NON-DISSIPATIVE LARGE-EDDY SIMULATION OF HIGH-PRESSURE TRANSCRITICAL TURBULENT FLOWS: FORMULATION AND A PRIORI ANALYSIS

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Abstract

This work presents a filtered set of equations suitable for the large-eddy simulation of high-pressure transcritical turbulent flows. The formulation is derived from a novel kinetic-energy- and pressure-equilibrium-preserving numerical framework, recently proposed to provide physics-compatible (stable and non-dissipative) simulations of the problem. In particular, the compressible Navier-Stokes equations are required to describe the evolution of supercritical fluids along with adequate real-gas thermodynamic closures based, for example, on the Peng-Robinson equation of state. The novelty of this work focuses, therefore, on (i) deriving the filtered set of equations based on the kinetic-energy and pressure-equilibrium-preserving framework, (ii) identifying the sub-filtered unclosed terms, and (iii) performing exploratory assessments of the resulting framework. In the future, these results will potentially enable the design of physics-based sub-filter scale models for high-fidelity LES of high-pressure transcritical turbulent flows.

1 Introduction

The study of complex turbulent flows by means of large-eddy simulation (LES) approaches has become increasingly popular in many scientific and engineering applications. The underlying filtering operation of the approach enables to significantly reduce the spatio-temporal resolution requirements with respect to direct numerical simulation (DNS) by means of representing only large-scale motions. However, the small-scale stresses and their effects on the resolved flow field are not negligible, and therefore require supplementary modeling (Jofre et al 2019). This is especially challenging in the case of high-pressure transcritical flows due to the additional hydrodynamic scales arising from the large localized thermophysical variations across the pseudo-boiling region, which further complicates the modeling of the subfilter-scale (SFS) terms arising from the filtered equations of motion.

Only a limited number of studies have focused on LES modeling for trans/superecritical thermodynamic conditions. Selle and Ribert (2008) performed *a priori* and *a posteriori* analysis of closure models for homogeneous isotropic turbulence and jets under various thermodynamic regimes. While *a priori* analyses were encouraging, *a posteriori* studies provided poor results. Borghesi and Bellan (2015) performed a similar analysis for multi-species high-pressure turbulent mixing, and highlighted the need for dedicated LES models. Recently, Unnikrishnan et al (2022) have quantified the impact of SFS modeling on the filtered equation of state (EOS) for supercritical turbulent mixing. It is clear that more efforts are needed towards a complete and reliable LES formulation for trans/supercritical turbulent flows.

A physically-relevant LES also requires a non-dissipative underlying discretization, so that the sub-filter scale dissipation is entirely provided by the corresponding model. This can be achieved by kinetic-energy preserving (KEP) formulations in conjunction with summation-by-parts operators (Coppola et al 2019). In the case of high-pressure transcritical flows, it is also of fundamental importance to discretely mimic the property of pressure-equilibrium preservation (PEP), in order to avoid spurious pressure oscillations at the pseudo-interface. Recently, a novel method has been developed by Bernades et al (2023), where the PEP property is achieved by solving a pressure evolution equation, and the continuity and momentum equations are expanded according to a KEP splitting. The resulting method is stable without any numerical diffusion or stabilization procedure.

Given the novelty of the above-mentioned numerical formulation, in addition to the inherent challenges associated with transcritical LES, an *a priori* analysis of the pressure-based formulation is highly warranted to understand the relative importance of each of the unclosed terms, with the ultimate objective of deriving physics-based subfilter-scale models. Therefore, this work aims to (i) develop a filtered set of equations suitable for LES based on the novel numerical formulation, and (ii) characterize the properties of the resulting SFS terms by means of performing *a priori* analyses of transcritical wall-bounded turbulence from DNS data (Bernades et al 2023).

In this regard, the paper is organized as follows. First, in Section 2, the flow physics modeling and discretization framework of high-pressure transcritical turbulence is presented. Then, the LES formulation is described in Section 3, introducing the filtering approach, defining the filtered equations of motion, with the resulting subfilter-scale terms. Section 4 presents the filter selection applied on the DNS for *a priori* analysis. Finally, Section 4 reports concluding remarks and future directions.

2 Flow physics modeling

The turbulent flow motion of supercritical fluids is described by the following set of transport equations of mass, momentum and pressure (see Bernades et al (2023) for details)

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \tag{1}$$

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) = -\nabla P + \nabla \cdot \boldsymbol{\sigma}, \tag{2}$$

$$\frac{\partial P}{\partial t} + \mathbf{u} \cdot \nabla P + \rho c^2 \nabla \cdot \mathbf{u} = \tag{3}$$
$$= \frac{1}{\rho} \frac{\beta_v}{c_v \beta_T} (\boldsymbol{\sigma} : \nabla \otimes \mathbf{u} - \nabla \cdot \boldsymbol{q}),$$

where ρ is the density, $\mathbf{u}$ is the velocity vector, P is the pressure, $\boldsymbol{\sigma} = \mu \left(\nabla \mathbf{u} + \nabla \mathbf{u}^T \right) - (2\mu/3)(\nabla \cdot \mathbf{u}) \boldsymbol{I}$ is the viscous stress tensor with μ the dynamic viscosity and $\boldsymbol{I}$ the identity matrix, $c = 1/\sqrt{\rho \beta_s}$ is the speed of sound with $\beta_s = -(1/v) \left(\partial v / \partial P \right)_s$ the isentropic compressibility and $v = 1/\rho$ the specific volume, $\beta_v = (1/v) \left(\partial v / \partial T \right)_P$ is the volume expansivity with T the temperature, c_v is the isochoric specific heat capacity, $\beta_T = -(1/v) \left(\partial v / \partial P \right)_T$ is the isothermal compressibility, and $\boldsymbol{q} = -\kappa \nabla T$ is the Fourier heat conduction flux, with κ the thermal conductivity.

Real-gas thermodynamics

The thermodynamic space of solutions for the state variables pressure P, temperature T, and density ρ of a single substance is described by an equation of state. One popular choice for systems at high pressures is the Peng-Robinson equation of state, written as

$$P = \frac{R_u T}{(W/\rho) - b} - \frac{a}{(W/\rho)^2 + 2b(W/\rho) - b^2}, \tag{4}$$

where R_u is the universal gas constant and W is the molecular weight. The coefficients a and b take into account real-gas effects related to attractive forces and finite packing volume, respectively, and depend on the critical temperatures T_c, critical pressures P_c, and acentric factors ω. They are defined as

$$a = 0.457 \frac{(\mathrm{R_u} T_c)^2}{P_c} \left[1 + c \left(1 - \sqrt{T/T_c} \right) \right]^2, \tag{5}$$

$$b = 0.078 \frac{\mathrm{R_u} T_c}{P_c}, \tag{6}$$

where coefficient c is provided by

$$c = \begin{cases} 0.380 + 1.485\omega - 0.164\omega^2 + 0.017\omega^3 & \\ & \text{if } \omega > 0.49, \\ 0.375 + 1.542\omega - 0.270\omega^2 & \text{otherwise.} \end{cases}$$

This EOS needs to be supplemented with the corresponding high-pressure thermodynamic variables based on departure functions calculated as a difference between two states. In particular, their usefulness is to transform thermodynamic variables from ideal-gas conditions (low pressure only temperature dependent) to supercritical conditions (high pressure). The ideal-gas parts are calculated by means of the NASA 7-coefficient polynomial, while the analytical departure expressions to high pressures are derived from the Peng-Robinson equation of state.

High-pressure transport coefficients

The high pressures involved in the analyses conducted in this work prevent the use of simple relations for the calculation of the dynamic viscosity μ and thermal conductivity κ. In this regard, standard methods for computing these coefficients for Newtonian fluids are based on the correlation expressions mainly function of critical temperature T_c and density ρ_c, molecular weight W, acentric factor ω, association factor κ_a and dipole moment $\mathcal{M}$, and the NASA 7-coefficient polynomial; further details can be found in dedicated works like the one by Jofre & Urzay (2021).

Numerical method

Simulations of high-pressure transcritical turbulence are strongly susceptible to numerical instabilities due to the presence of nonlinear thermodynamic phenomena and large density gradients, which can trigger spurious pressure oscillations that may contaminate the solution and even lead to its divergence. Consequently, it is highly beneficial that the numerical schemes utilized, in addition to being KEP, attain the so-called PEP property (Bernades et al 2023b). The numerical scheme utilized in this work has been developed specifically to be simultaneously KEP and PEP. The latter property is achieved by solving a pressure evolution equation. A thorough description and validation of this method can be found in Bernades et al (2022, 2023b).

In brief, the transport equations are numerically solved by adopting a standard semi-discretization procedure; viz. they are first discretized in space and then integrated in time. In particular, spatial operators are treated using second-order central-differencing schemes, and time-advancement is performed by means of a third-order strong-stability preserving (SSP) Runge-Kutta explicit approach. The convective terms are expanded according to the Kennedy-Gruber-Pirozzoli (KGP) splitting, which has been recently assessed for high-pressure supercritical fluids turbulence (Bernades et al 2022). As a result, the method utilized (i) preserves kinetic energy by convection, (ii) is locally conservative for mass and momentum, (iii) preserves pressure equilibrium and (iv) yields stable and robust numerical simulations without adding any numerical diffusion to the solution or stabilization procedures.

3 Large-eddy simulation framework

This section presents (i) the filtering approach and (ii) the filtered equations of fluid motion, whose SFS and unclosed terms are identified.

The filtering approach

In the classical LES formalism, any flow variable f is decomposed into a large-scale contribution $\overline{f}$ and a small-scale contribution $f^{'}$, i.e., $f = \overline{f} + f^{'}$. The filtered part $\overline{f}$ is defined as follows

$$\overline{f}(x) = \int_{\Omega} G(x,\xi) f(\xi) d\xi, \tag{7}$$

where $\mathbf{x}$ and ξ are vectors in the flow domain Ω. The filter kernel G depends on the parameter Δ called the filter width, which satisfies the condition

$$\int_{\Omega} G(x,\xi) d\xi, = 1 \tag{8}$$

for every x and Ω. For compressible flows, Favre (1983) introduced a related filter operation

$$\widetilde{f} = \frac{\overline{\rho f}}{\overline{\rho}}, \tag{9}$$

which leads to the decomposition $f = \widetilde{f} + f^{''}$.

Typical filters commonly used in large-eddy simulation correspond to the top-hat (also referred to as spatial or box filter), Gaussian and spectral cut-off filters (Vreman et al 1994). The symbol $\bar{\Delta}_i$ denotes the filter width in the i-direction, whereas $\bar{\Delta}$ is defined as

$$\bar{\Delta} = \left(\bar{\Delta}_1 \bar{\Delta}_2 \bar{\Delta}_3\right)^{1/3}. \tag{10}$$

Filtered equations of fluid motion

LES formulations based on a real-gas EOS are inherently non-trivial due to the non-linearity of the thermodynamic relations at play. In this work, inspired by recent efforts (Unnikrishnan et al 2022) and based on the proposed novel scheme by Bernades et al (2023b), the LES equations are carefully derived based on the classical low-pass filtering formalism. Interestingly, previously unknown terms arise from the analysis, which will require specific modeling efforts. In this regard, it is also worth to emphasize that transcritical turbulent wall-bounded flow physics profoundly differs from that observed in subcritical cases, most notably due to the presence of a strong baroclinic instability and, as a consequence, to the failure of standard scaling transformations for the velocity at the wall.

The LES equations are written for the transported variable vector $\boldsymbol{\Psi} = [\rho, \rho\mathbf{u}, P]$, which in terms of Favre-averaging is written as $\overline{\boldsymbol{\Psi}} = \left[\overline{\rho}, \overline{\rho}\widetilde{\mathbf{u}}, \overline{P}\right]$. Assuming that differentiation and filtering commute, the LES equations describing the motion of supercritical fluid turbulence correspond to the following set of low-pass filtered equations

$$\frac{\partial \overline{\rho}}{\partial t} + \nabla \cdot (\overline{\rho}\widetilde{\mathbf{u}}) = 0, \tag{11}$$

$$\frac{\partial (\overline{\rho}\widetilde{\mathbf{u}})}{\partial t} + \nabla \cdot (\overline{\rho}\widetilde{\mathbf{u}}\widetilde{\mathbf{u}}) + \nabla \overline{P} - \nabla \cdot \breve{\boldsymbol{\sigma}} = -\alpha_1 + \alpha_2, \tag{12}$$

$$\frac{\partial \overline{P}}{\partial t} + \widetilde{\mathbf{u}} \cdot \nabla \overline{P} + \overline{\rho}\breve{c}^2 \nabla \cdot \widetilde{\mathbf{u}} - \frac{1}{\overline{\rho}} \frac{\breve{\beta}_v}{\breve{c}_v \breve{\beta}_T} (\breve{\boldsymbol{\sigma}} : \nabla \otimes \widetilde{\mathbf{u}} - \nabla \cdot \breve{\boldsymbol{q}}) = \alpha_3 + \alpha_4 + \alpha_5, \tag{13}$$

where $\overline{\rho}$ and $\overline{P}$ are the filtered density and pressure variables, respectively, and $\widetilde{\mathbf{u}}$ corresponds to the Favre-filtered velocity vector. Equations (11)-(13) are presented such that the left-hand sides correspond to the governing equations, Eqs. (1)-(3), expressed with filtered variables $\overline{\boldsymbol{\Psi}}$. Instead, the right-hand sides contain the so-called subfilter-terms, which represent the effect of the unresolved scales (Vreman 1995) and cannot be expressed by the filtered flow variables.

In detail, the α_i terms in the equations above correspond to the following expressions

$$\alpha_1 = \nabla \cdot \overline{\rho}\boldsymbol{\tau}, \tag{14a}$$

$$\alpha_2 = \nabla \cdot (\overline{\boldsymbol{\sigma}} - \breve{\boldsymbol{\sigma}}), \tag{14b}$$

$$\alpha_3 = (\widetilde{\mathbf{u}} \nabla \cdot \overline{P} - \overline{\mathbf{u} \nabla \cdot P}), \tag{14c}$$

$$\alpha_4 = (\overline{\rho}\breve{c}^2 \nabla \cdot \widetilde{\mathbf{u}} - \overline{\rho c^2 \nabla \cdot \mathbf{u}}), \tag{14d}$$

$$\alpha_5 = [\overline{\frac{1}{\rho} \frac{\beta_v}{c_v \beta_T} (\boldsymbol{\sigma} : \nabla \otimes \mathbf{u} - \nabla \cdot \boldsymbol{q})} - \frac{1}{\overline{\rho}} \frac{\breve{\beta}_v}{\breve{c}_v \breve{\beta}_T} (\breve{\boldsymbol{\sigma}} : \nabla \otimes \widetilde{\mathbf{u}} - \nabla \cdot \breve{\boldsymbol{q}})], \tag{14e}$$

where the variables denoted by $\breve{\cdot}$ mean that the functional form of the DNS term remains, but these variables are calculated from $\overline{\boldsymbol{\Psi}}$ instead of $\boldsymbol{\Psi}$ (Selle & Ribert 2008).

Mass equation. By definition, the Favre-averaged mass equation, Eq. (11), does not generate any SFS term as the filtered product $\rho\mathbf{u}$ is equivalent to $\overline{\rho}\widetilde{\mathbf{u}}$.

Momentum equation. The filtered momentum equation, Eq. (12) generates two unclosed terms. First, the α_1 SFS from the non-linear convective term, referred to as turbulent stress tensor, which is written as

$$\overline{\rho}\boldsymbol{\tau} = \overline{\rho}\left(\widetilde{\mathbf{u}\mathbf{u}} - \widetilde{\mathbf{u}}\widetilde{\mathbf{u}}\right), \tag{15}$$

and corresponds to the interaction between subfilter and large scales, and consequently its closure requires modeling.

Second, the resulting subfilter-term from the viscous stress tensor α_2 results from the nonlinearity of the viscous term and the fact that the Favre filter and partial derivatives do not commute, which is typically neglected in high-Reynolds-number flows at low-pressure conditions. In fact, *a priori* tests confirm that it is an order of magnitude smaller than the first term

(Vreman 1995), where $\breve{\boldsymbol{\sigma}} = f(\widetilde{\mathbf{u}}, \breve{T})$. Nevertheless, due to the strong non-linearities arisen in transcritical regimes in the vicinity of the pseudoboiling line, this term cannot be neglected and needs to be closed (Borghesi et al 2015) with $\overline{\boldsymbol{\sigma}} = \overline{f(\mathbf{u}, T)}$.

Pressure equation. The filtered pressure equation has been previously analyzed by Zang et al (1992) in an ideal-gas framework. In this case, the resulting subfilter-terms are:

- α_3 is the pressure-velocity subfilter-term representing the effect of sub-filter turbulence on the conduction of heat at the resolved scales;
- α_4 represents the pressure-dilatation due to compressibility effects, which vanishes if the flow is divergence-free with constant density. In this case, $\breve{c} = f(\overline{\rho}, \overline{P})$;
- α_5 contains the sub-filter terms associated with the viscous, Fourier $\breve{\boldsymbol{q}} = f(\overline{\rho}, \breve{T})$ and thermophysical quantities, where $\breve{\beta_v} = f(\overline{\rho}, \overline{P})$, $\breve{\beta_T} = f(\overline{\rho}, \overline{P})$ and $\breve{c_v} = f(\overline{\rho}, \overline{P}, \breve{T})$. Unlike total energy-based formulations, the traditional subfilter fluxes, such as the Fourier tensor (Zang et al 1992) $\overline{\rho}\boldsymbol{Q} = \overline{\rho}\left(\widetilde{\mathbf{u}T} - \widetilde{\mathbf{u}}\widetilde{T}\right)$, do not appear in the pressure equation.

Equation of state. The Peng-Robinson equation of state relates the thermodynamic variables, i.e., $P = P(\rho, T)$. Hence, the filtered equation reads

$$\overline{P} = \overline{P(\rho, T)} = \\ = \overline{\frac{R_u T}{(W/\rho) - b} - \frac{a}{(W/\rho)^2 + 2b(W/\rho) - b^2}}. \quad (16)$$

Analogously to the filtered conservation equations, the EoS needs to be rearranged based on known filtered variables, i.e., $P(\overline{\rho}, \breve{T})$, as follows

$$\overline{P} = P(\overline{\rho}, \breve{T}) + \alpha_6, \quad (17)$$

where in this case temperature $\breve{T} = f(\overline{P}, \overline{\rho})$ is expressed as a function of filtered density and pressure from transported variables $\boldsymbol{\Psi}$, with the filtered coefficient related to attractive forces defined as $\breve{a} = f(\breve{T})$. As a result, Eq. (17) generates an additional unclosed term α_6, which can be expressed as

$$\alpha_6 = \overline{P(\rho, T)} - P(\overline{\rho}, \breve{T}). \quad (18)$$

4 A priori analysis

The *a priori* analyses are based on the DNS of transcritical channel flow computed by Bernades et al (2023). The system operates with N_2 at a supercritical bulk pressure of $P_b/P_c = 2$ and confined between bottom (bw) and top (tw) isothermal walls, separated in this case at a distance $H = 2\delta$ with $\delta = 100\,\mu$m the channel half-height, at $T_{bw}/T_c = 0.75$ and $T_{tw}/T_c = 1.5$, respectively. This configuration forces the fluid to undergo a transcritical trajectory by operating within a thermodynamic region across the pseudoboiling line. The friction Reynolds number selected at the bottom wall is $\mathrm{Re}_{\tau,bw} = \rho_{bw} u_{\tau,bw} \delta / \mu_{bw} = 100$ to ensure fully-developed turbulent flow conditions. The corresponding dimensional parameters are: dynamic viscosity $\mu_{bw} = 1.6 \cdot 10^{-4}\,\mathrm{Pa} \cdot \mathrm{s}$, density $\rho_{bw} = 839.4\,\mathrm{kg/m^3}$, and friction velocity $u_{\tau,bw} = 1.9 \cdot 10^{-1}\,\mathrm{m/s}$. The computational domain is $4\pi\delta \times 2\delta \times 4/3\pi\delta$ in the streamwise (x), wall-normal (y), and spanwise (z) directions, respectively. The grid is uniform in the streamwise and spanwise directions with resolutions in wall units (based on bw values) equal to $\Delta x^+ = 9.8$ and $\Delta z^+ = 3.3$, and stretched toward the walls in the vertical direction with the first grid point at $y^+ = y u_{\tau,bw}/\nu_{bw} = 0.1$ and with sizes in the range $0.4 \leq \Delta y^+ \leq 2.3$. Thus, this arrangement corresponds to a grid size of $128 \times 128 \times 128$ points. Based on the estimates provided by Jofre and Urzay (2021), the characteristic length scale for density gradients in this case is approximately $10\times$ larger than the Kolmogorov scale, therefore the latter is the driving factor to select mesh resolution. The selected grid size is thus assumed to resolve all the relevant flow scales. The simulation strategy starts from a linear velocity profile with random fluctuations, which is advanced in time to reach turbulent steady-state conditions after approximately five flow-through-time (FTT) units; based on the bulk velocity u_b and the length of the channel $L_x = 4\pi\delta$, a FTT is defined as $t_b = L_x/u_b \sim \delta/u_\tau$. In this regard, flow statistics are collected for roughly 10 FTTs once steady-state conditions are achieved.

Based on this dataset, several filter widths have been assessed based on the top-hat filter, which is typically used within high-pressure frameworks (Selle & Ribert, 2008 and Borghesi & Bellan, 2015). The cutoff is defined to attain a significantly large part of the small scales, i.e., at least 80% of turbulent kinetic energy (TKE) is defined in this case. As a result, $\bar{\Delta}/\Delta = 2$ is the largest filter width to accomplish these requirements. Based on Sagaut & Grohens (1999), the top-hat filter differential operator can be expressed as a function of a Taylor series as

$$\overline{\theta} = \theta + \frac{\bar{\Delta}^2}{24}\nabla^2\theta + \frac{\bar{\Delta}^4}{1920}\nabla^4\theta + \mathcal{O}(\Delta^6), \quad (19)$$

where θ is a random variable and $\overline{\theta}$ is the filtered variable. To this extent, Figure 1 depicts the normalized turbulent kinetic energy (TKE) at different filter widths and for different values of y^+ away from the viscous region. It is observed that the TKE slowly increases at a filter width above $\bar{\Delta}/\Delta = 4$. This phenomenon appears to be linked to the spatial order of the explicit filter utilized.

Second, before tackling the problem from a modeling standpoint, DNS results are compared with a filtered DNS. In this regard, Figure 2 shows the contours of u^+ for DNS case and with filtered DNS at $\bar{\Delta}/\Delta = 2$. The loss of resolution on the small scales of the flow can be clearly seen, which becomes more pronounced for larger filter widths.

5 Conclusions

This work has proposed a large-eddy simulation framework suitable to high-pressure transcritical fluid turbulence derived from a novel physics-compatible formulation, which is kinetic-energy- and pressure-equilibrium-preserving. The equations have been developed based on a low-pass filtering formalism, and the corresponding unclosed terms have been identified and their expressions described.

In particular, the mathematical framework derived has identified six unclosed terms: (i) two arising from the momentum conservation equation, (ii) three from the pressure transport equation, and (iii) one from the EoS. In this regard, with the objective of initially assessing the importance of the unclosed terms identified, an exploratory *a priori* analysis has been performed by filtering DNS data from a high-pressure transcritical channel flow with a filter width of $\bar{\Delta}/\Delta = 2$ to ensure that approximately 80% of turbulent kinetic energy is captured.

Ongoing work is, therefore, focused on quantifying the relative importance of the unclosed terms as a function of filter width. Moreover, to gain further insight into the structure of the unclosed stress tensor in terms of magnitude, shape and orientation, it will be carefully analyzed by leveraging the methodology developed by Jofre et al 2019. These results will be additionally compared against the structure provided by classical existing models, such as the constant-coefficient Smagorinsky, the scale-similarity approach, and the more recent minimum-dissipation strategies (Rozema et al 2015).

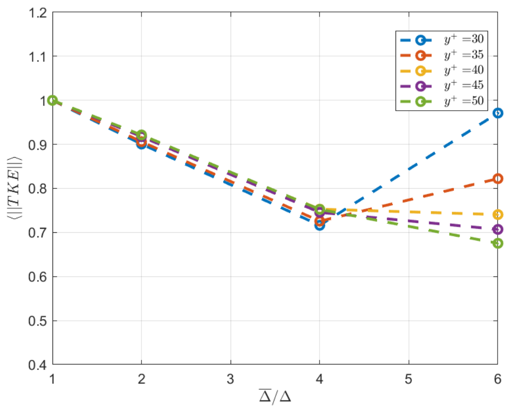

Figure 1: Normalized turbulent kinetic energy vs. filter width $\bar{\Delta}/\Delta$ at different y^+ levels (bottom/cold wall).

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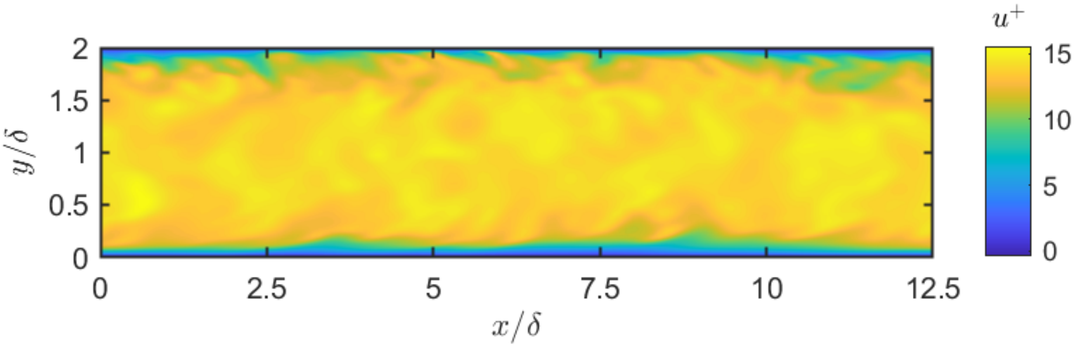
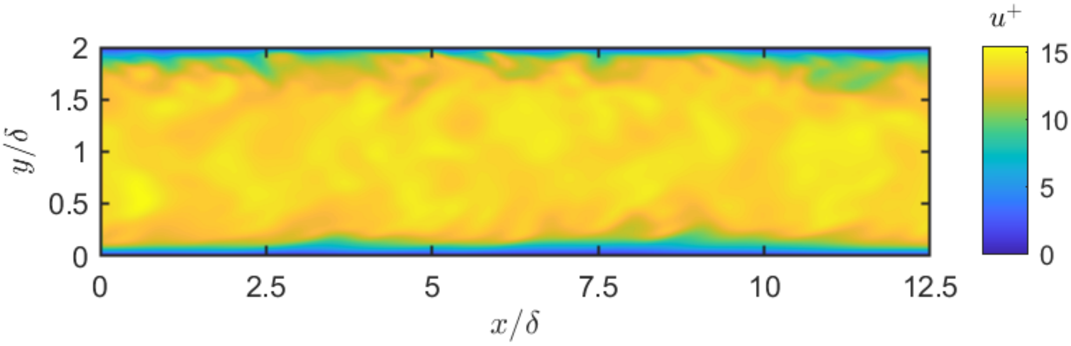


(a)



(b)

Figure 2: Snapshot of instantaneous streamwise velocity in wall units u^+ on a x-y slice for (a) DNS and (b) filtered DNS with top-hat filter with $\bar{\Delta}/\Delta = 2$.

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