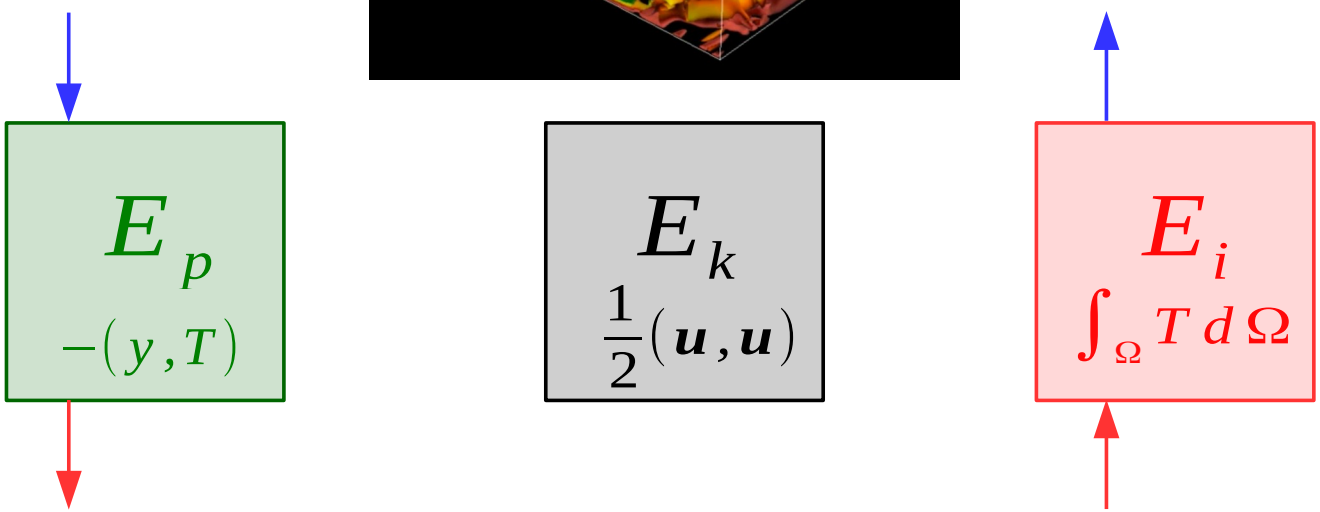
E_k
$\frac{1}{2}(\boldsymbol{u},\boldsymbol{u})$

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

Buoyancy-driven flows

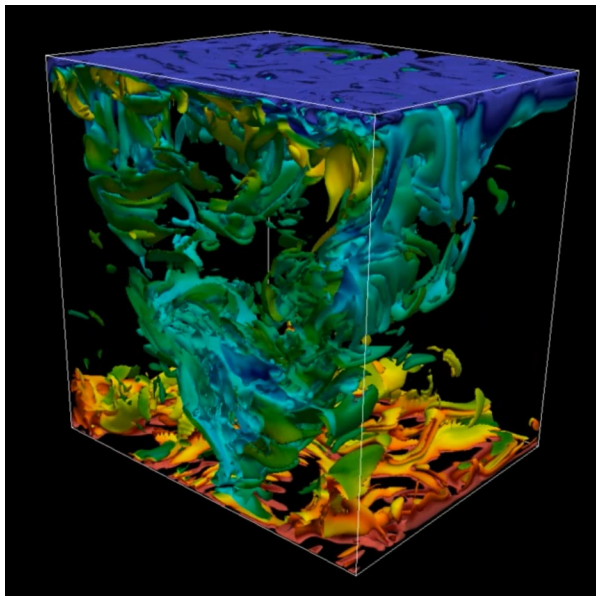
Energy-exchanges

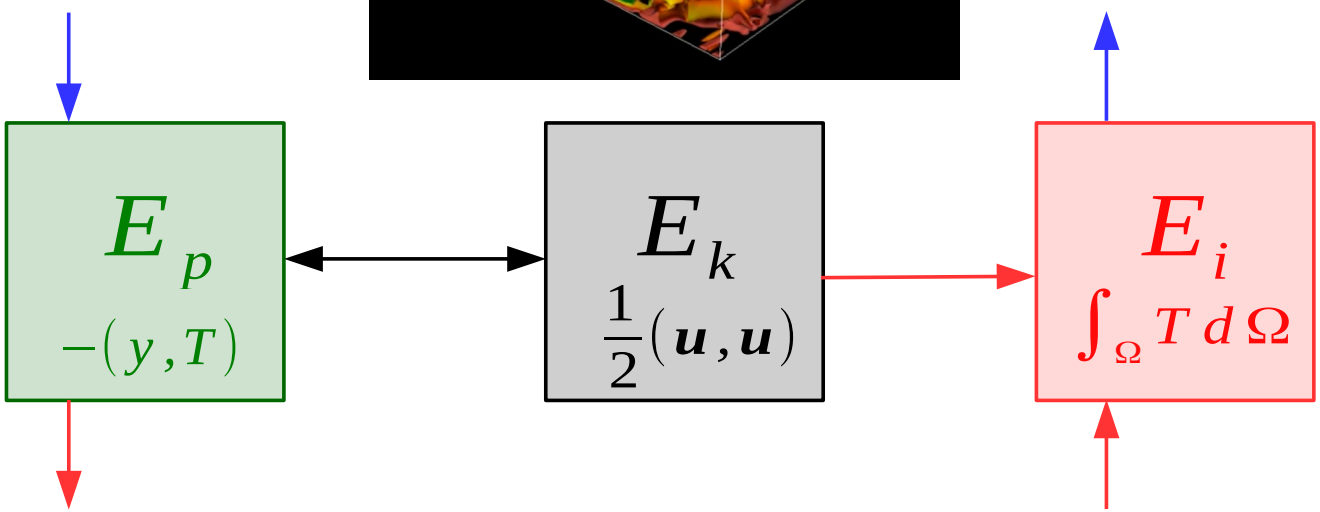




Buoyancy-driven flows

Energy-exchanges





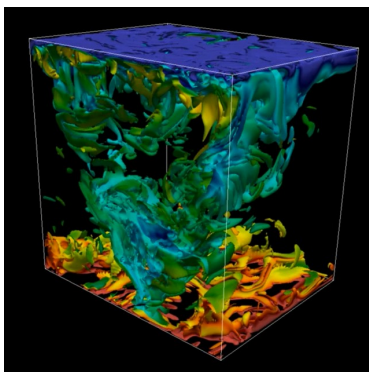
Buoyancy-driven flows

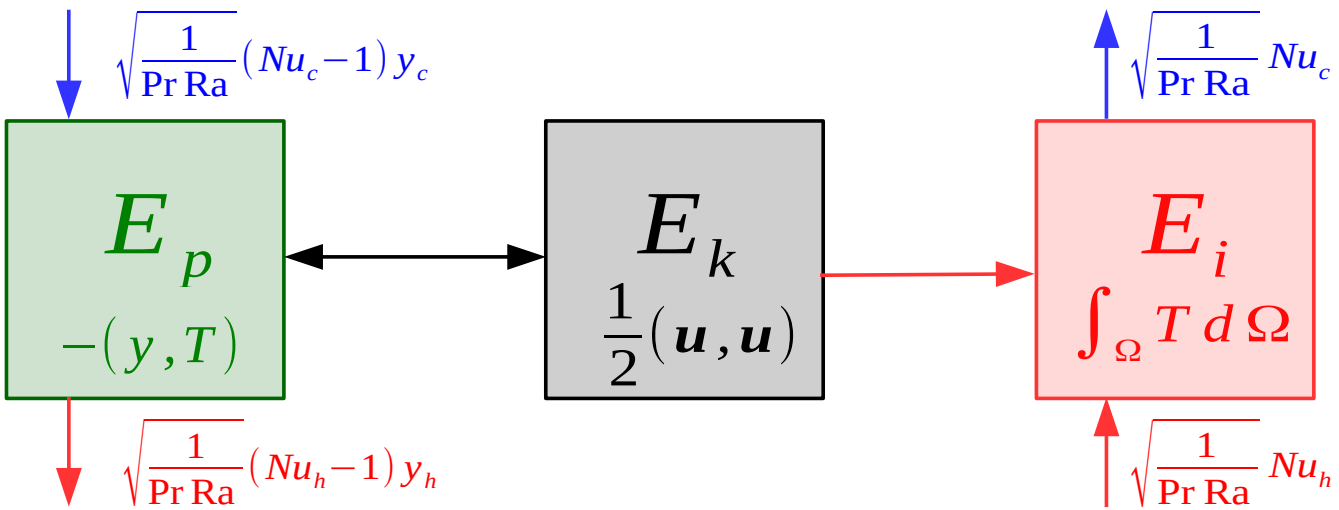
Continuous formulation

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u} = \sqrt{\frac{\mathrm{Pr}}{\mathrm{Ra}}}\nabla^2\boldsymbol{u} - \nabla p + T\,\boldsymbol{e}_y \qquad \nabla\cdot\boldsymbol{u} = 0$$

Boussinesq

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





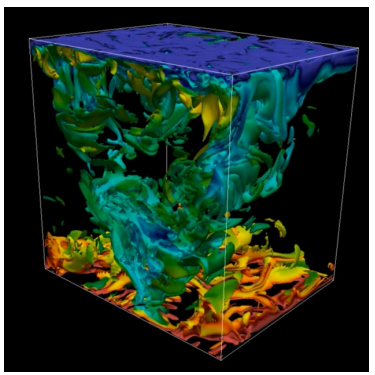
Buoyancy-driven flows

Continuous formulation

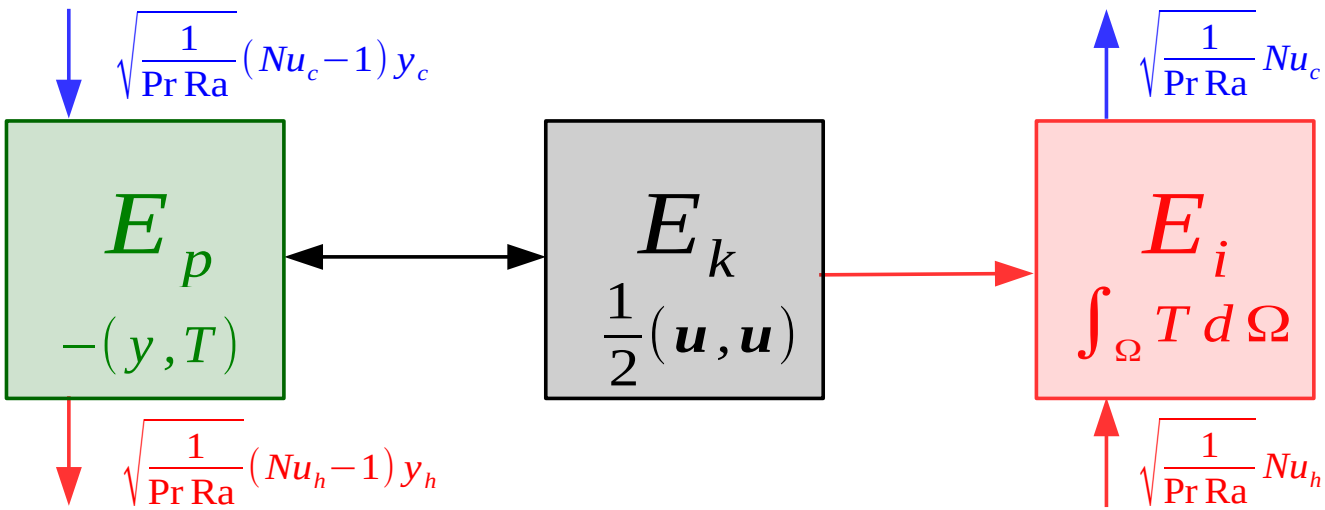
$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u} = \sqrt{\frac{\mathrm{Pr}}{\mathrm{Ra}}}\nabla^2\boldsymbol{u} - \nabla p + T\,\boldsymbol{e}_y \qquad \nabla\cdot\boldsymbol{u} = 0$$

Boussinesq

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



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



Buoyancy-driven flows

Continuous formulation

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

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

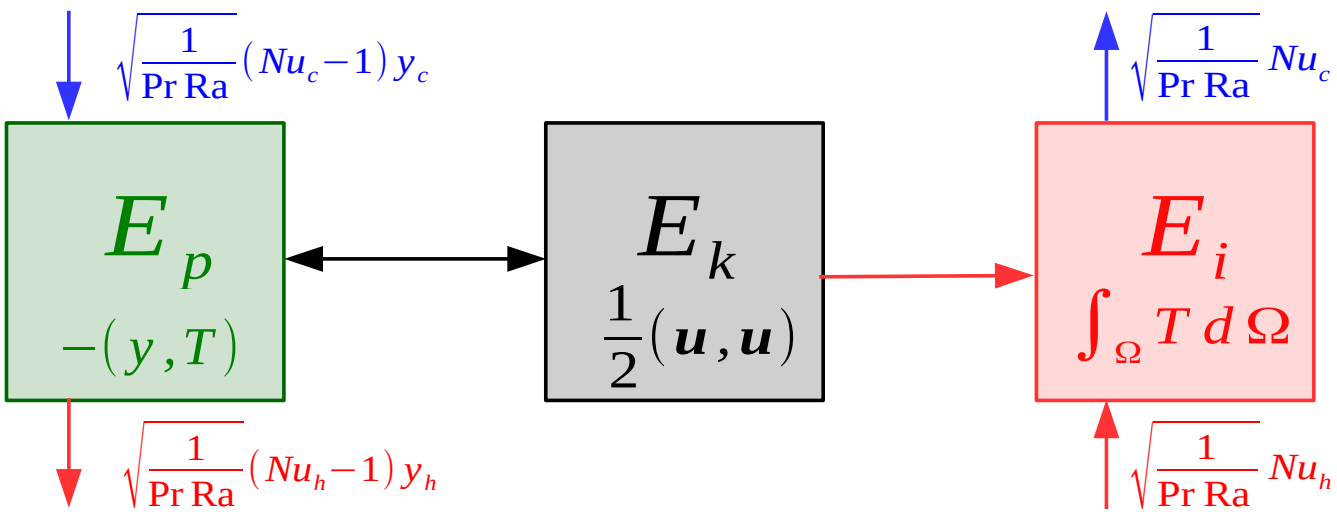
$$\frac{\partial T}{\partial t}+(\boldsymbol{u}\cdot\nabla)T=\sqrt{\frac{1}{\mathrm{Pr}\,\mathrm{Ra}}}\nabla^2 T$$

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

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

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

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



Buoyancy-driven flows

Continuous formulation

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

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

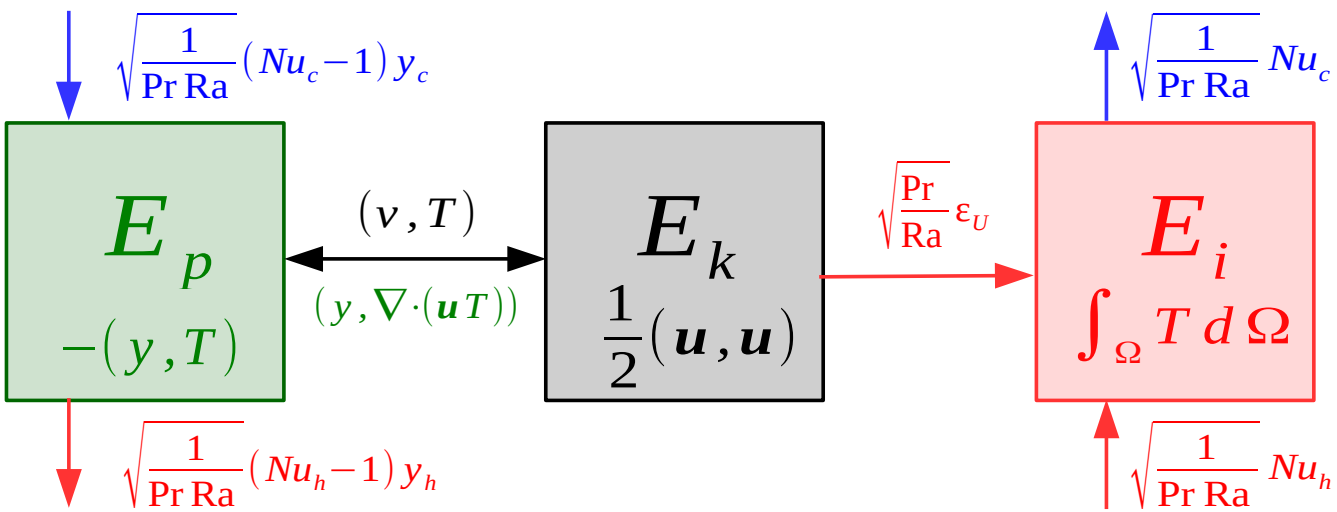
$$\frac{\partial T}{\partial t}+(\boldsymbol{u}\cdot\nabla)T=\sqrt{\frac{1}{\mathrm{Pr}\,\mathrm{Ra}}}\nabla^2 T$$

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

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

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

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



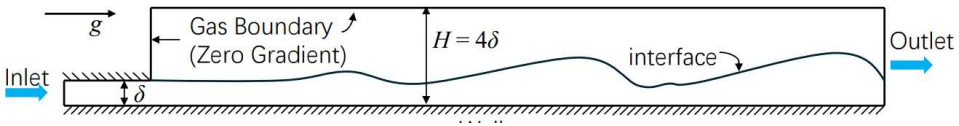
Multiphase flows

Continuous formulation

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

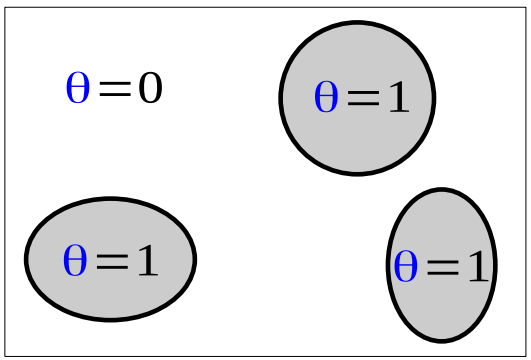
$$\frac{\partial\theta}{\partial t}+(\vec{u}\cdot\nabla)\theta=0$$

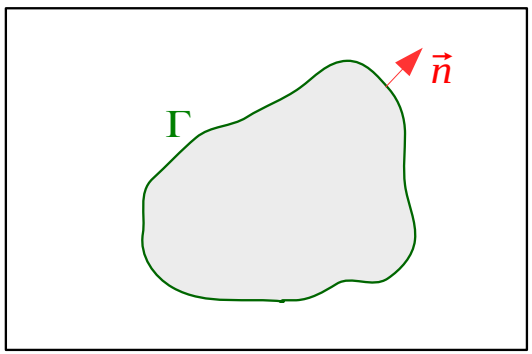
$$\kappa=-\nabla\cdot\vec{n}\quad\text{where}\quad\vec{n}=\frac{\nabla\theta}{|\nabla\theta|}$$











Multiphase flows

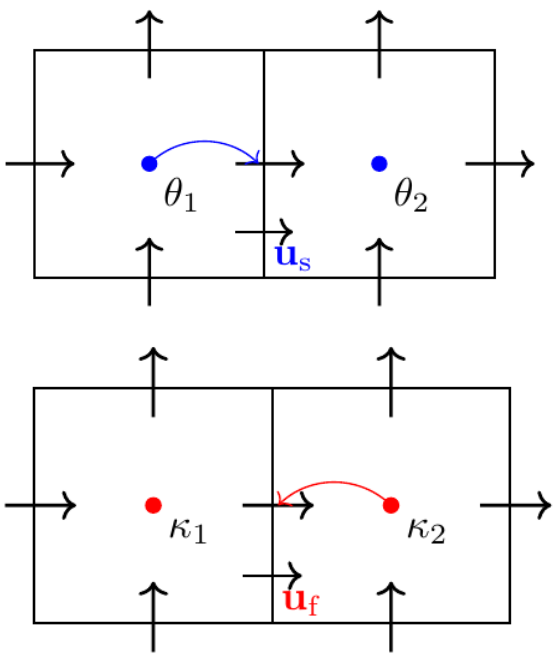
Conservative discrete formulation

Surface tension

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

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

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



Journal of Computational Physics 400 (2020) 108991

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

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), ESEIAAT, Carrer Colom 11, 08222 Terrassa (Barcelona), Spain

ARTICLE INFO

Article history:
Received 10 April 2019
Received in revised form 14 August 2019
Accepted 23 September 2019
Available online 30 September 2019

Keywords:
Multiphase flow
Symmetry-preserving
Mimetic
Conservative level set
Energy-preserving

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.

© 2019 Elsevier Inc. All rights reserved.

Multiphase flows

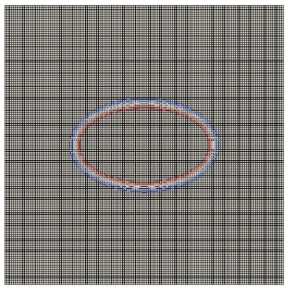
Conservative discrete formulation

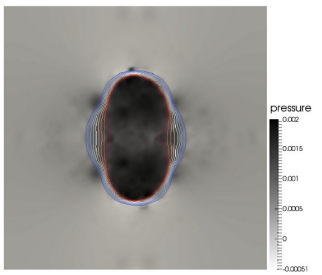
Surface tension

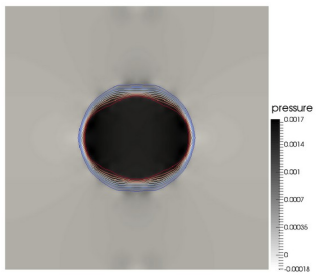
$$\rho\frac{\partial\vec{u}}{\partial t}+\rho(\vec{u}\cdot\nabla)\vec{u}=\nabla\cdot(2\mu\,S(\vec{u}))-\nabla p+\gamma\,\kappa\cdot\vec{n} \qquad \nabla\cdot\vec{u}=0$$

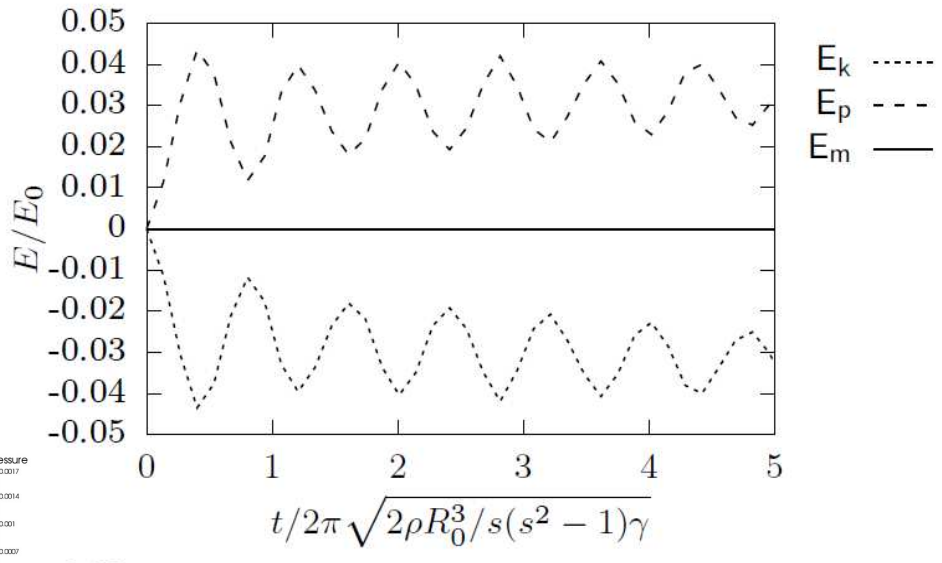
$$\frac{\partial\theta}{\partial t}+(\vec{u}\cdot\nabla)\theta=0$$

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









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)

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

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)

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

$\mu^{\phi} = \dfrac{\delta E^{\phi}[\phi]}{\delta\phi}$ Variational derivative

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

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)

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

Associated energy

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

Variational derivative

$$\frac{dE^{\phi}}{dt} = \langle \mu^{\phi}, \partial_t\phi\rangle = -\langle \mu^{\phi}, \mathscr{L}_{\boldsymbol{u}}\phi\rangle$$

$$\langle \boldsymbol{u}, \boldsymbol{f}^{\phi}\rangle = \langle \mu^{\phi}, \mathscr{L}_{\boldsymbol{u}}\phi\rangle$$

Energy balance

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

A new general framework for multiphysics

Application to buoyancy-driven flows

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

Associated force

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

Lie derivative

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

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

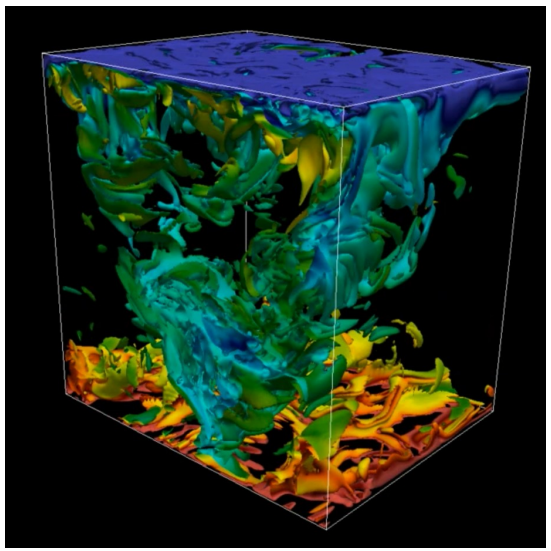
$E^{\phi}[\phi]$ Associated energy

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

$$\frac{dE^{\phi}}{dt} = \langle \mu^{\phi}, \partial_t\phi\rangle = -\langle \mu^{\phi}, \mathscr{L}_{\boldsymbol{u}}\phi\rangle$$

$\langle \boldsymbol{u}, \boldsymbol{f}^{\phi}\rangle = \langle \mu^{\phi}, \mathscr{L}_{\boldsymbol{u}}\phi\rangle$ Energy balance

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



A new general framework for multiphysics

Application to buoyancy-driven flows

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

Associated force

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

Lie derivative

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

Scalar (0-forms)

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

Density-like (3-forms)

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

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

Variational derivative

$$E^\rho[\rho] = \int_\Omega \rho\, g\, y\, d\Omega$$

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

$$\frac{dE^\phi}{dt} = \langle \mu^\phi, \partial_t\phi\rangle = -\langle \mu^\phi, \mathscr{L}_{\boldsymbol{u}}\phi\rangle$$

$$\langle \boldsymbol{u}, \boldsymbol{f}^\phi\rangle = \langle \mu^\phi, \mathscr{L}_{\boldsymbol{u}}\phi\rangle$$

Energy balance

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

A new general framework for multiphysics

Application to buoyancy-driven flows

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

Associated force

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

Lie derivative

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

Scalar (0-forms)

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

Density-like (3-forms)

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

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

Variational derivative

$$E^\rho[\rho] = \int_\Omega \rho\, g\, y\, d\Omega$$

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

$$\frac{dE^\phi}{dt} = \langle \mu^\phi, \partial_t\phi\rangle = -\langle \mu^\phi, \mathscr{L}_{\boldsymbol{u}}\phi\rangle$$

$$\langle \boldsymbol{u}, \boldsymbol{f}^\phi\rangle = \langle \mu^\phi, \mathscr{L}_{\boldsymbol{u}}\phi\rangle$$

Energy balance

$$\begin{aligned}\langle \mu^\rho, \mathscr{L}_{\boldsymbol{u}}\rho\rangle &= \langle \mu^\rho, \nabla\cdot(\boldsymbol{u}\rho)\rangle \\ &= -\langle \nabla\mu^\rho, \boldsymbol{u}\rho\rangle \\ &= -\langle \boldsymbol{u}, \rho\nabla\mu^\rho\rangle\end{aligned}$$

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

A new general framework for multiphysics

Application to buoyancy-driven flows

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

Associated force

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

Lie derivative

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

Scalar (0-forms)

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

Density-like (3-forms)

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

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

Variational derivative

$$E^\rho[\rho] = \int_\Omega \rho\, g\, y\, d\Omega$$

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

$$\frac{dE^\phi}{dt} = \langle \mu^\phi, \partial_t\phi\rangle = -\langle \mu^\phi, \mathscr{L}_{\boldsymbol{u}}\phi\rangle$$

$$\langle \boldsymbol{u}, \boldsymbol{f}^\phi\rangle = \langle \mu^\phi, \mathscr{L}_{\boldsymbol{u}}\phi\rangle$$

Energy balance

$$\langle \mu^\rho, \mathscr{L}_{\boldsymbol{u}}\rho\rangle = \langle \mu^\rho, \nabla\cdot(\boldsymbol{u}\rho)\rangle = -\langle \nabla\mu^\rho, \boldsymbol{u}\rho\rangle = -\langle \boldsymbol{u}, \rho\nabla\mu^\rho\rangle$$

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

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

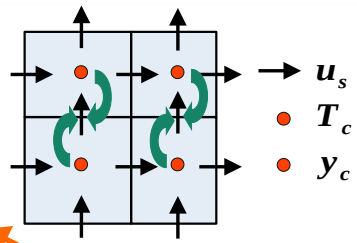
A new general framework for multiphysics

Buoyancy-driven flows on staggered grids

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

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

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



Cell-to-face interpolation

$$E_h^{\rho}[\boldsymbol{\rho}_c] := g\,\boldsymbol{\rho}_c \cdot \Omega_c \boldsymbol{y}_c$$

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

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

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

$$\begin{aligned}\langle \mu^{\rho}, \mathscr{L}_{\boldsymbol{u}} \rho \rangle &= \langle \mu^{\rho}, \nabla \cdot (\boldsymbol{u}\rho) \rangle \\ &= -\langle \nabla \mu^{\rho}, \boldsymbol{u}\rho \rangle \\ &= -\langle \rho \nabla \mu^{\rho}, \boldsymbol{u} \rangle\end{aligned}$$

$$\langle \boldsymbol{a}_c, \boldsymbol{b}_c \rangle_c := \boldsymbol{a}_c \cdot \Omega_c \boldsymbol{b}_c \qquad M = -(\Omega_s G)^T$$

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

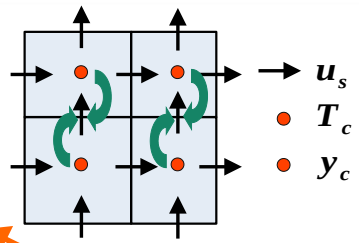
A new general framework for multiphysics

Buoyancy-driven flows on staggered grids

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

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

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



Cell-to-face interpolation

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

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

$$\boldsymbol{\mu}_c^{\rho} \cdot C_c(\boldsymbol{u}_s)\rho_c = \boldsymbol{\mu}_c^{\rho} \cdot M U_s \Pi_{cs} \boldsymbol{\rho}_c = -(G\,\boldsymbol{\mu}_c^{\rho}) \cdot \Omega_s U_s \Pi_{cs} \boldsymbol{\rho}_c = -((\Pi_{cs}\boldsymbol{\rho}_c) \odot (G\,\boldsymbol{\mu}_c^{\rho})) \cdot \Omega_s \boldsymbol{u}_s$$

$$\langle \mu^{\rho}, \mathscr{L}_{\boldsymbol{u}} \rho \rangle = \langle \mu^{\rho}, \nabla \cdot (\boldsymbol{u}\rho) \rangle = -\langle \nabla \mu^{\rho}, \boldsymbol{u}\rho \rangle = -\langle \rho \nabla \mu^{\rho}, \boldsymbol{u} \rangle$$

$$\langle \boldsymbol{a}_c, \boldsymbol{b}_c \rangle_c := \boldsymbol{a}_c \cdot \Omega_c \boldsymbol{b}_c \qquad M = -(\Omega_s G)^T$$

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

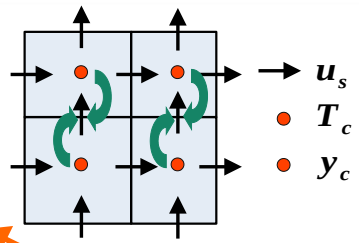
A new general framework for multiphysics

Buoyancy-driven flows on staggered grids

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

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

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



Cell-to-face interpolation

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

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

$$\boldsymbol{\mu}_c^{\rho} \cdot C_c(\boldsymbol{u}_s)\rho_c = \boldsymbol{\mu}_c^{\rho} \cdot M U_s \Pi_{cs} \boldsymbol{\rho}_c = -(G\,\boldsymbol{\mu}_c^{\rho}) \cdot \Omega_s U_s \Pi_{cs} \boldsymbol{\rho}_c = -((\Pi_{cs}\boldsymbol{\rho}_c) \odot (G\,\boldsymbol{\mu}_c^{\rho})) \cdot \Omega_s \boldsymbol{u}_s$$

$$\langle \mu^{\rho}, \mathscr{L}_{\boldsymbol{u}} \rho \rangle = \langle \mu^{\rho}, \nabla \cdot (\boldsymbol{u}\rho) \rangle = -\langle \nabla \mu^{\rho}, \boldsymbol{u}\rho \rangle = -\langle \rho \nabla \mu^{\rho}, \boldsymbol{u} \rangle$$

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

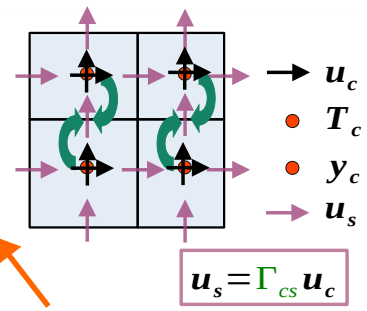
A new general framework for multiphysics

Buoyancy-driven flows on collocated grids

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

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

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



Cell-to-face interpolation

$$E_h^{\rho}[\boldsymbol{\rho}_c] := g\boldsymbol{\rho}_c \cdot \Omega_c \boldsymbol{y}_c$$

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

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

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

$$\begin{aligned} \langle \mu^{\rho}, \mathscr{L}_{\boldsymbol{u}} \rho \rangle &= \langle \mu^{\rho}, \nabla \cdot (\boldsymbol{u}\rho) \rangle \\ &= -\langle \nabla \mu^{\rho}, \boldsymbol{u}\rho \rangle \\ &= -\langle \rho \nabla \mu^{\rho}, \boldsymbol{u} \rangle \end{aligned}$$

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

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

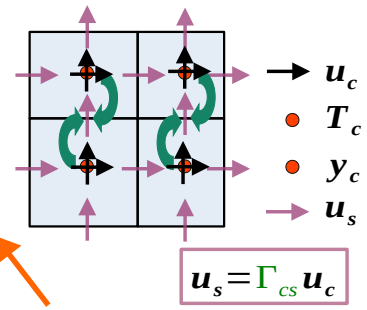
A new general framework for multiphysics

Buoyancy-driven flows on collocated grids

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

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

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



Cell-to-face interpolation

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

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

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

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

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

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

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

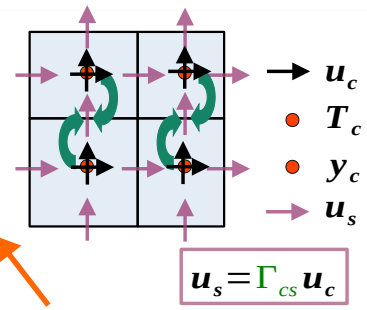
A new general framework for multiphysics

Buoyancy-driven flows on collocated grids

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

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

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



Cell-to-face interpolation

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

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

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

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

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

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

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

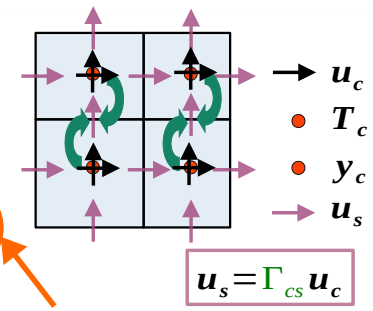
A new general framework for multiphysics

Buoyancy-driven flows on collocated grids

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

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

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



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

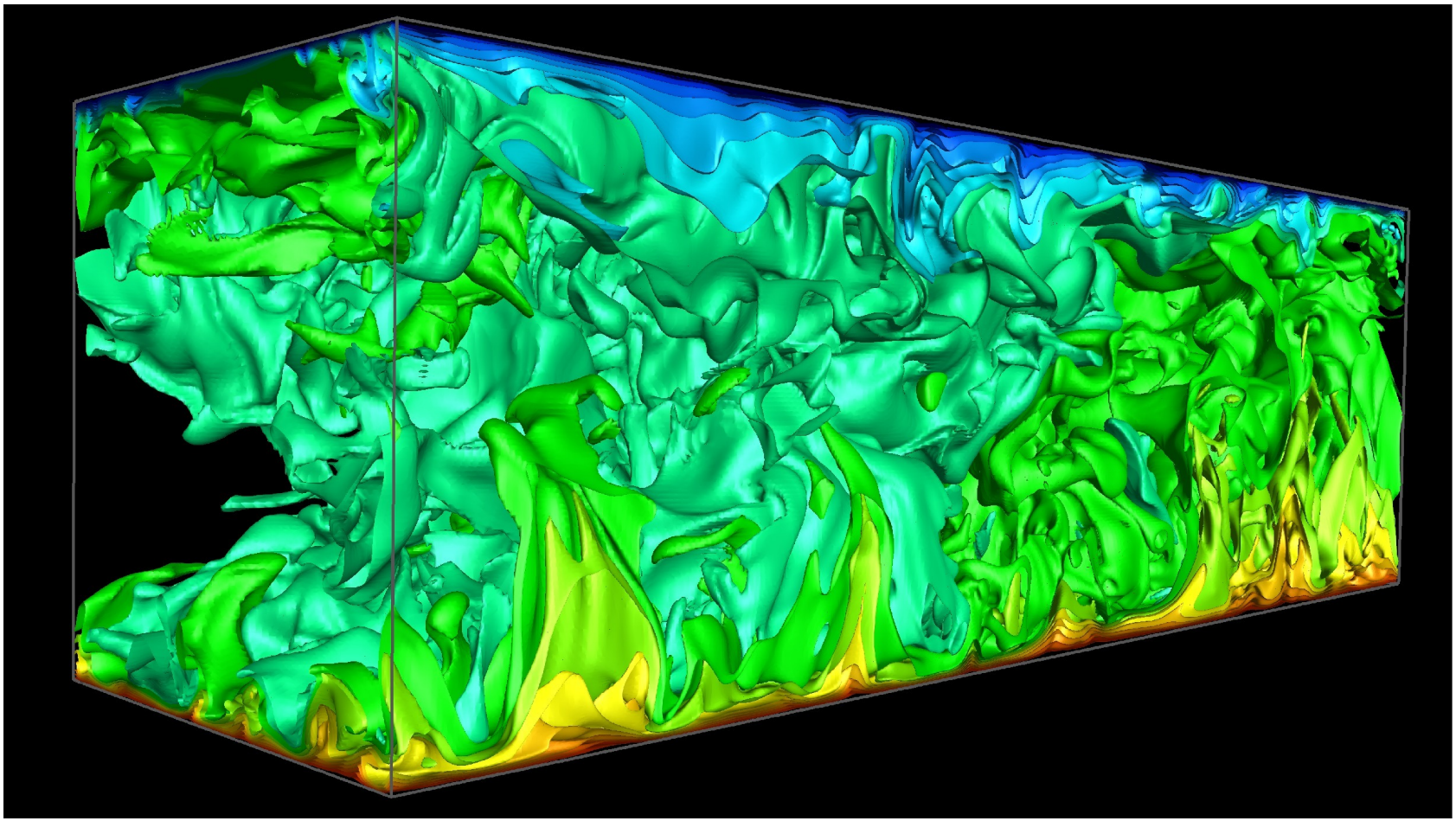
$\mathscr{L}_{\boldsymbol{u}}$ Lie derivative

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

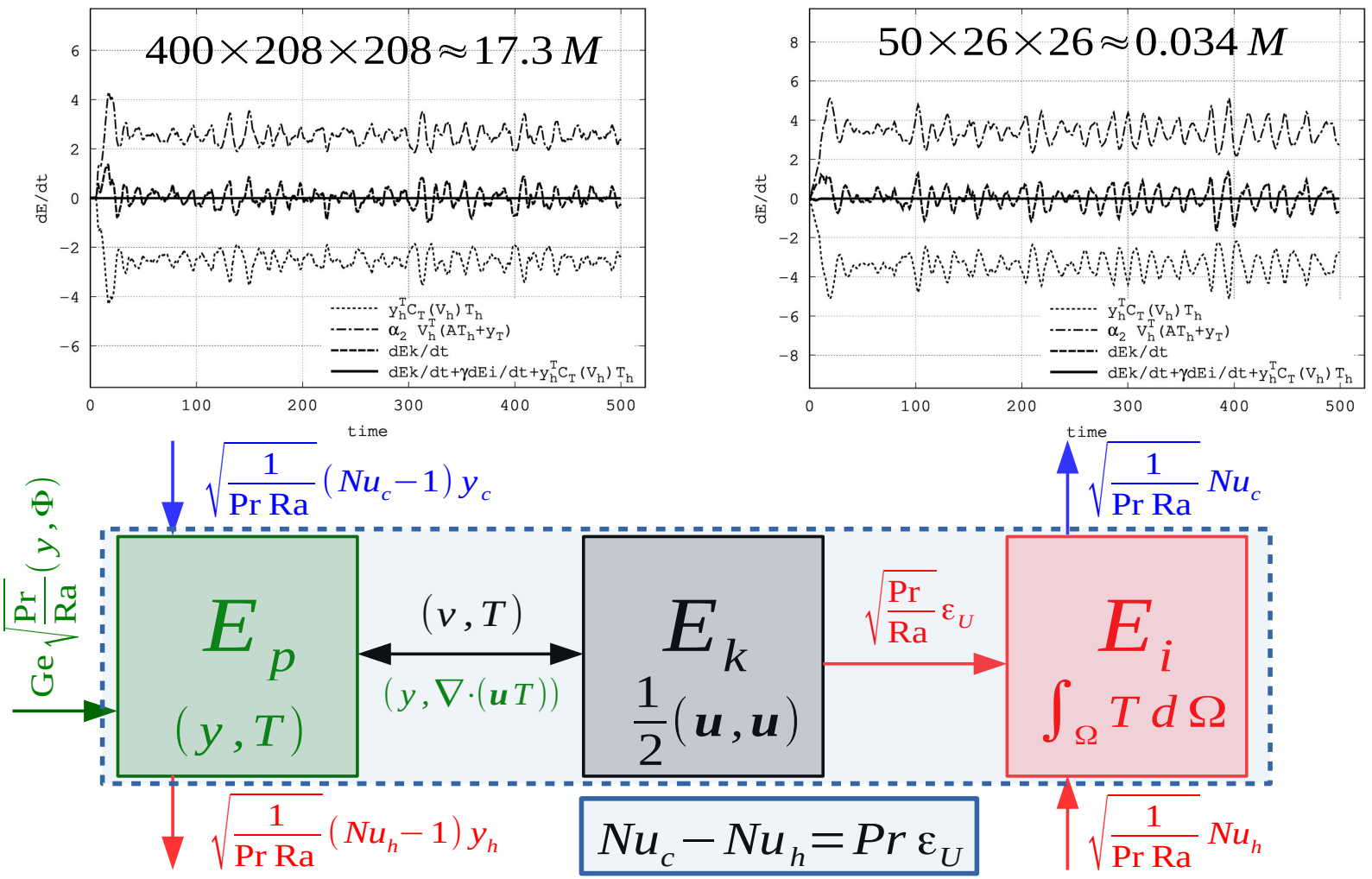
Leitmotiv: transport equation and its associated force **cannot** be discretized independently!!!

Buoyancy-driven flows

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

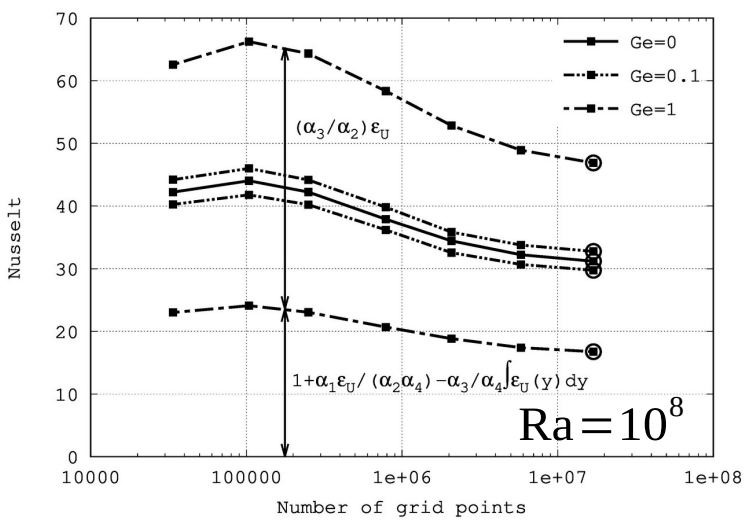


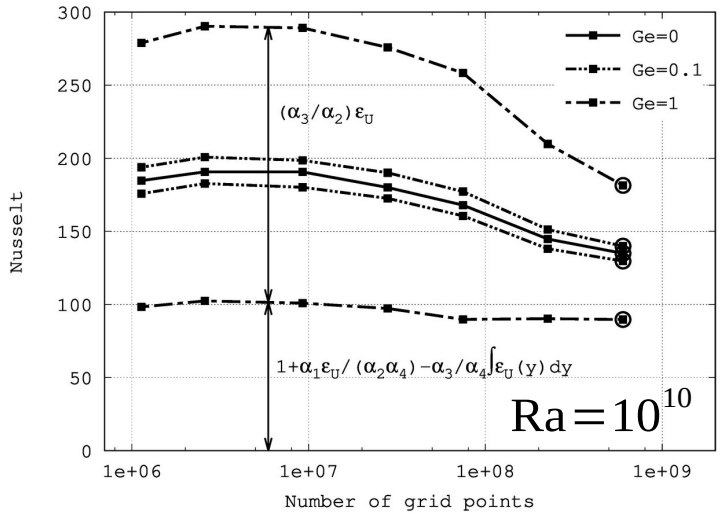
Buoyancy-driven flows[6]

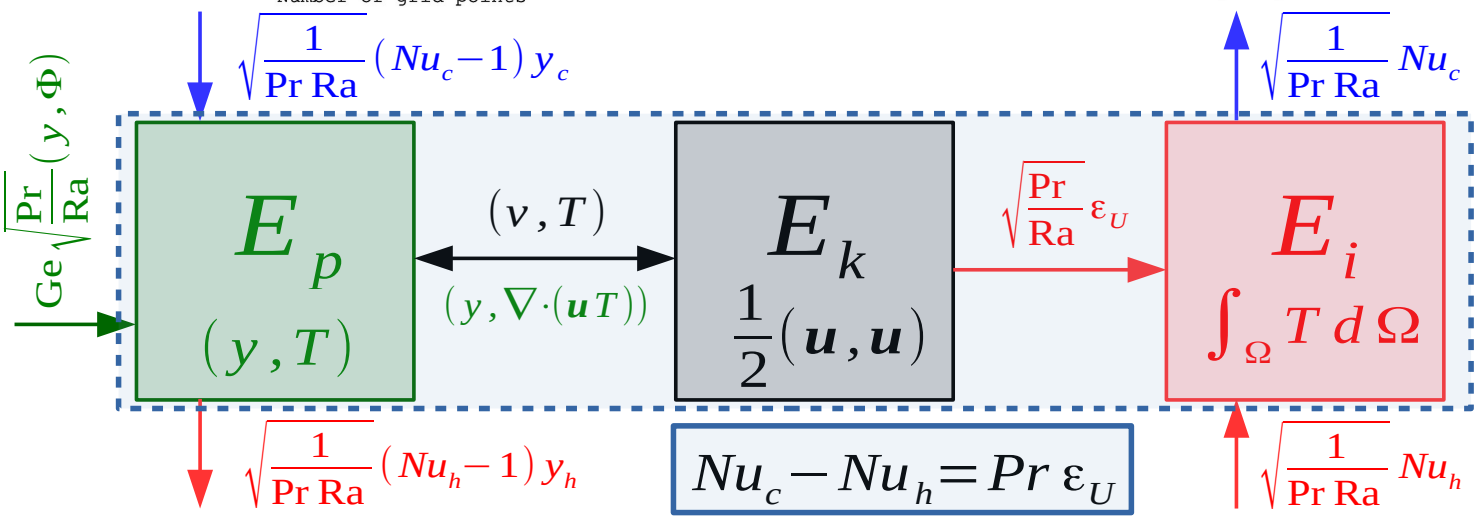


[6] B.Sanderse, F.X.Trias. *Energy-consistent discretization of viscous dissipation with application to natural convection flow*, **Computers & Fluids**, 286:106473, 2025.

Buoyancy-driven flows[6]

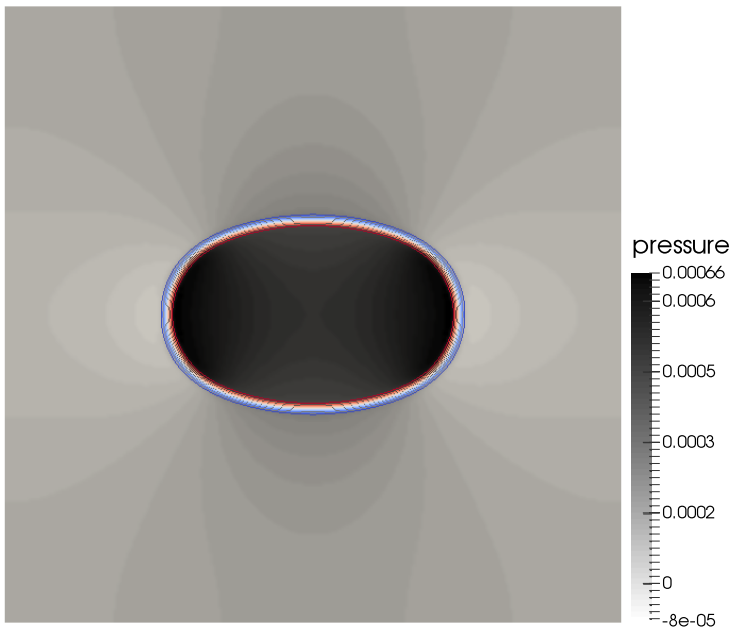




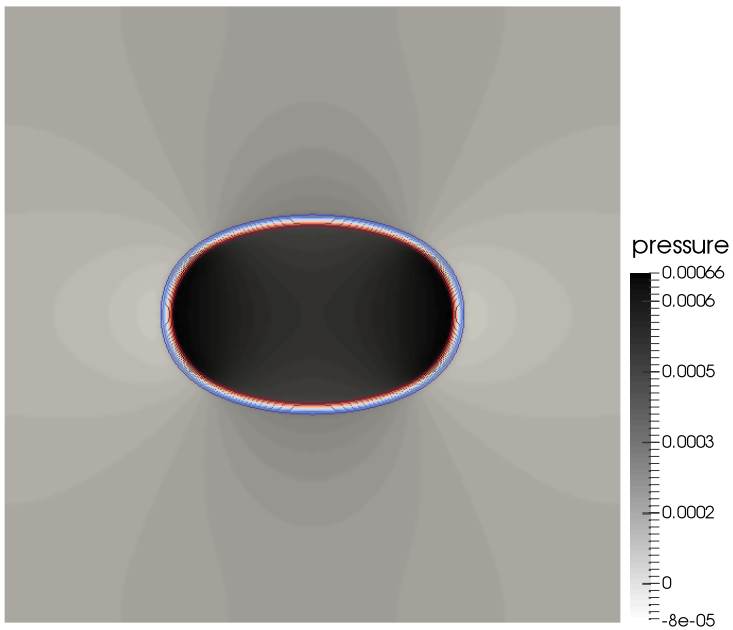


[6] B.Sanderse, F.X.Trias. *Energy-consistent discretization of viscous dissipation with application to natural convection flow*, **Computers & Fluids**, 286:106473, 2025.

Multiphase flows[6]



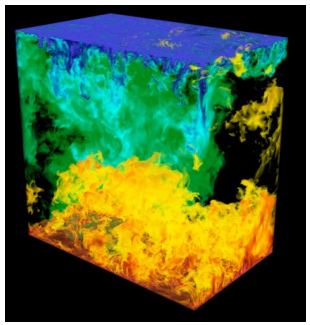
Non-symmetry-preserving!



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

HPC on modern supercomputers



SGS models

Numerical Methods

HPC (High Performance Computing)

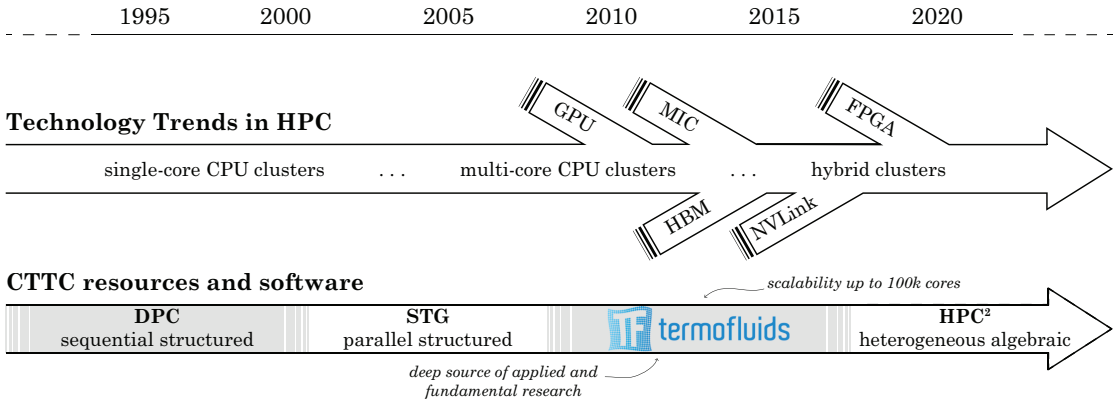
DNS

LES

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. *HPC^2 - a fully portable algebra-dominant framework for heterogeneous computing. Application to CFD*. **Computers & Fluids**, 173:285-292, 2018

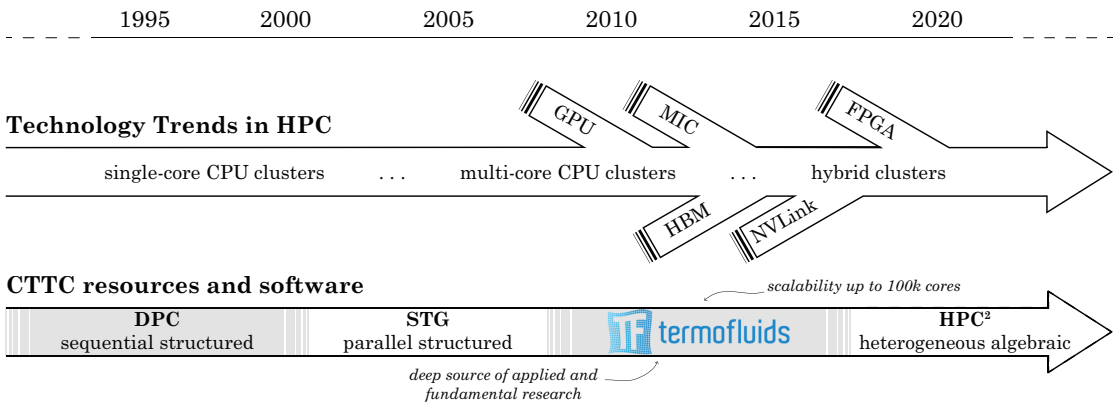
[8] À.Alsalti-Baldellou, X.Álvarez-Farré, F.X.Trias, A.Oliva. *Exploiting spatial symmetries for solving Poisson's equation*. **Journal of Computational Physics** 486:112133, 2023.

[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

Research question #3:

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



HPC^2: portable, algebra-based framework for heterogeneous computing is developed[7]. 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. *HPC^2 - 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	Discrete
$\frac{\partial \boldsymbol{u}}{\partial t} + C(\boldsymbol{u}, \boldsymbol{u}) = \nu \nabla^2 \boldsymbol{u} - \nabla p$	$\Omega \frac{d \boldsymbol{u}_h}{dt} + \mathrm{C}(\boldsymbol{u}_h)\, \boldsymbol{u}_h = \mathrm{D} \boldsymbol{u}_h - \mathrm{G} \boldsymbol{p}_h$
$\nabla \cdot \boldsymbol{u} = 0$	$\mathrm{M} \boldsymbol{u}_h = \boldsymbol{0}_h$
$\langle \boldsymbol{a}, \boldsymbol{b} \rangle = \int_\Omega \boldsymbol{a} \boldsymbol{b} d\Omega$	$\langle \boldsymbol{a}_h, \boldsymbol{b}_h \rangle_h = \boldsymbol{a}_h^T \Omega \boldsymbol{b}_h$
$\langle C(\boldsymbol{u}, \varphi_1), \varphi_2 \rangle = -\langle C(\boldsymbol{u}, \varphi_2), \varphi_1 \rangle$	$\mathrm{C}(\boldsymbol{u}_h) = -\mathrm{C}^T(\boldsymbol{u}_h)$
$\langle \nabla \cdot \boldsymbol{a}, \varphi \rangle = -\langle \boldsymbol{a}, \nabla \varphi \rangle$	$\Omega \mathrm{G} = -\mathrm{M}^T$
$\left\langle \nabla^2 \boldsymbol{a}, \boldsymbol{b} \right\rangle = \left\langle \boldsymbol{a}, \nabla^2 \boldsymbol{b} \right\rangle$	$\mathrm{D} = \mathrm{D}^T \quad def -$

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

Continuous

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

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

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

$$\langle C(\boldsymbol{u}, \varphi_1), \varphi_2 \rangle = -\langle C(\boldsymbol{u}, \varphi_2), \varphi_1 \rangle$$
$$\langle \nabla \cdot \boldsymbol{a}, \varphi \rangle = -\langle \boldsymbol{a}, \nabla \varphi \rangle$$
$$\left\langle \nabla^2 \boldsymbol{a}, \boldsymbol{b} \right\rangle = \left\langle \boldsymbol{a}, \nabla^2 \boldsymbol{b} \right\rangle$$

Discrete

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

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

Minimal set of kernels:

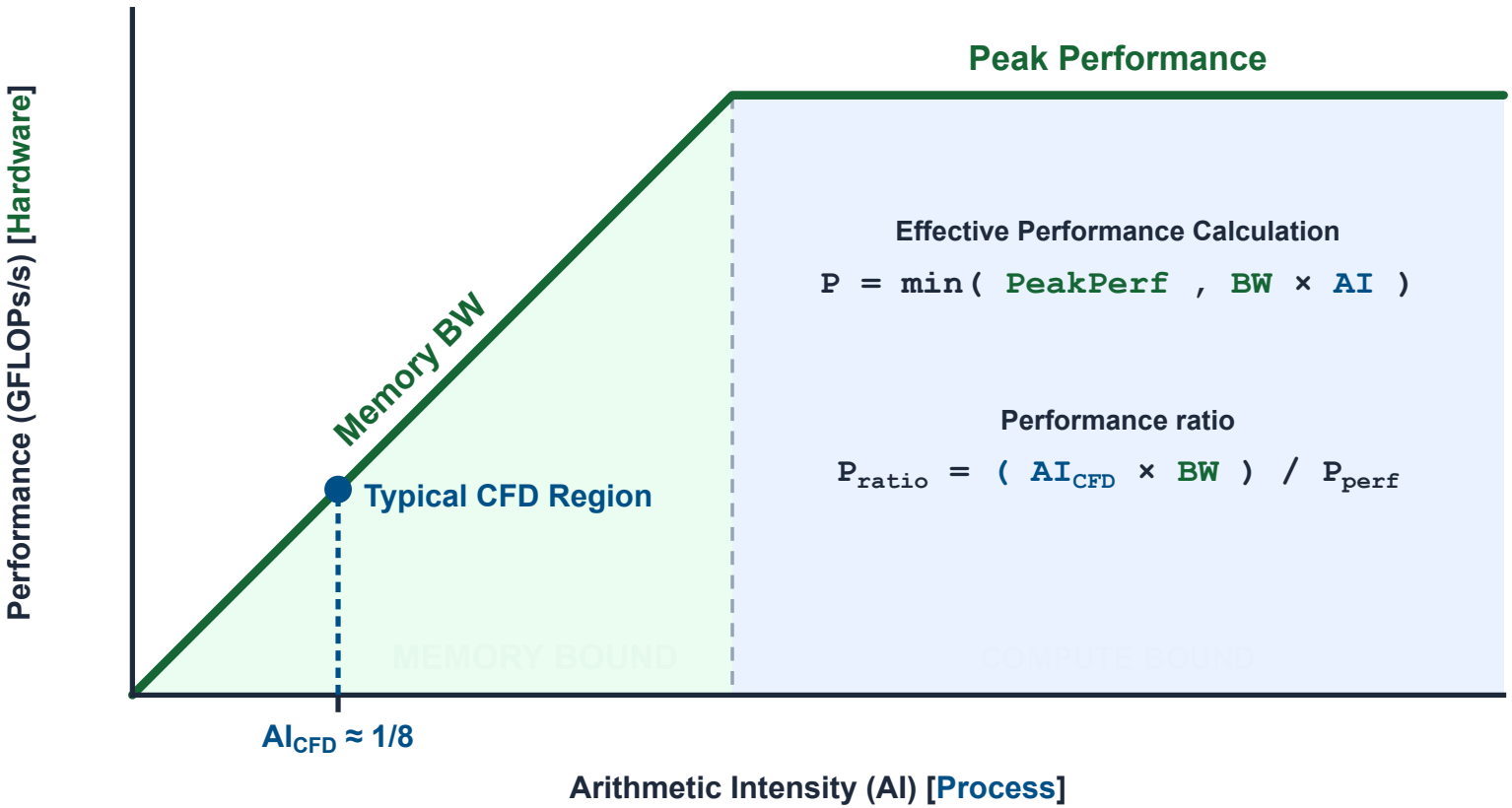
$$\texttt{SpMV}: \quad \boldsymbol{y} \leftarrow A\boldsymbol{x}$$
$$\texttt{axpy}: \quad \boldsymbol{z} \leftarrow a\boldsymbol{x} + b\boldsymbol{y}$$
$$\texttt{dot}: \quad r \leftarrow \boldsymbol{x} \cdot \boldsymbol{y}$$

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

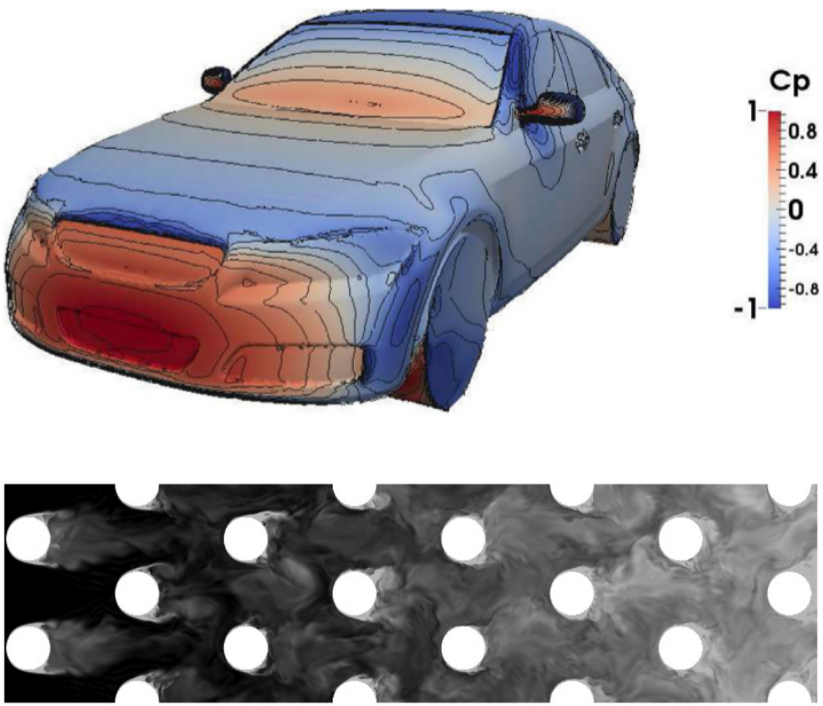
SpMV : $\boldsymbol{y} \leftarrow A\boldsymbol{x}$

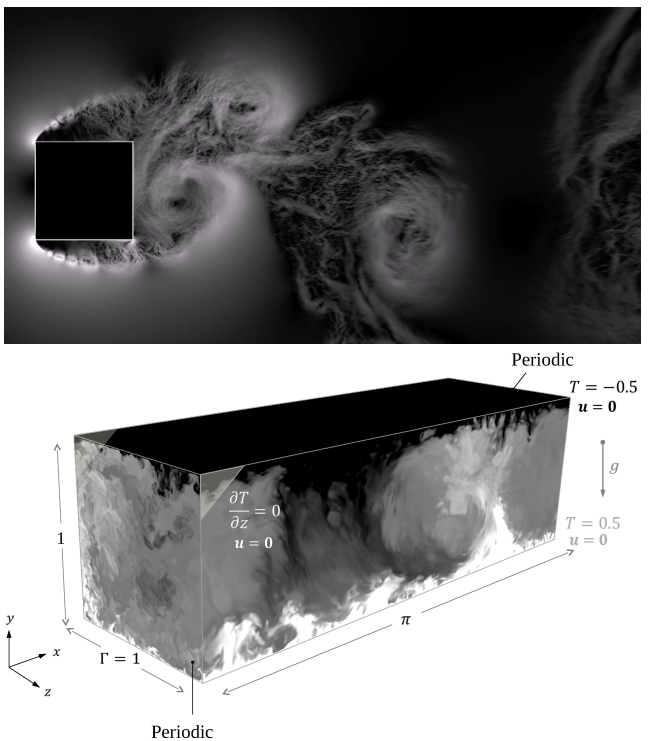
axpy : $\boldsymbol{z} \leftarrow a\boldsymbol{x} + b\boldsymbol{y}$

dot : $r \leftarrow \boldsymbol{x} \cdot \boldsymbol{y}$



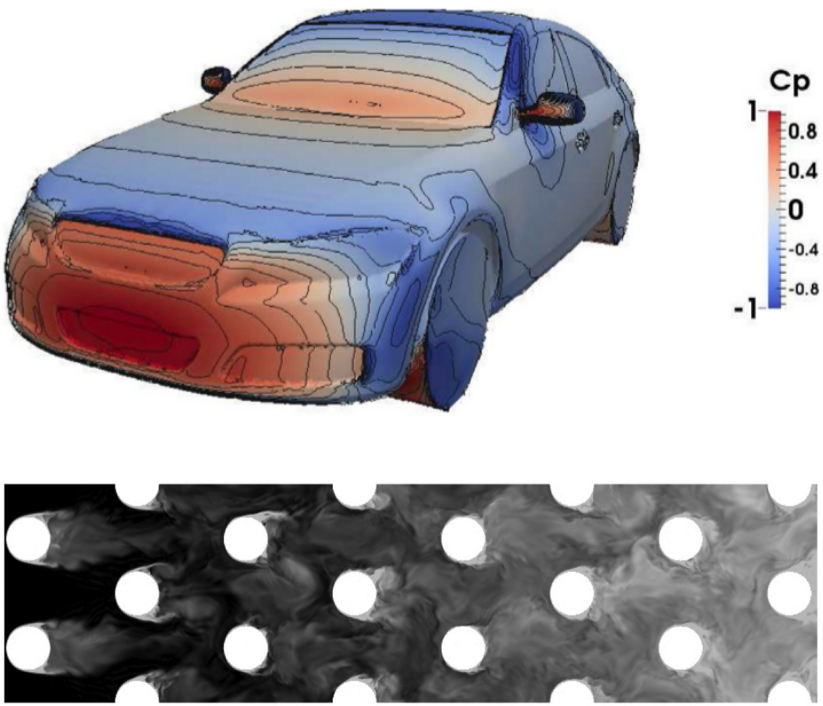
Algebra-based approach naturally leads to portability, to simple and analyzable formulations and opens the door to new strategies[10,11] to improve its performance...



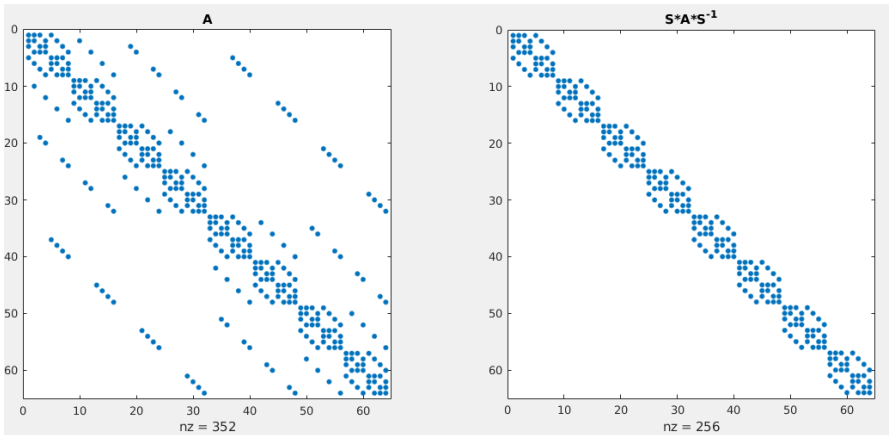


[10] À.Alsalti-Baldellou, X.Álvarez-Farré, F.X.Trias, A.Oliva. *Exploiting spatial symmetries for solving Poisson's equation*. **Journal of Computational Physics** 486:112133, 2023.

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...



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



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

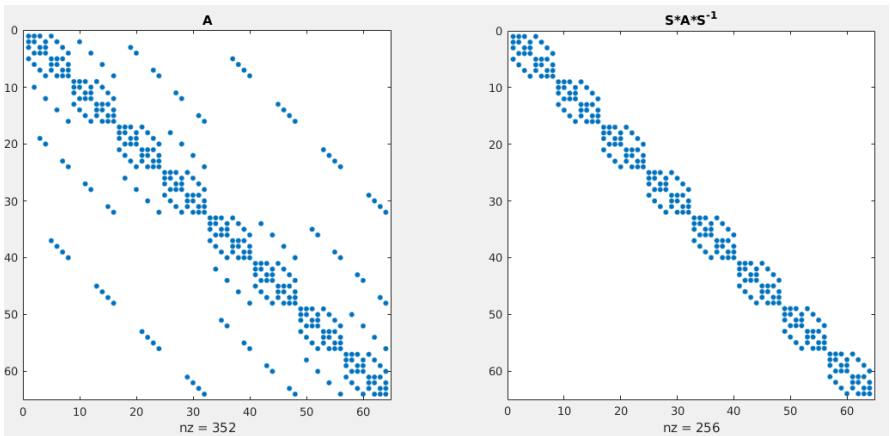
[10] À.Alsalti-Baldellou, X.Álvarez-Farré, F.X.Trias, A.Oliva. *Exploiting spatial symmetries for solving Poisson's equation*. **Journal of Computational Physics** 486:112133, 2023.

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...

Benefits for Poisson solver are 3-fold:

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

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



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

[10] 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.

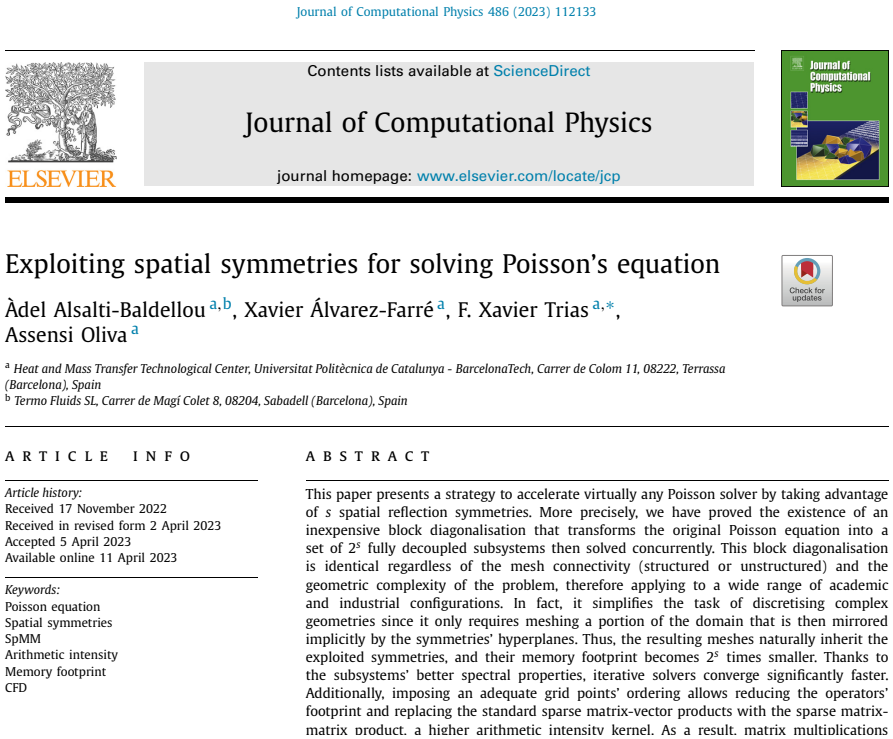
Algebra-based approach naturally leads to portability, to simple and analyzable formulations and opens the door to new strategies[10,11] to improve its performance...

Benefits for Poisson solver are 3-fold:

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

→ Overall speed-up up to **x2-x3** ✓

→ Memory reduction of ≈**2** ✓



Journal of Computational Physics 486 (2023) 112133

Contents lists available at ScienceDirect

Journal of Computational Physics

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

Exploiting spatial symmetries for solving Poisson's equation

Àdel Alsalti-Baldellou [a,b], Xavier Álvarez-Farré [a], F. Xavier Trias [a,*], Assensi Oliva [a]

[a] Heat and Mass Transfer Technological Center, Universitat Politècnica de Catalunya - BarcelonaTech, Carrer de Colom 11, 08222, Terrassa (Barcelona), Spain
[b] Termo Fluids SL, Carrer de Magí Colet 8, 08204, Sabadell (Barcelona), Spain

ARTICLE INFO

Article history:
Received 17 November 2022
Received in revised form 2 April 2023
Accepted 5 April 2023
Available online 11 April 2023

Keywords:
Poisson equation
Spatial symmetries
SpMM
Arithmetic intensity
Memory footprint
CFD

ABSTRACT

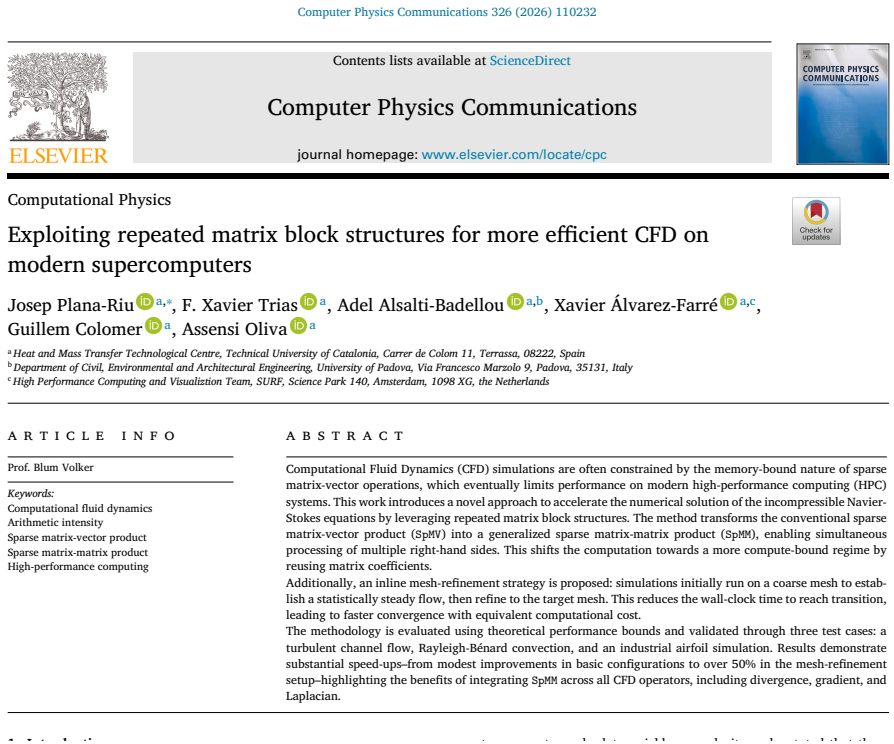
This paper presents a strategy to accelerate virtually any Poisson solver by taking advantage of s spatial reflection symmetries. More precisely, we have proved the existence of an inexpensive block diagonalisation that transforms the original Poisson equation into a set of 2^s fully decoupled subsystems then solved concurrently. This block diagonalisation is identical regardless of the mesh connectivity (structured or unstructured) and the geometric complexity of the problem, therefore applying to a wide range of academic and industrial configurations. In fact, it simplifies the task of discretising complex geometries since it only requires meshing a portion of the domain that is then mirrored implicitly by the symmetries' hyperplanes. Thus, the resulting meshes naturally inherit the exploited symmetries, and their memory footprint becomes 2^s times smaller. Thanks to the subsystems' better spectral properties, iterative solvers converge significantly faster. Additionally, imposing an adequate grid points' ordering allows reducing the operators' footprint and replacing the standard sparse matrix-vector products with the sparse matrix-matrix product, a higher arithmetic intensity kernel. As a result, matrix multiplications

[10] 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.

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?



Computer Physics Communications 326 (2026) 110232

Contents lists available at ScienceDirect

Computer Physics Communications

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

Computational Physics

Exploiting repeated matrix block structures for more efficient CFD on modern supercomputers

Josep Plana-Riu [a,*], F. Xavier Trias [a], Adel Alsalti-Badellou [a,b], Xavier Álvarez-Farré [a,c], Guillem Colomer [a], Assensi Oliva [a]

[a] Heat and Mass Transfer Technological Centre, Technical University of Catalonia, Carrer de Colom 11, Terrassa, 08222, Spain
[b] Department of Civil, Environmental and Architectural Engineering, University of Padova, Via Francesco Marzolo 9, Padova, 35131, Italy
[c] High Performance Computing and Visualiztion Team, SURF, Science Park 140, Amsterdam, 1098 XG, the Netherlands

ARTICLE INFO

Prof. Blum Volker

Keywords:
Computational fluid dynamics
Arithmetic intensity
Sparse matrix-vector product
Sparse matrix-matrix product
High-performance computing

ABSTRACT

Computational Fluid Dynamics (CFD) simulations are often constrained by the memory-bound nature of sparse matrix-vector operations, which eventually limits performance on modern high-performance computing (HPC) systems. This work introduces a novel approach to accelerate the numerical solution of the incompressible Navier-Stokes equations by leveraging repeated matrix block structures. The method transforms the conventional sparse matrix-vector product (SpMV) into a generalized sparse matrix-matrix product (SpMM), enabling simultaneous processing of multiple right-hand sides. This shifts the computation towards a more compute-bound regime by reusing matrix coefficients.

Additionally, an inline mesh-refinement strategy is proposed: simulations initially run on a coarse mesh to establish a statistically steady flow, then refine to the target mesh. This reduces the wall-clock time to reach transition, leading to faster convergence with equivalent computational cost.

The methodology is evaluated using theoretical performance bounds and validated through three test cases: a turbulent channel flow, Rayleigh-Bénard convection, and an industrial airfoil simulation. Results demonstrate substantial speed-ups–from modest improvements in basic configurations to over 50% in the mesh-refinement setup–highlighting the benefits of integrating SpMM across all CFD operators, including divergence, gradient, and Laplacian.

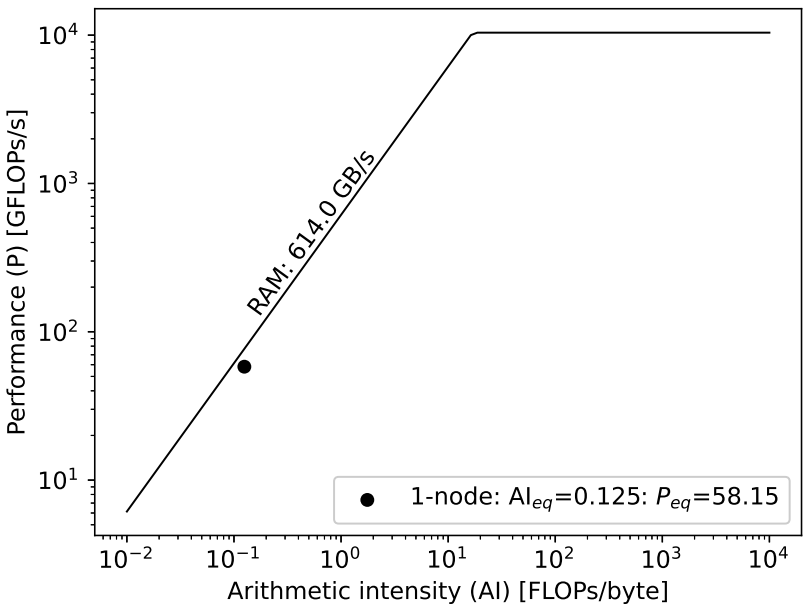
[10] À.Alsalti-Baldellou, X.Álvarez-Farré, F.X.Trias, A.Oliva. *Exploiting spatial symmetries for solving Poisson's equation*. **Journal of Computational Physics** 486:112133, 2023.

[11] 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.

Performance analysis

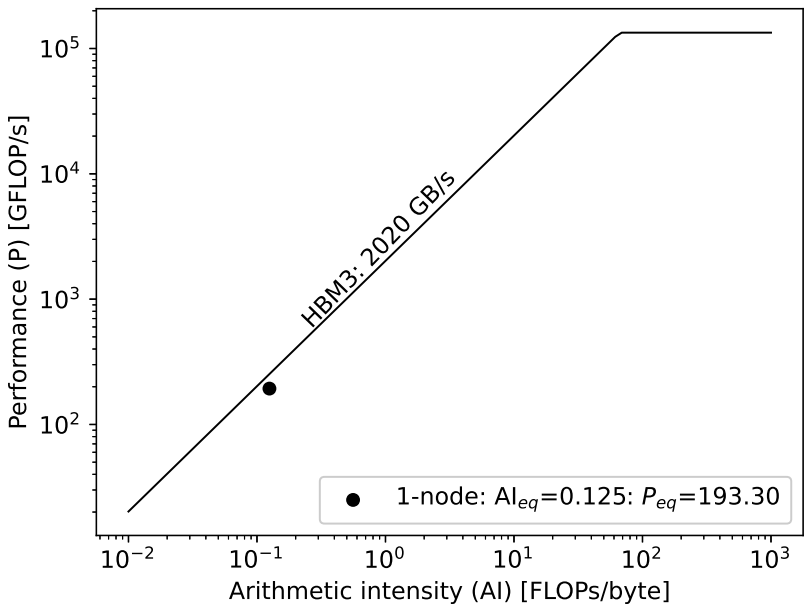
Roofline

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**

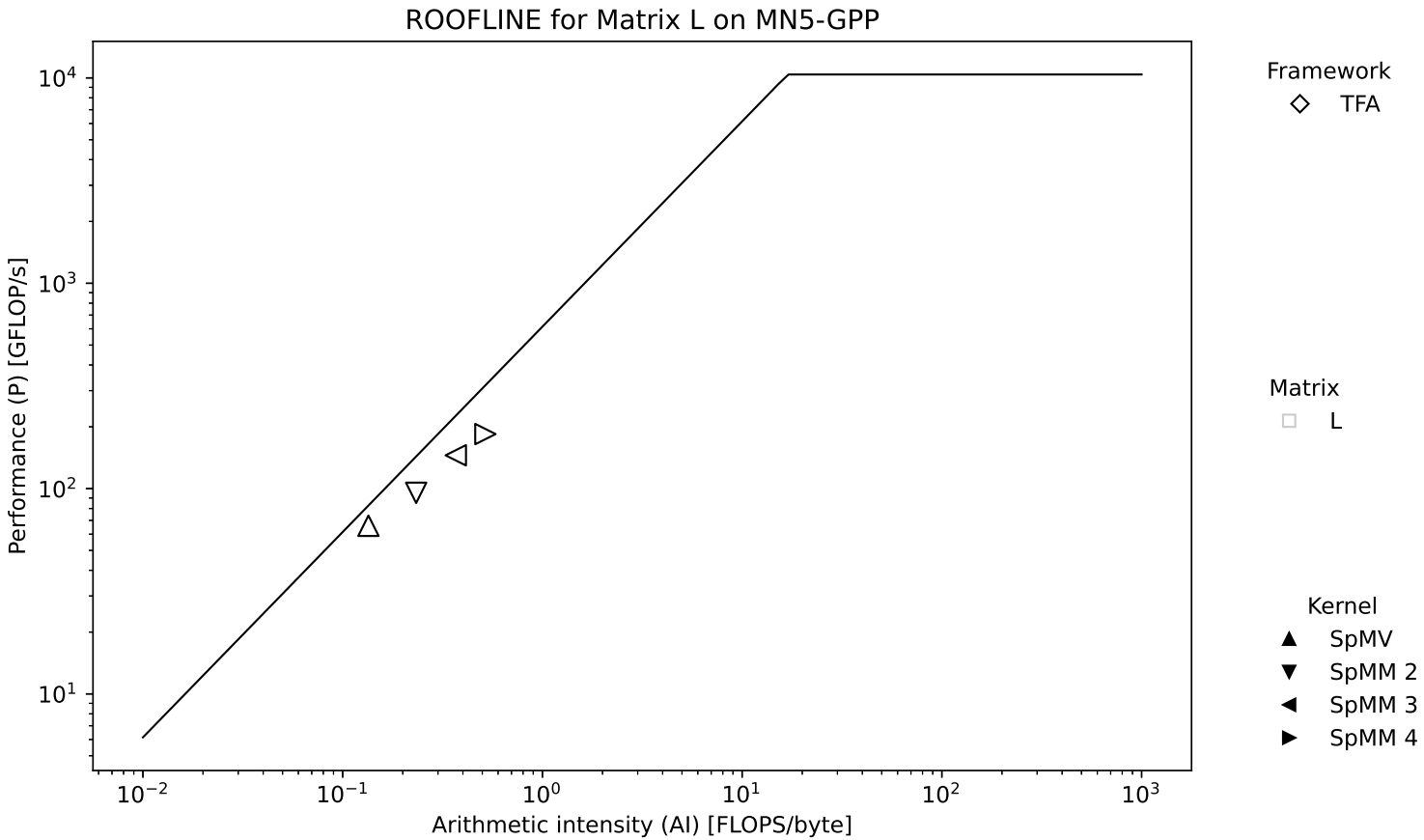
MareNostrum 5-ACC



- 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

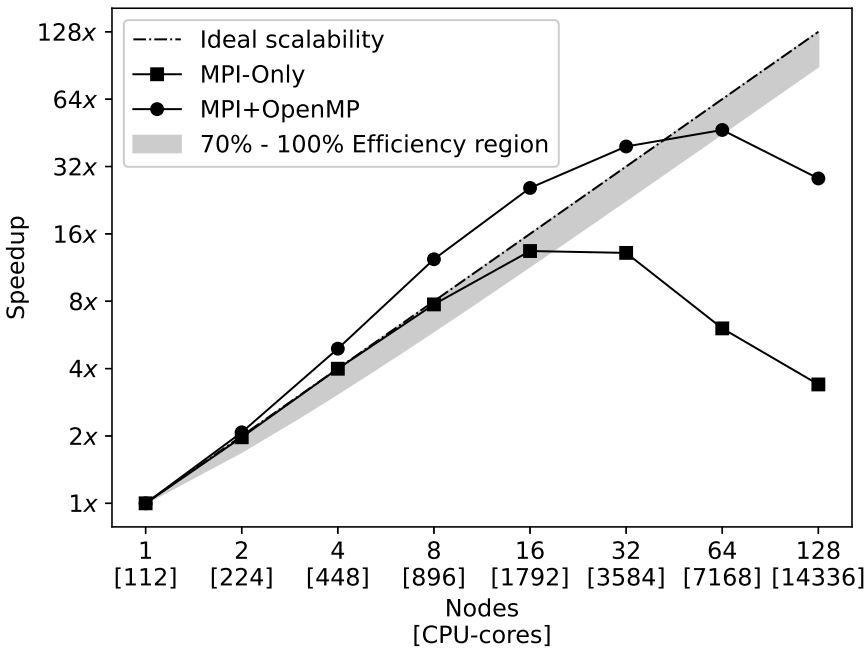
Roofline: SpMV versus SpMM



Performance analysis

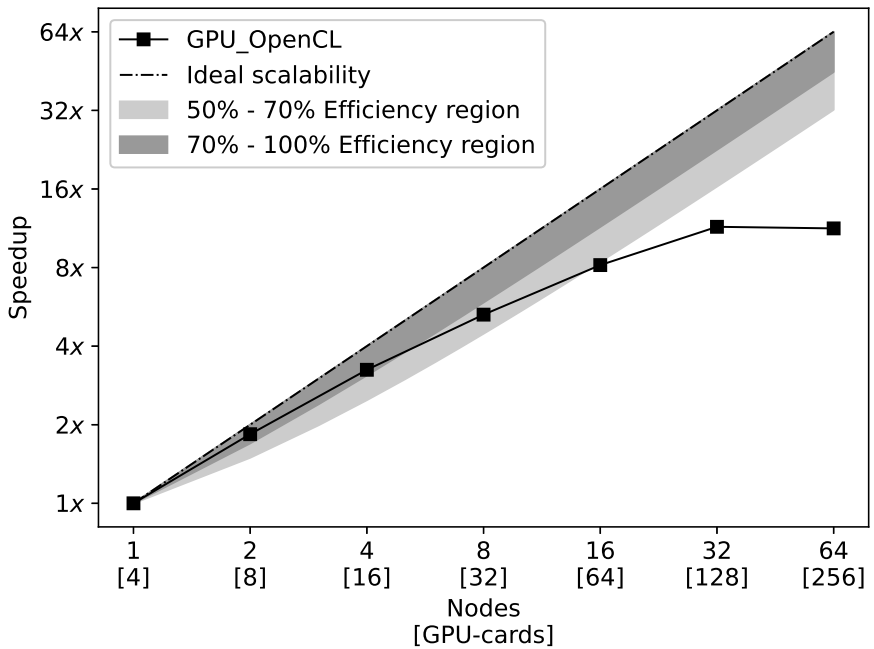
Strong scaling

MareNostrum 5-GPP



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

MareNostrum 5-ACC

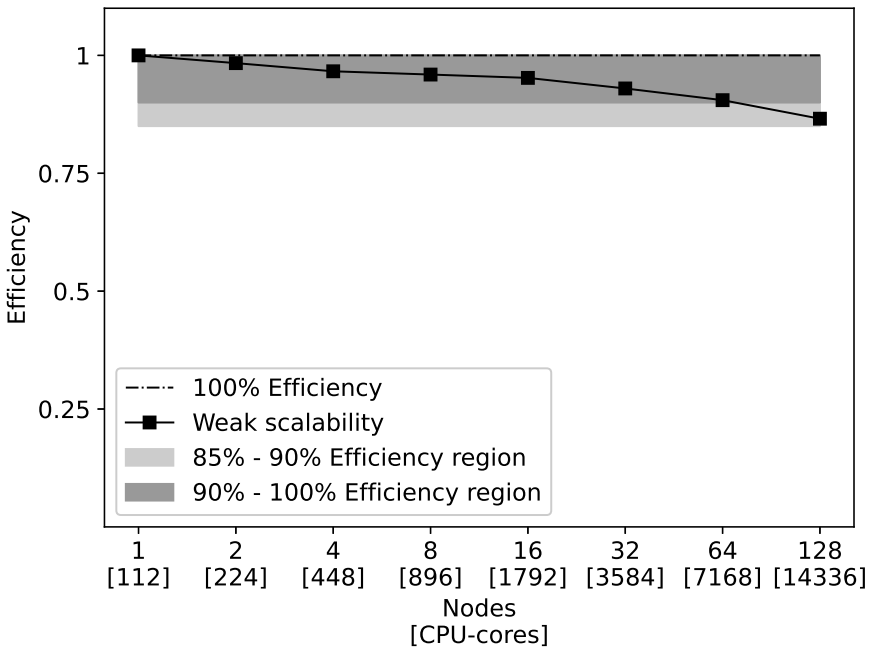


- $500 \times 1000 \times 340 \approx 170M$ CVs
- $42.5M$ CVs (1 node) $\longrightarrow$ $664k$ (64 nodes) per GPU

Performance analysis

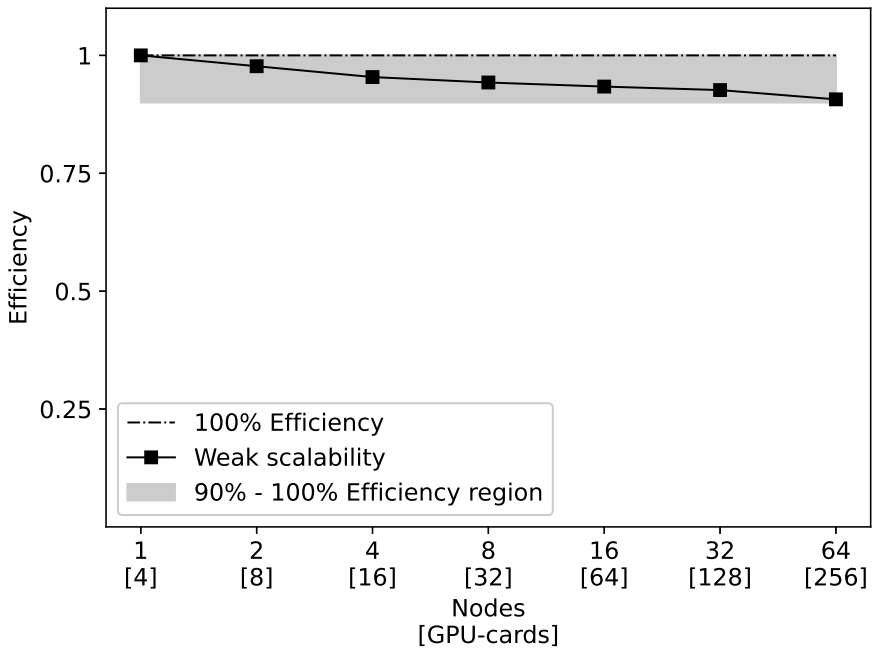
Weak scaling

MareNostrum 5-GPP



- $350 \times 480 \times 350 \approx 58.8M$ CVs per node
- $58.8M$ CVs (1 node) $\rightarrow$ $7.52B$ CVs (128 nodes)

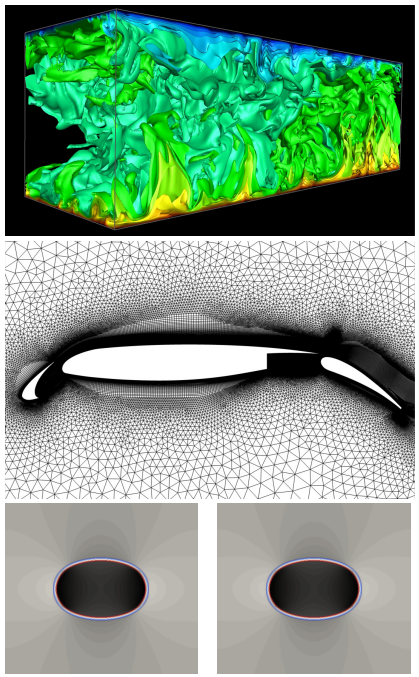
MareNostrum 5-ACC



- $500 \times 1000 \times 340 \approx 170M$ CVs per node
- $170M$ CVs (1 node) $\rightarrow$ $10.88B$ (64 nodes) per GPU

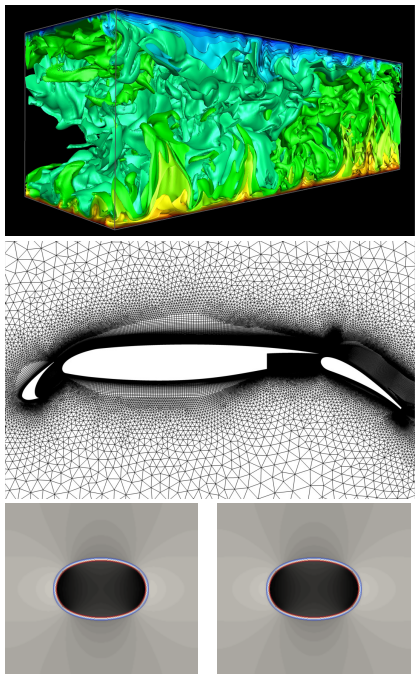
Take-away messages

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



Take-away messages

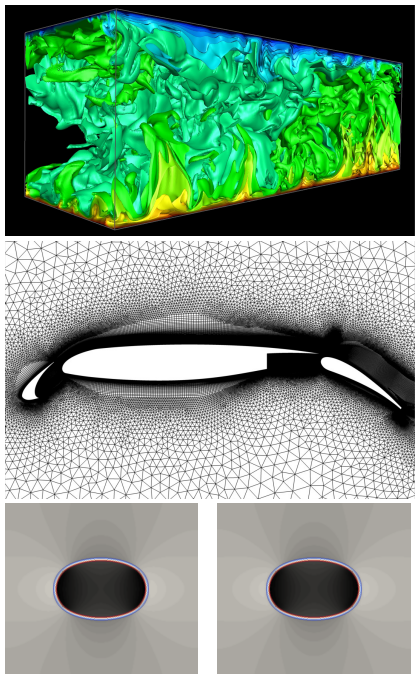
- **Preserving symmetries** is the key point for **reliable LES/DNS** simulations also for industrial problems.
- We usually focus on quadratic invariants (kinetic energy) but **energy exchanges** are also crucial.



Take-away messages

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

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

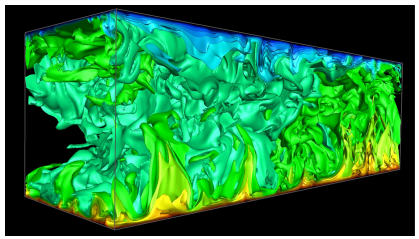


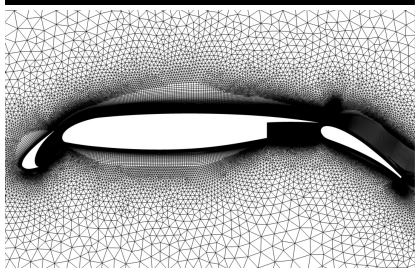
Take-away messages

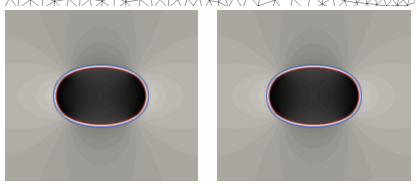
- **Preserving symmetries** is the key point for **reliable LES/DNS** simulations also for industrial problems.
- We usually focus on quadratic invariants (kinetic energy) but **energy exchanges** are also crucial.
- Transport equations and their associated forces **cannot be discretized independently**.

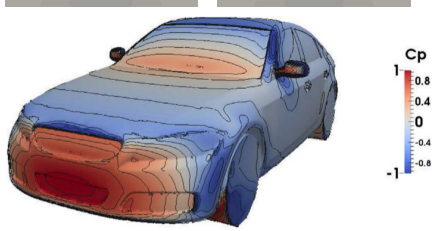
$$\boxed{\{E^{\phi}[\phi], \mathcal{L}_{\mathbf{u}}\} \implies \mathbf{f}^{\phi}}$$

- Algebra-based formulations naturally provide **portability** and **analyzability**, and open the door to **new performance strategies**.







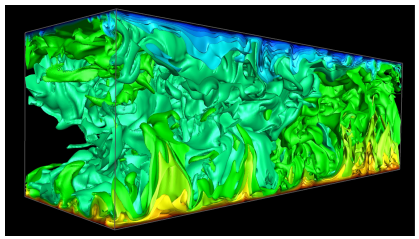


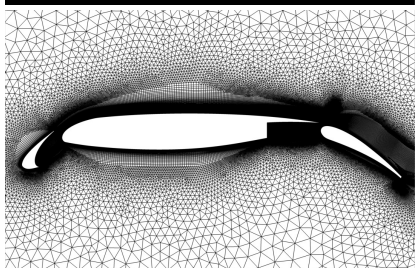
Take-away messages

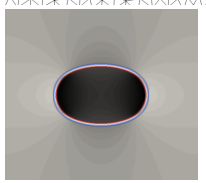
- **Preserving symmetries** is the key point for **reliable LES/DNS** simulations also for industrial problems.
- We usually focus on quadratic invariants (kinetic energy) but **energy exchanges** are also crucial.
- Transport equations and their associated forces **cannot be discretized independently**.

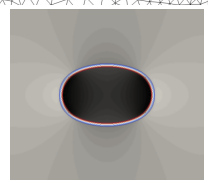
$$\boxed{\{E^{\phi}[\phi], \mathcal{L}_{\mathbf{u}}\} \implies \mathbf{f}^{\phi}}$$

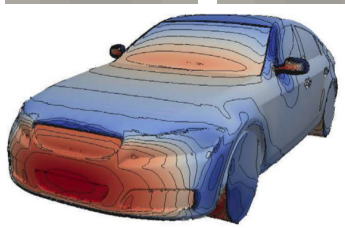
- Algebra-based formulations naturally provide **portability** and **analyzability**, and open the door to **new performance strategies**.
- **Open-source** platforms help to share and disseminate ideas.
  https://github.com/janneshopman/RKSymFoam











OpenFOAM

Thank you for your attention

