Approximate Deconvolution Reduced Order Modeling

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Abstract

This paper proposes a large eddy simulation reduced order model (LES-ROM) framework for the numerical simulation of convection-dominated flows. In this LES-ROM framework, the proper orthogonal decomposition (POD) is used to define the ROM basis and a ROM differential filter is used to define the large ROM structures. An approximate deconvolution (AD) approach is used to solve the ROM closure problem and develop a new AD-ROM. This AD-ROM is tested in the numerical simulation of the three-dimensional flow past a circular cylinder at a Reynolds number $Re = 1000$.

Keywords: Reduced order model, proper orthogonal decomposition, large eddy simulation, approximate deconvolution, spatial filter.

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1. Introduction

Reduced order models (ROMs) are an efficient approach to the numerical simulation of fluid flow, since they can reduce the computational time of a direct numerical simulation (DNS) by orders of magnitude while preserving key features of the flow. ROMs have been successfully used in numerous applications, such as fluid flow optimization and control, cardiovascular flows,

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7 or geophysical flows (see, e.g., the surveys in [1, 2, 3, 4, 5, 6]). The proper
8 orthogonal decomposition (POD) is one of the most successful methods for
9 ROM development. An accurate numerical simulation is used in POD to ex-
10 tract the dominant structures, which are then used in a Galerkin approxima-
11 tion of the underlying equations [3, 7]. In this paper, POD will be exclusively
12 used to construct the ROMs.

13 Standard ROMs are extremely efficient and relatively accurate for laminar
14 flows. They generally fail, however, in the numerical simulation of convection-
15 dominated flows [8, 9, 10, 11, 12, 13, 14, 15]. Indeed, to ensure a low compu-
16 tational cost, only the first few POD modes are generally used in the ROM.
17 The resulting low-dimensional ROM, however, generally yields poor results
18 in the numerical simulation of convection-dominated flows, often in the form
19 of numerical oscillations (see, e.g., [3, 4, 8, 9, 14, 16, 17, 18]). In the ROM
20 literature, a common explanation for this failure of standard ROMs is the vi-
21 olation of the concept of energy cascade [3, 8, 9, 14, 18, 19]. Indeed, in [20] it
22 was shown that the concept of energy cascade is also valid in a POD setting:
23 The main role of the neglected POD modes is to drain energy from the ROM.
24 Thus, since standard ROMs fail to account for this transfer of energy from
25 resolved to unresolved POD modes, they generally yield inaccurate results.

26 Over the years, numerous models for the effect of the neglected POD
27 modes have been devised (see, e.g., [8, 9, 10, 13, 14, 19, 21, 22]). Although a
28 survey of these approaches is beyond the scope of this paper, some of the most
29 recent developments can be found in, e.g., [9, 13, 14, 23, 24] and references
30 therein. Many of these models are similar to the large eddy simulation (LES)
31 closure models. Indeed, to model the effect of the neglected POD modes,
32 some authors start with the filtered equations and propose closure models
33 for ROMs, just as in LES (see, e.g., [3, 8, 20]). Other authors, however, do
34 not employ filtering and the LES analogy to develop models for the neglected
35 POD modes (see, e.g., [9, 17, 18, 19]). For the sake of brevity, in what follows
36 we will use *ROM closure model* as a generic term for models of neglected POD
37 modes [3, 9, 17, 18, 19, 20, 23, 24].

38 Since the analogy between ROM and LES closure modeling is relevant to
39 the model that we propose in this paper, we include next a “time capsule” of
40 LES closure modeling. Of course, we only include the LES developments that
41 are relevant to our paper; for more details, we refer the reader to specialized
42 texts, e.g., [25, 26, 27, 28].

43 The idea in LES is straightforward. Instead of approximating the flow
44 variables, the LES models aim at approximating the spatially filtered flow

45 variables, which can be discretized on significantly coarser spatial meshes.
 46 However, since the underlying Navier-Stokes equations are nonlinear, filtering
 47 them yields a system of equations that is not closed. Closing the spatially
 48 filtered Navier-Stokes equations, which is commonly known as the *closure*
 49 *problem*, represents the main challenge faced by LES.

50 There are many closure models used in LES. Following Sagaut’s terminol-
 51 ogy [28], these LES closure models could be divided into two categories: (i)
 52 functional closure models and (ii) structural closure models. Chronologically,
 53 the functional closure models were developed first and the structural closure
 54 models were put forth later.

55 The *functional* LES closure models (chapters 5 and 6 in [28]) follow from
 56 phenomenological arguments and aim at modeling the physical effect of the
 57 sub-filter scales (i.e., the scales [below](#) the spatial filter radius). The main tool
 58 used in developing these functional closure models is Kolmogorov’s statistical
 59 theory of turbulence and the resulting energy cascade, which postulates that
 60 the main role of the sub-filter scales is to drain energy out of the LES model.
 61 In the functional closure models, this is generally achieved by adding an eddy
 62 viscosity to the molecular viscosity of the system. Probably the most popular
 63 example in this class is the Smagorinsky model [29].

64 The second type of closure models is *structural LES* closure models (chap-
 65 ter 7 in [28]). These closure models are generally derived through mathemat-
 66 ical rather than phenomenological arguments, e.g., formal series expansions.
 67 One of the most popular models in this class is the approximate deconvolution
 68 (AD) model [30, 31, 32], which uses the deconvolution approaches developed
 69 in the image processing and inverse problems communities to recover the
 70 original signal from a blurred filtered signal.

71 The ROM closure model development was similar to the LES closure
 72 modeling development. Just as in LES, the first ROM closure models have
 73 been of the functional type. These functional ROM closure models have
 74 generally used some sort of stabilization procedure to model the effect of the
 75 discarded POD modes. Probably the first functional ROM closure model
 76 has been the mixing length model pioneered by Lumley and his group [8].
 77 This model was followed by more accurate ROM closure models, such as
 78 the Smagorinsky model [33, 34, 35], the variational multiscale model [14, 22]
 79 and the dynamic subgrid-scale model [14]. As already mentioned, a physical
 80 motivation for the approach used to develop these functional ROM closure
 81 models is the concept of energy cascade [20]. We emphasize that, just as in
 82 the LES case, these functional ROM closure models do not employ an explicit

83 spatial filter; instead, they use phenomenological arguments to model the
84 effect of the discarded POD modes.

85 To our knowledge, structural ROM closure models have not been pro-
86 posed yet. Again, this is not surprising, since in LES the structural closure
87 models were developed much later than the functional closure models. We
88 believe that the main reason why structural ROM closure models have not
89 been proposed is that the concept of *explicit spatial filtering* (which is central
90 in the development of structural LES closure models) has not been exploited
91 yet in the ROM field.

92 In this paper, we take a first step in this direction and propose a structural
93 ROM closure model. To this end, we first outline an LES-ROM framework
94 that employs explicit ROM spatial filtering to develop new ROMs in which
95 the term that needs to be modeled (i.e., the ROM stress tensor) is explic-
96 itly defined. We emphasize that, in this LES-ROM framework, we carry
97 out explicit spatial filtering at a ROM level, not at the input data level.
98 Thus, the new LES-ROMs can use either DNS input data (as we do in this
99 paper, see Section 2 and Section 5) or LES input data (see discussion in
100 Section 6). Within the LES-ROM framework, we use the AD method to put
101 forth a new structural ROM closure model, the AD-ROM. Specifically, given
102 the approximation of the filtered ROM variables, we use AD to obtain an
103 approximation of the original unfiltered ROM variables and solve the ROM
104 closure problem. Since the AD problem is notoriously ill-posed, we use a
105 regularization method from image processing and inverse problems to obtain
106 stable AD approximations.

107 *Previous Relevant Work.* The LES-ROM framework that we use in this paper
108 has been also utilized in, e.g., [3, 8, 14]. We emphasize that, to our knowledge,
109 the LES-ROM framework has only been used *implicitly*, to motivate various
110 functional ROM closure models [3, 8]. In this paper, we take a completely
111 different approach and *explicitly* use the LES-ROM framework (specifically,
112 the ROM stress tensor) to develop a structural ROM closure model, the
113 AD-ROM.

114 In ROMs, spatial filtering has been used as a preprocessing step, to filter
115 out the noise in the snapshot data, i.e., in the generation of the POD modes
116 (see, e.g., Section 5 in [36] for a survey of relevant work). We emphasize,
117 however, that our approach is *fundamentally different*, since we *explicitly* use
118 spatial filters in the *actual ROMs*, i.e., we modify the mathematical model,
119 not the input data. To our knowledge, explicit ROM spatial filtering has

only be used in [14, 37, 38].

In this paper, we exclusively use ROM spatial filtering to develop the LES-ROM framework and the AD-ROM. A different filtering approach was used in [23]: Instead of ROM spatial filtering, the authors used *ROM ensemble averaging* to develop the ensemble averaged ROM, called the Galerkin-Reynolds equation (see equation (7) in [23]). The ensemble averaged ROM proposed in [23] has, in our opinion, great potential. We emphasize, however, that the LES-ROM that we propose in this paper and the ensemble averaged ROM proposed in [23] are *fundamentally different*. The LES-ROM employs the LES methodology to develop a dynamical system for the spatial averages of the ROM velocity. The ensemble averaged ROM, on the other hand, is reminiscent of RANS formalism and consists of a dynamical system for the ensemble average of the ROM coefficients.

The rest of the paper is organized as follows: In Section 2, we briefly discuss the POD and the standard ROM. In Section 3, we outline the LES-ROM framework. In Section 4, we use this LES-ROM framework to develop the new AD-ROM. In Section 5, we present numerical results for the new AD-ROM for a 3D flow past a circular cylinder at Reynolds number $Re = 1000$. Finally, in Section 6 we draw conclusions and present an outlook of future work.

2. Reduced Order Modeling

In this section, the POD, the standard Galerkin ROM and the centering trajectory are briefly presented. The *Navier-Stokes equations (NSE)* are used as mathematical model:

$$\mathbf{u}_t - \frac{2}{Re} \nabla \cdot \mathbb{D}(\mathbf{u}) + \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p = \mathbf{0}, \quad (1)$$

$$\nabla \cdot \mathbf{u} = 0, \quad (2)$$

where $\mathbf{u}$ is the velocity, p the pressure, Re the Reynolds number and $\mathbb{D}(\mathbf{u}) := (\nabla \mathbf{u} + (\nabla \mathbf{u})^\top)/2$ is the deformation tensor of $\mathbf{u}$. In this paper, the NSE (1)–(2) are supplemented with the initial condition $\mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0(\mathbf{x})$ and steady Dirichlet boundary conditions.

Remark 2.1 (Viscous Term Formulation). *In the NSE (1), we used the viscous term formulation*

$$\frac{2}{Re} \nabla \cdot \mathbb{D}(\mathbf{u}) = \frac{1}{Re} \nabla \cdot \left[\nabla \mathbf{u} + (\nabla \mathbf{u})^\top \right]. \quad (3)$$

151 When $\nabla \cdot \mathbf{u} = 0$, the viscous term formulation (3) is identical to the standard
 152 formulation

$$\frac{1}{Re} \nabla \cdot \nabla \mathbf{u} = \frac{1}{Re} \Delta \mathbf{u}. \quad (4)$$

153 As noted in Section 3.3.1 of [39], however, the finite element (FE) discretiza-
 154 tions of the two formulations are usually not identical.

155 Both the continuous version and the FE discretization of the alternative
 156 viscous term formulation (3) are carefully discussed in Section 3.11.3, Section
 157 3.12.1 and Section 3.13.1 of [39]. We only note that, since $\mathbb{D}(\mathbf{u}) = \mathbb{D}(\mathbf{u})^\top$,
 158 the following inequality (which is equation (3.11-11) of [39]) holds:

$$\left(2\mathbb{D}(\mathbf{u}), \nabla \mathbf{u} \right) = \left(\mathbb{D}(\mathbf{u}), \nabla \mathbf{u} + (\nabla \mathbf{u})^\top \right) = 2 \left(\mathbb{D}(\mathbf{u}), \mathbb{D}(\mathbf{u}) \right) \geq 0. \quad (5)$$

159 Inequality (5) and Korn's inequality (see Theorem 3.77 in [40]) imply that
 160 the matrix corresponding to the FE discretization of (3) in $\mathbf{H}_0^1$ is positive
 161 definite.

162 In the remainder of the paper, we use the alternative viscous term formu-
 163 lation (3).

164 2.1. Proper Orthogonal Decomposition (POD)

165 One of the most popular reduced order modeling techniques is the POD,
 166 which we exclusively use to generate all the ROMs in this paper. We briefly
 167 describe POD next. For more details, the reader is referred to, e.g., [3, 4, 7].
 168 The POD starts with the snapshots $\{\mathbf{u}_h^1, \dots, \mathbf{u}_h^{N_s}\}$, which are numerical ap-
 169 proximations of the NSE at N_s different time instances. For all the ROMs in
 170 this paper, we use DNS data to build the snapshots. Specifically, we utilize
 171 the FE approximations of the NSE as snapshots (see Section 5 for details).
 172 We emphasize, however, that other numerical methods can be used instead.
 173 The POD seeks a low-dimensional basis that approximates the snapshots
 174 optimally with respect to a certain norm. In this paper, we choose the com-
 175 monly used L^2 -norm. The solution of the minimization problem is equivalent
 176 to the solution of the eigenvalue problem

$$\mathbf{Y} \mathbf{Y}^\top \mathbf{M}_h \boldsymbol{\varphi}_j = \lambda_j \boldsymbol{\varphi}_j, \quad j = 1, \dots, N, \quad (6)$$

177 where $\boldsymbol{\varphi}_j$ and λ_j denote the vector of the FE coefficients of the POD basis
 178 functions and the POD eigenvalues, respectively, $\mathbf{Y}$ denotes the snapshot

matrix, whose columns correspond to the FE coefficients of the snapshots, $\mathbf{M}_h$ denotes the FE mass matrix, and N is the dimension of the FE space $\mathbf{X}^h$ [41]. The eigenvalues are real and non-negative, so they can be ordered as follows:

$$\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_N \geq 0. \quad (7)$$

The POD basis consists of the normalized functions $\{\boldsymbol{\varphi}_j\}_{j=1}^r$, which correspond to the first $r \ll N$ largest eigenvalues. Thus, the POD space is defined as $\mathbf{X}^r := \text{span}\{\boldsymbol{\varphi}_1, \dots, \boldsymbol{\varphi}_r\}$.

The centering trajectory method is popular in ROM development [3]. In this approach, the snapshots $\{\mathbf{u}_h^1, \dots, \mathbf{u}_h^{N_s}\}$ are replaced by $\{\mathbf{u}_h^1 - \mathbf{U}, \dots, \mathbf{u}_h^{N_s} - \mathbf{U}\}$, where $\mathbf{U} = \frac{1}{N_s} \sum_{i=1}^{N_s} \mathbf{u}_h^i$ is the centering trajectory and $\mathbf{u}_h^i - \mathbf{U}$ are the snapshot fluctuations. Thus, the POD basis functions are computed from the snapshot fluctuations $\mathbf{u}_h^i - \mathbf{U}$, $i = 1, \dots, N_s$. The centering trajectory method is especially useful for problems that have steady nonhomogeneous Dirichlet boundary conditions, such as the boundary conditions in the 3D flow past a cylinder investigated in Section 5. Since in this case the snapshot fluctuations $\mathbf{u}_h^i - \mathbf{U}$, $i = 1, \dots, N_s$ satisfy homogeneous Dirichlet boundary conditions, the centering trajectory method avoids the challenges posed by the nonhomogeneous boundary conditions in ROMs (see, however, [42] for alternative approaches). In what follows, we will use the centering trajectory approach. We emphasize, however, that the new AD-ROM that we develop in what follows works equally well when the centering trajectory is not used.

2.2. The Galerkin ROM (G-ROM)

To develop the standard Galerkin ROM, we start by considering the ROM velocity approximation, $\mathbf{U}_r$, defined as follows:

$$\mathbf{U}_r(\mathbf{x}, t) = \mathbf{U}(\mathbf{x}) + \sum_{j=1}^r a_j(t) \boldsymbol{\varphi}_j(\mathbf{x}) = \mathbf{U}(\mathbf{x}) + \mathbf{u}_r(\mathbf{x}, t), \quad (8)$$

where $\{a_j(t)\}_{j=1}^r$ are the sought time-varying POD coefficients, $\mathbf{U}$ is the centering trajectory defined in Section 2.1, and $\mathbf{u}_r(\mathbf{x}, t) = \sum_{j=1}^r a_j(t) \boldsymbol{\varphi}_j(\mathbf{x})$ is the ROM velocity fluctuation. We use the POD basis, the fact that the POD modes are weakly divergence-free (just as the snapshots), and a Galerkin approximation of the NSE to obtain the standard *Galerkin ROM (G-ROM)* [3]: $\forall i = 1, \dots, r$,

$$\left(\frac{\partial \mathbf{U}_r}{\partial t}, \boldsymbol{\varphi}_i \right) + \frac{2}{Re} \left(\mathbb{D}(\mathbf{U}_r), \nabla \boldsymbol{\varphi}_i \right) + \left(\mathbf{U}_r \cdot \nabla \mathbf{U}_r, \boldsymbol{\varphi}_i \right) = 0. \quad (9)$$

209 The G-ROM (9) yields the following autonomous dynamical system for the
 210 vector of time coefficients, $\mathbf{a}(t)$:

$$\dot{\mathbf{a}} = \mathbf{b} + \mathbf{A} \mathbf{a} + \mathbf{a}^\top \mathbf{B} \mathbf{a}, \quad (10)$$

211 where $\mathbf{b}$, $\mathbf{A}$, and $\mathbf{B}$ correspond to the constant, linear, and quadratic terms
 212 in the numerical discretization of the NSE (1)–(2), respectively. The initial
 213 conditions are obtained by projection:

$$a_j(0) = (\mathbf{u}_0 - \mathbf{U}, \boldsymbol{\varphi}_j), \quad j = 1, \dots, r. \quad (11)$$

214 The finite dimensional system (10) can be written componentwise as follows:
 215 For all $i = 1, \dots, r$,

$$\dot{a}_i(t) = b_i + \sum_{m=1}^r A_{im} a_m(t) + \sum_{m=1}^r \sum_{n=1}^r B_{imn} a_m(t) a_n(t), \quad (12)$$

216 where

$$b_i = -(\mathbf{U} \cdot \nabla \mathbf{U}, \boldsymbol{\varphi}_i) - \frac{2}{Re} \left(\frac{\nabla \mathbf{U} + \nabla \mathbf{U}^\top}{2}, \nabla \boldsymbol{\varphi}_i \right), \quad (13)$$

$$A_{im} = -(\mathbf{U} \cdot \nabla \boldsymbol{\varphi}_m, \boldsymbol{\varphi}_i) - (\boldsymbol{\varphi}_m \cdot \nabla \mathbf{U}, \boldsymbol{\varphi}_i) - \frac{2}{Re} \left(\frac{\nabla \boldsymbol{\varphi}_m + \nabla \boldsymbol{\varphi}_m^\top}{2}, \nabla \boldsymbol{\varphi}_i \right), \quad (14)$$

$$B_{imn} = -(\boldsymbol{\varphi}_m \cdot \nabla \boldsymbol{\varphi}_n, \boldsymbol{\varphi}_i). \quad (15)$$

217 3. Large Eddy Simulation ROM (LES-ROM) Framework

218 Numerous ROM closure modeling approaches have been proposed to ad-
 219 dress the inaccuracy (and numerical instability) of the standard G-ROM (see,
 220 e.g., [4, 13, 14] and references therein). In this paper, we take a different ap-
 221 proach and develop an LES-ROM framework that is centered around explicit
 222 ROM spatial filtering.

223 In Section 3.1, we present a continuous ROM spatial filter and two discrete
 224 ROM spatial filters. In Section 3.2, we use this explicit ROM spatial filtering
 225 to develop the LES-ROM framework.

226 3.1. Explicit ROM Spatial Filtering

227 To develop the new LES-ROM framework, we use the explicit *differential*
 228 *filter (DF)*. We present the continuous formulation of the DF in Section 3.1.1,
 229 and two of its discrete formulations in Section 3.1.2 and Section 3.1.3.

230 The DF has been pioneered in LES by Germano [43, 44]. Later, it was
 231 also used in a ROM context to develop regularized ROMs: The ROM-DF
 232 was first used in [37] for the 1D Kuramoto–Sivashinsky equation in a periodic
 233 setting. The ROM-DF was subsequently used in [38] for the 3D NSE in a
 234 general non-periodic setting.

235 3.1.1. Continuous Differential Filter (C-DF)

236 The *continuous differential filter (C-DF)* has been extensively used to
 237 develop LES models [45]. It is defined as follows (see, e.g., Section 2.2.6
 238 in [45]): Let δ be the radius of the C-DF. For all $\Phi \in \mathbf{L}^2(\Omega)$, find $\bar{\Phi} \in \mathbf{L}^2(\Omega)$
 239 such that

$$-\delta^2 \Delta \bar{\Phi} + \bar{\Phi} = \Phi \quad \text{in } \Omega \quad (16)$$

$$\bar{\Phi} = \mathbf{0} \quad \text{on } \partial\Omega. \quad (17)$$

240 The C-DF (16)–(17) is a linear spatial filter, which employs an elliptic oper-
 241 ator to smooth the input variables and eliminate the small scales (i.e., high
 242 frequencies) [25].

243 The following lemma was proved in [46]:

244 **Lemma 3.1.** *The C-DF (16)–(17) is a self-adjoint operator on $\mathbf{L}^2(\Omega)$.*

245 **PROOF.** Consider $\Phi, \Psi \in \mathbf{L}^2(\Omega)$. By the definition of the C-DF, we have

$$-\delta^2 \Delta \bar{\Psi} + \bar{\Psi} = \Psi \quad \text{in } \Omega \quad (18)$$

$$\bar{\Psi} = \mathbf{0} \quad \text{on } \partial\Omega. \quad (19)$$

246 Multiplying (18) by $\bar{\Phi}$, integrating by parts, and using (17), we obtain

$$\delta^2 \left(\nabla \bar{\Psi}, \nabla \bar{\Phi} \right) + \left(\bar{\Psi}, \bar{\Phi} \right) = \left(\Psi, \bar{\Phi} \right) \quad \text{in } \Omega. \quad (20)$$

247 Multiplying (16) by $\bar{\Psi}$, integrating by parts, and using (19), we obtain

$$\delta^2 \left(\nabla \bar{\Phi}, \nabla \bar{\Psi} \right) + \left(\bar{\Phi}, \bar{\Psi} \right) = \left(\Phi, \bar{\Psi} \right) \quad \text{in } \Omega. \quad (21)$$

248 Equations (20) and (21) prove the lemma. $\square$

249 *3.1.2. FE Differential Filter (FE-DF)*

250 The *FE differential filter (FE-DF)* is defined as follows [25, 45]: Let δ be
 251 the radius of the FE-DF. For all $\mathbf{u}^h \in \mathbf{X}^h$ (where $\mathbf{X}^h$ is the FE space), find
 252 $\overline{\mathbf{u}^h}^h \in \mathbf{X}^h$ such that

$$-\delta^2 \Delta \overline{\mathbf{u}^h}^h + \overline{\mathbf{u}^h}^h = \mathbf{u}^h \quad \text{in } \Omega \quad (22)$$

$$\overline{\mathbf{u}^h}^h = \mathbf{0} \quad \text{on } \partial\Omega, \quad (23)$$

253 which yields the following linear system:

$$(\mathbf{M}_h + \delta^2 \mathbf{S}_h) \overline{\mathbf{U}^h}^h = \mathbf{M}_h \mathbf{U}^h, \quad (24)$$

254 where $\mathbf{M}_h \in \mathbb{R}^{N \times N}$ is the FE mass matrix, $\mathbf{S}_h \in \mathbb{R}^{N \times N}$ is the FE stiffness
 255 matrix, $\overline{\mathbf{U}^h}^h \in \mathbb{R}^N$ is the vector of FE coefficients of the output filtered
 256 variable $\overline{\mathbf{u}^h}^h$, and $\mathbf{U}^h \in \mathbb{R}^N$ is the vector of FE coefficients of the input
 257 variable $\mathbf{u}^h$.

258 *3.1.3. ROM Differential Filter (ROM-DF)*

259 The *ROM differential filter (ROM-DF)* is defined as follows: Let δ be the
 260 radius of the ROM-DF. For all $\mathbf{u}^r \in \mathbf{X}^r$, find $\overline{\mathbf{u}^r}^r \in \mathbf{X}^r$ such that

$$-\delta^2 \Delta \overline{\mathbf{u}^r}^r + \overline{\mathbf{u}^r}^r = \mathbf{u}^r \quad \text{in } \Omega \quad (25)$$

$$\overline{\mathbf{u}^r}^r = \mathbf{0} \quad \text{on } \partial\Omega, \quad (26)$$

261 which yields the following linear system:

$$(\mathbf{M}_r + \delta^2 \mathbf{S}_r) \overline{\mathbf{a}^r}^r = \mathbf{a}^r, \quad (27)$$

262 where $\mathbf{M}_r \in \mathbb{R}^{r \times r}$ is the POD mass matrix with entries $(\mathbf{M}_r)_{ij} = (\varphi_j, \varphi_i)$,
 263 $\mathbf{S}_r \in \mathbb{R}^{r \times r}$ is the POD stiffness matrix with entries $(\mathbf{S}_r)_{ij} = (\nabla \varphi_j, \nabla \varphi_i)$,
 264 $\overline{\mathbf{a}^r}^r \in \mathbb{R}^r$ is the vector of POD coefficients of the output filtered variable $\overline{\mathbf{u}^r}^r$,
 265 and $\mathbf{a} \in \mathbb{R}^r$ is the vector of POD coefficients of the input variable $\mathbf{u}^r$.

266 We emphasize that the computational cost of the ROM-DF is much lower
 267 than the computational cost of the FE-DF, since the former yields a very
 268 small $r \times r$ linear system, whereas the latter yields a much larger, $N \times N$
 269 linear system.

270 3.2. Large Eddy Simulation ROM (LES-ROM)

271 To develop the LES-ROM, we use the standard LES approach [25, 26,
272 27, 28, 47]:

- 273 1. Filter the NSE to obtain the *spatially filtered NSE (SF-NSE)*.
- 274 2. Use the SF-NSE and the ROM approximation to obtain the LES-ROM.

275 The motivation for using the above strategy in the LES field is straightfor-
276 ward: The SF-NSE are a system of equations for the filtered flow variables,
277 which can be approximated on the given coarse mesh more accurately than
278 the original, unfiltered flow variables. In this paper, we use a similar argu-
279 ment to develop the LES-ROM framework: Since the spatial structures in
280 the SF-NSE are larger than the spatial structures in the NSE, we expect
281 that, for a fixed target numerical accuracy of the ROM, the SF-NSE require
282 fewer POD modes than the NSE. This, of course, is advantageous from a
283 computational point of view in challenging, realistic applications.

284 In the remainder of this section, we first present the derivation of the
285 SF-NSE and the associated closure problem. Then, we outline the general
286 LES-ROM framework. In Section 4, we use this LES-ROM framework to
287 develop the new AD-ROM.

288 We filter the NSE (1) with the continuous ROM differential filter, C-DF,
289 and assume that differentiation and filtering commute (see, e.g., Chapter 9
290 in [25]):

$$\frac{\partial \bar{\mathbf{u}}}{\partial t} - \frac{2}{Re} \nabla \cdot \mathbb{D}(\bar{\mathbf{u}}) + \overline{\mathbf{u} \cdot \nabla \mathbf{u}} + \nabla \bar{p} = \mathbf{0}. \quad (28)$$

291 Next, we project (28) onto a space of weakly divergence-free functions ϕ to
292 obtain the weak formulation of the *spatially filtered NSE (SF-NSE)*:

$$\left(\frac{\partial \bar{\mathbf{u}}}{\partial t}, \phi \right) + \frac{2}{Re} \left(\mathbb{D}(\bar{\mathbf{u}}), \nabla \phi \right) + \left(\overline{\mathbf{u} \cdot \nabla \mathbf{u}}, \phi \right) = 0. \quad (29)$$

293 **Remark 3.1.** *The standard SF-NSE generally include a pressure term. Since*
294 *we used weakly divergence-free test functions ϕ , the pressure term from (28)*
295 *dropped out of (29). We used this approach since the POD basis functions*
296 *employed in our ROMs are weakly divergence-free. Thus, the SF-NSE (29),*
297 *although nonstandard, are better suited to our ROM framework.*

298 Of course, in LES one cannot simply discretize the SF-NSE (29), since
 299 these equations are not closed. Thus, one first needs to address the *closure*
 300 *problem*, i.e., to model the filtered nonlinearity $\overline{\mathbf{u} \cdot \nabla \mathbf{u}}$ in terms of the filtered
 301 velocity $\overline{\mathbf{u}}$:

$$\overline{\mathbf{u} \cdot \nabla \mathbf{u}} = \text{function}(\overline{\mathbf{u}}). \quad (30)$$

302 The *closure model* is the explicit dependence on $\overline{\mathbf{u}}$ of the filtered nonlinearity
 303 $\overline{\mathbf{u} \cdot \nabla \mathbf{u}}$ in equation (30). Once the closure problem is addressed, the SF-
 304 NSE (29) yield the *LES model*:

$$\left(\frac{\partial \overline{\mathbf{u}}}{\partial t}, \phi \right) + \frac{2}{Re} \left(\mathbb{D}(\overline{\mathbf{u}}), \nabla \phi \right) + \left(\text{function}(\overline{\mathbf{u}}), \phi \right) = \mathbf{0}. \quad (31)$$

305 Of course, the LES model (31) needs to be discretized. We use a ROM
 306 approximation and obtain the *LES-ROM*: $\forall i = 1, \dots, r$,

$$\left(\frac{\partial \mathbf{W}_r}{\partial t}, \varphi_i \right) + \frac{2}{Re} \left(\mathbb{D}(\mathbf{W}_r), \nabla \varphi_i \right) + \left(\text{function}(\mathbf{W}_r), \varphi_i \right) = \mathbf{0}, \quad (32)$$

307 where $\mathbf{W}_r$ is the ROM approximation of the filtered velocity $\overline{\mathbf{u}}$ in (31).

308 **Remark 3.2.** *In the LES literature, the ROM closure problem generally*
 309 *takes a form that is different from (30). In this paper, however, we use*
 310 *the equivalent form in (30), since just as in LES [25, 28, 45], it makes the*
 311 *derivation of the AD-ROM in Section 4 straightforward.*

312 *For completeness, however, we outline the derivation of the standard for-*
 313 *mulation of the LES closure problem. First, in the NSE, we use the fact that*
 314 $\nabla \cdot \mathbf{u} = 0$ *to rewrite the nonlinear term as follows: $\mathbf{u} \cdot \nabla \mathbf{u} = \nabla \cdot (\mathbf{u} \mathbf{u})$. Thus,*
 315 *the SF-NSE (29) can be written as*

$$\left(\frac{\partial \overline{\mathbf{u}}}{\partial t}, \phi \right) + \frac{2}{Re} \left(\mathbb{D}(\overline{\mathbf{u}}), \nabla \phi \right) + \left(\overline{\nabla \cdot (\mathbf{u} \mathbf{u})}, \phi \right) = \mathbf{0}. \quad (33)$$

316 *Next, we decompose the nonlinearity in (33) as follows:*

$$\overline{\mathbf{u} \mathbf{u}} = \overline{\mathbf{u}} \overline{\mathbf{u}} + \left(\overline{\mathbf{u} \mathbf{u}} - \overline{\mathbf{u}} \overline{\mathbf{u}} \right) = \overline{\mathbf{u}} \overline{\mathbf{u}} + \boldsymbol{\tau}, \quad (34)$$

317 *where, following the LES terminology [25, 28], the stress tensor*

$$\boldsymbol{\tau} = \overline{\mathbf{u} \mathbf{u}} - \overline{\mathbf{u}} \overline{\mathbf{u}} \quad (35)$$

318 is the subfilter-scale stress tensor. Thus, the SF-NSE (33) take the form

$$\left(\frac{\partial \bar{\mathbf{u}}}{\partial t}, \phi\right) + \frac{2}{Re} \left(\mathbb{D}(\bar{\mathbf{u}}), \nabla \varphi_i\right) + \left(\nabla \cdot (\bar{\mathbf{u}} \bar{\mathbf{u}}), \phi\right) + \left(\nabla \cdot \boldsymbol{\tau}, \phi\right) = \mathbf{0}. \quad (36)$$

319 We emphasize that equation (36) can be regarded as the standard weak for-
 320 mulation for the NSE for $\bar{\mathbf{u}}$ (not $\mathbf{u}$), plus the extra term $(\nabla \cdot \boldsymbol{\tau}, \phi)$. The
 321 closure problem for the SF-NSE (36) is

$$\boldsymbol{\tau} = \text{function}(\bar{\mathbf{u}}). \quad (37)$$

322 Equation (37) is the form generally used in the LES literature for the closure
 323 problem.

324 4. Approximate Deconvolution ROM (AD-ROM)

325 Most ROM closure models have generally used some sort of stabilization
 326 procedure, e.g., [8, 9, 10, 13, 14, 18, 19, 21, 22, 23, 48]. A physical motivation
 327 for this popular approach is given in [20], where it is shown that the concept
 328 of energy cascade is also valid in a POD setting. Thus, the role of the ROM
 329 closure model is to drain energy out of the system.

330 In this paper, we use a fundamentally different, novel ROM closure mod-
 331 eling strategy that centers around the concept of *approximate deconvolution*
 332 (*AD*). In LES, the AD models have been pioneered in a series of papers
 333 by Adams and Stolz [30, 31, 32, 49]. These AD models are based on the
 334 *deconvolution* idea, which is central in *image processing* and *inverse prob-*
 335 *lems* [50, 51, 52]: Given an approximation of the filtered input signal, find
 336 an approximation of the input itself. In LES, the deconvolution is used as
 337 follows: Given the available approximation of the filtered velocity, the decon-
 338 volution is used to obtain an approximation of the unfiltered velocity, which
 339 is then used to solve the LES closure problem.

340 In this paper, we use the LES-ROM framework developed in Section 3.2
 341 to construct a novel AD-ROM. In Section 4.1, we present the deconvolution
 342 procedure. In Section 4.2, we use this deconvolution to develop the new
 343 AD-ROM.

344 4.1. Approximate Deconvolution

345 For clarity of presentation, let us denote with G the explicit ROM spatial
 346 filter used to develop the LES-ROM framework in Section 3.2. We assume

347 that an approximation of the filtered velocity

$$\bar{\mathbf{u}} := G \mathbf{u} \quad (38)$$

348 is available. The goal in the ROM deconvolution problem is to find an approx-
 349 imation of the original flow variable, $\mathbf{u}$, so that the ROM closure problem (30)
 350 can be solved.

351 Since G is invertible, at first glance, one just has to use an *exact decon-*
 352 *volution (ED)*, i.e., employ the inverse of the filter G in (38) to solve the
 353 deconvolution problem:

$$\mathbf{u}^{ED} = G^{-1} \bar{\mathbf{u}} = \mathbf{u}. \quad (39)$$

354 It is well-known in the inverse problem community that the ED is generally
 355 a bad idea because the inverse problem (38) is *ill-posed*: small changes in
 356 the data can lead to large changes in the solution [45, 50, 52]. Indeed, in-
 357 verting the operator G in (39) results in division by small coefficients of the
 358 high-frequency components of the operator G . Thus, any changes in the in-
 359 put (38) translate into large unphysical oscillations in the output (39) [50, 52].
 360 The ED (39) was carefully investigated in Section 5.2 of [53], where it was
 361 shown that, as expected, for input signals ($\mathbf{u}$) of different types, adding noise
 362 to the filtered signal ($\bar{\mathbf{u}}$) and then using the ED (39) results in inaccurate
 363 approximations ($\mathbf{u}^{ED}$), usually in the form of numerical oscillations.

364 To avoid the numerical oscillations in the ED (39), we use one of the
 365 *regularized deconvolution* methods developed in the image processing and
 366 inverse problems communities [50, 51, 52]. Following the LES terminology,
 367 we call this method *approximate deconvolution (AD)*. Since this paper is
 368 the first investigation of the new AD-ROM, we employ one of the simplest
 369 regularized deconvolutions used in the image processing and inverse problems
 370 communities, the *Lavrentiev regularization*:

$$\mathbf{u}^{AD} = \left(G + \mu I \right)^{-1} \bar{\mathbf{u}}, \quad (40)$$

371 where I is the identity operator and μ is a regularization parameter.

372 The AD (40) was carefully investigated in Section 5.4 in [53], where it
 373 was shown that it performs much better than the ED (39): For input signals
 374 of different types, noise was added to the filtered signal ($\bar{\mathbf{u}}$), and the ED
 375 and AD were compared. The AD (40) produced much better results than
 376 the ED (39): The latter increased the amplitude of the noise added to the

377 filtered input signal, which, in turn, yielded spurious numerical oscillations.
 378 The former, on the other hand, significantly decreased the amplitude of the
 379 noise and yielded relatively accurate results.

380 **Remark 4.1 (AD vs ED).** *We emphasize that these results are not sur-*
 381 *prising at all. Indeed, they reflect the reality in the inverse problems and*
 382 *image processing communities, where it is well known that the ED produces*
 383 *inaccurate results, and the AD should be used instead. However, both the AD*
 384 *and ED were carefully investigated in [53], since, to our knowledge, this was*
 385 *the first investigation of deconvolution in the ROM field.*

386 4.2. Approximate Deconvolution ROM (AD-ROM)

387 The AD approximation (40) is used to close the LES model (31): $\forall i =$
 388 $1, \dots, r,$

$$\left(\frac{\partial \bar{\mathbf{u}}}{\partial t}, \boldsymbol{\varphi}_i \right) + \frac{2}{Re} \left(\mathbb{D}(\bar{\mathbf{u}}), \nabla \boldsymbol{\varphi}_i \right) + \left(\overline{\mathbf{u}^{AD} \cdot \nabla \mathbf{u}^{AD}}, \boldsymbol{\varphi}_i \right) = \mathbf{0}. \quad (41)$$

389 At first glance, to obtain an LES-ROM, one would simply replace the filtered
 390 velocity $\bar{\mathbf{u}}$ in (41) with a ROM approximation

$$\mathbf{W}_r = \mathbf{U} + \sum_{j=1}^r a_j \boldsymbol{\varphi}_j = \mathbf{U} + \mathbf{w}_r. \quad (42)$$

391 **Remark 4.2.** *Note that the coefficients a_j in the $\mathbf{w}_r$ expansion (42) are dif-*
 392 *ferent from the coefficients a_j used in the $\mathbf{u}_r$ expansion (8). We use the same*
 393 *notation, however, to ensure consistency with the traditional ROM notation.*
 394

395 We emphasize that approximation (42) is not appropriate. Indeed, since the
 396 POD basis functions were obtained from the numerical discretization of the
 397 *unfiltered* NSE, they can only approximate the *unfiltered* flow velocity, $\mathbf{u}$:

$$\mathbf{u} \approx \mathbf{U}_r = \mathbf{U} + \mathbf{u}_r. \quad (43)$$

398 Thus, the *filtered* flow velocity in (41) should be approximated as

$$\bar{\mathbf{u}} \approx \overline{\mathbf{U}_r} \stackrel{(43)}{=} \overline{\mathbf{U}} + \overline{\mathbf{u}_r}. \quad (44)$$

399 Furthermore, to be able to approximate $\bar{\mathbf{u}}$ in the ROM space $\mathbf{X}^r$, we make
 400 the following ansatz:

$$\bar{\mathbf{u}}_r \approx \mathbf{w}_r = \sum_{j=1}^r a_j \boldsymbol{\varphi}_j. \quad (45)$$

401 Thus, the filtered velocity $\bar{\mathbf{u}}$ in (41) should be replaced with

$$\mathbf{W}_r = \bar{\mathbf{U}} + \bar{\mathbf{u}}_r \stackrel{(45)}{\approx} \bar{\mathbf{U}} + \mathbf{w}_r. \quad (46)$$

402 We emphasize that, although approximations (42) and (46) are similar in
 403 that they both use ansatz (45), they are different in one important aspect:
 404 Approximation (42) *assumes* that the *filtered* centering trajectory $\bar{\mathbf{U}}$ can be
 405 approximated by the unfiltered centering trajectory $\mathbf{U}$ and the POD basis,
 406 whereas approximation (46) does not make this assumption.

407 Next, we present the ROM approximation of $\mathbf{u}^{AD}$ in (41):

$$\begin{aligned} \mathbf{u}^{AD} &\approx G^{-1} \bar{\mathbf{u}} \stackrel{(43)}{\approx} G^{-1} \bar{\mathbf{U}}_r \stackrel{(45)}{\approx} G^{-1} (\bar{\mathbf{U}} + \mathbf{w}_r) = \mathbf{U} + G^{-1} \mathbf{w}_r \\ &\stackrel{(40)}{\approx} \mathbf{U} + \left(G + \mu I \right)^{-1} \mathbf{w}_r. \\ &= \mathbf{U} + \mathbf{w}_r^{AD}, \end{aligned} \quad (47)$$

408 where $\mathbf{w}_r^{AD}$ is a ROM approximation of the unfiltered flow velocity.

409 Using the ROM approximations (46) and (47) in the LES model (41), we
 410 obtain the *approximate deconvolution ROM (AD-ROM)*:

$$\begin{aligned} \left(\frac{\partial(\bar{\mathbf{U}} + \mathbf{w}_r)}{\partial t}, \boldsymbol{\varphi}_i \right) &+ \frac{2}{Re} \left(\mathbb{D}(\bar{\mathbf{U}} + \mathbf{w}_r), \nabla \boldsymbol{\varphi}_i \right) \\ &+ \left(\overline{(\mathbf{U} + \mathbf{w}_r^{AD}) \cdot \nabla (\mathbf{U} + \mathbf{w}_r^{AD})}, \boldsymbol{\varphi}_i \right) = \mathbf{0}. \end{aligned} \quad (48)$$

411 Furthermore, since the C-DF is self-adjoint (see Lemma 3.1), the AD-ROM (48)
 412 can be written in the following equivalent form:

$$\begin{aligned}
 & \left(\frac{\partial \vec{U}}{\partial t} + \frac{\partial \mathbf{w}_r}{\partial t}, \varphi_i \right) + \frac{2}{Re} \left(\mathbb{D}(\mathbf{U}), \nabla \overline{\varphi}_i \right) + \frac{2}{Re} \left(\mathbb{D}(\mathbf{w}_r), \nabla \varphi_i \right) \\
 & + \left(\mathbf{U} \cdot \nabla \mathbf{U}, \overline{\varphi}_i \right) + \left(\mathbf{w}_r^{AD} \cdot \nabla \mathbf{U}, \overline{\varphi}_i \right) + \left(\mathbf{U} \cdot \nabla \mathbf{w}_r^{AD}, \overline{\varphi}_i \right) \\
 & + \left(\mathbf{w}_r^{AD} \cdot \nabla \mathbf{w}_r^{AD}, \overline{\varphi}_i \right) = 0.
 \end{aligned} \tag{49}$$

413 We note that the alternative AD-ROM formulation (49) is better suited for
 414 discretization than the standard AD-ROM formulation (48), since it avoids
 415 the spatial filtering of the vectors and tensors involving the centering tra-
 416 jectory ($\mathbf{U}$), which can be challenging in a ROM setting. Thus, in the
 417 numerical investigation in Section 5, we will use the alternative AD-ROM
 418 formulation (49).

419 **Remark 4.3.** *At first glance, the approach used in the derivation of the al-*
 420 *ternative formulation of the AD-ROM in (49) (i.e., using the self-adjointness*
 421 *of the C-DF) is reminiscent of other approaches used in LES. For example,*
 422 *using test functions that are multiplied by the inverse of the C-DF and then*
 423 *using the self-adjointness of the C-DF was essential in the proof of the well-*
 424 *posedness of the Rational LES model (see discussion on page 161 in [25]).*
 425 *The same approach was later used to develop a new type of AD-LES models*
 426 *in [46, 54, 55]. We emphasize, however, that there is a fundamental differ-*
 427 *ence between the AD-ROM (49) and the AD-LES in [46, 54, 55]: To develop*
 428 *the alternative AD-ROM formulation (49), we first multiplied by the stan-*
 429 *dard test function and then we used the self-adjointness of the C-DF to move*
 430 *the filtering operator from the terms involving the centering trajectory to the*
 431 *test function. We note that the filtered test functions that appear in (49)*
 432 *do not constitute a challenge in our ROM setting, since they can be pre-*
 433 *computed and stored. However, for the discretization of the AD-LES models*
 434 *in [46, 54, 55] with standard numerical methods (e.g., FE), storing all the*
 435 *filtered basis functions is not possible in realistic settings with a large number*
 436 *of degrees of freedom. Thus, for the AD-LES models in [46, 54, 55], one has*
 437 *first to use test functions that are multiplied by the inverse of the C-DF and*

438 *only then use the self-adjointness of the C-DF. The price paid, however, is*
 439 *that fourth-order differential operators need to be discretized in these AD-LES*
 440 *models [46, 55].*

441 4.3. Spatial Filtering for the AD-ROM

442 To use the AD-ROM (49) in actual numerical simulations, the continuous
 443 C-DF (16)–(17) needs to be replaced by one of its two discrete variants: the
 444 FE-DF (22)–(23) or the ROM-DF (25)–(26).

445 4.3.1. ROM-DF Spatial Filtering

446 With this choice, the AD-ROM (49) can be written as the following dy-
 447 namical system:

$$\dot{\mathbf{a}} = \mathbf{b} + \mathbf{A} \mathbf{a} + \mathbf{A}^{AD} \mathbf{a}^{AD} + (\mathbf{a}^{AD})^\top \mathbf{B}^{AD} \mathbf{a}^{AD}, \quad (50)$$

448 which can be written componentwise as follows: For all $i = 1, \dots, r$,

$$\begin{aligned} \dot{a}_i(t) &= b_i + \sum_{m=1}^r A_{im} a_m(t) + \sum_{m=1}^r A_{im}^{AD} a_m^{AD}(t) \\ &+ \sum_{m=1}^r \sum_{n=1}^r B_{imn}^{AD} a_m^{AD}(t) a_n^{AD}(t), \end{aligned} \quad (51)$$

449 where

$$b_i = -(\mathbf{U} \cdot \nabla \mathbf{U}, \overline{\boldsymbol{\varphi}}_i^r) - \frac{2}{Re} \left(\frac{\nabla \mathbf{U} + \nabla \mathbf{U}^\top}{2}, \nabla \overline{\boldsymbol{\varphi}}_i^r \right), \quad (52)$$

$$A_{im} = -\frac{2}{Re} \left(\frac{\nabla \boldsymbol{\varphi}_m + \nabla \boldsymbol{\varphi}_m^\top}{2}, \nabla \boldsymbol{\varphi}_i \right), \quad (53)$$

$$A_{im}^{AD} = -(\mathbf{U} \cdot \nabla \boldsymbol{\varphi}_m, \overline{\boldsymbol{\varphi}}_i^r) - (\boldsymbol{\varphi}_m \cdot \nabla \mathbf{U}, \overline{\boldsymbol{\varphi}}_i^r), \quad (54)$$

$$B_{imn}^{AD} = -(\boldsymbol{\varphi}_m \cdot \nabla \boldsymbol{\varphi}_n, \overline{\boldsymbol{\varphi}}_i^r), \quad (55)$$

450 and the vector $\mathbf{a}^{AD} = \{a_m^{AD}\}_{m=1}^r$ in (51) is the solution of the following linear
 451 system:

$$\left((1 + \mu) \mathbf{M}_r + \delta^2 \mathbf{S}_r \right) \mathbf{a}^{AD} = \left(\mathbf{M}_r + \delta^2 \mathbf{S}_r \right) \mathbf{a}. \quad (56)$$

4.3.2. FE-DF Spatial Filtering

To our knowledge, the only investigation of the FE-DF in a ROM setting has been carried out in [56]. In this paper, we outline only the FE-DF features that are relevant to the AD-ROM (49). For more details, we refer the reader to [56].

ROM filtering with the FE-DF relies on the fact that the ROM space ($\mathbf{X}^r$) is a subspace of the FE space ($\mathbf{X}^h$). Indeed, each POD basis function $\boldsymbol{\varphi}_i$, $i = 1, \dots, r$ has a unique FE representation:

$$\boldsymbol{\varphi}_i = \sum_{j=1}^N c_{ji} \mathbf{h}_j, \quad (57)$$

where $\{\mathbf{h}_j\}_{j=1}^N$ are the FE basis functions. (We note in passing that it is precisely representation (57) that allows the offline stage assembly of the vectors, matrices and tensors in standard ROMs.)

The FE-DF is used in the AD-ROM (49) in two instances: To compute $\overline{\boldsymbol{\varphi}}_i^h$ and $\mathbf{w}_r^{AD}$. Next, we briefly outline the approach used to compute these terms.

To compute $\overline{\boldsymbol{\varphi}}_i^h$, we use the representation (57) for both $\boldsymbol{\varphi}_i$ and $\overline{\boldsymbol{\varphi}}_i^h$:

$$\boldsymbol{\varphi}_i = \sum_{j=1}^N c_{ji} \mathbf{h}_j \quad \text{and} \quad \overline{\boldsymbol{\varphi}}_i^h = \sum_{j=1}^N \bar{c}_{ji} \mathbf{h}_j. \quad (58)$$

Thus, the equation $\overline{\boldsymbol{\varphi}}_i^h \stackrel{(22)}{=} (I - \delta^2 \Delta)^{-1} \boldsymbol{\varphi}_i$ yields the following linear systems: $\forall i = 1, \dots, r$,

$$(\mathbf{M}_h + \delta^2 \mathbf{S}_h) \bar{\mathbf{c}}_i = \mathbf{M}_h \mathbf{c}_i, \quad (59)$$

where $\mathbf{M}_h$ and $\mathbf{S}_h$ are the FE mass and stiffness matrices defined in Section 3.1.2, and $\bar{\mathbf{c}}_i = \{\bar{c}_{ji}\}_{j=1}^N$ and $\mathbf{c}_i = \{c_{ji}\}_{j=1}^N$ are the vectors of coefficients in (58), which need to be computed and stored in the offline stage to be used in the AD-ROM in the online stage.

To compute $\mathbf{w}_r^{AD}$, we need to solve the following equation:

$$\mathbf{w}_r^{AD} \stackrel{(22),(40)}{=} \left((I - \delta^2 \Delta)^{-1} + \mu I \right)^{-1} \mathbf{w}_r, \quad (60)$$

474 which is equivalent to

$$\begin{aligned} \mathbf{w}_r^{AD} + \mu (I - \delta^2 \Delta) \mathbf{w}_r^{AD} &= (I - \delta^2 \Delta) \mathbf{w}_r \\ &\stackrel{(45),(57)}{=} \sum_{j=1}^r a_j \sum_{i=1}^N c_{ij} (I - \delta^2 \Delta) \mathbf{h}_i. \end{aligned} \quad (61)$$

475 We emphasize that (61) needs to be solved in $\mathbf{X}^h$, since the FE-DF is defined
476 in $\mathbf{X}^h$. There are two natural approaches to solve (61):
477

478 (i) In the first approach, we simply let

$$\mathbf{w}_r^{AD} = \sum_{i=1}^N \alpha_i \mathbf{h}_i \quad (62)$$

479 in (61), which yields the following $N \times N$ linear system:

$$\left((1 + \mu) \mathbf{M}_h + \mu \delta^2 \mathbf{S}_h \right) \boldsymbol{\alpha} = \sum_{j=1}^r a_j \left((\mathbf{M}_h + \delta^2 \mathbf{S}_h) \mathbf{c}_j \right), \quad (63)$$

480 where $\boldsymbol{\alpha} = \{\alpha_j\}_{j=1}^N$ is the vector of coefficients in (62).
481

482 (ii) In the second approach for solving (61), we let

$$\mathbf{w}_r^{AD} = \sum_{j=1}^r a_j \sum_{i=1}^N c_{ij}^{AD} \mathbf{h}_i = \sum_{j=1}^r a_j \boldsymbol{\varphi}_j^{AD}, \quad (64)$$

483 where $\boldsymbol{\varphi}_j^{AD}$ is defined as

$$\boldsymbol{\varphi}_j^{AD} = \sum_{i=1}^N c_{ij}^{AD} \mathbf{h}_i. \quad (65)$$

484 We emphasize that $\boldsymbol{\varphi}_j^{AD}$ belongs to the FE space $\mathbf{X}^h$, but does not necessarily
485 belong to the ROM space $\mathbf{X}^r$. To solve (61), we simply solve the following r
486 linear systems of dimension $N \times N$ in the offline stage:

$$\left((1 + \mu) \mathbf{M}_h + \mu \delta^2 \mathbf{S}_h \right) \mathbf{c}_j^{AD} = \left(\mathbf{M}_h + \delta^2 \mathbf{S}_h \right) \mathbf{c}_j, \quad j = 1, \dots, r, \quad (66)$$

487 where $\mathbf{c}_j^{AD} = \{c_{ij}^{AD}\}_{i=1}^N$ is the vector of coefficients in (64).
488

489 Comparing approaches (i) and (ii) in terms of computational efficiency,
 490 we draw the following conclusions: In approach (i), there is no extra storage
 491 required, but the $N \times N$ linear system (63) needs to be solved at each time
 492 step in the online stage. In approach (ii), the r linear systems (66) are
 493 solved only once, in the offline stage, after which the r vectors $\mathbf{c}_j^{AD}$, $j =$
 494 $1, \dots, r$ (corresponding to $\boldsymbol{\varphi}_j^{AD}$ in (65)) are used to assemble and store the
 495 $r \times r$ matrices and $r \times r \times r$ tensor corresponding to the nonlinearity in the
 496 AD-ROM (49). Since the extra storage requirements in approach (ii) are
 497 relatively low for the small r that we use in this paper, in Section 5 we utilize
 498 this approach instead of approach (i), which has a significantly higher CPU
 499 cost.

500 Using approach (ii), the AD-ROM (49) can be written as the following
 501 dynamical system:

$$\dot{\mathbf{a}} = \mathbf{b} + (\mathbf{A} + \mathbf{A}^{AD}) \mathbf{a} + \mathbf{a}^\top \mathbf{B}^{AD} \mathbf{a}, \quad (67)$$

502 which can be written componentwise as follows: For all $i = 1, \dots, r$,

$$\dot{a}_i(t) = b_i + \sum_{m=1}^r \left(A_{im} + A_{im}^{AD} \right) a_m(t) + \sum_{m=1}^r \sum_{n=1}^r B_{imn}^{AD} a_m(t) a_n(t), \quad (68)$$

503 where

$$b_i = -(\mathbf{U} \cdot \nabla \mathbf{U}, \overline{\boldsymbol{\varphi}}_i^h) - \frac{2}{Re} \left(\frac{\nabla \mathbf{U} + \nabla \mathbf{U}^\top}{2}, \nabla \overline{\boldsymbol{\varphi}}_i^h \right), \quad (69)$$

$$A_{im} = -\frac{2}{Re} \left(\frac{\nabla \boldsymbol{\varphi}_m + \nabla \boldsymbol{\varphi}_m^\top}{2}, \nabla \boldsymbol{\varphi}_i \right), \quad (70)$$

$$A_{im}^{AD} = -(\mathbf{U} \cdot \nabla \boldsymbol{\varphi}_m^{AD}, \overline{\boldsymbol{\varphi}}_i^h) - (\boldsymbol{\varphi}_m^{AD} \cdot \nabla \mathbf{U}, \overline{\boldsymbol{\varphi}}_i^h), \quad (71)$$

$$B_{imn}^{AD} = -(\boldsymbol{\varphi}_m^{AD} \cdot \nabla \boldsymbol{\varphi}_n^{AD}, \overline{\boldsymbol{\varphi}}_i^h). \quad (72)$$

504 5. Numerical Tests

505 **Goals** The main goal of this section is to assess the performance of the AD-
 506 ROM (49) in the numerical simulation of a 3D flow past a circular cylinder
 507 at Reynolds number $Re = 1000$. Since the AD-ROM is an LES-ROM, we
 508 follow the standard approach used in LES model assessment, which we briefly

509 describe next (see, e.g., [25, 28] for details). To investigate a new LES model,
510 the following models are generally tested on the same coarse mesh: (i) the
511 new LES model; (ii) the under-resolved solver (i.e., the NSE code without an
512 LES model); (iii) the filtered DNS data (which serves as a benchmark); and
513 (iv) the current state-of-the-art LES model. The new LES model is expected
514 to perform significantly better than the under-resolved solver and to show
515 some improvement over the current state-of-the-art LES model.

516 To assess the performance of the new AD-ROM, we follow the standard
517 LES approach described above. Thus, we also use the spatially filtered DNS
518 results as a benchmark. Furthermore, we also include G-ROM (9) results as
519 a ROM counterpart of the under-resolved solver used in the LES assessment.
520 Finally, we also make a brief qualitative comparison of the new AD-ROM
521 with the eddy viscosity ROMs (EV-ROMs) [8, 14] (which, to our knowledge,
522 are the current state-of-the-art LES-ROMs) and the regularized ROMs (Reg-
523 ROMs) [38]. Just as in the standard LES model assessment, we expect the
524 new AD-ROM to perform significantly better than the G-ROM and show
525 some improvement over the EV-ROMs and Reg-ROMs.
526

527 **Computational Domain** In this section, the x -axis represents the stream-
528 wise direction, the y -axis represents the normal direction, and the z -axis
529 represents the spanwise direction. Furthermore, u denotes the streamwise
530 velocity component (associated with the x -axis), v denotes the normal ve-
531 locity component (associated with the y -axis), and w denotes the spanwise
532 velocity component (associated with the z -axis).

533 The computational domain is cylindrical and is centered around the z -
534 axis, i.e., along the spanwise direction. The cylinder of diameter D is also
535 centered around the z -axis. The diameter of the cylindrical computational
536 domain is $15D$ and its spanwise length is $2D$. The free-stream flow is in the
537 positive x -direction. The same computational domain was used in [14, 35]
538 (see Fig. 9 and Appendix A in [35]).
539

540 **Criteria** The qualitative behavior of the ROMs is judged according to the
541 following six criteria [14]: (i) the kinetic energy spectrum; (ii) the mean
542 velocity; (iii) the Reynolds stresses; (iv) the root mean square (rms) values of
543 the velocity fluctuations; (v) the time evolution of the POD coefficients; and
544 (vi) the Strouhal number. The first four criteria are statistics that measure
545 the temporal and spatial average behavior of the ROMs, whereas the fifth
546 criterion measures the instantaneous behavior of the ROMs. We also include
547 a computational efficiency assessment for all the ROMs. Next, we briefly

548 present these criteria.

549 For all statistics, we use the averaging operator $\langle \cdot \rangle = \langle \cdot \rangle_{tyz}$, which consists
 550 of averaging in time (over the time interval $[0, 300]$) and in the y - and z -
 551 directions. Specifically, to compute $\langle q \rangle_{tyz}$ for a given quantity q , for each
 552 fixed point x , we have

$$\langle q \rangle_{tyz}(x) = \frac{1}{T L_y L_z} \sum_{t,y,z} q(x, y, z, t), \quad (73)$$

553 where T is the total time length (i.e., $T = 300$), L_y is the dimension of
 554 the computational domain in the y -direction, and L_z is the dimension of the
 555 computational domain in the z -direction. Since the numerical results with
 556 spatial averaging in the xz -direction are qualitatively similar to those with
 557 spatial averaging in the yz -direction, we do not include them in the paper.

559 *Energy Spectrum:* All energy spectra are calculated from the average ki-
 560 netic energy of the nodes in the cube with side 0.1 centered at the probe
 561 (0.9992, 0.3575, 1.0625).

563 *Mean Velocity Components:* The following mean velocity components are
 564 plotted: $\langle u \rangle$ (the mean streamwise velocity), $\langle v \rangle$ (the mean normal velocity),
 565 and $\langle w \rangle$ (the mean spanwise velocity).

567 *Reynolds Stresses:* The following Reynolds stresses are plotted: $\langle u - \langle u \rangle, v - \langle v \rangle \rangle$ (the xy-component of the Reynolds stress), $\langle u - \langle u \rangle, w - \langle w \rangle \rangle$ (the xz-component of the Reynolds stress), and $\langle v - \langle v \rangle, w - \langle w \rangle \rangle$ (the yz-component of the Reynolds stress).
 570

572 *RMS Values of Velocity Fluctuations:* The following rms values of velocity
 573 fluctuations are plotted: $\langle u \rangle_{rms} = \langle u - \langle u \rangle, u - \langle u \rangle \rangle$ (the rms of the stream-
 574 wise velocity fluctuations), $\langle v \rangle_{rms} = \langle v - \langle v \rangle, v - \langle v \rangle \rangle$ (the rms of the normal
 575 velocity fluctuations), and $\langle w \rangle_{rms} = \langle w - \langle w \rangle, w - \langle w \rangle \rangle$ (the rms of the span-
 576 wise velocity fluctuations).

578 *Strouhal Number:* The Strouhal number (St) is computed as [57, 58]

$$St = \frac{f D}{U_\infty}, \quad (74)$$

579 where f is the shedding frequency, U_∞ is the freestream velocity (i.e., the
 580 velocity at the inlet), and D is the diameter of the cylinder. Since we have
 581 limited the scope of this paper to just velocity ROMs, we do not consider a
 582 ROM representation of the pressure field. Hence we do not calculate the lift

583 and drag coefficient spectra. Thus, we compute the shedding frequency f as
 584 the frequency corresponding to the first spike in the energy spectrum (see
 585 discussion on page 410 in [59]).

586

587 **Numerical Methods** We investigate all ROMs in the numerical simulation
 588 of 3D flow past a circular cylinder at $\text{Re} = 1000$. The Reynolds number is
 589 computed using the diameter (D) of the cylinder as the length scale and
 590 the freestream velocity (U_∞) as the velocity scale. A parallel CFD solver is
 591 employed on the time interval $[0, 300]$ to generate the DNS data. Details on
 592 the numerical discretization are presented in [57, 58, 60].

593 We obtain the POD basis by collecting 1000 snapshots of the DNS ve-
 594 locity field (u, v, w) over the time interval $[0, 75]$ and applying the method of
 595 snapshots developed in [7]. These POD modes are then interpolated onto a
 596 structured quadratic FE triangulation with nodes coinciding with the nodes
 597 used in the original DNS finite difference discretization. All the ROMs use
 598 the first $r = 6$ POD modes, which capture 84% of the energy of the velocity
 599 fluctuations. As temporal discretization, all the ROMs employ the explicit
 600 Euler method with a time step $\Delta t = 7.5 \times 10^{-4}$. (We note that decreasing
 601 the time step by a factor of 10 does not significantly change the numeric-
 602 al results.) As spatial discretization, all the ROMs use piecewise quadratic
 603 Lagrange FEs. Finally, all the ROMs are investigated on the time interval
 604 $[0, 300]$.
 605

606 **Model Parameters** In Section 4.3, we discussed two possible discretiza-
 607 tions of the C-DF: the ROM-DF and the FE-DF. Since in our preliminary
 608 numerical tests the FE-DF yielded more accurate results than the ROM-DF,
 609 in this section we use the FE-DF and the resulting AD-ROM formulation in
 610 equations (67)–(72).

611 One of the most important parameters of the AD-ROM is the radius of
 612 the ROM spatial filter, δ . In our numerical investigation, we tried only three
 613 δ values: $\delta = 0.03$, $\delta = 0.3$ and $\delta = 0.4$. The low value (i.e., $\delta = 0.03$) yielded
 614 inaccurate results. The high values (i.e., $\delta = 0.3$ and $\delta = 0.4$) yielded similar
 615 results, significantly more accurate than the results for $\delta = 0.03$. Thus, in
 616 what follows, we present results for $\delta = 0.3$. We emphasize, however, that
 617 the value $\delta = 0.3$ does not represent an optimal value; it is just the best value
 618 of the very few we tried. To find the optimal value, numerous δ values (and
 619 different test problems) should be thoroughly investigated. We plan to carry
 620 out this investigation in a future study (see the discussion in Section 6).

Another important parameter of the AD-ROM is the regularization parameter μ used in the Lavrentiev regularization of the AD procedure. In the image processing and inverse problems communities, numerous approaches are proposed to determine the regularization parameters [50, 51, 52]. In our numerical investigation, for the fixed $\delta = 0.3$ value, we choose the μ value that ensures that the time average of the L^2 -norm of the AD-ROM solution is as close as possible to the time average of the L^2 -norm of the filtered DNS data. This approach yields the following optimal value: $\mu = 0.0285$.

5.1. Numerical Results

In Fig. 1, we plot the energy spectra of the AD-ROM and, for comparison purposes, of the G-ROM. The two energy spectra are compared with the spatially filtered DNS energy spectrum. The energy spectrum of the AD-ROM is significantly more accurate (i.e., closer to the filtered DNS energy spectrum) than the energy spectrum of the G-ROM. The latter overestimates the energy spectrum of the filtered DNS.

In Fig. 2, we plot the mean velocity components for different x values. Figure 2 yields the following conclusions: Both the AD-ROM and the G-ROM yield an accurate approximation of the streamwise velocity. The AD-ROM yields an accurate approximation of the mean normal velocity, but the G-ROM does not. Finally, both the AD-ROM and the G-ROM yield inaccurate approximations of the mean spanwise velocity.

In Fig. 3, we plot the Reynolds stresses for different x values. For all the Reynolds stresses, the AD-ROM yields accurate approximations, whereas the G-ROM yields inaccurate approximations.

In Fig. 4, we plot the rms values for different x values. For all the rms values, the AD-ROM yields accurate approximations, whereas the G-ROM yields inaccurate approximations.

The time evolutions of the ROM's POD basis coefficients a_1, a_2 and a_6 on the entire time interval $[0, 300]$ are shown in Fig. 5. We note that the other POD coefficients have a similar behavior. Thus, for clarity of exposition, we include only a_1, a_2 and a_6 . The G-ROM results are clearly inaccurate, since the coefficients' magnitudes are several times larger than that of the filtered DNS data. The AD-ROM yields significantly more accurate results for all the coefficients.

The Strouhal numbers predicted by the AD-ROM, G-ROM and filtered DNS are listed in Table 1. The Strouhal number predicted by the AD-ROM is slightly lower than the Strouhal number computed from the filtered DNS data

Table 1: Strouhal numbers predicted by ROMs.

	DNS	G-ROM	AD-ROM
St	0.2083	–	0.1888

because the AD-ROM’s shedding frequency is lower than the filtered DNS’ shedding frequency (see Fig. 1). We note that the G-ROM fails to predict a clear shedding frequency and, thus, cannot yield a Strouhal number.

Table 2: Offline and online CPU times (in seconds) of DNS and ROMs.

DNS	G-ROM offline	G-ROM online	AD-ROM offline	AD-ROM online
2.3e+06	5.9e+04	9.2e+01	6.1e+04	1.4e+02

To measure the computational efficiency of the AD-ROM (which is one of the main requirements for any successful ROM), we list in Table 2 its offline and online CPU times together with the G-ROM offline and online CPU times and the DNS CPU time. We draw the following conclusions from Table 2:

First, the AD-ROM online CPU time is on the same order as the G-ROM online CPU time. Both online CPU times are about four orders of magnitude lower than the DNS CPU time.

Second, the offline CPU times of both the AD-ROM and the G-ROM are about two orders of magnitude lower than the DNS CPU time. We note, however, that the AD-ROM and G-ROM offline CPU times are significantly higher than their corresponding online CPU times. Indeed, it is well known in the ROM community that in the offline stage, in order to assemble the vectors, matrices and tensors used in the dynamical systems formulation of the G-ROM, the underlying numerical discretization (e.g., FE discretization) needs to be used. Thus, the G-ROM offline CPU time is significant. We also note that, since we use the FE-DF in the numerical discretization of the AD-ROM (see Section 4.3), additional vectors and matrices need to be assembled. This makes the AD-ROM offline CPU time higher than the G-ROM offline CPU time.

Finally, we note that in the applications generally targeted by ROMs, the models are used numerous times and for long time intervals [2, 4, 5]. Thus,

in this type of applications, the bulk of the computational cost of the ROMs is paid in the online stage. Since, as mentioned above, the AD-ROM (and G-ROM) online CPU time is significantly lower than the DNS CPU time, we deem the AD-ROM as computationally efficient.

5.2. Comparison With Other ROMs

In Section 5.1, to assess the performance of the new AD-ROM, we compared it with the G-ROM and the filtered DNS data. Overall, the AD-ROM results were significantly more accurate than the G-ROM results. Thus, the AD-ROM satisfied the basic accuracy criterion of any successful ROM. Furthermore, the AD-ROM results were relatively close to the filtered DNS results, which prompted us to conclude that the AD-ROM was relatively accurate. A natural question, however, is how the AD-ROM’s accuracy compares with the accuracies of other ROMs for convection-dominated flows.

We emphasize that a thorough comparison of the AD-ROM with the plethora of ROMs for convection-dominated flows would require the numerical investigation of different types of ROM strategies for various computational settings and numerous parameter choices. Thus, while needed, this comparison is beyond the scope of this paper. We will, however, present next a brief qualitative comparison of the AD-ROM with two other representative classes of ROMs: the EV-ROMs [3, 8, 14] and the Reg-ROMs [37, 38]. Since both the test problem and the statistics used in [14, 38] are identical to those used in this paper, our qualitative comparison is meaningful.

Overall, the AD-ROM results are similar to those for the EV-ROMs in [14] and Reg-ROMs in [37, 38]: For example, the accuracy of the AD-ROM energy spectrum (see Fig. 1 in this paper) is similar to the accuracy of the energy spectra of the *best* EV-ROMs (see Fig. 3 in [14]) and *best* Reg-ROMs (see Fig. 2 in [38]). The AD-ROM’s accuracy is also similar to that of the best EV-ROMs and Reg-ROMs with respect to other statistics and time evolution of the ROM coefficients (compare, e.g., Fig. 5 in this paper, Fig. 7 and Fig. 8 in [14], and Fig. 6 in [38]).

We believe that the AD-ROM’s performance is impressive given that we did not use any explicit numerical dissipation mechanisms, which are generally expected for ROMs of convection-dominated flows. Indeed, we emphasize that the EV-ROMs include terms that allow explicit dissipation [3, 8, 14] and the Reg-ROMs increase the numerical stability by using explicit spatial filtering of various terms in the models [37, 38]. The AD-ROM, however, does not use any explicit dissipation mechanism. We followed this

720 approach in order to decouple the AD and dissipation effects, which, we
 721 believe, is necessary in the first step of a careful assessment the AD procedure
 722 in a ROM setting.

Figure 1: Kinetic energy spectrum of the spatially filtered DNS (blue) and ROMs (red):
 (a) the G-ROM, and (b) the AD-ROM.

Figure 2: Mean velocity components of the spatially filtered DNS and ROMs: (a) $\langle u \rangle$ (the mean streamwise velocity), (b) $\langle v \rangle$ (the mean normal velocity), and (c) $\langle w \rangle$ (the mean spanwise velocity).

Figure 3: Reynolds stresses of the spatially filtered DNS and ROMs: (a) $\langle u - \langle u \rangle, v - \langle v \rangle \rangle$ (the xy -component of the Reynolds stress), (b) $\langle u - \langle u \rangle, w - \langle w \rangle \rangle$ (the xz -component of the Reynolds stress), and (c) $\langle v - \langle v \rangle, w - \langle w \rangle \rangle$ (the yz -component of the Reynolds stress).

Figure 4: Rms values of the velocity fluctuations of the spatially filtered DNS and ROMs:
(a) $\langle u \rangle_{rms} = \langle u - \langle u \rangle, u - \langle u \rangle \rangle$ (the rms value of the streamwise velocity fluctuations),
(b) $\langle v \rangle_{rms} = \langle v - \langle v \rangle, v - \langle v \rangle \rangle$ (the rms value of the normal velocity fluctuations), and (c)
 $\langle w \rangle_{rms} = \langle w - \langle w \rangle, w - \langle w \rangle \rangle$ (the rms value of the spanwise velocity fluctuations).

Figure 5: Time evolution of the POD basis coefficients a_1 (first row), a_2 (second row) and a_6 (third row) of the spatially filtered DNS (blue) and ROMs (red): the AD-ROM (left column), and G-ROM (right column).

723 6. Conclusions and Future Work

724 We used explicit ROM spatial filtering to develop a large eddy simula-
 725 tion ROM (LES-ROM) framework. Within this LES-ROM framework, we
 726 proposed an approximate deconvolution ROM (AD-ROM). We assessed the
 727 AD-ROM in the numerical simulation of the 3D flow past a circular cylin-
 728 der at $Re = 1000$. The numerical investigation showed that the accuracy
 729 of the AD-ROM was significantly higher than the accuracy of the standard
 730 G-ROM and on the same order as the accuracy of the eddy viscosity ROMs
 731 (EV-ROMs) [14] and Reg-ROMs [38]. Finally, we emphasize that the CPU
 732 time of the AD-ROM was orders of magnitude lower than the CPU time of
 733 the DNS.

734 These first steps in the investigation of the LES-ROM framework and AD-
 735 ROM yielded encouraging results. We emphasize, however, that there are
 736 numerous open questions, both at a fundamental (theoretical and modeling)
 737 and practical (discretization) level. This is, of course, natural, since in the
 738 LES field the same issues have been tackled over decades. We believe that
 739 the following are some of the most stringent issues that need to be addressed
 740 in the LES-ROM framework (in general) and AD-ROM (in particular).

741 *LES-ROM Framework Open Questions.* We believe that the choice of the
 742 *explicit ROM spatial filter* used to develop the LES-ROM framework should
 743 be thoroughly investigated. Indeed, in the LES field, several spatial filters
 744 are commonly used, e.g., the Gaussian, box, sharp cutoff and differential
 745 filters (see [25, 28] for more details). The effect of spatial filtering on the
 746 resulting LES model is relatively well understood. In the ROM, however,
 747 to our knowledge, only two ROM spatial filters have been used so far: the
 748 ROM projection and the ROM differential filter. Their effect on the resulting
 749 ROMs has been investigated in [14, 37, 38, 53, 56]. We believe, however, that
 750 finding the best explicit ROM spatial filter for the LES-ROM framework is
 751 an important open question.

752 Once the ROM spatial filter is chosen, another open question for the LES-
 753 ROM framework is finding the *optimal filter radius*, δ . We emphasize that,
 754 although heuristic scalings (e.g., $\delta \sim h$, where h is the mesh size) are often
 755 used in LES, the optimal scaling is, to our knowledge, still an open question in
 756 the LES field [25, 28]. To answer this question in our LES-ROM framework,
 757 we will use the LES-ROM discretization error (which consists of the error of
 758 the standard numerical discretization, the filtering error [25, 45, 47] and the

ROM truncation [61]) to develop δ scalings, which we will then numerically investigate for different test problems.

In the derivation of the LES-ROM framework in Section 3, we assumed that the differentiation and spatial filtering operators commute. We note that in the LES field, this assumption fails in certain situations (for example, when the radius of the spatial filter, δ , is variable) [25, 28]. In this cases, the *LES-ROM commutation error*, i.e., the error made by using the above assumption, must be addressed. Using a variable δ seems appropriate for our LES-ROM framework as well, especially when the POD modes display highly localized spatial features. Thus, we plan to investigate the magnitude of the LES-ROM commutation error when a variable δ is used. If the commutation error is relatively large compared with the discretization and modeling errors, then we will use various strategies to model it, just as in LES [25].

LES: Before or After? A natural question is whether spatial filtering and LES should be used to generate the snapshot data (i.e., before the ROM is used) or only to develop the ROM. We believe that in realistic, turbulent flow applications, spatial filtering and LES should be used both in the data generation and the ROM development (i.e., both “before” and “after”). The same conclusion seems to be yielded by the numerical investigation of a flow past the Ahmed body at $Re = 300,000$ in [18], in which a standard LES model (the Smagorinsky model) was used to generate the snapshots and a functional ROM closure model was utilized to stabilize the ROM. Since this paper represents the first step in the investigation of the new AD-ROM, we decided to separate the spatial filtering effects in the data generation from those in the ROM development. Thus, in this paper we only considered the “after” case. However, for the numerical simulation of realistic, high Reynolds number flows, we plan to use spatial filtering and LES both in the data generation and ROM development (i.e., both “before” and “after”).

AD-ROM Open Questions. The choice of other *regularization methods* in the AD-ROM should be carefully investigated. Indeed, as a first step, in this paper we considered only one of the simplest regularization method, the Lavrentiev regularization. We plan, however, to investigate other regularization strategies, both variational and iterative [50, 51, 52].

Probably the most important research direction that we plan to pursue is to investigate the AD-ROM in the numerical simulation of *realistic turbulent flows that display recurrent structures* (see, e.g., [18, 24]). We emphasize, however, that in these challenging settings, the current AD-ROM should

probably be supplemented with a *numerical dissipation mechanism* (e.g., time relaxation [45]), just as in LES [30, 31, 32, 49]. In this paper we investigated the AD-ROM without any additional numerical dissipation mechanism. We believe that decoupling the AD and dissipation mechanisms was necessary in order to understand the effect of the former, which, to our knowledge, is new in a ROM setting. We note, however, that for higher Reynolds number flows, adding numerical dissipation would probably be needed in order to account for the subgrid-scale effects due to the inherently coarse meshes used in the data generation.

In our numerical investigation, the accuracy of the new AD-ROM was similar to that of the EV-ROMs [14] and Reg-ROMs [38]. We believe that this is impressive, given that the new AD-ROM did not use any explicit numerical dissipation mechanisms, whereas the other ROMs did. For high Reynolds number flows, we plan to add numerical dissipation (e.g., time relaxation) to the AD-ROM and perform a *thorough comparison with other types of ROMs* (e.g., EV-ROMs [3, 8, 14], Reg-ROMs [37, 38] and calibrated ROMs [62, 63, 64, 65]).

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