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LARGE EDDY SIMULATION OF SCO_2 FLOW WITH A DISCONTINUOUS GALERKIN METHOD

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ABSTRACT

We present large eddy simulations (LES) of heat transfer in sCO_2 at 8 MPa in a plane channel geometry with various temperature ranges. This presents a numerical challenge, as the density can vary by more than a factor 2. We use a pressure-based solver with a high-order discontinuous Galerkin discretization. The large eddy simulation is based on the Wall-averaged Local Eddy viscosity (WALE) model and a constant turbulent Prandtl number. We resolve the flow near the wall. Though our geometry allows for a structured grid, our numerical scheme is highly flexible with respect to unstructured meshes. We validate our LES with an isothermal flow, and with a simulation in a temperature range that is far from the pseudocritical line. The results for non-isothermal flow show that the LES can accurately predict the average velocity and temperature profiles, despite reducing the number of degrees of freedom by several orders of magnitude compared to the reference direct numerical simulation. This paper is a precursor to future work, in which we will present more extensive validation of the non-isothermal test case. Our results are a first step toward using a pressure-based discontinuous Galerkin solver for sCO_2 flows.

INTRODUCTION

There is a growing interest for using supercritical CO_2 in heat exchangers, but using such an innovative approach makes it harder to predict the efficiency based on previous experiments. Numerical simulations therefore seem an obvious approach, but unfortunately there are no reliable, affordable numerical models for heat transfer in supercritical CO_2. In this paper we investigate using a Large Eddy Simulation (LES) based on a discontinuous Galerkin (DG) method to predict the heat transfer in a heated infinite plane channel flow. Using an LES model greatly reduces the required computational resources compared to a more straightforward direct numerical simulation.

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GOVERNING EQUATIONS

The governing equations for sCO_2 flow with heat transfer are

$$\frac{\partial(\rho h)}{\partial t}+\nabla\cdot(mh)=\nabla\cdot(\lambda\nabla T),$$

$$\frac{\partial m}{\partial t}+\nabla\cdot(um)=\nabla\cdot\tau-\nabla p+F,$$

$$\frac{\partial \rho}{\partial t}+\nabla\cdot m=0,$$

where t is the time, ρ is the density, u is the velocity, $m=\rho u$ is the mass flux, h is the specific enthalpy, λ is the thermal conductivity, T is the temperature, and p is the pressure. We can neglect effect of the pressure gradient on the Fourier heat flux:

$$-\lambda\nabla T\approx-\frac{\lambda}{c_p}\nabla h,$$

where c_p is the specific heat capacity [1]. The viscous stress tensor is

$$\tau=\mu\left(\nabla u+(\nabla u)^{\mathrm{T}}-\frac{2}{3}(\nabla\cdot u)I\right).$$

That is, we leave out an the bulk viscosity (or 'volume viscosity'), as in all previous literature on supercritical fluids of which we are aware. There is no no good experimental data for the bulk viscosity.

To close the system of equations, we calculate the material properties ρ, α λ, μ, and T as a function of the computed specific enthalpy, evaluating the equations of state at a fixed thermodynamic pressure. In other words, we neglect the effect of turbulent pressure fluctuations on the material properties. This approach is valid because the pressure fluctuations are several orders of magnitude smaller than the absolute pressure.

We use the open-source CoolProp library to evaluate the material properties of CO_2 [2]. The data is based on [3] for the equation of state, [4] for the thermal conductivity (λ), and [5] for the dynamic viscosity (μ). The most important alternative to CoolProp is the proprietary REFPROP software library. There can be minor differences between CoolProp and REFPROP; in particular, the values for the thermal conductivity can differ by up to 1% [6]. We do not know which is more accurate, and we have not investigated this topic further.

CoolProp is too slow to be called directly in a high-performance CFD code, so we approximate all material properties with cubic B-splines. (See, e.g., [7].) We refine the B-splines locally as follows. We start with a very coarse approximation with only a few interpolation points. This spline interpolation is refined by looping over each segment, checking whether the segment deviates too much from the actual value, and adding an extra point if necessary. This refinement procedure is repeated until the maximum relative deviation at any point is at most 10^{-4}.

NUMERICAL METHOD

This section summarizes the numerical method. We only sketch the outlines of our approach.

Numerical schemes for fluid dynamics fall roughly into two broad categories. First, there are compressible solvers, which are used extensively for simulating high-Mach number flow. These methods can deal with strong density gradients and varying material properties. The problem is that they calculate a thermodynamic pressure from an equation of state. This thermodynamic relation is highly sensitive in supercritical CO_2: small changes in the density imply large changes in the pressure, which makes stable calculations infeasible with contemporary computational resources.

The second type of numerical methods is designed for incompressible flows. They usually assume a constant density, or postulate that the density gradients are small. These assumptions do not hold for sCO_2 in a heat exchanger. We have therefore modified an incompressible solver to deal with the strongly varying density gradients.

A pressure-correction method is used to march the solution forward in time [8]. This is a type of splitting scheme, meaning that we solve the transport equations one by one at each time step. We first march h forward in time, then update ρ as a function of h, and subsequently solve for the mass flux and pressure. We do not need to iterate within a time step: each equation is solved once. This is in line with most previous literature on the simulation of supercritical fluids in periodic, non-developing domains (e.g., [1]); flow in developing domains usually does require iteration (e.g., [9] and [10]). We also monitor the errors in the pressure-correction splitting scheme by calculating the difference between the discrete pressure vectors in two consecutive time steps; their relative difference is approximately 0.01 to 0.02 in the L_2-norm.

We solve for the specific enthalpy (h), the mass flux (m) and the hydraulic pressure (p). This hydraulic pressure is only unique up to a constant; we do not compute the absolute pressure from an equation of state. The main challenges in developing the numerical scheme were connected to the strong density variations of the sCO_2, since most literature on incompressible fluids assumes a constant density. We adjusted the standard pressure-correction scheme to take the temporal derivative of the density into account.

In a discontinuous Galerkin method, the approximated quantity is modeled as a weighted sum of basis functions, each of which has support on one element in the mesh. The numerical solution is therefore generally discontinuous across element interfaces. We use a modal function set, meaning that the solution space in an element is the span of all polynomials up to a particular order. This is to be contrasted with a nodal DG method, where the function space within an element is the tensor product of one-dimensional Legendre sets. The polynomials bases for the unknowns are always of the same order.

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We use a standard symmetric interior penalty method for the Fourier heat flux in the enthalpy equation [11], which is one of several discretizations of the diffusive terms in the transport equations. We include the spatial derivative of the density into this penalty method. The penalty parameter is based on [12]. We modified this discretization so that it could also be applied to the viscous stress in the momentum equations. This is similar to what is done for hyperbolic systems in compressible flows [13]. The Cartesian components of the mass flux are coupled implicitly, that is, we solve for all directions of the mass flux in a single linear system.

The convective terms for the density, enthalpy and momentum equations are all treated with the same upwind discretization, based on the Lax-Friedrichs flux.

SUBGRID-SCALE MODEL

We use a Wall-Averaged Local Eddy viscosity (WALE) LES model for the momentum equations, which prescribes an subgrid scale viscosity of

$$\nu_{\mathrm{SGS}}=\left(C_w\Delta\right)^2\frac{|\widetilde{S}^{\mathrm{d}}|_{\mathrm{Frob}}^3}{|\widetilde{S}|_{\mathrm{Frob}}^5+|\widetilde{S}^d|_{\mathrm{Frob}}^{5/2}},$$

where Δ is the LES filter width,

$$\widetilde{S}_{ij}=\frac{1}{2}\left(\widetilde{g}_{ij}+\widetilde{g}_{ji}\right),$$

$$\widetilde{S}_{ij}^d=\frac{1}{2}\left(\widetilde{E}_{ij}+\widetilde{E}_{ji}\right)-\frac{1}{3}\widetilde{E}_{mn}\widetilde{E}_{mn}\delta_{ij},$$

$\widetilde{E}_{ij}:=\widetilde{g}_{ik}\widetilde{g}_{kj}$ and $\widetilde{g}_{ij}:=\partial\widetilde{u}_i/\partial r_j$.

Here $\widetilde{u}$ is the filtered (resolved) velocity, $r=[x,y,z]$ is the position vector, and $|.|_{\mathrm{Frob}}$ denotes the Frobenius norm of a matrix (i.e., the square root of the sum of the squares of the elements). See [14] and [15] for a motivation for this LES model.

A turbulent Prandtl number accounts for the subgrid-scale effects in the enthalpy equation. That is, the subgrid scale thermal conductivity is modeled as

$$\left(\frac{\lambda}{c_p}\right)_{SGS}=\frac{\nu_{SGS}}{Pr_{SGS}}\widetilde{\rho},$$

where $\widetilde{\rho}$ is the filtered (resolved) density. This removes small-scale structures in the enthalpy field, thereby making a numerical simulation feasible. We use a simple constant model, where $\mathrm{Pr}_{\mathrm{SGS}}$ is fixed at a constant value. It is usually chosen in the range [0.3,0.9]. (See, e.g., [16].) In our case, setting $\mathrm{Pr}_{\mathrm{SGS}}=0.7$ removes enough small-scale effects to stabilize the numerical scheme. We do not investigate the effect of using other values. We suspect that an LES is less sensitive to the turbulent Prandtl number than a RANS calculation would be, because we believe that the primary goal of a subgrid model is not to model the physics accurately, but rather to stabilize the flow without overly distorting the large-scale structures. In fact, inaccurate subgrid models can yield accurate results, and vice versa. (See, e.g., [17]). Nevertheless, investigating the effect of the turbulent Prandtl number is certainly an interesting venue for other work.

IMPLEMENTATION

We developed an in-house computational fluid dynamics (CFD) code 'DG Flows' that implements our discontinuous Galerkin method. It is written in Fortran 2003/2008, and has been in development since late 2015. It has also been used to model the flow and heat transfer of molten salt, and to investigate experimental large-eddy simulation techniques.

We use the MPI-based PETSc software library to solve the linear systems that arise from the discretizations [18]. In particular, we use a conjugate gradient method with an incomplete Cholesky preconditioner for the pressure equation, and a GMRES method with an incomplete LU preconditioner for the enthalpy and momentum equations. The linear systems are solved up to a certain tolerance r_{tol}, meaning that the norms of the preconditioned residuals are at most r times the norm of the right-hand-side vector. We set $r_{tol}=10^{-6}$ for the enthalpy, the pressure, and the momentum equations.

To parallelize the calculation, the mesh is partitioned with the METIS software library, which is based on a multilevel recursive-bisection, multilevel k-way, and multi-constraint partitioning scheme [19]. We use a simple block-Jacobi scheme to distribute the linear solver over the processes.

RESULTS FOR PLANE CHANNEL FLOW

We test the numerical method and the LES model in a plane channel geometry. We show (i) an isothermal test case, (ii) a simulation with heat transfer at a temperature far from the critical point, and (iii) a simulation with heat transfer close to the pseudocritical point. In each case, the domain is $\Omega=[0,(4/3)\pi\delta]\times[-\delta,\delta]\times[0,2\pi\delta]$, where δ is the channel half-width. We impose no-slip boundary conditions at $y=\pm\delta$, and periodic boundary conditions in the *x*- and *z*-directions. The flow is in the *z*-direction. We add the constraint $\int_\Omega p\,\mathrm{d}r=0$ to ensure that the pressure is uniquely defined. We keep the body force in the flow direction (F_3) constant, so that the time-averaged wall shear stress ($\langle\tau_w\rangle=F_3\delta$) is known a priori. The friction velocity is $u_\tau=\sqrt{\langle\tau_w\rangle/\rho}$ and the Reynolds stress is $\mathrm{Re}_\tau=\delta u_\tau/\nu$. We average the quantities of interest over time and in the x- and z-directions.

Isothermal Channel Flow

For the isothermal case we let $\mathrm{Re}_\tau=180$, so that the results can be compared to the DNS data from [20], which was performed at $\mathrm{Re}_\tau=178.13$. We use a second-order polynomial basis in the boundary elements, and gradually increase this to a fourth-order polynomial basis for elements in the bulk. We used 0.41M degrees of freedom per direction of the mass flux, whereas [20] used 4.0M. Figure 1 shows that the LES overpredicts the velocity by approximately 5%. Note that the bulk velocity is approximately proportional to Re_τ.

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Channel Flow with sCO_2 far from Pseudocritical Point

The second test case is a heated plane channel flow with supercritical CO_2. We aim to reproduce the DNS data from [21], which was obtained with a compressible, DG-based solver at a Mach number of 0.2. They found that the turbulent pressure fluctuations are small at this Mach number, which justifies a comparison with our simulation with a low-Mach approximation, though there is of course a discrepancy in the material properties, which do not depend on the pressure in our simulation. The thermodynamic pressure is 8.0 MPa, and temperatures at the boundaries are fixed at $T=335\,\mathrm{K}$ at $y=-\delta$, and $T=345\,\mathrm{K}$ at $y=\delta$. This temperature range is far from the pseudocritical point. The bulk Reynolds number is defined as $\mathrm{Re}_{\mathrm{bulk}}=u_{\mathrm{bulk}}\,\delta/\,\nu_{\mathrm{ref}}$, where u_{bulk} is the bulk velocity, and ν_{ref} is the kinematic viscosity at the thermodynamic reference point of (8.0Mpa, 340 K). In [21] the body force is dynamically adjusted to keep the bulk Reynolds number constant at 2800 throughout the simulation.

Since we do not know a priori what body force will result in the desired bulk Reynolds number, we estimate the Darcy friction factor (c_f) with the Colebrook-White relation for smooth pipes:

$$\frac{1}{\sqrt{c_f}}=-2\log_{10}\left(\frac{2.51}{\mathrm{Re}_{\mathrm{hydr}}\sqrt{c_f}}\right),$$

where $\mathrm{Re}_{\mathrm{hydr}}$ is the Reynolds number based on the hydraulic diameter. This gives an estimate $c_f\approx 0.0300$, which is used in the Darcy-Weisbach equation to estimate the required volumetric force in the flow direction:

$$F_3=c_f\frac{\rho}{2}\frac{u_{\mathrm{bulk}}^2}{D_{\mathrm{hydr}}},$$

where we evaluate the density at the thermodynamic reference point. The bulk Reynolds number was then checked *a posteriori*, showing that the body force needed to be increased by approximately 1% to achieve the desired bulk Reynolds number.

Figures 2, 3, and 4 compare the LES results with the DNS data in [21]. Figures 3 and 4 show a slight discrepancy in the thermodynamic properties, but this can be explained by the fact that we use a constant thermodynamic pressure to evaluate the density and temperature, that is, we do not take the effect of the pressure on T and ρ into account. Note that the error in the density at the boundaries is solely due to the low-Mach approximation, because our density is fixed by the boundary conditions for the temperature, whereas the density in the reference data can fluctuate with a varying pressure. Figure 4 shows a deviation of approximately 0.2% in density at the boundaries, which gives an indication of the error inherent in the low-Mach approximation. The error in the average density profile is not more than 0.2% anywhere else in the domain. Figure 2 shows that our LES predicts a slightly higher velocity near the hot wall, where the density is lower. The velocity profile in the compressible DNS simulation is less asymmetrical. Nevertheless, the DNS data and the LES for the average velocity profile differ by only 3%, despite the fact that we use only 0.46M degrees of freedom, whereas [21] used 198M.

Channel Flow with sCO_2 That Includes the Pseudocritical Line

We also perform an LES of a heated channel flow in a temperature range that is close to the pseudocritical point. The thermodynamic pressure is 8 MPa, and the boundary conditions for the temperature are $T=311\,\mathrm{K}$ at $y=-\delta$, and $T=305\,\mathrm{K}$ at $y=+\delta$. Note that the thermal expansion ratio at this pressure is highest at $T=308\,\mathrm{K}$, so that the temperature range includes the pseudocritical line, and the material properties vary strongly. We use a constant body force F, such that $\mathrm{Re}_{\tau}=180$ on average over the two boundaries. Unfortunately we do not have reference data with which to validate our results for this test case.

Figure 6 shows the average temperature profile. Compared to the simulation far from the pseudocritical point (Figure 3), the temperature is more homogeneous in the bulk of the fluid, indicating a better mixing, though the Reynolds number is the approximately same. Figure 7 shows that the density differs by more than a factor of between the two planes, which explains the strongly skewed velocity profile in Figure 5.

CONCLUSION

The results indicate that a large eddy simulation with a discontinuous Galerkin method can simulate turbulent flow of sCO_2 with heat transfer. This is achieved with far fewer degrees of freedom than a direct numerical simulation (DNS) would require, which opens the door to investigating the flows at moderate Reynolds numbers in engineering applications where DNS is still unattainable.

In future work we plan to validate our results for flow near the pseudocritical point. We will also investigate the efficacy of various LES models for heat transfer in supercritical fluids. In particular, it is not clear whether using a constant turbulent Prandtl number can accurately predict heat transfer deterioration. We also do not know how accurate the LES predictions are when a gravity force is included in the simulation.

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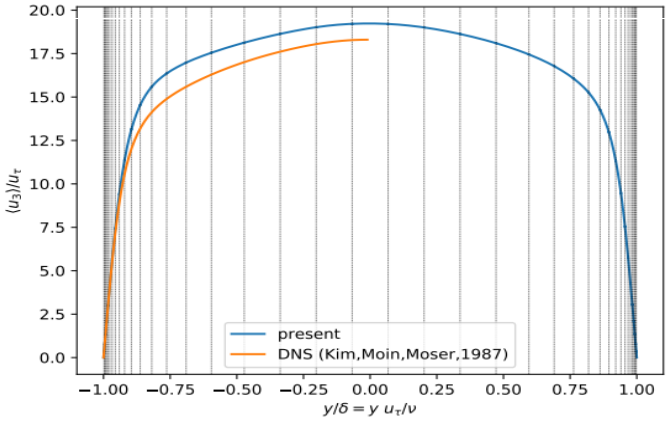

Figure 1: Average velocity profiles for the current LES and the DNS data from [20]. The gray vertical lines indicate the boundaries of the elements.

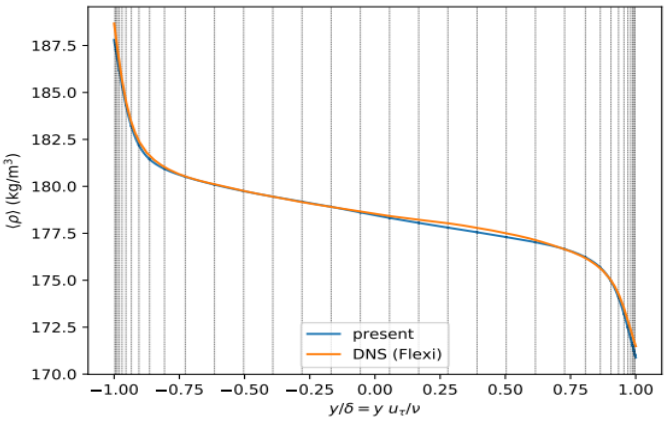

Figure 4: Average density profiles for the current LES and the DNS data from [21]. The gray vertical lines indicate the boundaries of the elements.

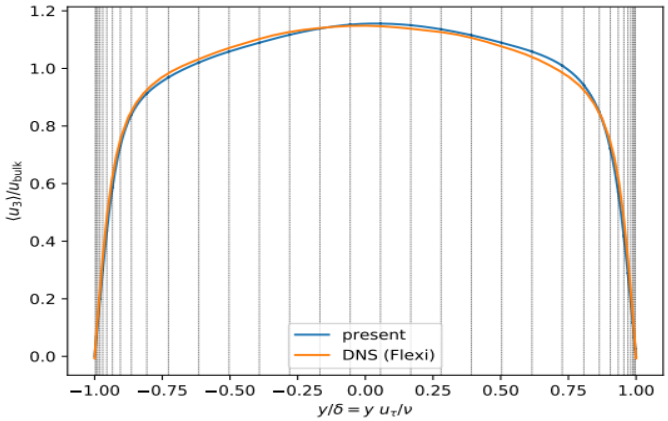

Figure 2: Average velocity profiles for the current LES and the DNS data from [21]. The gray vertical lines indicate the boundaries of the elements.

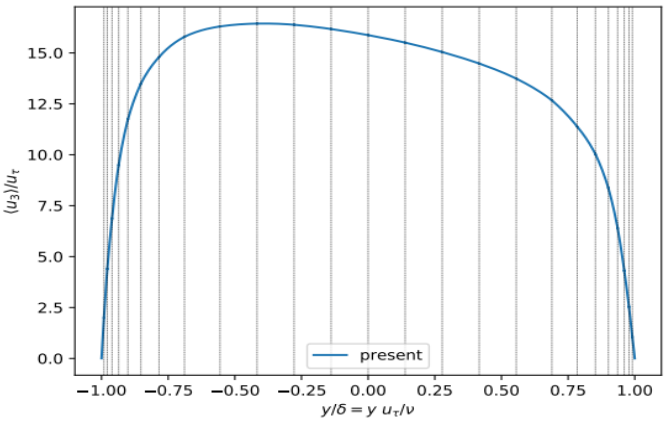

Figure 5: Average velocity profile for the LES near the pseudocritical point. The gray vertical lines indicate the boundaries of the elements.

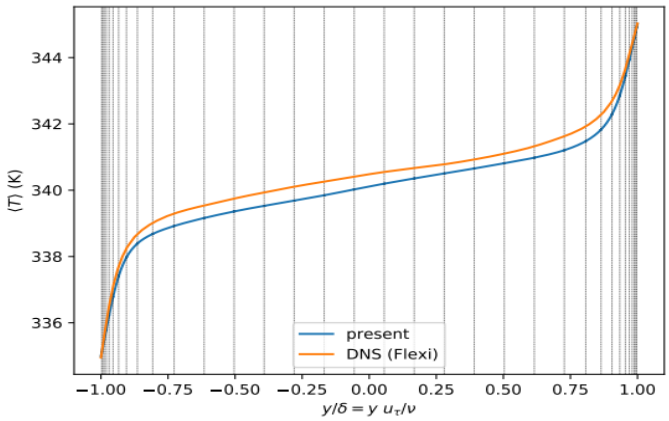

Figure 3: Average temperature profiles for the current LES and the DNS data from [21]. The gray vertical lines indicate the boundaries of the elements.

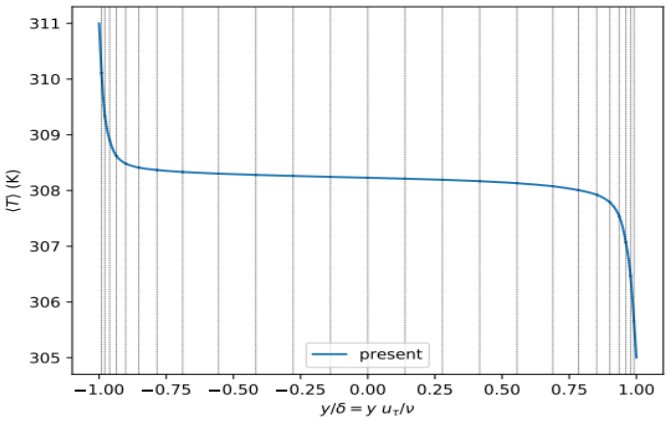

Figure 6: Average temperature profile for the LES near the pseudocritical point. The gray vertical lines indicate the boundaries of the elements.

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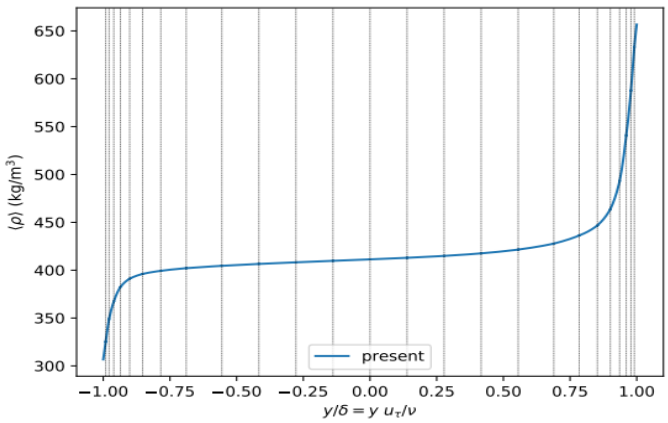

Figure 7: Average density profile for the LES near the pseudocritical point. The gray vertical lines indicate the boundaries of the elements.

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