Large Eddy Simulation of sCO2 with a Discontinuous Galerkin Method

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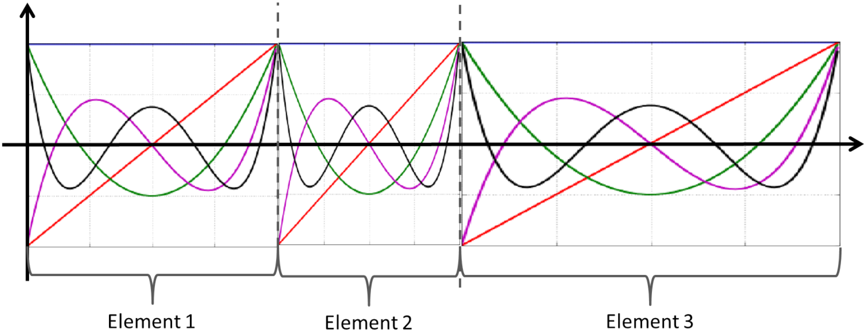
Discontinuous Galerkin

Basis functions

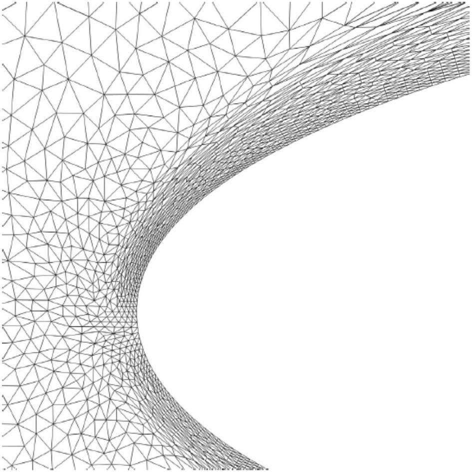
- basis functions in Element k: $\{\phi_i^{(k)}\}_i = \{\phi_1^{(k)}, \phi_2^{(k)}, \phi_3^{(k)}, \ldots\}$
- approximation in Element k:
  $f \approx \sum_i c_i^{(k)} \phi_i^{(k)} = c_1^{(k)} \phi_1^{(k)} + c_2^{(k)} \phi_2^{(k)} + \ldots$

arbitrarily high polynomial orders ("high-order finite volume")



Discontinuous Galerkin

inhomogeneous and unstructured meshes



([1])

[1] F. Bassi, L. Botti, A. Colombo, A. Crivellini, C. De Bartolo, N. Franchina, A. Ghidoni, and S. Rebay (2015). “Time Integration in the Discontinuous Galerkin code MIGALE - Steady Problems”. In: *Notes on Numerical Fluid Mechanics and Multidisciplinary Design* 128, pp. 179–204

Compressible vs. Incompressible Solvers

Incompressible Solvers (pressure-based)

- ✔ Highly mature numerical methods and computer codes.

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- ✘ Very expensive and sensitive to errors, because
  - it accounts for heat generation due to friction and compression;
  - all fluid properties depend on the density ρ and the enthalpy H.
  - determining the pressure by $p = p(\rho, H)$ is very sensitive to errors;
  - the flow compresses the fluid $\Rightarrow \rho$ increases $\Rightarrow p$ increases.
    There is a finite speed of sound.
    This is not the physics at low Ma;

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$\Rightarrow$ **high resolution, and 'stiff' linear systems.**

Low-Mach Solver

Transport equations in the limit $\mathrm{Ma} \to 0$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \qquad \text{mass}$$

$$\frac{\partial m_i}{\partial t} + \nabla \cdot (\mathbf{u}\ m_i) = \frac{\partial}{\partial x_j}\tau_{ij} - \frac{\partial p}{\partial x_i} \qquad \text{momentum}$$

$$\frac{\partial \rho h}{\partial t} + \nabla \cdot (\mathbf{u}\ \rho h) = \nabla \cdot ((\lambda / c_p) \nabla h) \qquad \text{enthalpy}$$

The fluid properties $(\rho, \nu, \lambda, \dots)$ only depend on the enthalpy h.

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- ✔ Assumtions are valid for heat transfer in sCO2 for many flows.
- ✔ Pressure-based $\Rightarrow$ no speed of sound $\Rightarrow$ larger time steps.
- ✘ Less straightforward than the fully compressible formulation. Numerical methods are less mature, especially for finite elements.

The pressure-correction method

The Algorithm

1. Solve the enthalpy transport equation.
2. Solve the momentum transport equation.
3. Solve a Poisson equation ($-\Delta\phi = \dots$).
4. Correct the pressure and the mass flux (with ϕ).

This is a time-splitting method: the transport equations are solved one by one in each time step. **This is much cheaper than a compressible solver.**

Our method is stable without iterating within a time step, with **full second-order temporal accuracy**.

Unresolved issues with Low-Mach Solvers: An Example

What enthalpy/energy variable to choose?

Solving for the volumetric enthalpy $H = \rho h$ [J/m^3]

✔ The temporal derivative is easy:

$$\frac{\partial H}{\partial t} \approx \frac{1}{\delta t}\left(H^{n+1} - H^{n}\right) \ .$$

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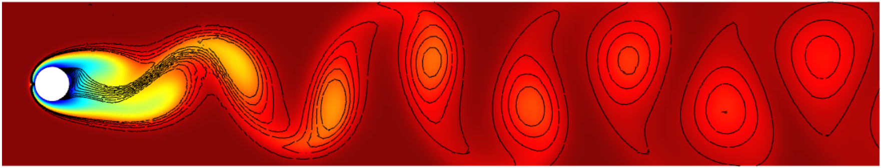
The term $(\rho h)^{n+1}$ is nonlinear, because ρ^{n+1} is a function of h^{n+1}.

Heated Vortex Shedding: a DNS Example



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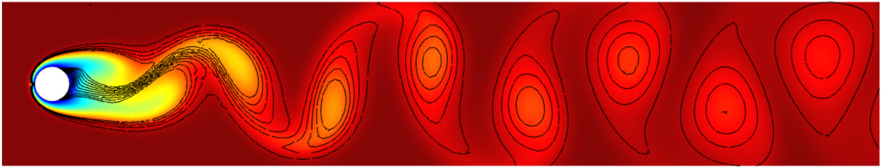

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Flow past a circilar wire

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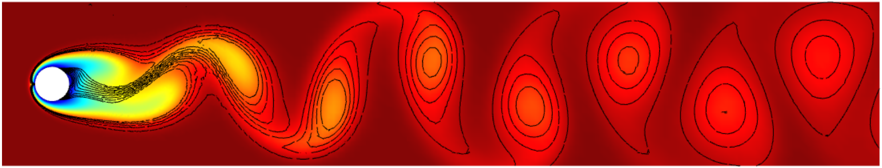

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Flow past a circilar wire

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- Heating the wire alters ρ and μ
- The shedding frequencies can be compared to experimental data. Our results agree to within 1%.

Large Eddy Simulation (LES): the idea

The code is very similar to a DNS solver.

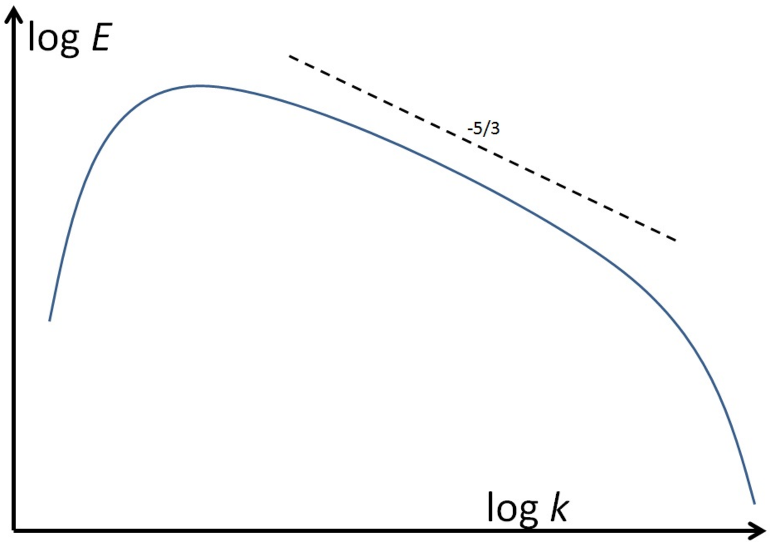
- The same governing equations, but add extra viscosity:

$$\nu \leftarrow \nu + \nu_{\mathrm{SGS}} \ .$$

  ν_{SGS} is the sub-grid-scale viscosity.
- This surpresses small-scale vortices that cannot be simulated.
- ν_{SGS} is based on the velocity field.

Large Eddy Simulation (LES): the idea

Large scales vs. small scales: energy spectrum



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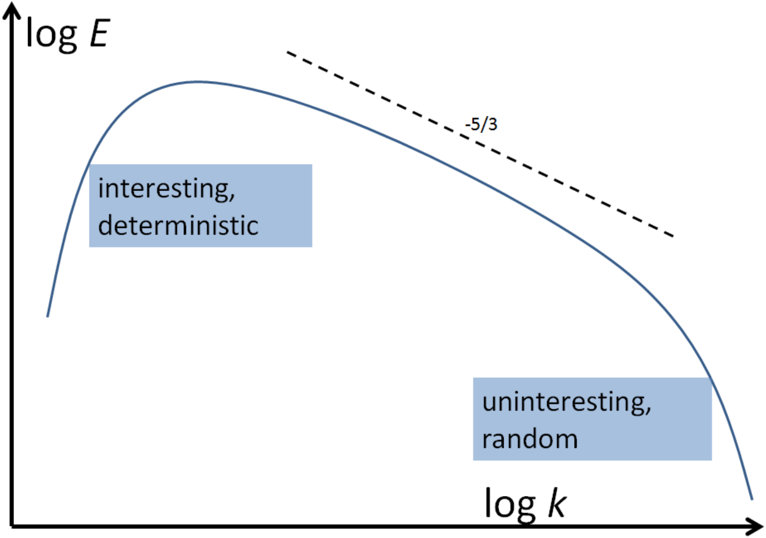
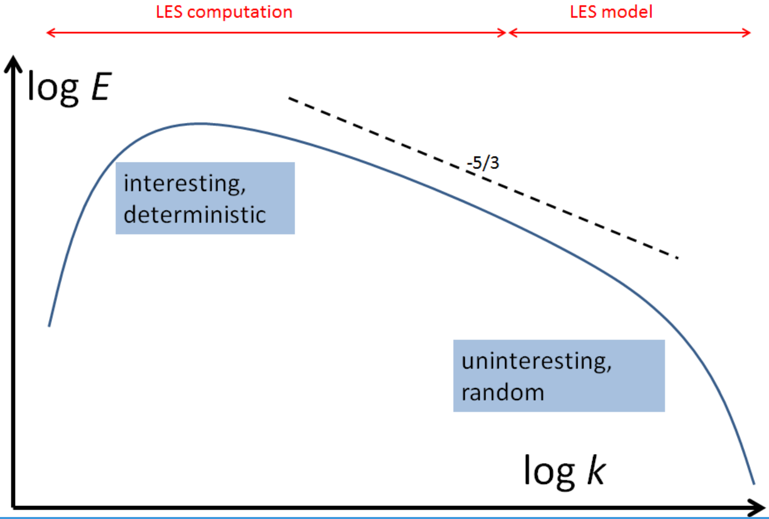


Large Eddy Simulation (LES): the idea

- Compute large movements, model small scales.
- **Isolate the deterministic part.**



Examples of LES models

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The Smagorinsky model

- Simple, and traditionally by far the most widely used.
- Linear in the rate of strain: $\nu_{\mathrm{SGS}} \propto |S|$

$$S = \nabla \mathbf{u} + \nabla \mathbf{u}^{\top} - \frac{2}{3}(\nabla \cdot \mathbf{u}) I \tag{1}$$

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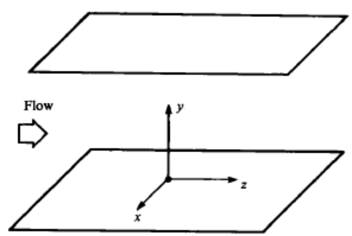
The WALE model

- WALE: Wall-adapted Local Eddy Viscosity.
- Non-linear in the rate of strain.
  ν_{SGS} is a function of both both $\nabla \mathbf{u}$ and $\nabla \mathbf{u} \cdot (\nabla \mathbf{u})^{\top}$
- Constructed to get the correct scaling near a wall: $\nu_{\mathrm{SGS}} \propto (y^{+})^{3}$.

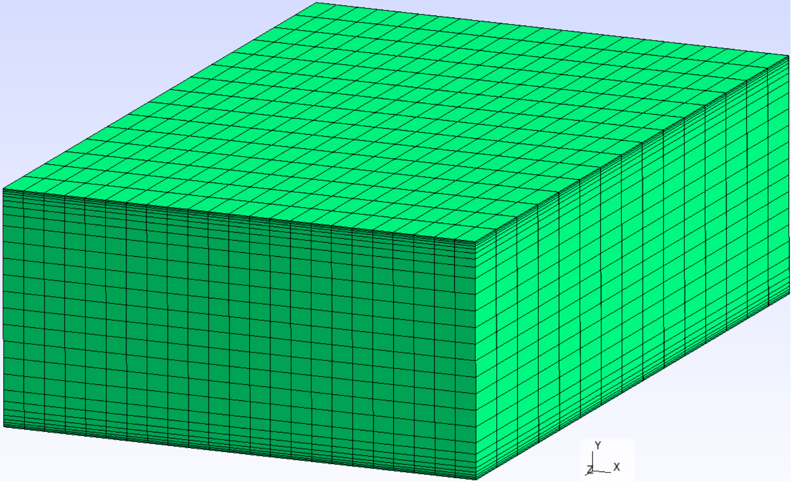
Start 'Simple': Plane Channel Flow

The most basic wall-bounded flow



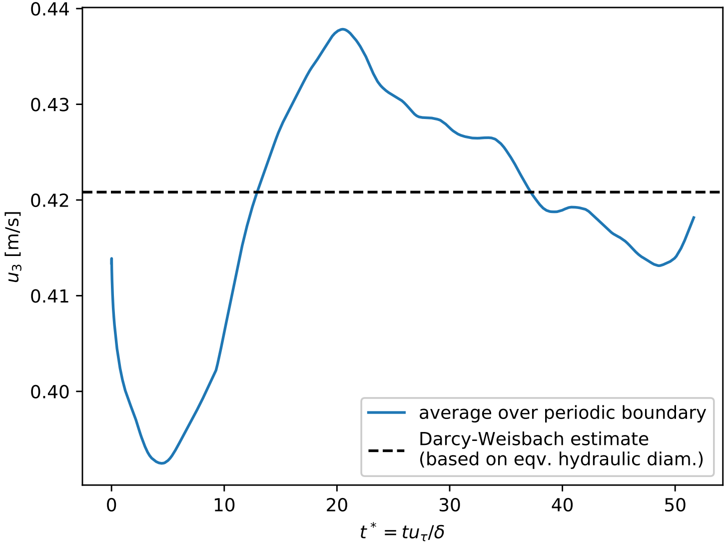
- Still far from trivial.
- Bedrock for first DNS papers, and a large part of LES literature.
- New papers are being published all the time.
- There are experimental results, but DNS is better.

LES with DG: Isothermal Results



LES for isothermal Flow: Converge to statistical average

Mass flow:



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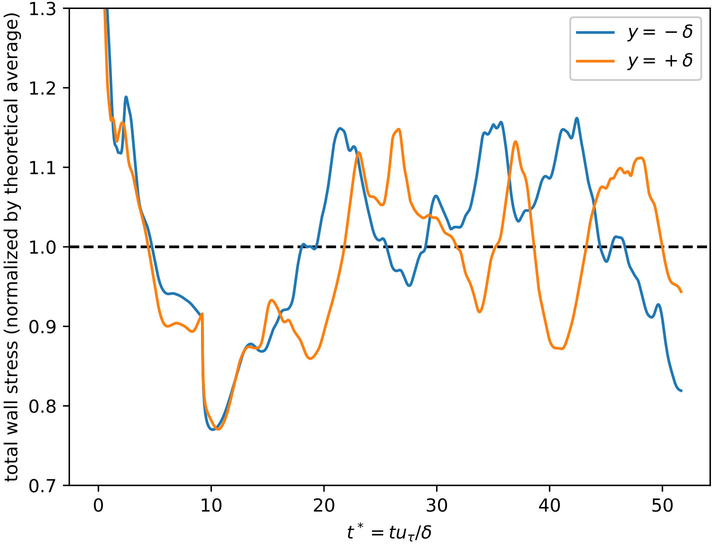
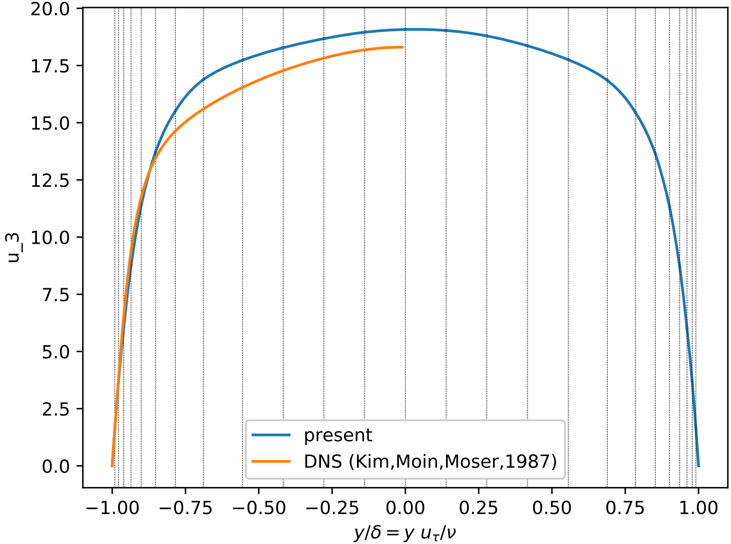
Wall stress:



LES for isothermal Flow: Average velocity profile



LES with DG: Isothermal Results

- Friction Reynolds number: $\mathrm{Re}_\tau = 180$
- 1 wall unit = δ/Re_τ
- Kolmogorov length ≈ 2 wall units
- **LES** (present case):
  - **# DOFs: 0.1 M**
  - max. element size: ~ 23 wall units
  - Completely general method, for all geometries.
- **DNS** (Kim, Moin, and Moser,1987)[2]:
  - **# DOFs: 4 M**
  - max. element size: 4.4 wall units
  - Highly specialized code and method for this particular geometry.
- Domain shape and averaging time: same for DNS and LES

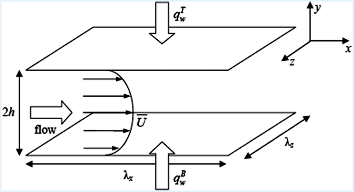
[2] J. Kim, P. Moin, and R. Moser (1987). "Turbulence statistics in fully developed channel flow at low Reynolds number". In: *Journal of Fluid Mechanics* 177.-1, p. 133. DOI: 10.1017/S0022112087000892

LES with DG: Isothermal results

- stresses are not great
- velocity is OK ($\sim 10\%$ off)
- I adjusted the mesh and the LES filter width independently. The error is mainly due to LES model, not the discretization.
- The simulation is very well resolved. . . too well resolved.

Channel Flow with sCO2: Compare LES to DNS

The most basic wall-bounded flow



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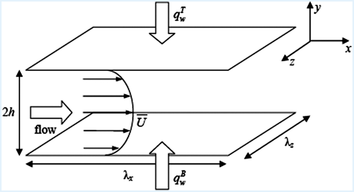

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- degrees of freedom: 198M

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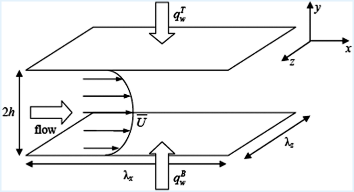

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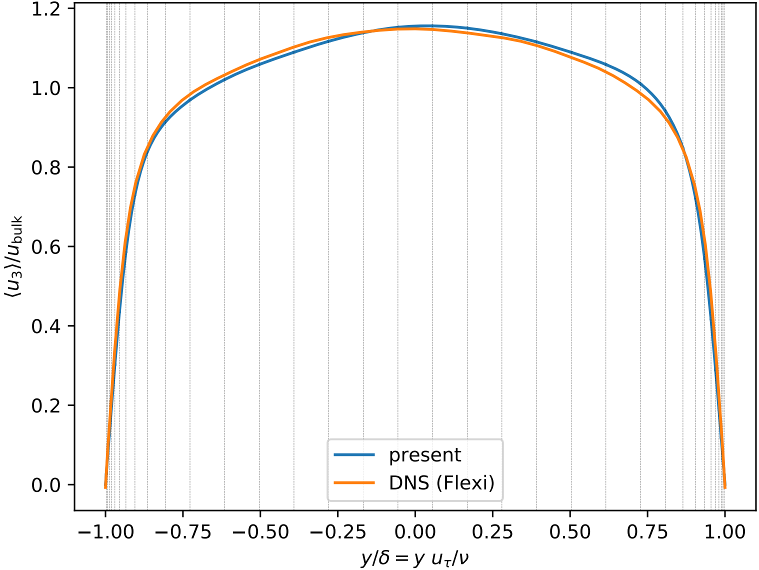
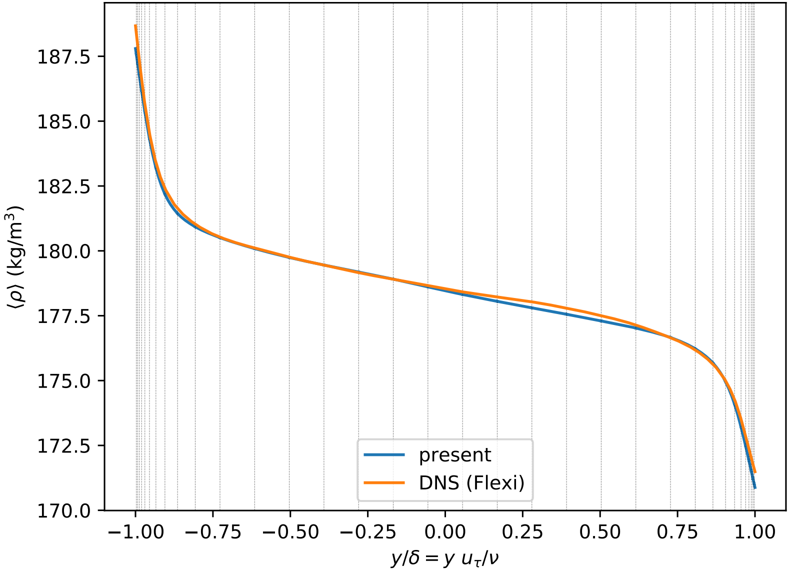
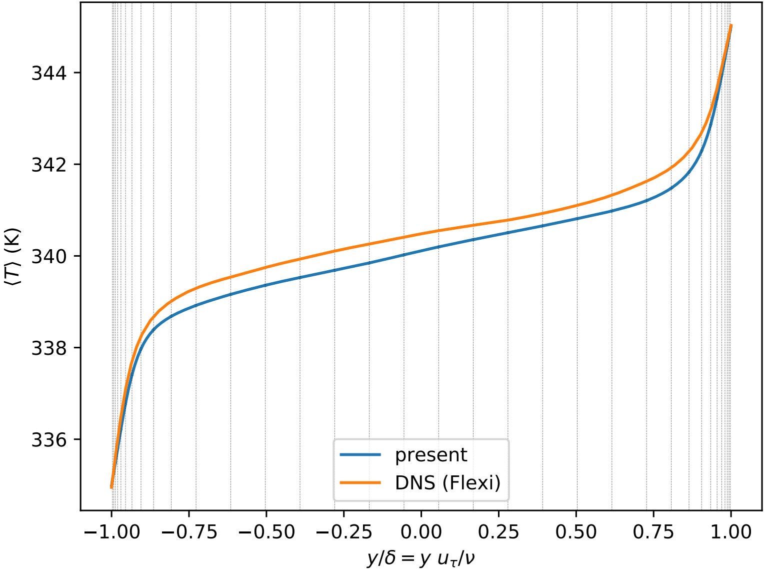
LES for sCO2 Channel Flow: Average Velocity



LES for sCO2 Channel Flow: Average Temperature



LES for sCO2 Channel Flow: Average Density



LES for sCO2 Channel Flow: How well do our results compare?

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- The difference in Mach number is probably more significant than the modeling errors and the numerical errors.

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LES is a physical model.

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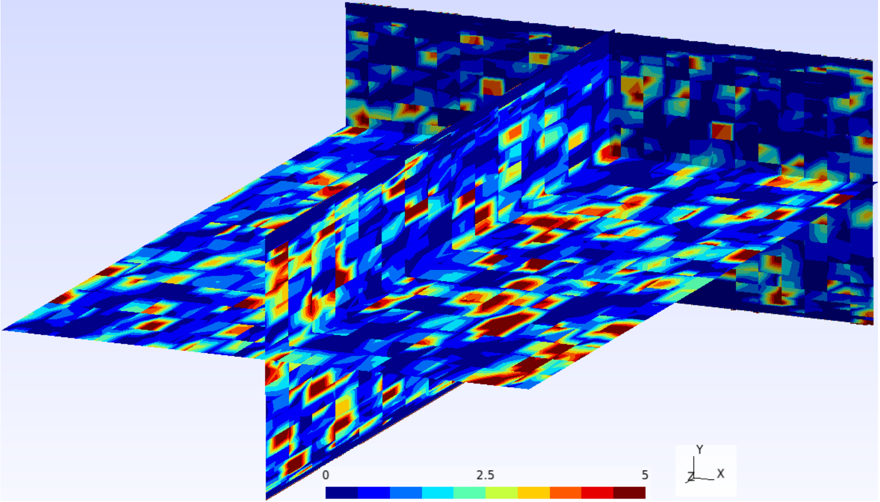
- Some models correlate much better (e.g., the self-similarity model), but often perform worse.
- Highly effective models (e.g., WALE) often have artificial motivations.
  Another example: The QR model is new, promising, and *purely* designed to stabilize the numerical method.

Comparing ν_{WALE} to ν_{Smag}

$\nu_{\text{WALE}}/\nu_{\text{Smag}}$ is totally erratic.



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1. Using a pressure-based low-Mach solver is much better than pushing a density-based compressible solver to $\mathrm{Ma} = 0.2$.
2. Large Eddy Simulation can work wonders for the computational cost, even if the underlying model is not accurate.
3. If you want 'just want results' for heat transfer in sCO2, then consider implementing a few new LES ideas into an established code.

Acknowledgements

I am grateful to

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Thank you!

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