Centre Tecnològic de Transferència de Calor
UNIVERSITAT POLITÈCNICA DE CATALUNYA

Structure-preserving multiphysics simulations

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

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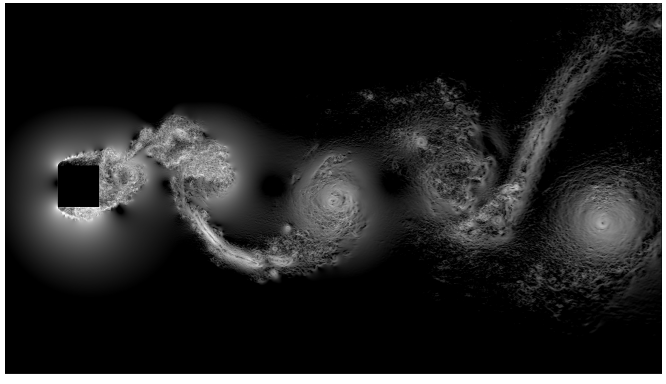

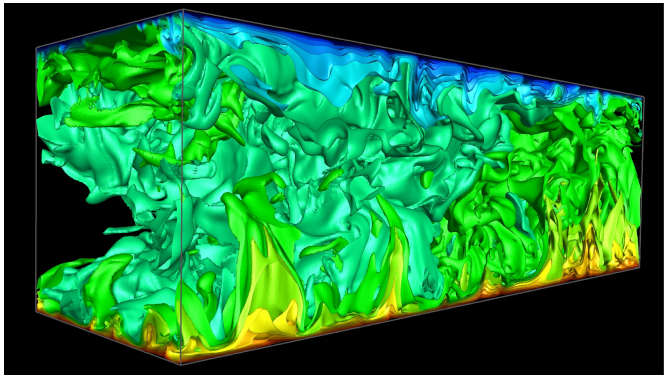

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UNIVERSITAT POLITÈCNICA DE CATALUNYA

Structure-preserving multiphysics simulations using portable algebraic kernels

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

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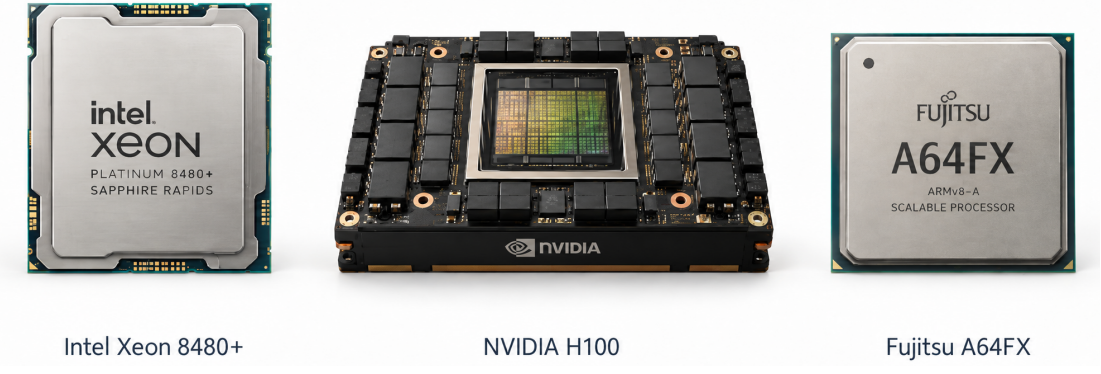
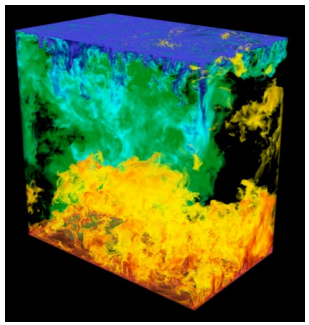


Intel Xeon 8480+ NVIDIA H100 Fujitsu A64FX

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

For canonical **academic** flows...



DNS

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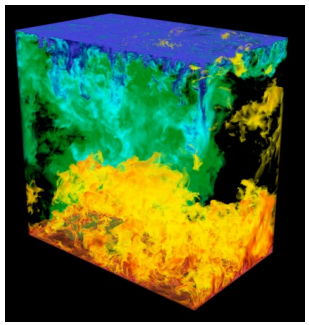
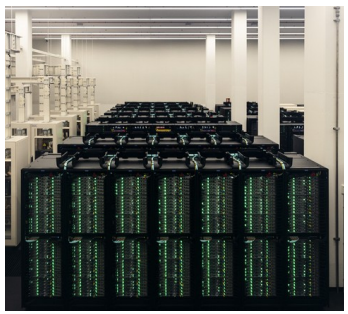


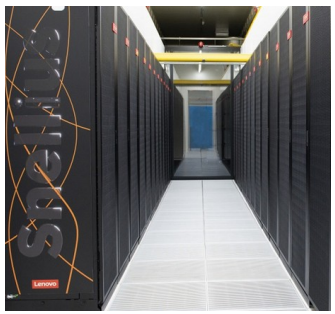
DNS

MareNostrum 5-ACC
(Barcelona)



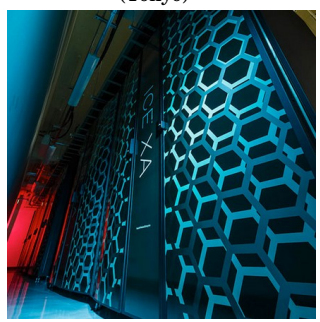
rank #8
1120 nodes with:
2× Intel Shappire Rapids 8460
1× NVIDIA Hopper 64 GB HBM
1× Infiniband NDR200

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

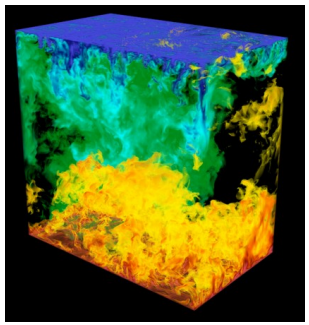




HPC (High Performance Computing)

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

For canonical **academic** flows...



How to properly discretize NS?

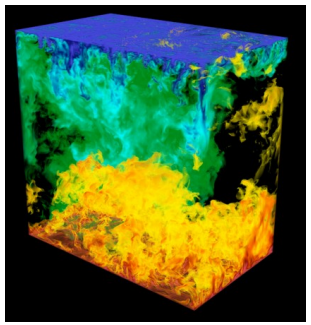
DNS

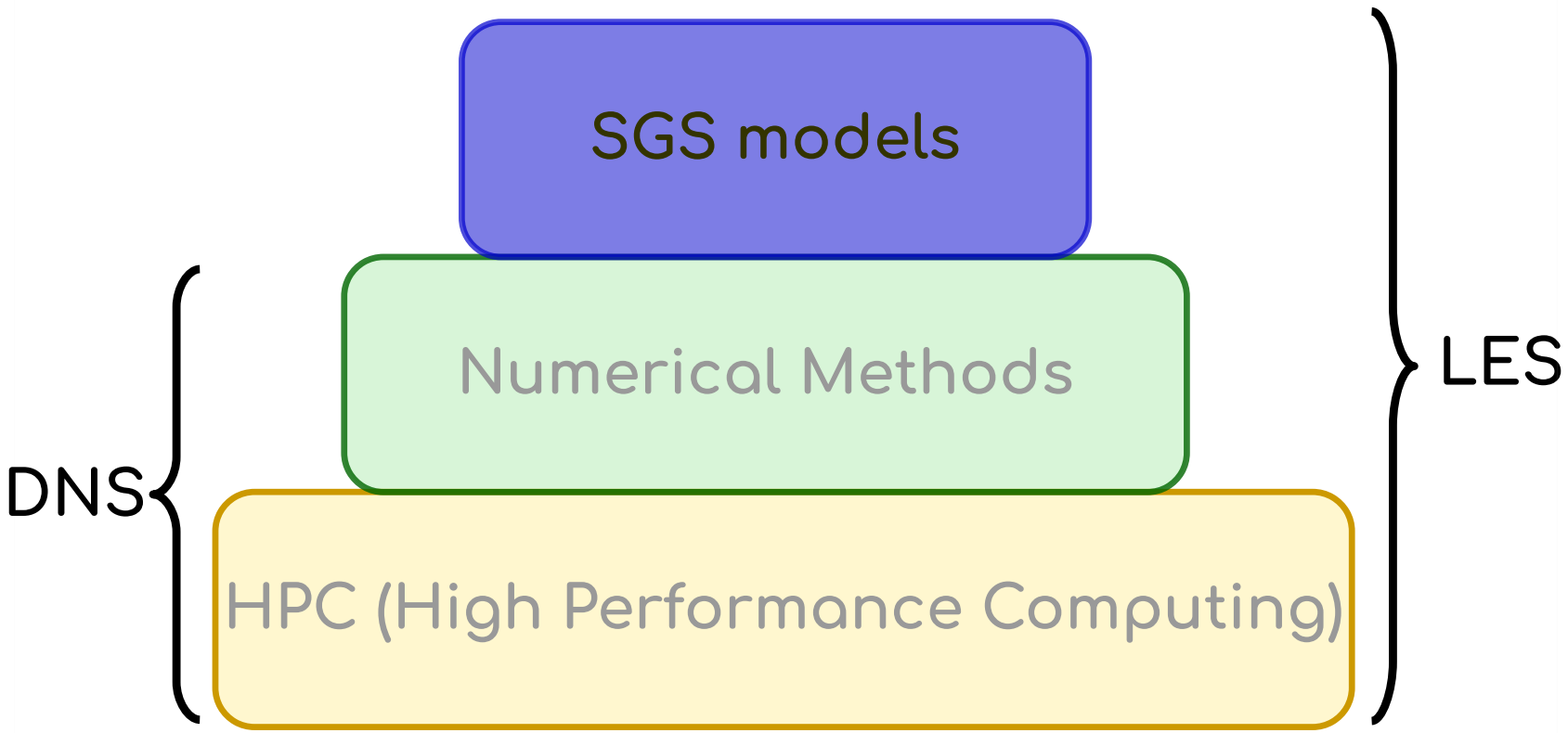
- Numerical Methods
- HPC (High Performance Computing)

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

For canonical **academic** flows...

How to properly model SGS?





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

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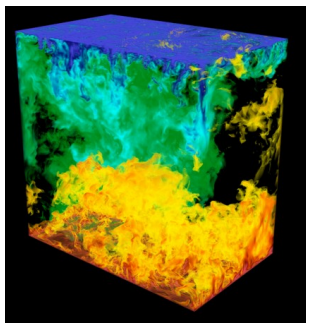
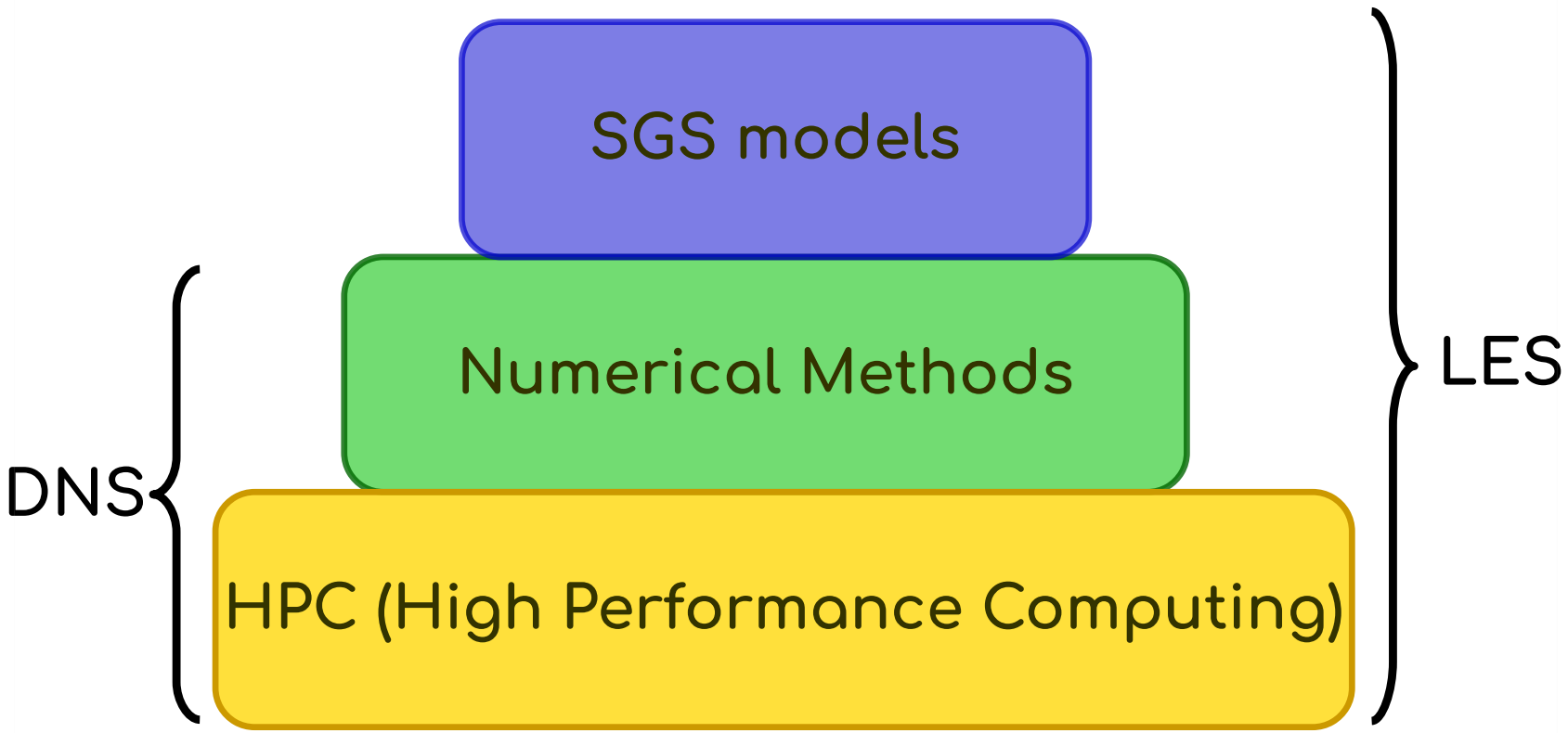
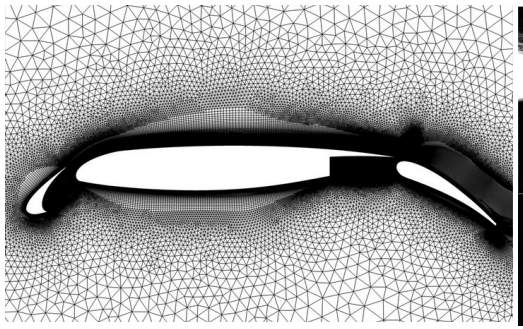
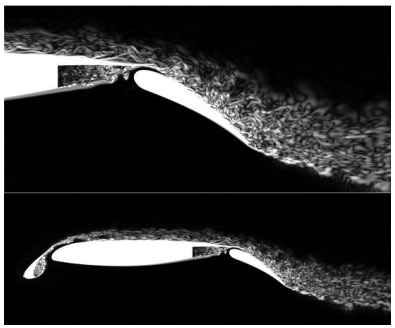


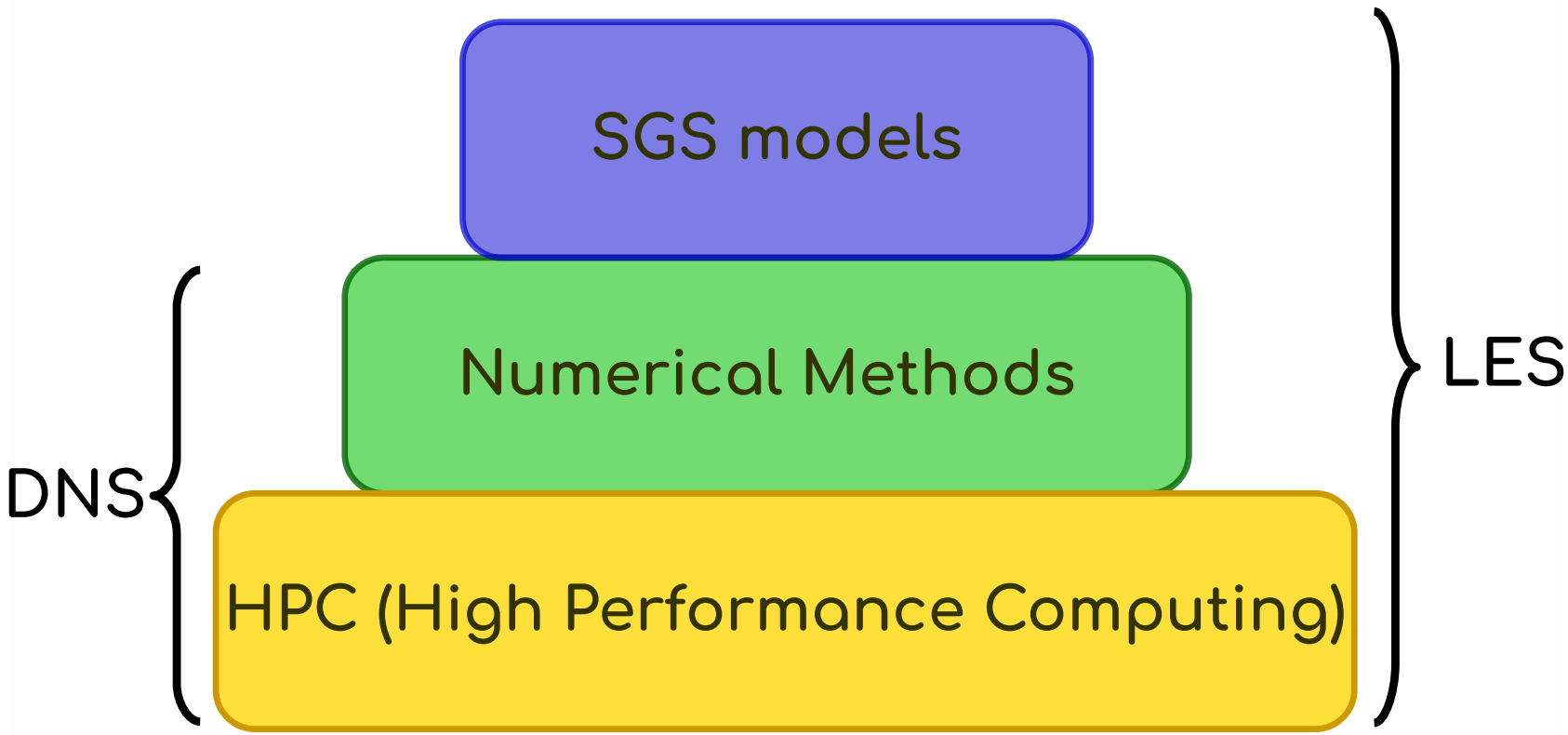


General motivation: (very) large-scale DNS/LES

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







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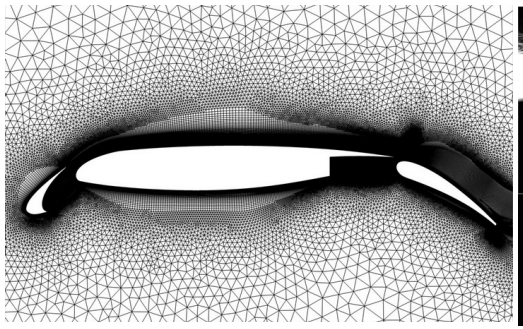
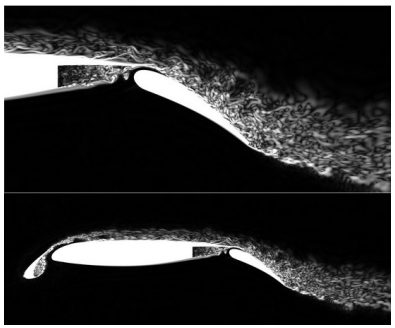
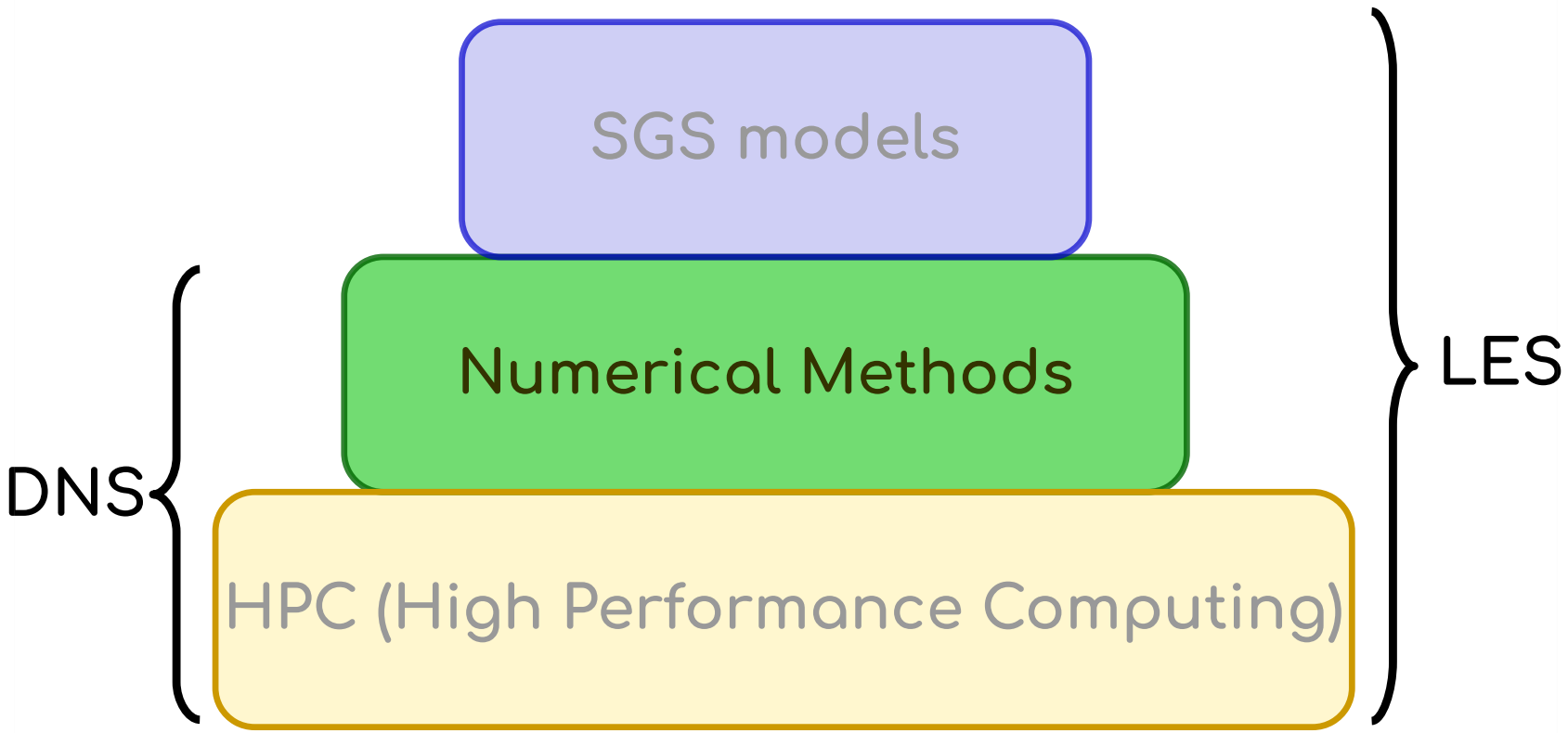


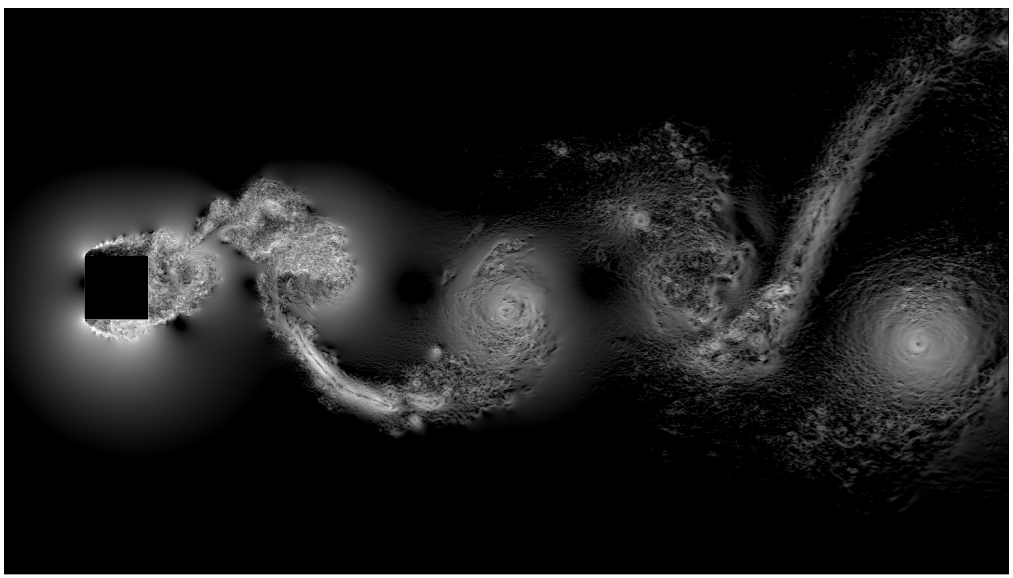


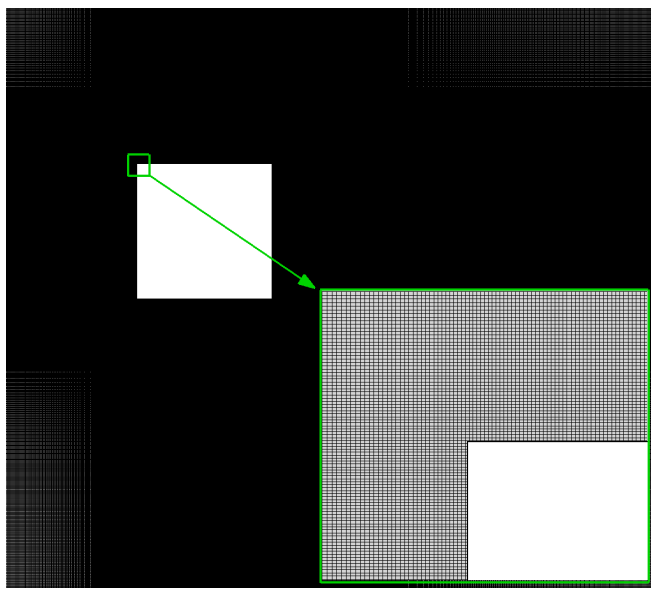


Numerical methods for DNS/LES

Research question #1:

- Can we construct numerical discretizations of the Navier-Stokes equations suitable for **complex geometries**, such that the **symmetry properties** are exactly preserved?





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

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

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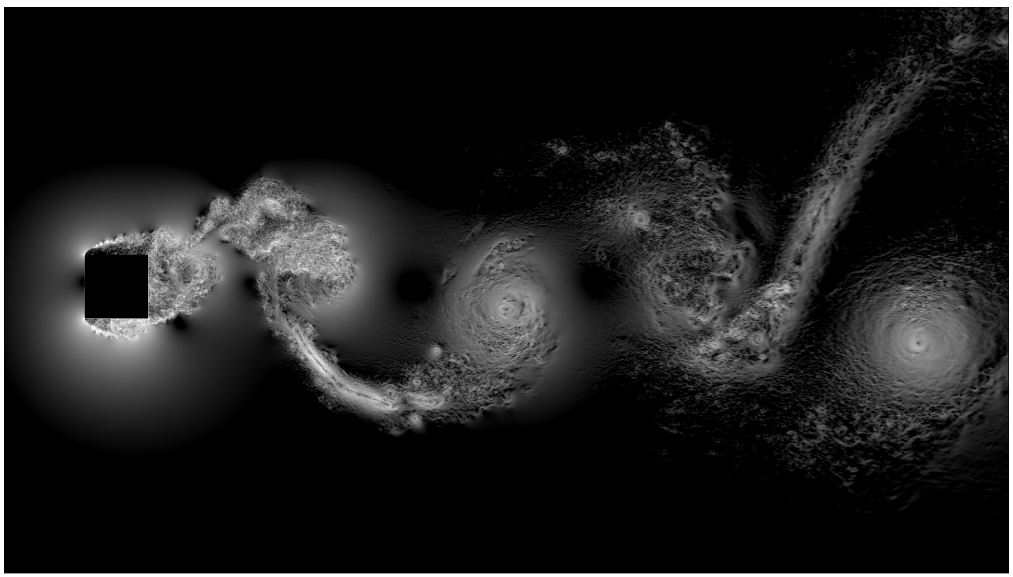

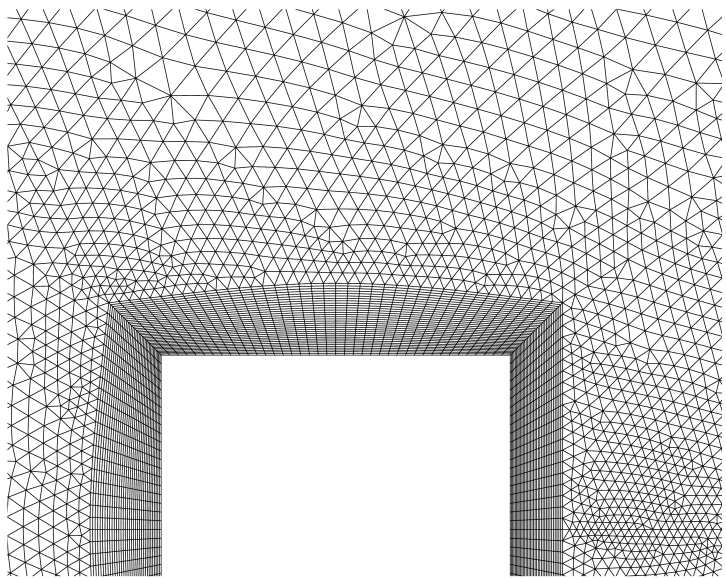

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Symmetry-preserving discretization

Continuous

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

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

Symmetry-preserving discretization

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Discrete

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

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

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

Symmetry-preserving discretization

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

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

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

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

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

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

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Discrete

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

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

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

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

Why a collocated formulation?

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



SIEMENS





eDF

OpenFOAM®



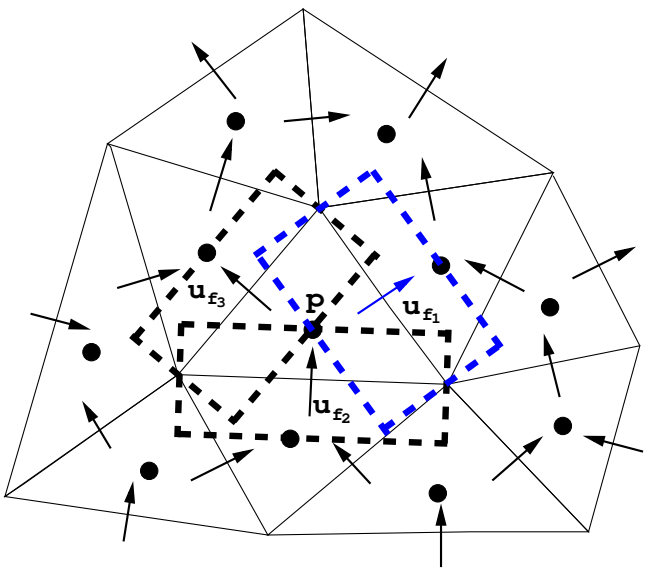
GPL

GPL Free Software

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

In staggered meshes

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



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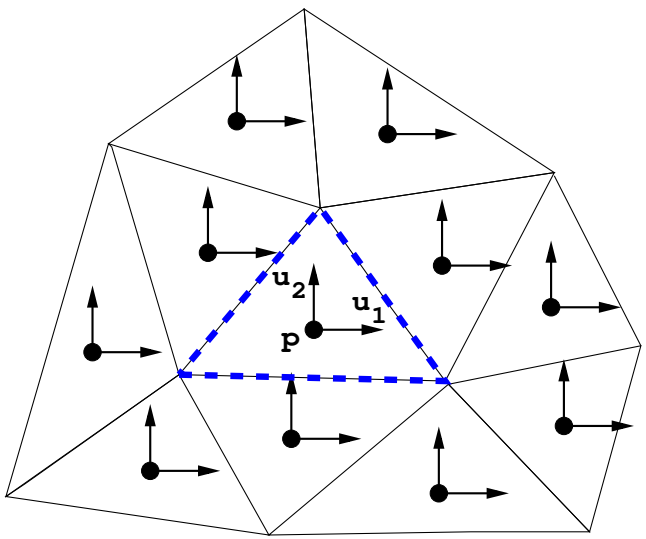
$$\Omega_c \frac{d\boldsymbol{u}_c}{dt} + \mathrm{C}(\boldsymbol{u}_s)\,\boldsymbol{u}_c = \mathrm{D}\boldsymbol{u}_c - \mathrm{G}_c\boldsymbol{p}_c; \quad \mathrm{M}_c\boldsymbol{u}_c = \mathbf{0}_c$$

In collocated meshes

- p-$\boldsymbol{u}_c$ coupling is cumbersome ✗
- $\mathrm{C}(\boldsymbol{u}_s)$ 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

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

F.X. Trias [a,b], O. Lehmkuhl [a,c], A. Oliva [a,*,1], C.D. Pérez-Segarra [a], R.W.C.P. Verstappen [b]

[a] Heat and Mass Transfer Technological Center, Technical University of Catalonia, ETSEIAT, c/ Colom 11, 08222 Terrassa, Spain
[b] Johann Bernoulli Institute for Mathematics and Computing Science, University of Groningen, P.O. Box 407, 9700 AK Groningen, The Netherlands
[c] Termo Fluids, S.L., c/ Magí Colet 8, 08204 Sabadell, Spain

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

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

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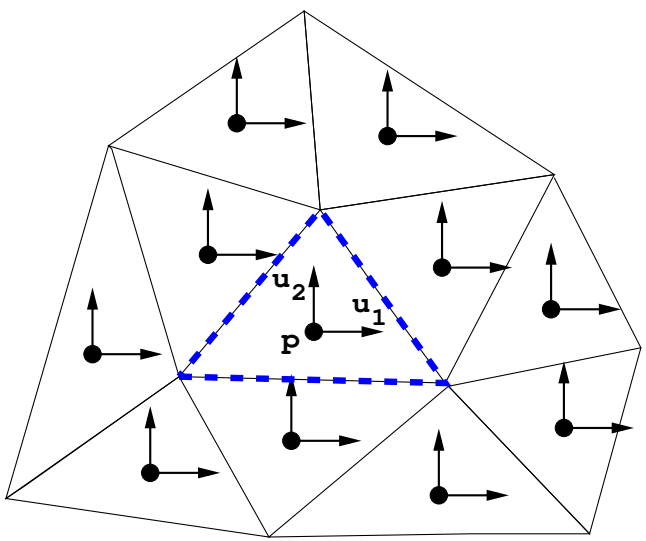

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A symmetry-preserving second-order time-accurate PISO-based method

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

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

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Available online 27 April 2021

ABSTRACT

A new conservative symmetry-preserving second-order time-accurate PISO-based pressure-velocity coupling for solving the incompressible Navier-Stokes equations on unstructured collocated grids is presented in this paper. This new method for implicit time stepping is an extension of the conservative symmetry-preserving incremental-pressure projection method for explicit time stepping and unstructured collocated

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

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- $\mathrm{C}(\boldsymbol{u}_s)$ and D easy to discretize ✓
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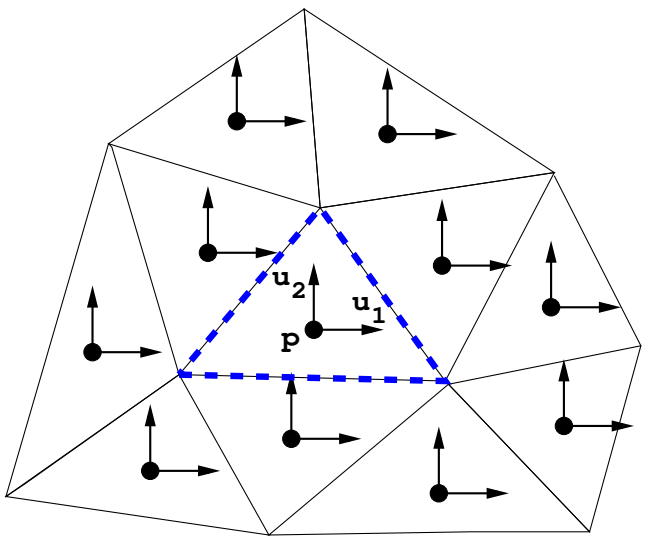
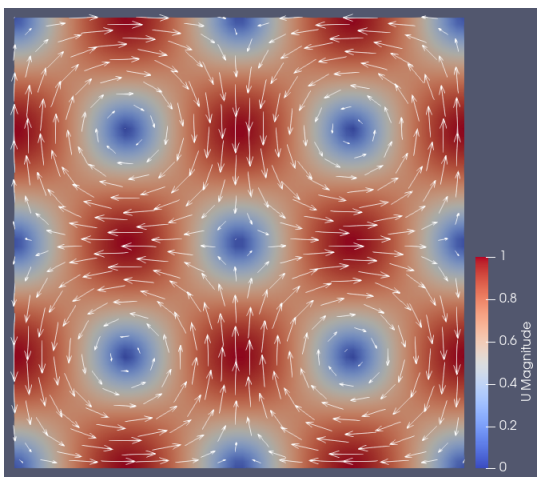
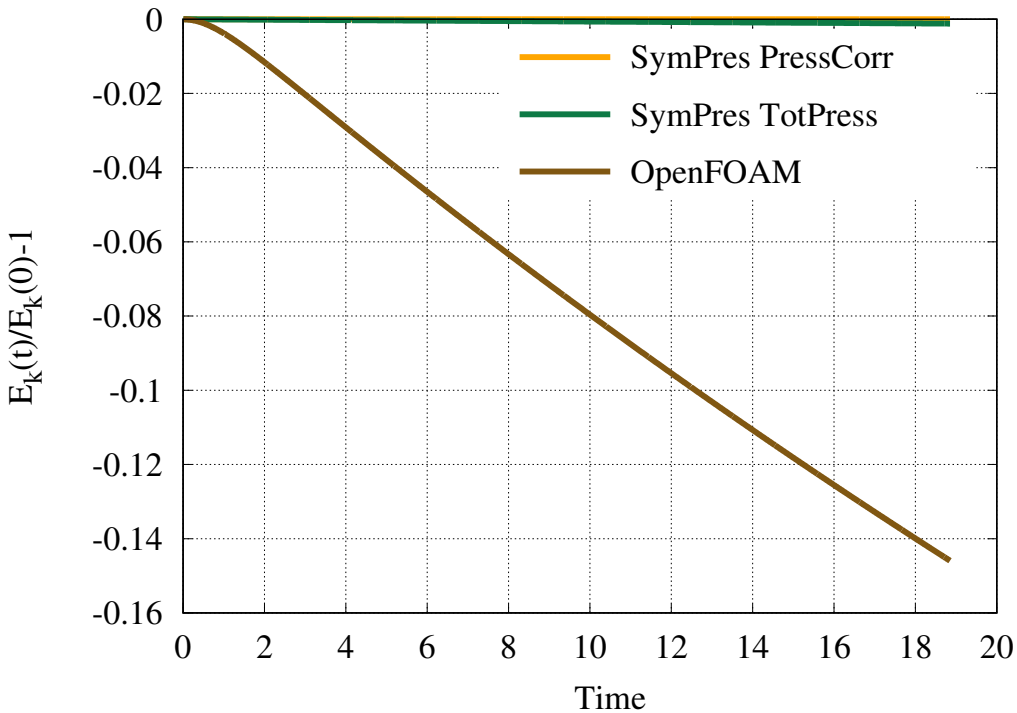


Pressure-velocity coupling on collocated grids

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

OpenFOAM





Results for an inviscid Taylor-Green vortex[3]

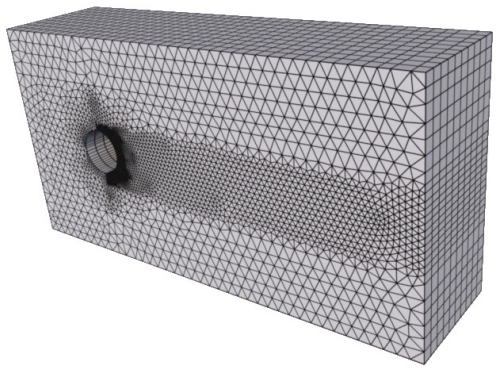
[3] E.Komen, J.A.Hopman, E.M.A.Frederix, F.X.Trias, R.W.C.P.Verstappen. *A symmetry-preserving second-order time-accurate PISO-based method*, **Computers & Fluids**, 225:104979, 2021.

Pressure-velocity coupling on collocated grids

Summary

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

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



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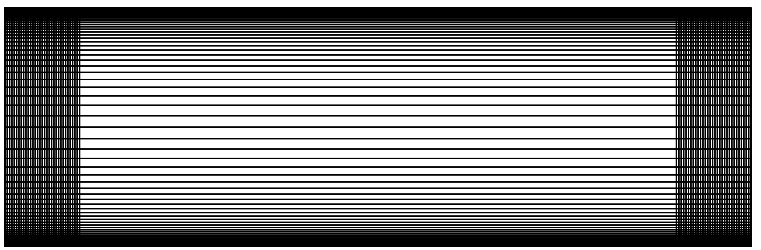

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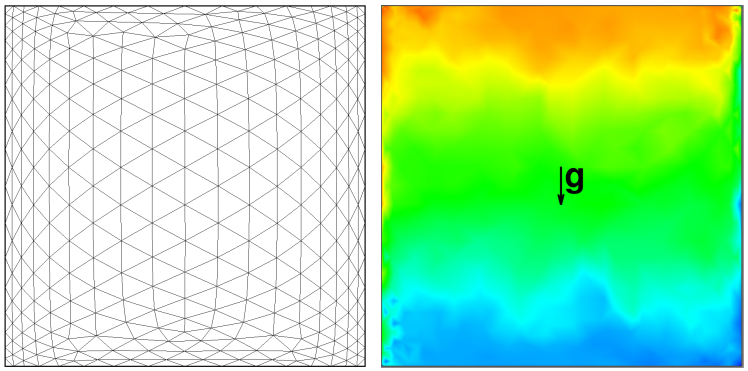

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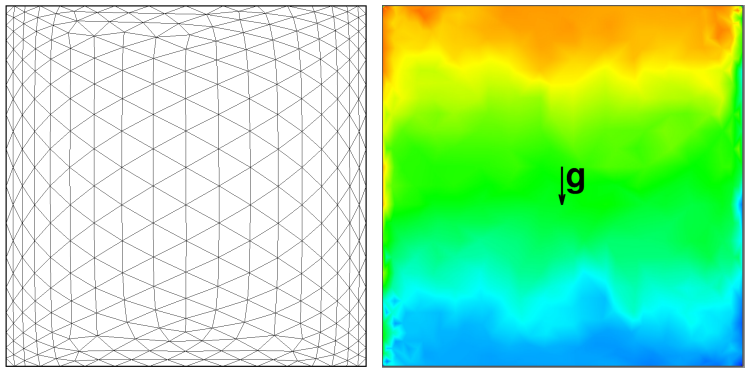

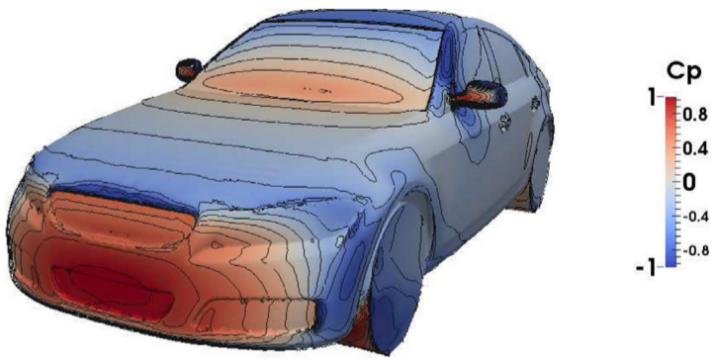

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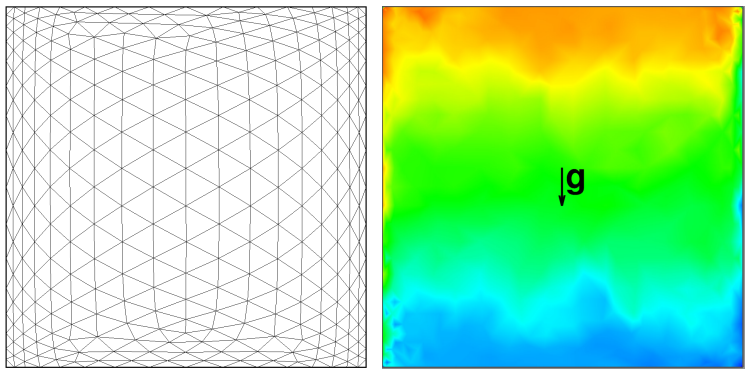

OpenFOAM

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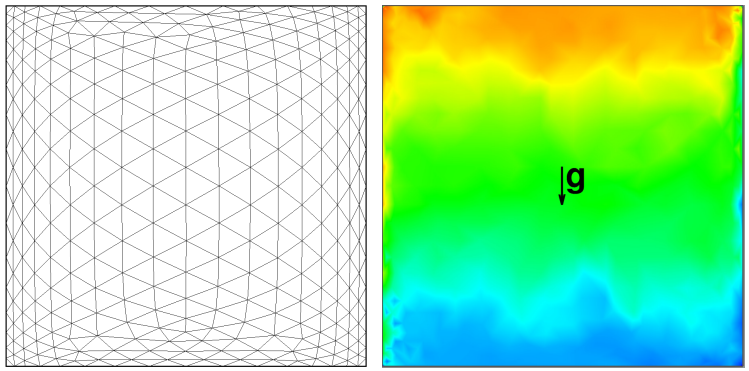

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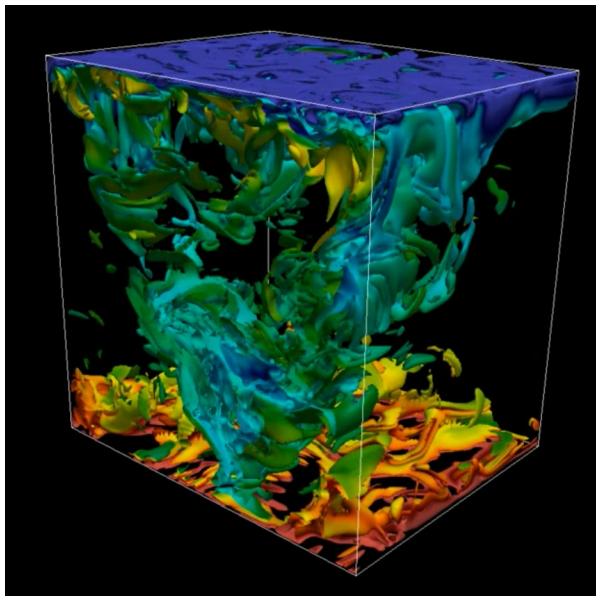
OpenFOAM

Research question #2:

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

Buoyancy-driven flows

Energy-exchanges



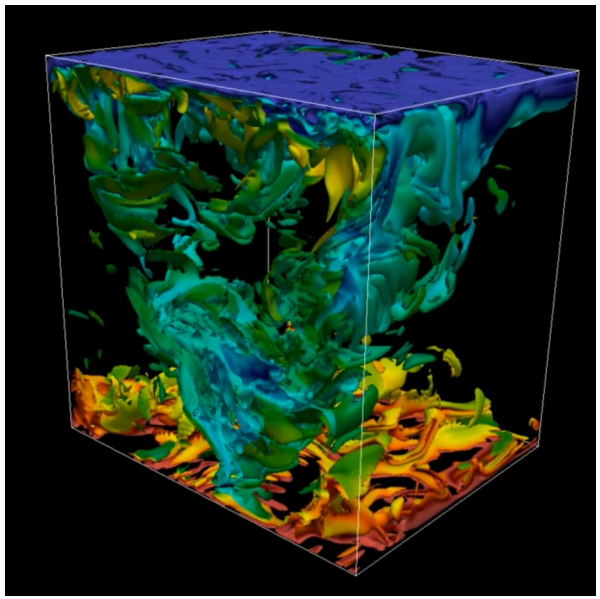
E_p
$-(y,T)$

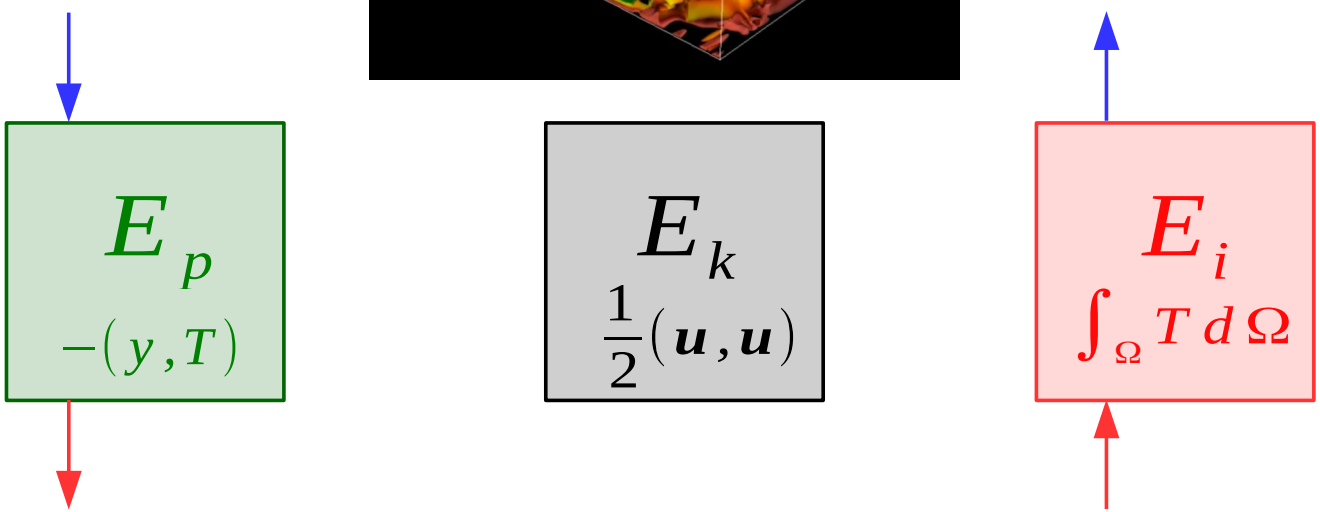
E_k
$\frac{1}{2}(\boldsymbol{u},\boldsymbol{u})$

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

Buoyancy-driven flows

Energy-exchanges





Buoyancy-driven flows

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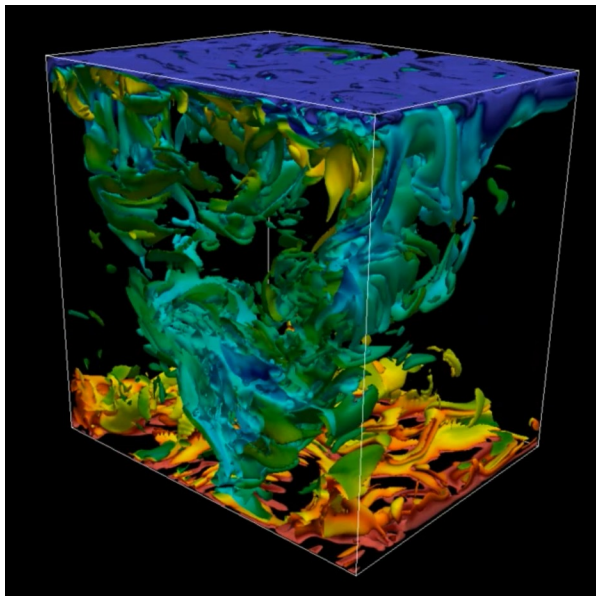
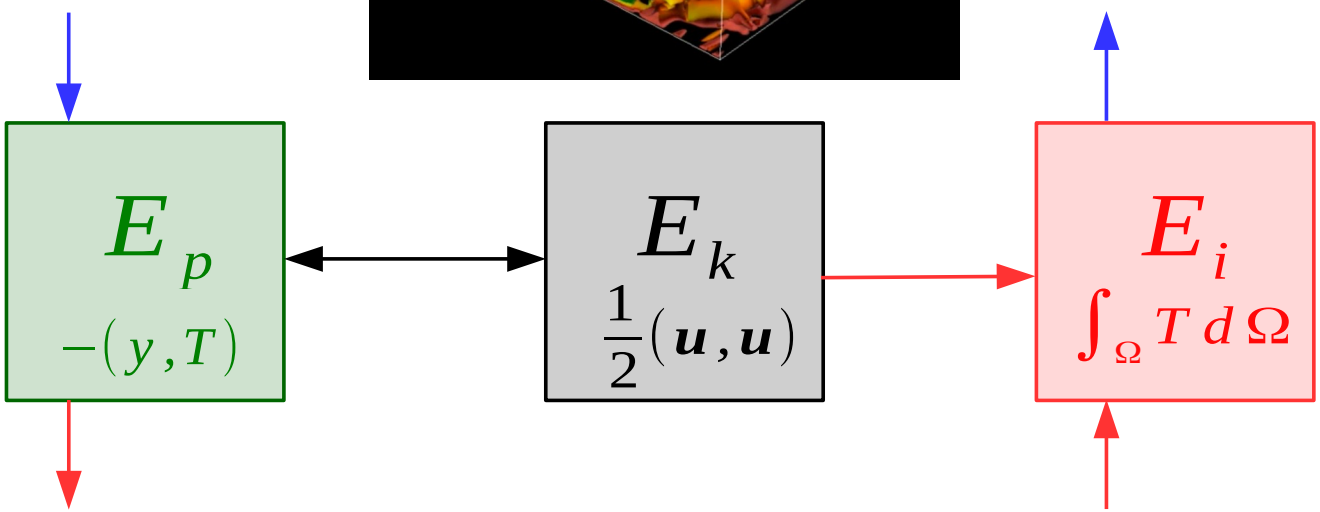




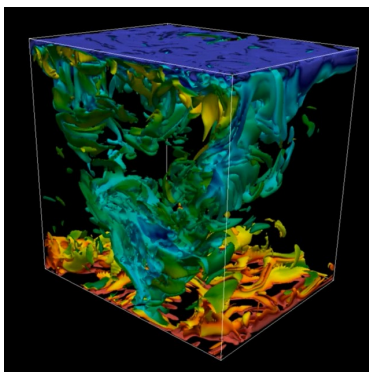
Buoyancy-driven flows

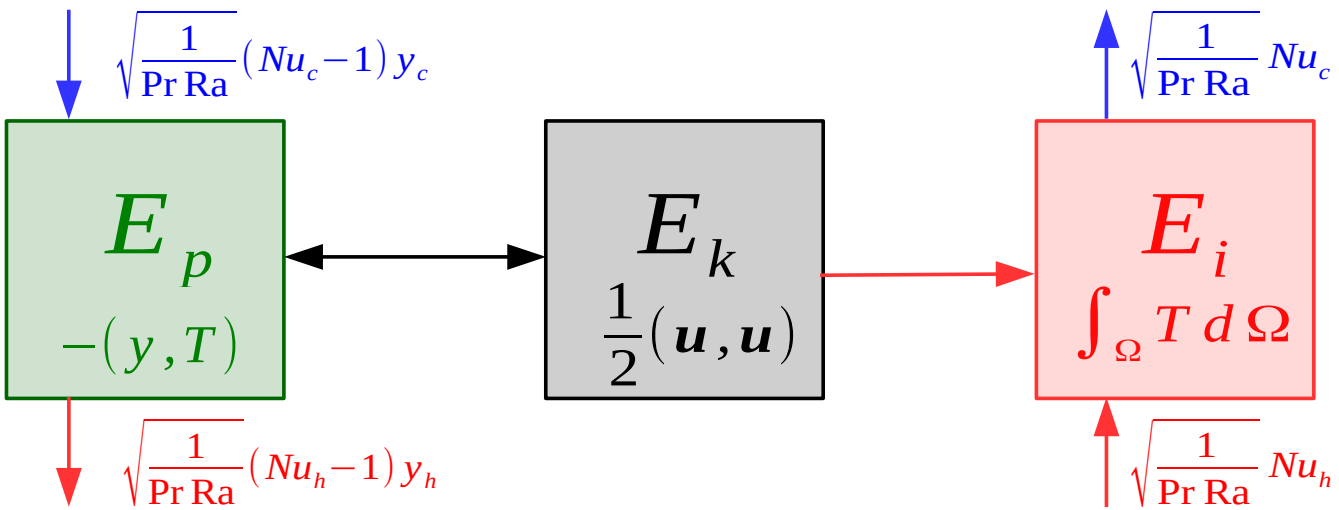
Continuous formulation

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

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

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





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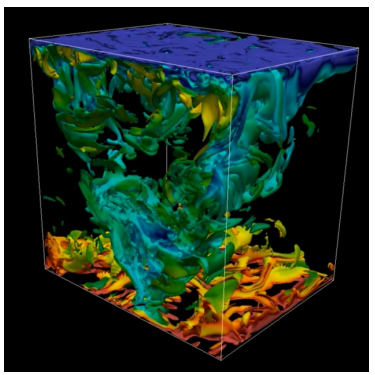
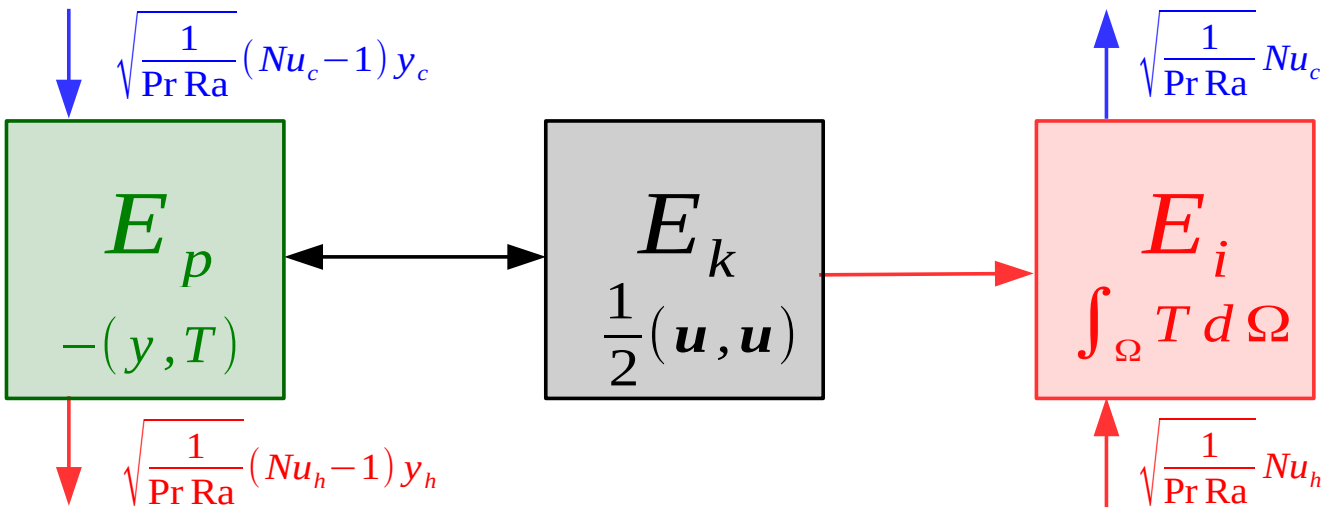


$$\frac{dE_p}{dt} = (y, \nabla\cdot(\boldsymbol{u}T)) - \sqrt{\frac{1}{\mathrm{Pr}\,\mathrm{Ra}}}(y, \nabla^2 T)$$



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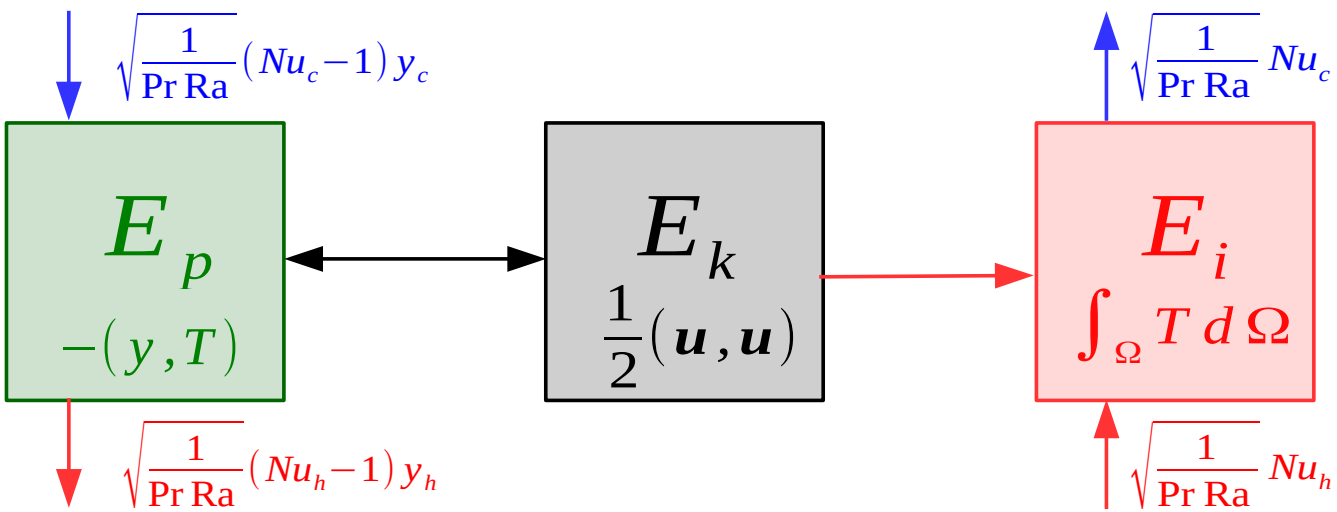
$$\Phi = \|\nabla \boldsymbol{u}\|^2 \quad \varepsilon_U = \int_\Omega \Phi\, d\Omega$$

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

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

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



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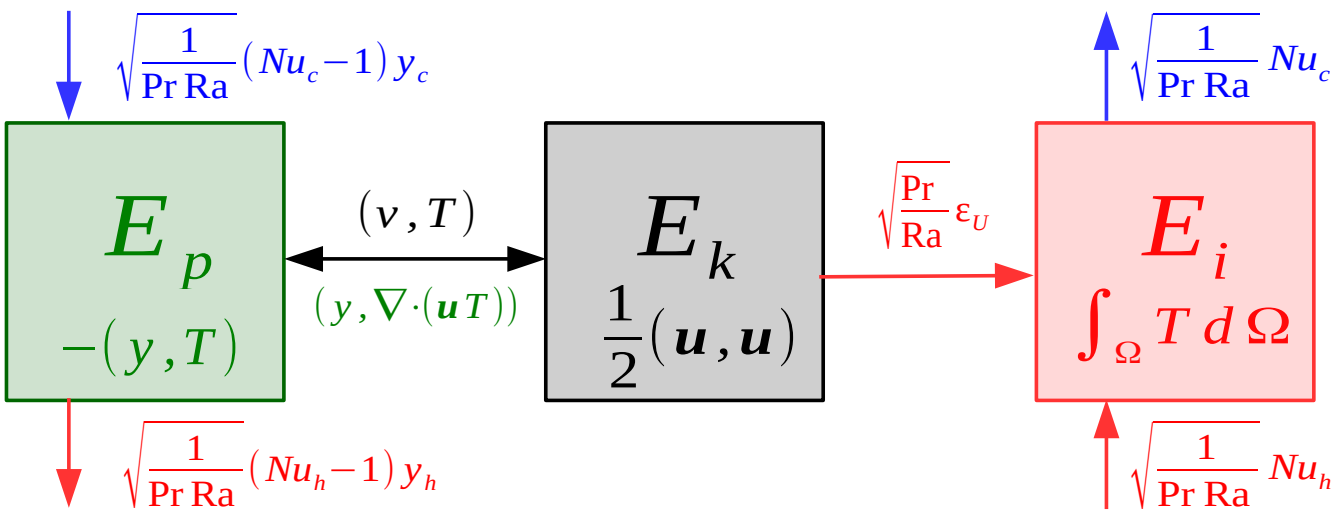


Multiphase flows

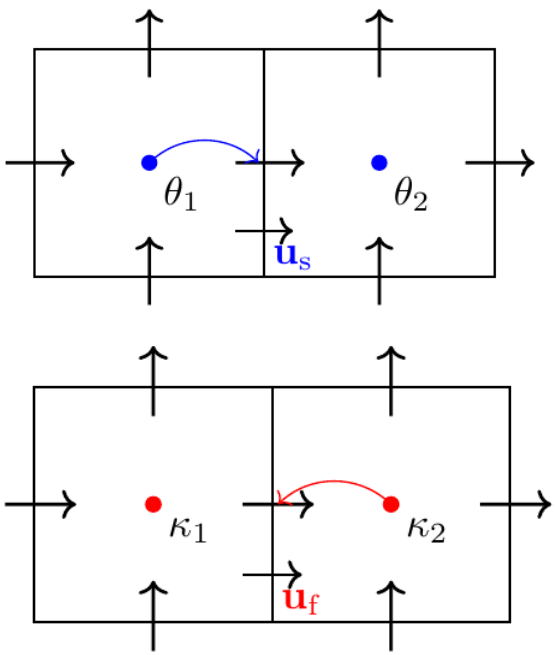
Conservative discrete formulation

Surface tension

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

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

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



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An energy-preserving level set method for multiphase flows

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ABSTRACT

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

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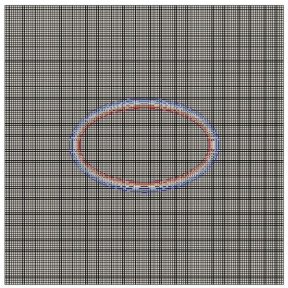

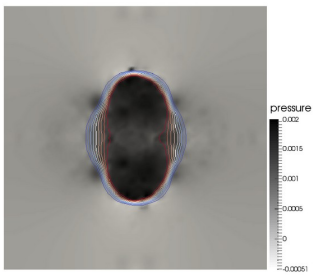

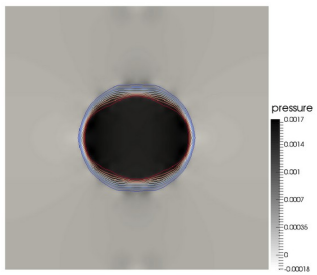

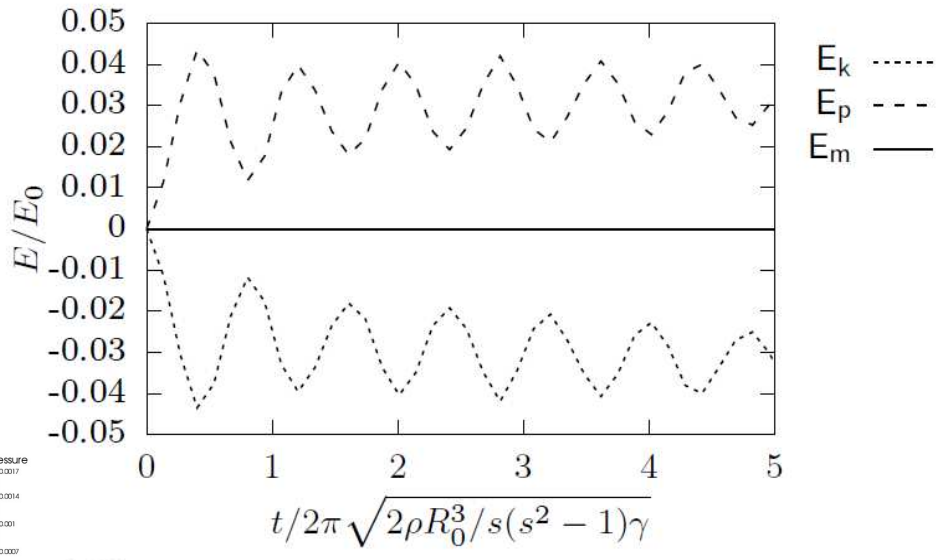

Mechanical energy (kinetic+potential) **is preserved**!

A new general framework for multiphysics

Variational formulation

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

Associated force

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

Lie derivative

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

Scalar (0-forms)

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

Density-like (3-forms)

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

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Application to buoyancy-driven flows

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

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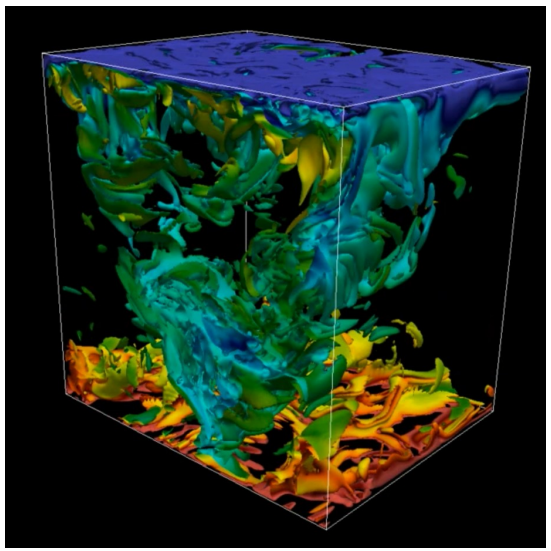

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$$E^\rho[\rho] = \int_\Omega \rho\, g\, y\, d\Omega$$

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

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

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

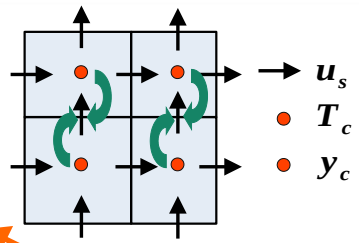
A new general framework for multiphysics

Buoyancy-driven flows on staggered grids

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

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

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



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A new general framework for multiphysics

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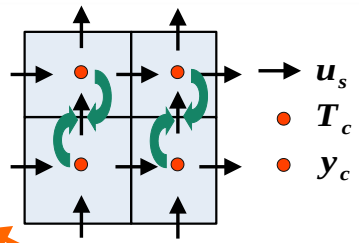

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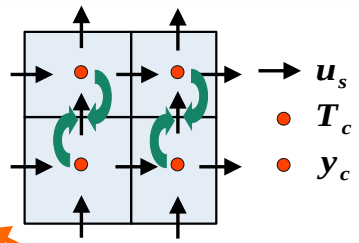

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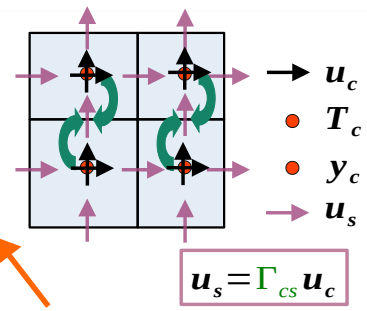

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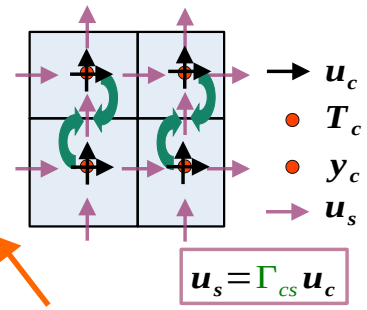

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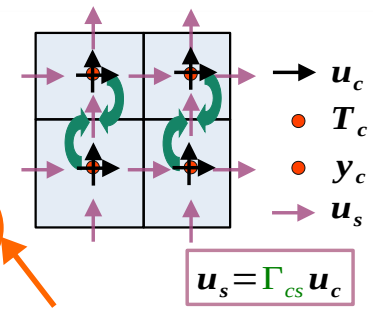

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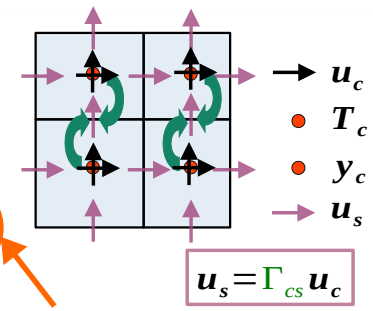

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A new general framework for multiphysics

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

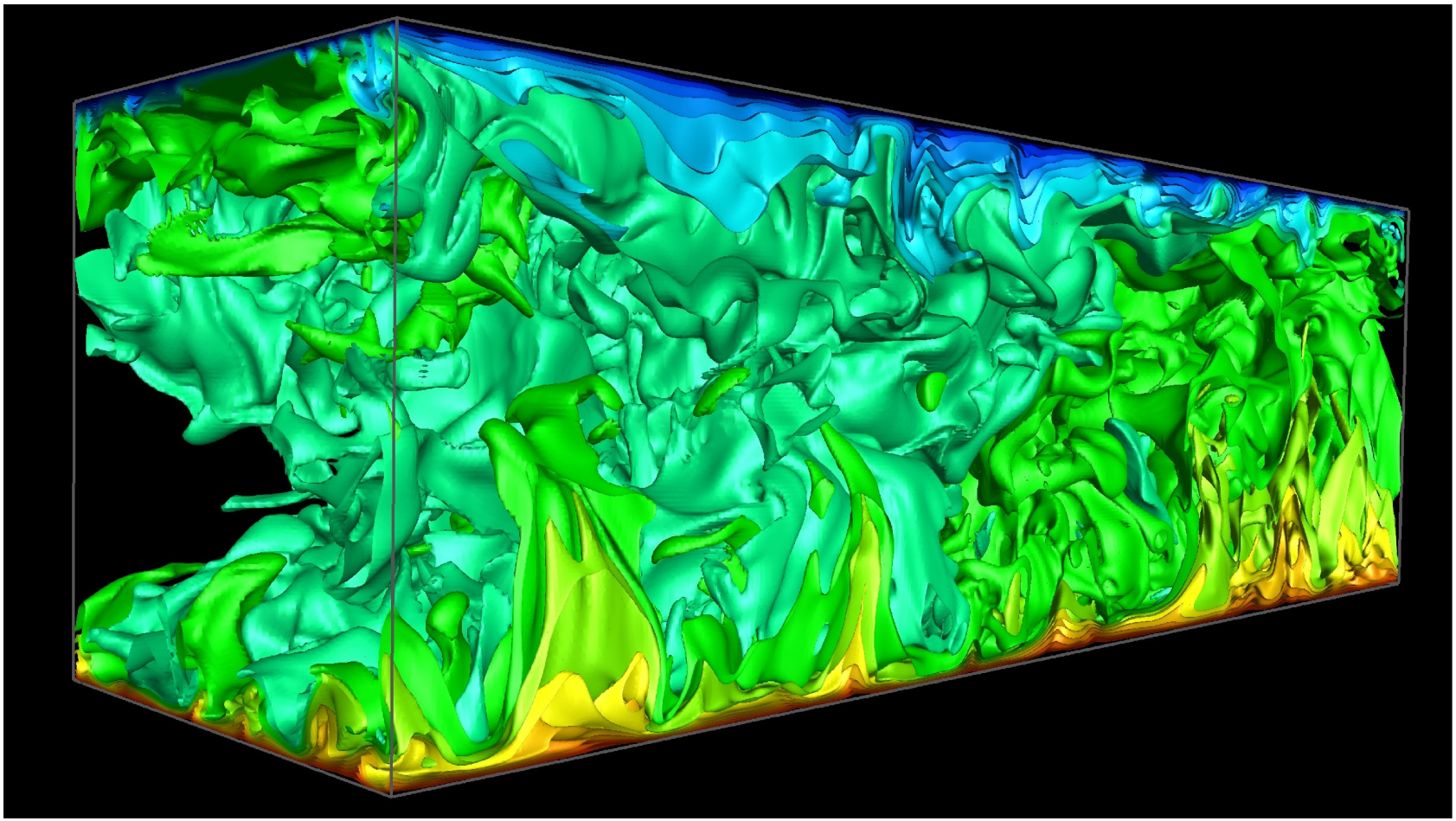
$\mathscr{L}_{\boldsymbol{u}}$ Lie derivative

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

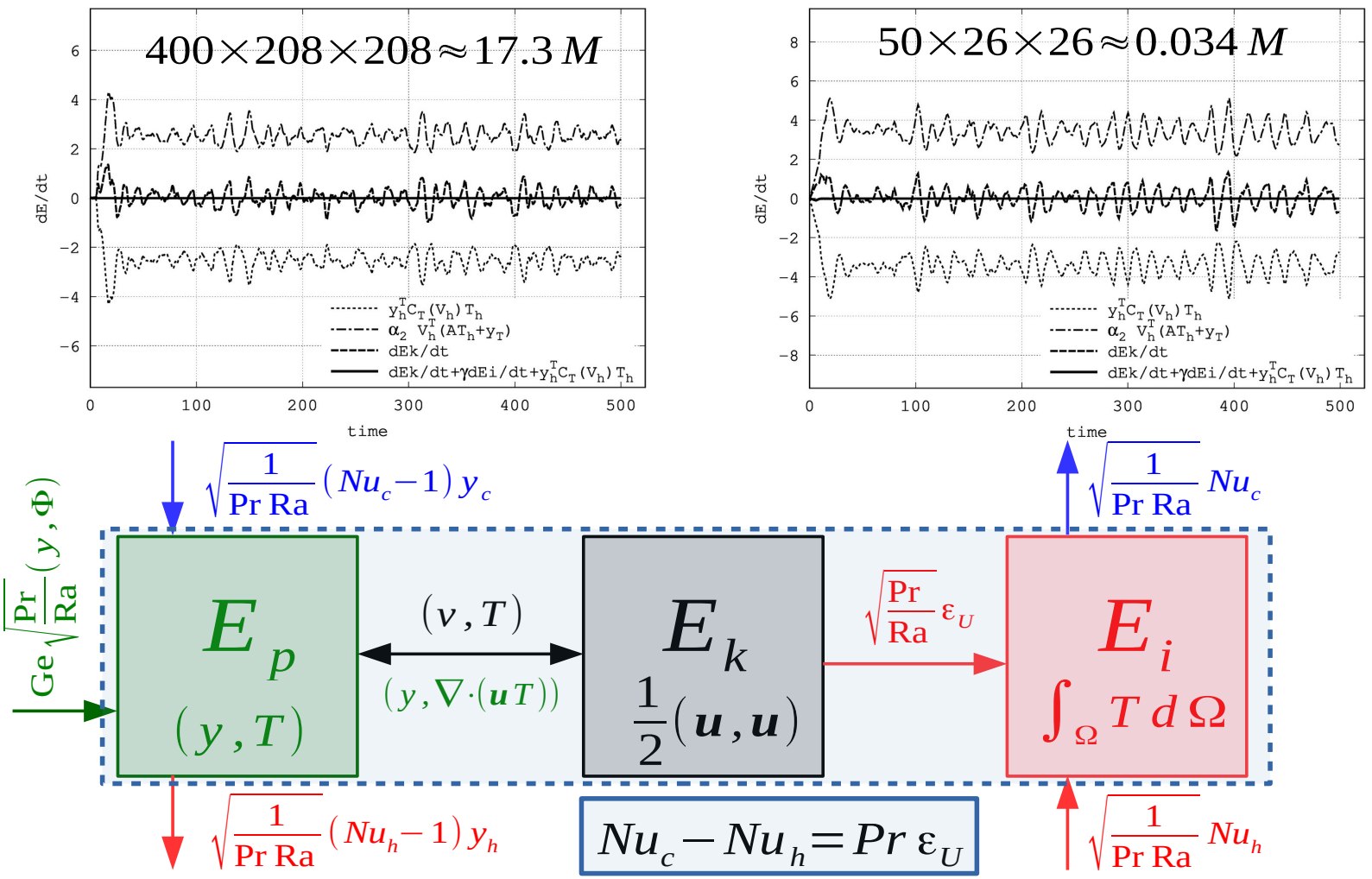
Leitmotiv: transport equation and its associated force **cannot** be discretized independently!!!

Buoyancy-driven flows

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



Buoyancy-driven flows[4]



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

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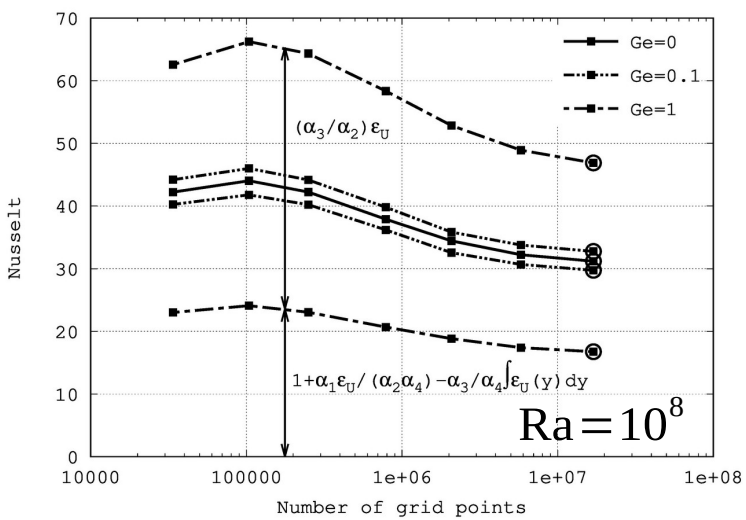

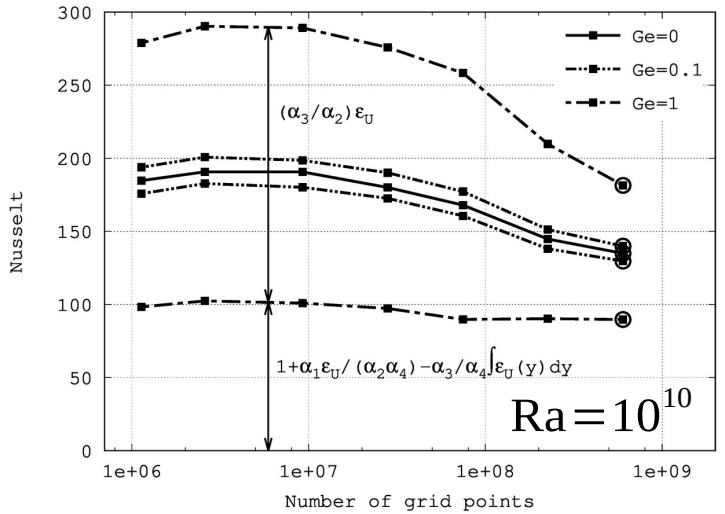

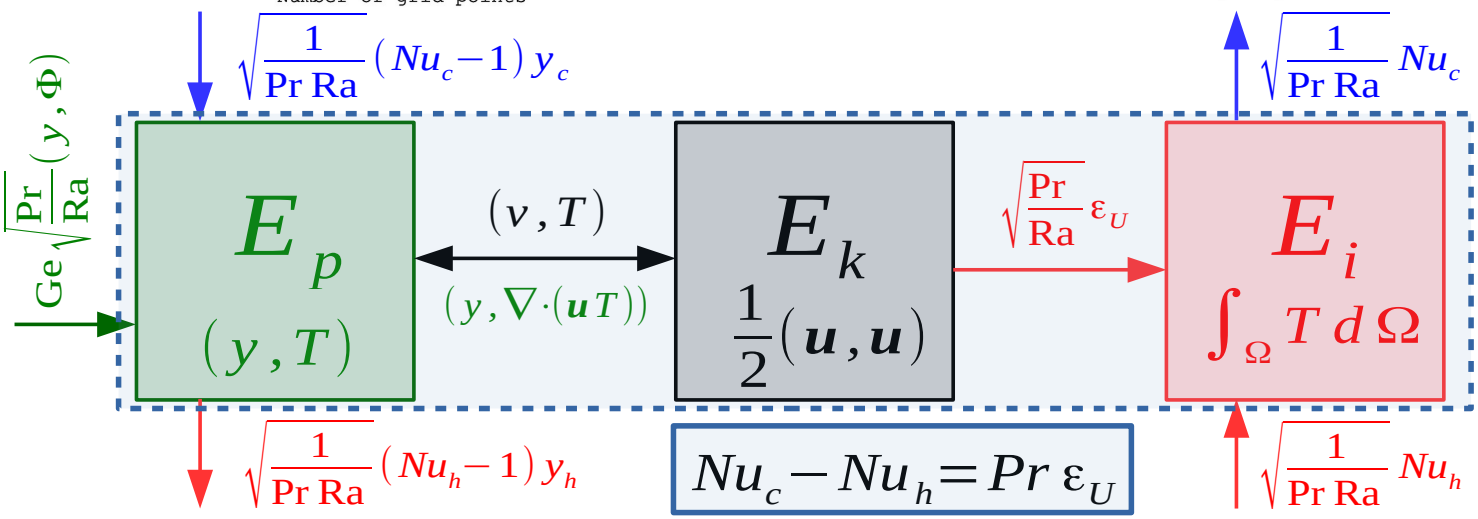

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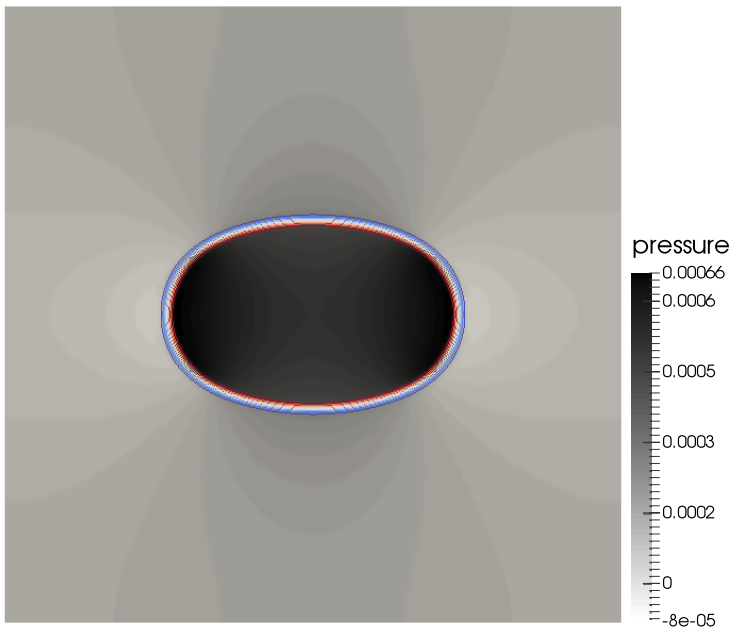
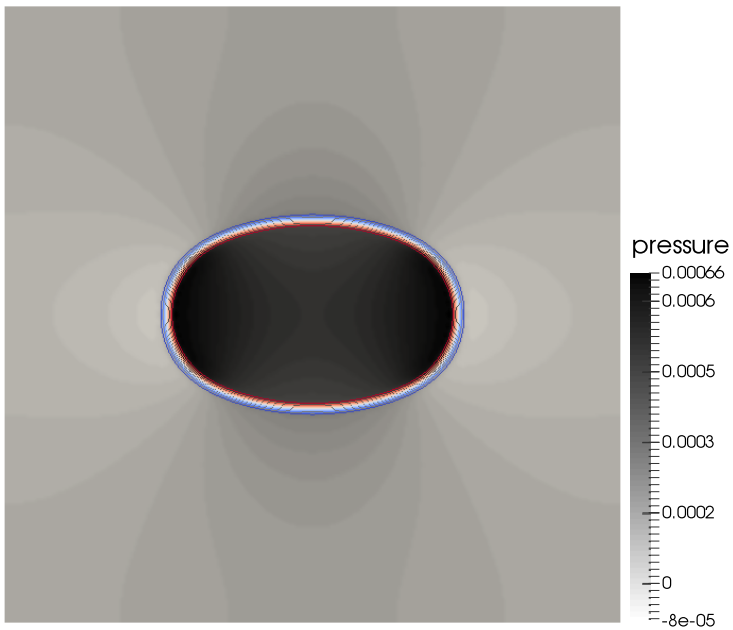
Multiphase flows[4]



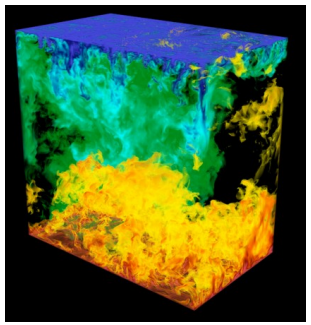
Non-symmetry-preserving!



Symmetry-preserving!

[4] 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)

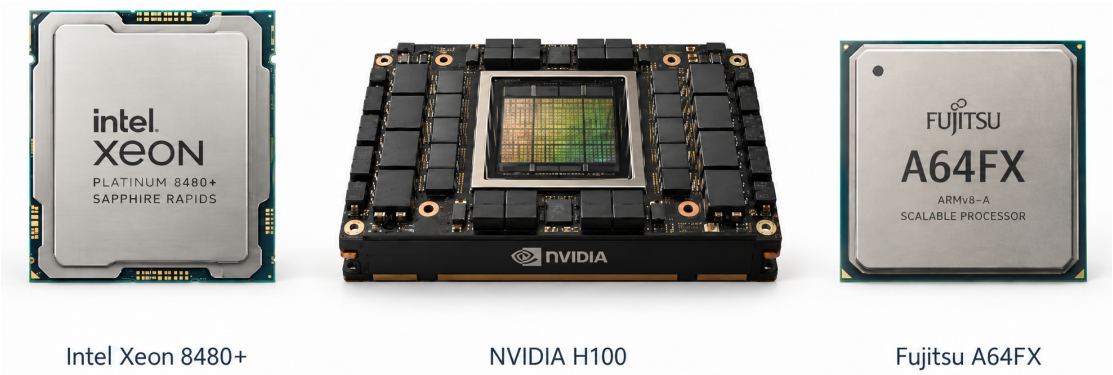
DNS

LES

HPC on modern supercomputers

Research question #3:

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



Intel Xeon 8480+ NVIDIA H100 Fujitsu A64FX

[5] 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

[6] 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.

[7] 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.

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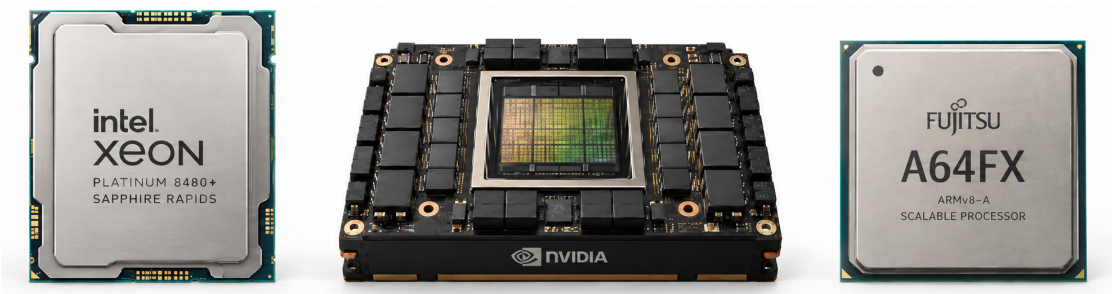

Intel Xeon 8480+ NVIDIA H100 Fujitsu A64FX

HPC^2: portable, algebra-based framework for heterogeneous computing is developed[5]. 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[6,7].

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

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

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

$$\left\langle \nabla^2 \boldsymbol{a}, \boldsymbol{b} \right\rangle = \left\langle \boldsymbol{a}, \nabla^2 \boldsymbol{b} \right\rangle$$

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:

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

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

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

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

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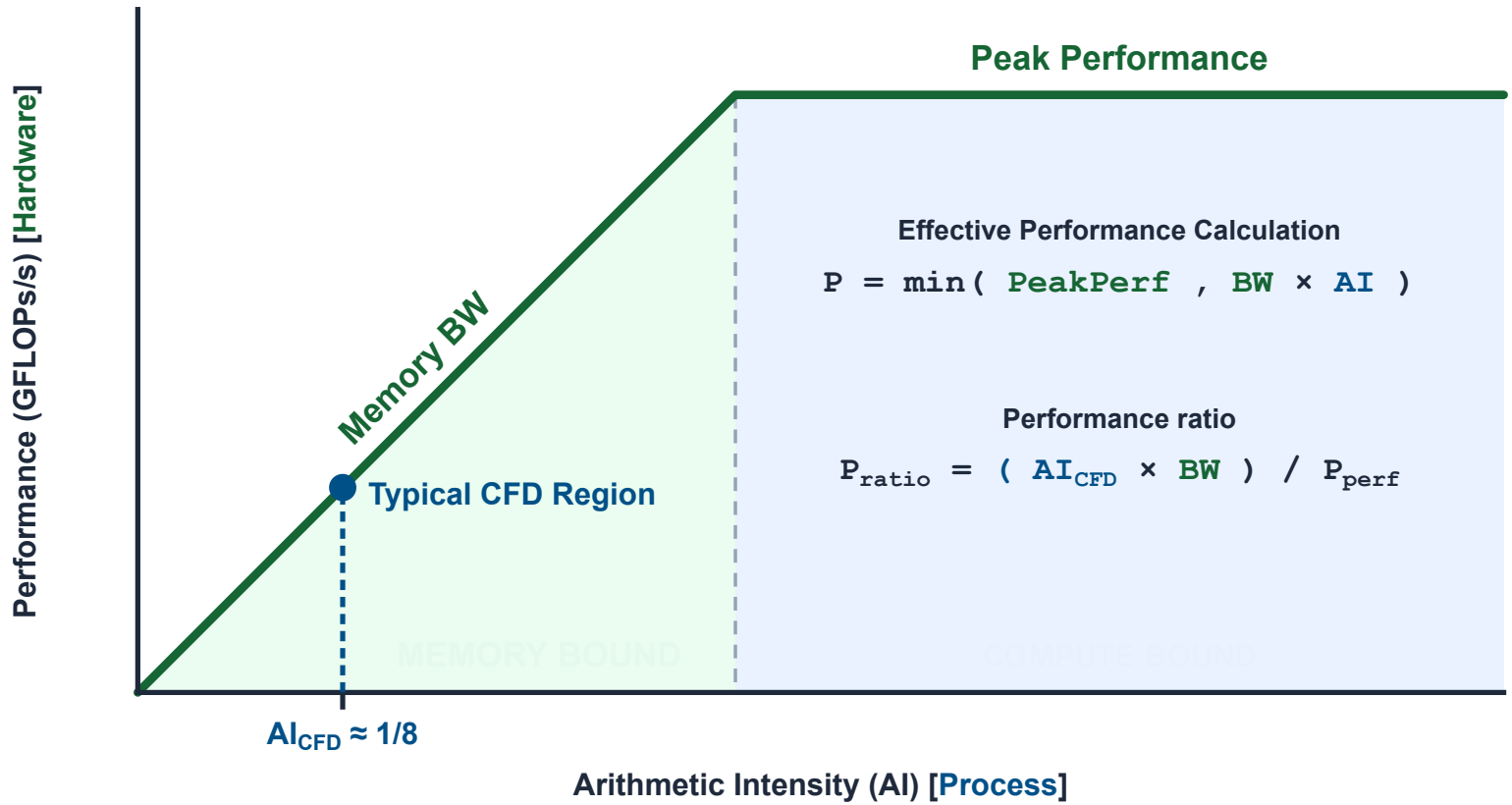
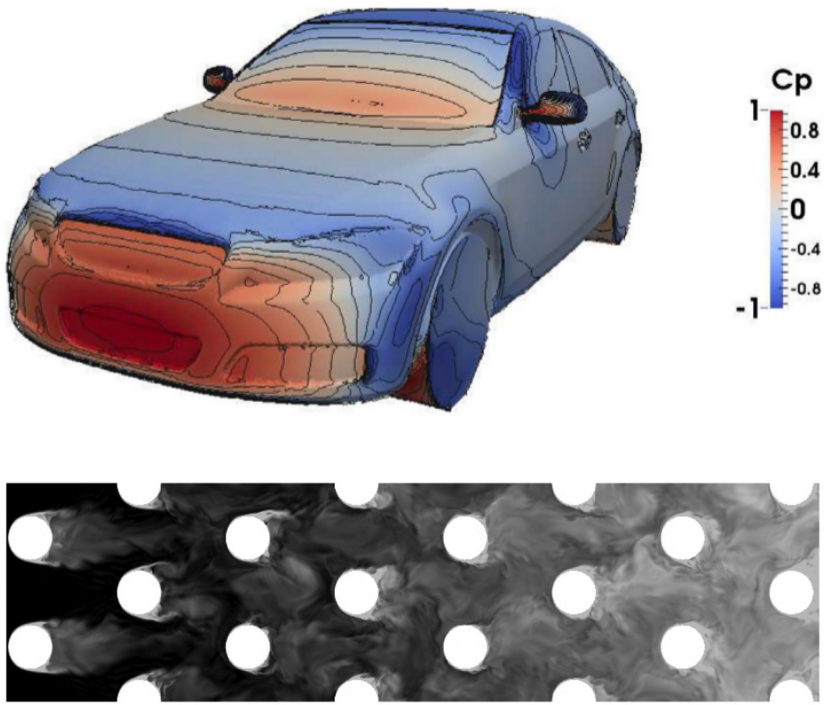
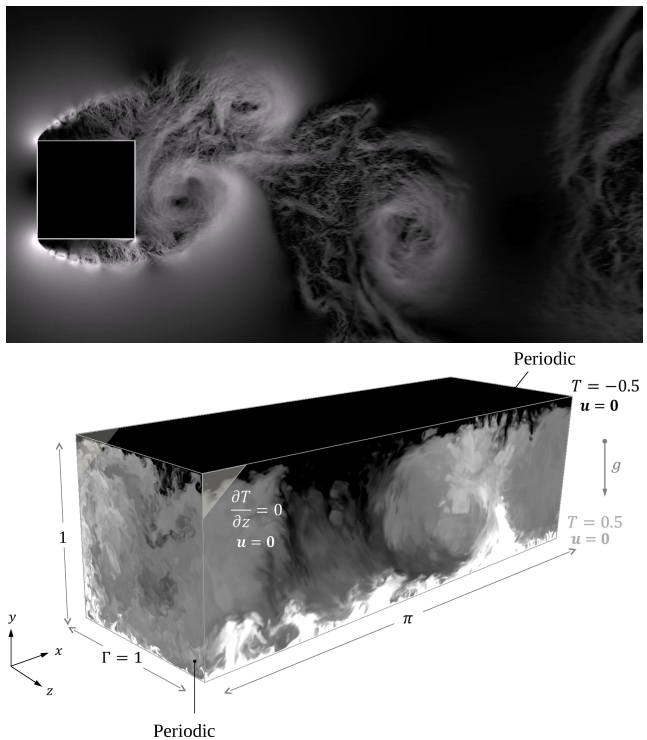


Algebra-based approach naturally leads to portability, to simple and analyzable formulations and opens the door to new strategies[8] to improve its performance...





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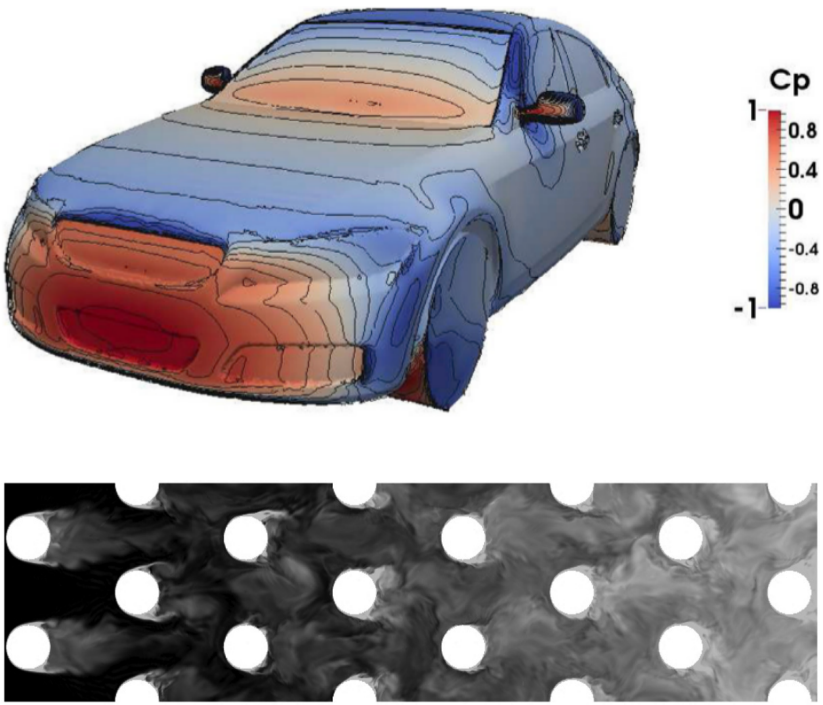
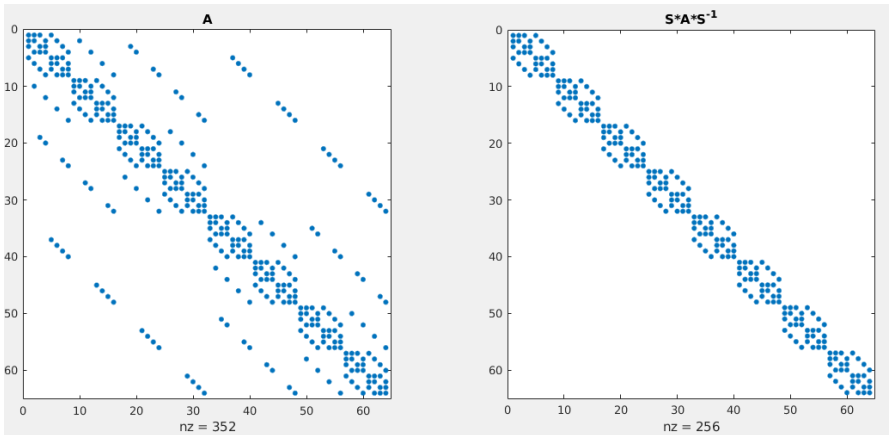


$$\hat{L} = SLS^{-1} = I \otimes L_{inn} + diag(\boldsymbol{d})$$



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

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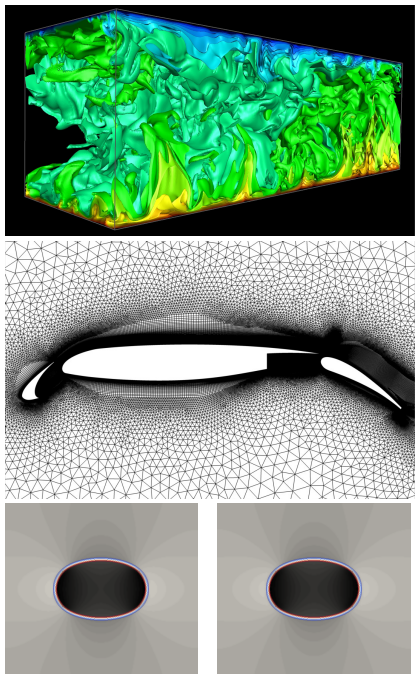

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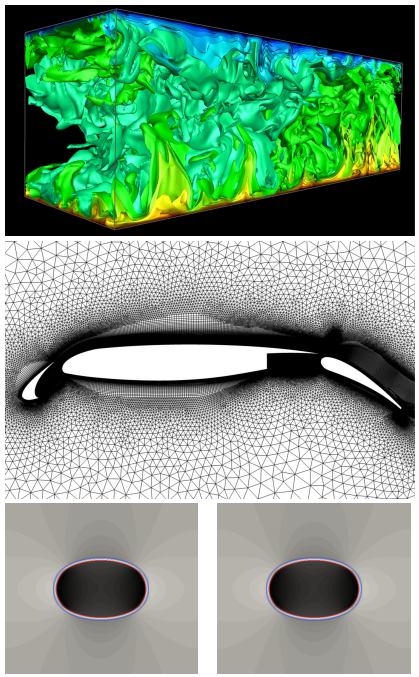

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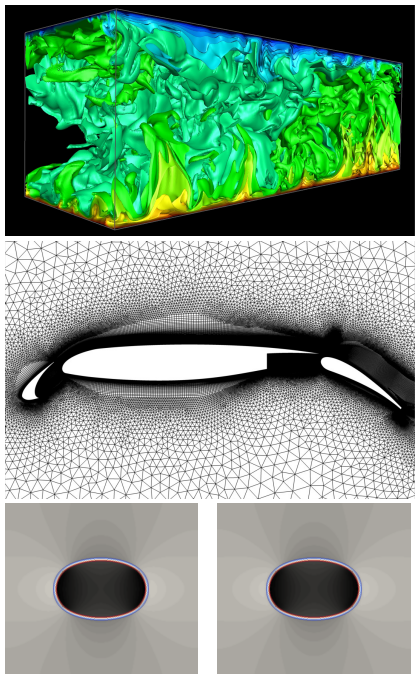

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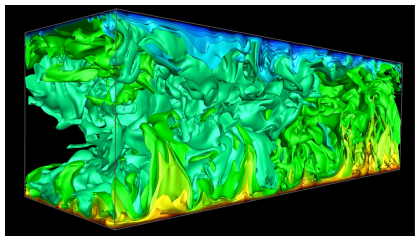

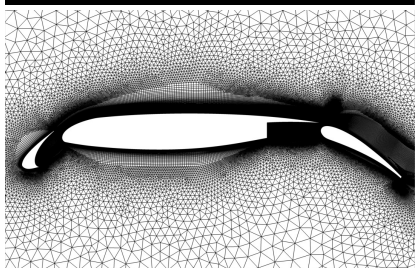

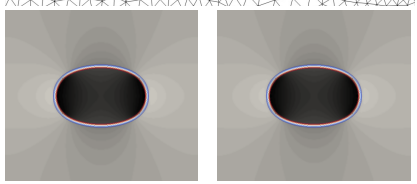

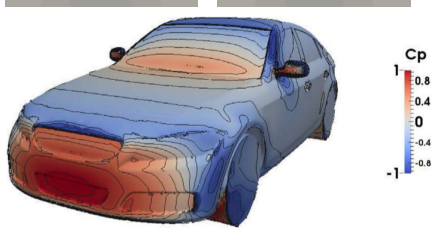

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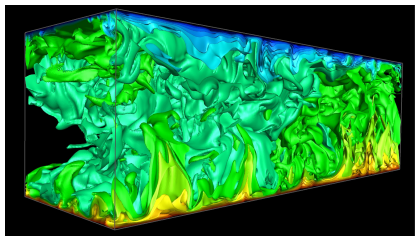
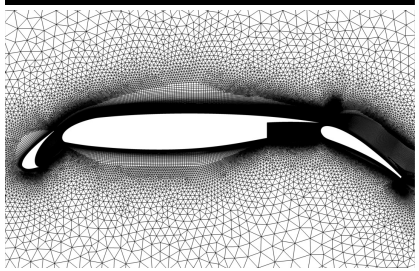
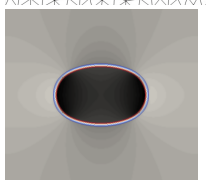
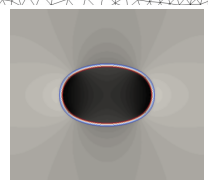
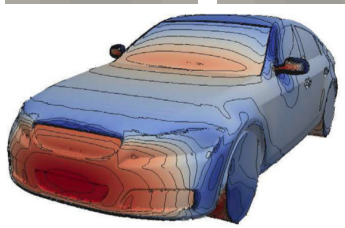
- **Open-source** platforms help to share and disseminate ideas.
  https://github.com/janneshopman/RKSymFoam

OpenFOAM

Thank you for your attention

