Large-eddy models from variational principles

Master's Thesis

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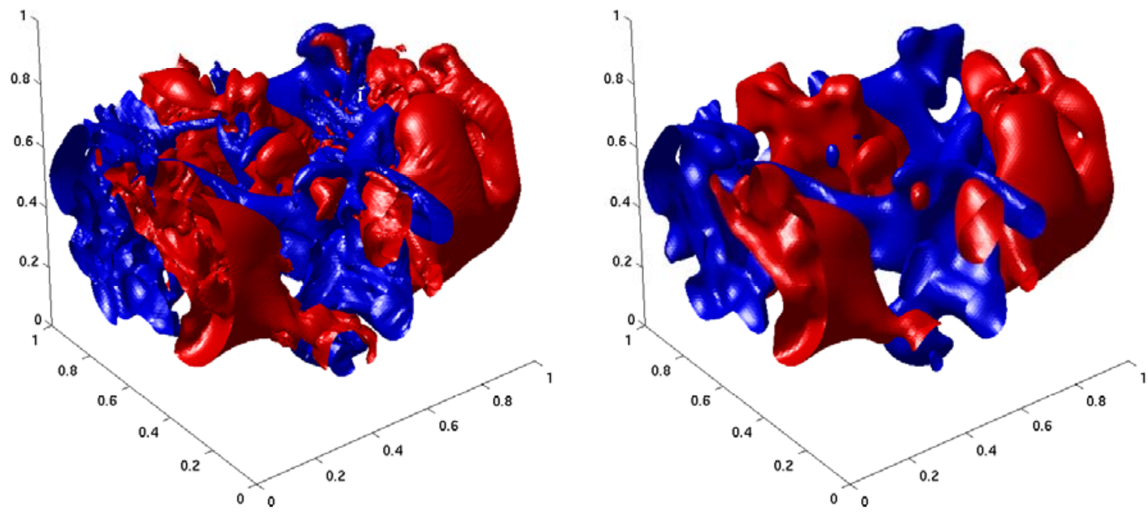
August 25, 2003



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August 25, 2003

I dedicate this work to my father. I hope that a successful surgery will take place soon, such that he is able to restart his beloved job as a farmer.

Abstract

We present a variational approach to structure the design of subgrid models in large-eddy simulation and the treatment of the flow near a solid wall. The variational approach consists of three successive stages. First, a variational principle for the considered equation expressed in the fluid parcel labels of the full velocity field is modified to yield a variational principle expressed in the fluid parcel labels of the filtered velocity field instead. A structured method to perform this modification is presented. Moreover, a filter is selected. Then, the unknowns - depending on the selected variational principle and filter - present in the given smoothed equations that result from a general variational principle and filter have to be determined. Finally, a treatment of the flow near a solid wall results from the variational approach and the physical consideration that the influence of that wall is negligible far from the wall. The wall treatment implies the natural constraint, no normal flow through the boundary, and boundary conditions which depend on the selected variational principle and filter. Moreover, a preliminary investigation is presented of employing a filter with a variable instead of constant filter width. The variational approach is illustrated for the incompressible Euler equations.

Preface

This report is the concluding work of my master's project performed at the Numerical Analysis and Computational Analysis group of Prof.dr.ir. Jaap van der Vegt, at the Mathematics department of the University of Twente. It contains the work performed predominantly in the final 6,5 weeks of my master's project. For the work carried out in the preceding 4,5 months, I refer to the unfinished previous final report. Besides some preparatory investigations for the work presented here, the previous research includes direct numerical simulations and large-eddy simulations of the one dimensional unforced and forced Burgers equation, both with a first and second order LDG-method and a second and fourth order FV-method.

I would like thank everyone who contributed in any way to the research for my master's project or the great five years I had in Twente. In particular, I would like to thank the guys of the turbulence meetings, in special Fedderik van der Bos and Chris Klaij, for their enthusiastic assistance, comments and discussions. Subsequently, I would like to thank my supervisors, Onno Bokhove and Bernard Geurts, for their enthousiastic supervision and for offering me plenty of challenges. Furthermore, I am gratefull to Prof.dr. D.D. Holm from Los Alamos National Laboratory for his readiness to participate in my graduation committee, his reviewing of this report and our discussions on the work. Finally, I would like to thank everyone who gave me understanding and support at the end.

Contents

1 Introduction

Modeling of complex flows is a topic of considerable research effort, as flows in typical environmental and engineering applications are very complicated. For simple flows, e.g., low Reynolds number flows in a simple geometry, a direct numerical simulation is often possible and captures all dynamically relevant features of the flow. For more complex flows, though, computational costs are (too) high. Hence, methods that capture only the large scales of the flow are introduced. Large-eddy simulation [12] is a prominent example of such methods. In large-eddy simulation the dynamics of the large scales of a flow are resolved, whereas the influence of the smaller scales on these large scales is modeled. The fundamental idea behind the modeling of the small scales in large-eddy simulation is that small scales tend to be more homogeneous and universal than the larger ones [11]. Moreover, small features are inclined to be less affected by the geometry.

For simple flows, large-eddy simulation performs well, and progress has been made for more complex flows [11]. However, plenty of challenges lie ahead for application of large-eddy simulation in technological applications. A major problem is that structures in the flow near a wall become very small. To be able to capture these detailed features with the large-eddy approach, the resolution near the wall needs to be very high, which induces high computational costs. Therefore, an explicit modeling of the flow near the wall is desirable [4]. Moreover, the tendency to similarity of the small, unresolved features gives hope for simple so-called subgrid models, which are applicable to many different flows. In spite of this, in the course of time numerous subgrid models have been developed for different situations [15]. To recover the uncomplicated structure of the basic ideas of large eddy simulation, it is desirable to introduce a fundamental basis for developing subgrid models. To construct this basis, a variational approach is selected. The aim of this work can thus be encapsulated by

Structuring the design of subgrid models and *treatment of the flow near a solid wall* by means of a *variational approach.*

The variational approach consists of three parts. In the first part, a filter and a variational principle suitable to derive an LES equation are selected. In the second part, the resulting regularized equations are given for an arbitrary Lagrangian and filter. The third part of the variational approach treats the modeling of the flow near a solid wall. The variational approach is compared with the traditional large-eddy approach in figure 1.

The outline of this report is as follows. First, a one dimensional example variational principle is presented at the end of this chapter, devoted to readers unfamiliar with variational principles. Then, in chapter 2 the variational approach is presented. Next, the approach is illustrated in chapter 3. Finally, in chapter 4 this work is summarized and recommendations for future research are given.

The main goal of this report is to enable the reader to derive subgrid models and to introduce wall modeling by means of the variational approach. Therefore, much attention is paid to detailed calculations and less emphasis lies on the interpretation of derived the subgrid models.

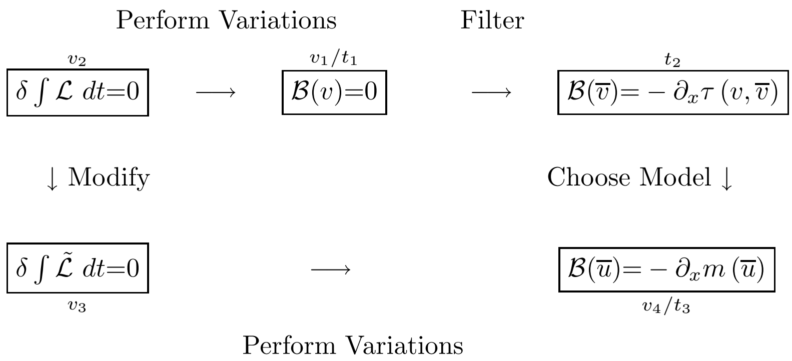

Figure 1: This schematic compares the traditional LES approach, $(t_1)-(t_3)$, with the variational approach, $(v_1)-(v_4)$. The 1D-case is conveyed for simplicity. Traditionally, the considered DNS equation, (t_1), e.g., Burgers for $\mathcal{B}(v)=\partial_t v+\partial_x\left(\frac{1}{2}v^2\right)=0$ with v velocity, is filtered (overbar). Using linearity of filter and commutivity of filtering with differentiation [5], and rearranging terms results in (t_2), where τ is the turbulent stress tensor, e.g., for Burgers equation $\tau=\frac{1}{2}\left[\overline{v^2}-\overline{v}^2\right]$, and $\overline{v}$ is the filtered solution of (t_1). To close this filtered equation, a subgrid model is introduced, e.g., the Bardina model: $m=\frac{1}{2}\left[\overline{\overline{u}^2}-\overline{\overline{u}}^2\right]$, and $\overline{u}$ is the solution of the resulting *LES equation in conservative or divergence form* (t_3) and we hope $\overline{u}\approx\overline{v}$ hopefully [5]) The variational approach starts with a variational principle, (v_2) , from which the DNS equation (v_1) can be derived, slightly modifies this principle (v_3), and after taking variations a smoothed equation results. Using the filter relations, it can be rewritten into an *LES equation*, $\mathcal{B}(\overline{u}){=}f\left(\overline{u}\right)$, which usually can be rewritten into the LES conservative form template (v_4). The (v_4/t_3)-box has two labels to emphasize that the obtained LES equations are presumably different.

The rest of this chapter concerns a one dimensional example of a variational principle. The aim of this example is to acquaint readers who are unfamiliar with variational principles. If the reader knows about calculus of variations, this section may be skipped.

The density, ρ, and filtered velocity, $\overline{u}$, are determined by the Lagrangian fluid particle label, a, by

$$\rho = \partial_x a \quad \text{and} \tag{1.1a}$$
$$\overline{u} = -\partial_t a/\partial_x a. \tag{1.1b}$$

The example variational principle we consider reads [10]

$$0=\delta\int_t \mathcal{L}\left(\rho\left(a\right),u\left(a\right);p\right)\ dt \equiv \lim_{\varepsilon\to 0}\frac{1}{\varepsilon}\int_t \mathcal{L}\left(\rho\left(a+\varepsilon\delta a\right),u\left(a+\varepsilon\delta a\right);p+\varepsilon\delta p\right)\ -\mathcal{L}\left(\rho\left(a\right),u\left(a\right);p\right)\ dt, \tag{1.2a}$$

with Lagrangian $\mathcal{L}$ given by

$$\mathcal{L}=\int_S\left(\tfrac{1}{2}\overline{u}u-p\left(\rho-1\right)\right)dx. \tag{1.3a}$$

Here, δ means taking *arbitrary* variations with respect to the two parameters governing this variational principle (1.3), which are a and p. This becomes visible from substitution of (1.1a) and (1.1b) in (1.3). Next, taking δ within the integrals, performing variations and rearranging terms yields

$$0=\int\left(\tfrac{1}{2}u\delta\overline{u}+\tfrac{1}{2}\overline{u}\delta u-p\delta\rho-\left(\rho-1\right)\delta p\right)\ dxdt. \tag{1.4}$$

To continue, we first need to express δu in $\delta \overline{u}$ and we therefore need to define a relation between the filtered velocity $\overline{u}$ and the full velocity u. Let us choose as an example the Helmholtz filter, for which $u = \overline{u} - \alpha^2 \partial_{xx} \overline{u}$. Taking variations of this relation between filtered and full velocity yields

$$\delta u = \delta \overline{u} - \alpha^2 \left(\partial_{xx} \delta \overline{u} \right), \tag{1.5}$$

as from definition (1.2a) follows that taking variations commutes with differentiation. Substituting (1.5) in $\int \frac{1}{2} \overline{u} \, \delta u \, dxdt$ yields

$$\int \tfrac{1}{2} \overline{u} \delta \overline{u} - \alpha^2 \overline{u} \left(\partial_{xx} \delta \overline{u} \right) \, dxdt = \int \tfrac{1}{2} \left(\overline{u} - \alpha^2 \partial_{xx} \overline{u} \right) \delta \overline{u} \, dxdt = \int \tfrac{1}{2} u \delta \overline{u} \, dxdt, \tag{1.6}$$

where the first step follows from integrating by parts twice and the second step results from substitution of (1.5). Note that we assume here that boundary terms arising upon integrating by parts vanish. Substituting the result in (1.4) yields

$$0 = \int \left(u \delta \overline{u} - p \, \delta \rho - (\rho - 1) \, \delta p \right) \, dxdt. \tag{1.7}$$

The next step is to express $\delta \overline{u}$ and $\delta \rho$ in terms of δa. Therefore, taking δ (1.1b) yields

$$\delta \overline{u} = -\frac{1}{\partial_x a} \delta \left(\partial_t a \right) - \left(\partial_t a \right) \delta \left(\frac{1}{\partial_x a} \right). \tag{1.8}$$

Furthermore, $\delta \left(1/\partial_x a \right) = -1/\left(\partial_x a \right)^2 \delta \left(\partial_x a \right)$. Substituting this expression in (1.8), applying commutation of δ with differentiation and rearranging terms yields

$$\delta \overline{u} = -\frac{1}{\partial_x a} \left(\left(\partial_t \delta a \right) - \frac{\left(\partial_t a \right)}{\left(\partial_x a \right)} \left(\partial_x \delta a \right) \right). \tag{1.9}$$

Finally, substituting (1.1b) and (1.1a) results in

$$\delta \overline{u} = -\left(\partial_t \delta a + \overline{u} \partial_x \delta a \right) / \rho. \tag{1.10}$$

Substituting (1.10) and $\delta \rho = \partial_x \delta a$ in (1.7) and rearranging gives

$$0 = \int \left(-\frac{u}{\rho} \partial_t \delta a - \left(\frac{u \overline{u}}{\rho} + p \right) \partial_x \delta a - (\rho - 1) \, \delta p \right) \, dxdt. \tag{1.11}$$

Partial integration and assuming that boundary terms vanish then yields

$$0 = \int \left(\left[\partial_t \left(\frac{u}{\rho} \right) + \partial_x \left(\frac{u \overline{u}}{\rho} + p \right) \right] \delta a - (\rho - 1) \, \delta p \right) \, dxdt. \tag{1.12}$$

Since δa and δp are arbitrary, we must have

$$\partial_t \left(\frac{u}{\rho} \right) + \partial_x \left(\frac{u \overline{u}}{\rho} \right) + \partial_x p = 0 \quad \text{and} \quad \rho = 1. \tag{1.13}$$

Substituting this incompressibility constraint $\rho = 1$ in (1.13) yields the final equation of motion,

$$\partial_t u + \partial_x \left(u \overline{u} \right) + \partial_x p = 0. \tag{1.14}$$

Note that p is called a Lagrange multiplier [10]. This multiplier is introduced in the variational principle (1.3) to enforce the constraint $\rho - 1 = 0$.

2 Variational Approach

In this chapter, the variational approach to develop subgrid models is introduced. The approach consists of three parts. In the first part, an LES variational principle and filter are selected. This selection is discussed in section 2.1. In the second part, the regularized equations for a *periodic domain*, which result from the selected principle and filter, are derived by means of the variational framework. This variational framework is presented in section 2.2. In the third part, the variational framework is reconsidered for a domain with solid boundaries. The consequences of the presence of a solid wall are discussed in section 2.3. Moreover, a treatment of the flow near a solid wall is suggested. All analysis is performed for equations in two spatial dimensions.

2.1 Selection of Lagrangian and filter

The variational framework is applied to a selected LES variational principle and filter. First, the selection of filters is mentioned briefly. For appropriate choices of filter, we refer to the literature. To support the selection of the variational principle, a method is suggested to obtain an LES variational principle from the DNS variational principle. In addition, we provide the modelling steps involved. Finally, the scope to choose a variational principle is defined. The variational framework offers a systematic way to investigate the consequences of the choice of variational principle and filter (see next section).

We restrict to homogeneous, isotropic filters, i.e., filters which are independent of position and rotations in space. These filters can mathematically be represented by a convolution product [12]. A subset of these filters are the so-called differential filters [12, 2]. For differential filters not only the filter operator, defined by the convolution product, is known, but also the inverse operator, which is given by a linear differential operator. As parts of the analysis in this work are technically more straightforward for differential filters than for the remaining convolution filters, a distinction between these two types of filters is made whenever favorable.

As put forward in the introduction, any DNS variational principle is considered which is expressed in the velocity, $\mathbf{u}$, density, ρ, and pressure, p, of a fluid. Moreover, both the velocity and density are defined by the fluid parcel label that moves with the flow, $\mathbf{a_u}$, such that $\mathbf{u} = \mathbf{u}(\mathbf{a_u})$ and $\rho = \rho(\mathbf{a_u})$ [7]. Besides, by definition, $\mathbf{a_u}$ satisfies the advection law, $(\partial_t + \mathbf{u} \cdot \nabla)\mathbf{a_u} = \mathbf{0}$. A DNS variational principle can be formulated as[1]

$$0 = \delta \int_t \mathcal{L}(\rho(\mathbf{a_u}), \mathbf{u}(\mathbf{a_u}); p)\ dt \equiv \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \int_t \mathcal{L}(\rho(\mathbf{a_u} + \varepsilon\delta\mathbf{a_u}), \mathbf{u}(\mathbf{a_u} + \varepsilon\delta\mathbf{a_u}); p + \varepsilon\delta p)\ -\mathcal{L}(\rho(\mathbf{a_u}), \mathbf{u}(\mathbf{a_u}); p)\ dt, \tag{2.1}$$

where $\mathcal{L}$ is a Lagrangian functional. Now define a second fluid particle field, $\mathbf{a_{\overline{u}}}$, which moves with a filtered flow, $\overline{\mathbf{u}}$, i.e., $(\partial_t + \overline{\mathbf{u}} \cdot \nabla)\mathbf{a_{\overline{u}}} = \mathbf{0}$. Hence, $\overline{\mathbf{u}} = \overline{\mathbf{u}}(\mathbf{a_{\overline{u}}})$ and likewise, for the density of the filtered velocity field, $\hat{\rho}$, we have $\hat{\rho} = \hat{\rho}(\mathbf{a_{\overline{u}}})$.

The changes employed to derive an LES variational principle from the DNS variational principle (2.1) are:

1. expressing the DNS variational principle (2.1) in $\mathbf{a_{\overline{u}}}$ instead of $\mathbf{a_u}$. This fundamental modeling step is materialized by
   - expressing $\mathbf{u}$ in $\mathbf{a_{\overline{u}}}$ using the (theoretical) inverse filter relation, $\mathbf{u} = L^{-1}(\overline{\mathbf{u}})$,
   - and replacing the full velocity field density, $\rho(\mathbf{a_u})$, by the density of the filtered velocity field, $\hat{\rho}(\mathbf{a_{\overline{u}}})$.

   Consequently, the variational principle (2.1) becomes a *fundamental LES variational principle*,

$$0 = \delta \int_t \mathcal{L}(\hat{\rho}(\mathbf{a_{\overline{u}}}), \mathbf{u}(\mathbf{a_{\overline{u}}}); \overline{p})\ dt, \tag{2.2}$$

[1] According to [13] such a variational principle exists for any set of evolution equations, but its physical meaning might be disputable.

where δ now means arbitrary variations of $\mathbf{a}_{\overline{\mathbf{u}}}$ and $\overline{p}$.

2. (tentatively) neglecting terms in the fundamental LES variational principle (2.2) which arise after a decomposition of the velocity. The full velocity field can be decomposed into a filtered velocity field and its residual, $\mathbf{u} = \overline{\mathbf{u}} + \mathbf{u}'$. Hence, a DNS variational principle (2.1) and therefore the fundamental LES variational principle (2.2) typically contain $\mathbf{u}\cdot\mathbf{u}$. Substituting the decomposition in the nonlinear term and expanding terms yields $\mathbf{u}\cdot\mathbf{u} = \overline{\mathbf{u}}\cdot\overline{\mathbf{u}} + 2\overline{\mathbf{u}}\cdot\mathbf{u}' + \mathbf{u}'\cdot\mathbf{u}'$. We can obtain an LES variational principle by, for example, neglecting the terms $\overline{\mathbf{u}}\cdot\mathbf{u}'$ and $\mathbf{u}'\cdot\mathbf{u}'$ and hence only taking into account $\overline{\mathbf{u}}\cdot\mathbf{u}$. As $\mathbf{u}'$ can be substituted by $\mathbf{u} - \overline{\mathbf{u}}$, a fundamental LES variational principle on which a similar, second modeling step is performed can be expressed in the filtered and total velocity field as

$$0 = \delta \int_t \mathcal{L}\left(\hat{\rho}\left(\mathbf{a}_{\overline{\mathbf{u}}}\right), \overline{\mathbf{u}}\left(\mathbf{a}_{\overline{\mathbf{u}}}\right), \mathbf{u}\left(\mathbf{a}_{\overline{\mathbf{u}}}\right); \overline{p}\right)\ dt. \tag{2.3}$$

If, in addition to the fundamental modeling step described in item 1, terms are neglected, we refer to the variational principle as *reduced LES variational principle.* Note that this additional modeling step is optional.

To illustrate the method proposed here, the derivation of the basic LES variational principle and a reduced LES variational principle from an example DNS variational principle is presented in the next chapter.
The framework only allows variational principles of the form (2.3). Hence, if a variational principle is selected in a different way then proposed here, (2.3) defines the scope in which the LES variational principle can be chosen.
From (2.3) follows that an LES variational principle is fully expressed in the fluid parcel labels that move with the filtered flow, $\mathbf{a}_{\overline{\mathbf{u}}}$, and the pressure of the filtered flow, $\overline{p}$. Moreover, only the density of the filtered flow, $\hat{\rho}$, is present. Therefore, for ease of notation we denote henceforward $\mathbf{a} \equiv \mathbf{a}_{\overline{\mathbf{u}}}$, $\rho \equiv \hat{\rho}$ and $p \equiv \overline{p}$, unless stated otherwise. After the Lagrangian and filter are selected, the variational framework, as presented next, can be applied to them in order to obtain the resulting LES equations of motion.

2.2 Variational framework

In this section, the variational framework is introduced to derive regularized equations of motion on a periodic domain, from any variational principle of the form (2.3) and for an arbitrary filter. First, the exact definitions concerning an LES variational principle are given. Subsequently, the resulting smoothed equations are derived for two specific combinations of Lagrangian and filter. Then, this derivation of regularized equations is slightly extended, such that it is also applicable for the remaining combination of Lagrangian and filter. Next, we present a way in which the influence of a choice of filter or Lagrangian on the resulting equations of motion can be investigated systematically. Finally, the results of this section are summarized in (2.2.1).

The scaled density ρ is defined as

$$\rho \equiv \det\left(J\right), \tag{2.4}$$

where J is the Jacobian matrix of the mapping from Eulerian coordinates $\mathbf{x} \equiv \left(x^1, x^2\right)$ to label coordinates $\mathbf{a} \equiv \left(a^1, a^2\right)$. Its entries are given by

$$\left(J\right)^i_j \equiv \partial_j a^i, \tag{2.5}$$

where $\partial_j = \partial/\partial x^j$. Here i, j are in the range $\{1, 2\}$, as are all indices below. The inverse of J is denoted by J^{-1}, and the i, j^{th}-element of J^{-1} by $\left(J^{-1}\right)^i_j$. Moreover, in this work, the placement of indices, raised or lowered, is purely used as a rule: lowered indices sum with upper ones. If

$\mathbf{a}$ is now specified as the label coordinates of the *filtered* velocity field, $\overline{\mathbf{u}} \equiv (\overline{u}, \overline{v})$, these label coordinates satisfy the advection equation[2]

$$\partial_t a^i + \overline{u}^j \partial_j a^i = 0, \tag{2.6}$$

where t is time and $\partial_t = \partial/\partial t$.

Now the definitions are formulated, the regularized equations are derived for two special cases. In the first case, the selected Lagrangian does not contain the full velocity field. In the second case, a differential filter is selected, such that the full velocity field can be eliminated from the Lagrangian by substituting the inverse filter relation,

$$\mathbf{u} = L^{-1}(\overline{\mathbf{u}}). \tag{2.7}$$

The variational principle we consider then reads

$$0 = \delta \int_t \mathcal{L}(\mathbf{a}; p) \ dt, \tag{2.8}$$

where time integration is over the interval $[t_0, t_1]$, p a Lagrange multiplier introduced to enforce a constraint [10], and $\mathcal{L}$ any Lagrangian functional of the form

$$\mathcal{L}(\rho(\mathbf{a}), \overline{\mathbf{u}}(\mathbf{a}); p). \tag{2.9}$$

Here, ρ and p are the density and pressure respectively of the *filtered* velocity field $\overline{\mathbf{u}}$. The Lagrangian $\mathcal{L}$ depends on the fluid parcel labels $\mathbf{a}$ of the *filtered* velocity field and pressure p and hence δ denotes taking arbitrary variations with respect to $\mathbf{a}$ and p at fixed coordinates $\mathbf{x}$ and time t. Restriction to a Lagrangian of this form (2.9) is appropriate, as it allows a wide variety of regularized equations. Performing variations in (2.8) for any Lagrangian of the form (2.9) then yields

$$0 = \int_{S,t} \left(\frac{\delta \mathcal{L}}{\delta \overline{u}^k} \delta \overline{u}^k + \frac{\delta \mathcal{L}}{\delta \rho} \delta \rho + \frac{\delta \mathcal{L}}{\delta p} \delta p \right) d\mathbf{x} dt, \tag{2.10}$$

where $\int_{S,t}$ is an economic notation for both spatial integration over a periodic surface S and time integration over an interval $[t_0, t_1]$, and $\delta/\delta q$ denotes the functional derivative with respect to a function $q(\mathbf{a}, p)$ [14]. After some calculation, including partial integration in which boundary terms vanish due to periodicity, (2.10) results in

$$0 = \int_{S,t} \left(\rho \left(J^{-1}\right)_i^k \left[D_t \left(\frac{1}{\rho} \frac{\delta \mathcal{L}}{\delta \overline{u}^k} \right) + \frac{1}{\rho} \frac{\delta \mathcal{L}}{\delta \overline{u}^j} \partial_k \overline{u}^j - \partial_k \frac{\delta \mathcal{L}}{\delta \rho} \right] \delta a^i + \frac{\delta \mathcal{L}}{\delta p} \delta p \right) \ d\mathbf{x} dt, \tag{2.11}$$

where D_t denotes the time derivative at constant fluid label,

$$D_t \equiv \partial_t + \overline{\mathbf{u}} \cdot \nabla. \tag{2.12}$$

See Appendix B for details. As $\delta \mathbf{a}$ is arbitrary, (2.11) yields the smoothed equations of motion for any filter and any Lagrangian of the form (2.9),

$$D_t \left(\frac{1}{\rho} \frac{\delta \mathcal{L}}{\delta \overline{u}^k} \right) + \frac{1}{\rho} \frac{\delta \mathcal{L}}{\delta \overline{u}^j} \partial_k \overline{u}^j - \partial_k \frac{\delta \mathcal{L}}{\delta \rho} = 0. \tag{2.13}$$

Moreover, from (2.11) for arbitrary variations δp we obtain the condition

$$\frac{\delta \mathcal{L}}{\delta p} = 0. \tag{2.14}$$

[2] Note that this advection equation (2.6) can be derived from $\frac{\partial(a,b,\tau)}{\partial(x,y,t)} \frac{\partial(x,y,t)}{\partial(a,b,\tau)} = Id$, together with the following definition for the filtered velocity $\overline{\mathbf{u}} \equiv \partial \mathbf{x}/\partial \tau$. The former expression formulates the relation between the Jacobi matrices of the coordinate transformations from Eulerian coordinates $\mathbf{x}$ and time t to label coordinates $\mathbf{a}$ and Lagrangian time $\tau \equiv t$ and reversely, and Id denotes the identity matrix.

Note that these smoothed equations can be rewritten into *LES equations*, i.e., equations solely expressed in the filtered velocity, by using the filter operator and its (theoretical) inverse. If the inverse of a filter operator does not exist, an accurate inverse operator has to be constructed [3, 6]. usually in conservative form (v_4 figure 1).

As mentioned before, the above is only directly applicable to Lagrangians solely expressed in $\overline{\mathbf{u}}$ and an arbitrary filter, or differential filters in combination with any Lagrangian. However, a slight modification to the above derivation allows the extension to convolution filters. This alteration is presented below.

The variational principle of a Lagrangian of the type $\mathcal{L}_{\mathbf{u}}(\rho, \overline{\mathbf{u}}, \mathbf{u}; p)$ reads

$$0 = \delta \int_t \mathcal{L}_{\mathbf{u}}(\rho, \overline{\mathbf{u}}, \mathbf{u}; p)\ dt \tag{2.15a}$$

$$= \int_{S,t} \left(\frac{\delta \mathcal{L}_{\mathbf{u}}}{\delta \overline{u}^k} \delta \overline{u}^k + \frac{\delta \mathcal{L}_{\mathbf{u}}}{\delta u^i} \delta u^i + \frac{\delta \mathcal{L}_{\mathbf{u}}}{\delta \rho} \delta \rho + \frac{\delta \mathcal{L}_{\mathbf{u}}}{\delta p} \delta p \right) d\mathbf{x} dt, \tag{2.15b}$$

where the last step follows from straightforwardly taking variations. Comparison of (2.15*b*) with (2.10) shows that the only differences are the appearance of $\mathcal{L}_{\mathbf{u}}$ instead of $\mathcal{L}$, and an extra term involving $\delta\mathbf{u}$. This extra term can be rewritten into expressions containing $\delta\overline{\mathbf{u}}$ and $\delta\rho$ instead of $\delta\mathbf{u}$, if the relation between $\mathbf{u}$ and $\overline{\mathbf{u}}$ is finally taken into account:

$$\int_{S,t} \frac{\delta \mathcal{L}_{\mathbf{u}}}{\delta u^i} \delta u^i\ d\mathbf{x} dt \equiv \int_{S,t} A_i \delta \overline{u}^i + B \delta \rho\ d\mathbf{x} dt. \tag{2.16}$$

Here, $\mathbf{A}$ and B are functions of $\mathbf{u}$, $\overline{\mathbf{u}}$ and ρ, which are determined for a specific Lagrangian and filter by this relation (2.16). Resolving the unknown expressions $\mathbf{A}$ and B from (2.16) for convolution filters involves exchanging of integrals and possibly solving extra integral equations. Examples of these approaches are given in section 3.1.3 and 3.2.3 respectively. Substitution of (2.16) in (2.15), after rearrangements of terms, and comparison with (2.10) shows that for any variational principle (2.15*a*) and any filter, the form (2.10) can be derived, with functional derivatives given by

$$\frac{\delta \mathcal{L}}{\delta \overline{u}^i} = \frac{\delta \mathcal{L}_{\mathbf{u}}}{\delta \overline{u}^i} + A_i, \qquad \frac{\delta \mathcal{L}}{\delta \rho} = \frac{\delta \mathcal{L}_{\mathbf{u}}}{\delta \rho} + B \quad \text{and} \quad \frac{\delta \mathcal{L}}{\delta p} = \frac{\delta \mathcal{L}_{\mathbf{u}}}{\delta p}. \tag{2.17}$$

So along with the above specification of functional derivatives, the derivation from (2.10) to (2.11) applies. The resulting smoothed equations of motion and constraint for any Lagrangian of the form (**??**) and any convolution filter, are thus found by substituting (2.17) in (2.13),

$$D_t \left(\frac{1}{\rho} \frac{\delta \mathcal{L}_{\mathbf{u}}}{\delta \overline{u}^k} + \frac{A_k}{\rho} \right) + \left(\frac{1}{\rho} \frac{\delta \mathcal{L}_{\mathbf{u}}}{\delta \overline{u}^j} + \frac{A_j}{\rho} \right) \partial_k \overline{u}^j - \partial_k \left(\frac{\delta \mathcal{L}_{\mathbf{u}}}{\delta \rho} + B \right) = 0, \tag{2.18}$$

and (2.14),

$$\frac{\delta \mathcal{L}_{\mathbf{u}}}{\delta p} = 0. \tag{2.19}$$

Smoothed equations presented in the form (2.18) are rather beneficial for analyzing the consequences of chosen filters and Lagrangians. For a selected Lagrangian, (2.18) gives clear insight in the influence of the choice of filter on the resulting regularized equations. Moreover, a clear understanding is obtained of the influence of the choice of Lagrangian on the resulting smoothed equations. For sake of clarity: the terms which depend on the choice of filter are $\mathbf{A}$ and B, whereas the terms which do not depend on the choice of filter are given by the functional derivatives of $\mathcal{L}_{\mathbf{u}}$. The former can be seen from the definition of $\mathbf{A}$ and B, (2.16), and the latter from (2.15). Although for differential filters it is more straightforward to derive smoothed equations in the formulation (2.13), it might be desirable to derive equations in the formulation (2.18), such that more insight in the consequences of certain choices can be gained. To obtain (2.18) for differential filters, we first express $\delta\mathbf{u}$ in $\delta\overline{\mathbf{u}}$ and $\delta\rho$ by straightforward calculations on $\delta\mathbf{u} = \delta\left(L^{-1}(\overline{\mathbf{u}})\right)$. Substituting $\delta\left(L^{-1}(\overline{\mathbf{u}})\right)$ in the lhs (left hand side) of (2.16) and integrating by parts, yields an expression in the form rhs (right hand side) of (2.16). See section 3.1.4 and 3.2.4 for examples. In this way, the smoothed equations of motion for differential filters can be written in the form (2.18) as well.

2.2.1 Summary

The regularized equations of motion and constraint, resulting from definitions (2.4) − (2.6) along with an LES variational principle, given by (2.15a) and filter relation (2.7), are given by (2.18) and (2.19) respectively. These smoothed equations for any filter and Lagrangian contain two types of unknowns, which are the functional derivatives and the expressions $\mathbf{A}$ and B. The functional derivatives can easily be derived from (2.15). Resolving $\mathbf{A}$ and B from (2.16) requires more effort. Moreover, the form (2.18) gives a clear insight in the consequences of the choice of filter (acts upon $\mathbf{A}$ and B only), and Lagrangian (determines the functional derivatives and acts upon $\mathbf{A}$ and B), on the resulting equations of motion. For the special cases in which the selected Lagrangians does not contain the full velocity field, (2.9), or the full velocity field can be eliminated from the considered Lagrangian by substituting the inverse filter relation, (2.7), the equations of motion are given in a simpler form, (2.13). Computations to obtain the functional derivatives in this form are straightforward, but it does not provide insight in the consequences of choices.

In section 2.2, merely the outline to determine the unknowns in the resulting smoothed equation has been presented. As put forward, these unknowns depend on the choice of filter and Lagrangian. Hence, to obtain regularized equations of motion without unknowns, a choice of Lagrangian and filter is required in the end. As obviously not all possible choices of Lagrangians and filters can be treated in this work, several illustrating examples are provided in the next chapter to facilitate the reader.

2.3 Wall behavior

The previously derived variational framework for periodic domains is reviewed here for domains with solid boundaries. Boundary terms that appear upon integrating by parts in different places of the framework have to be considered, as they no longer vanish necessarily. Moreover, convolution filters become inhomogeneous and anisotropic due to the presence of a wall [12], which requires additional study on, for example, interchanging of integrals. First, in section 2.3.1 a treatment of the flow near a wall is proposed. Then, in section 2.3.2, boundary terms which are independent of the choice of filter and Lagrangian are presented. Moreover, boundary conditions resulting from the proposed wall treatment are presented. The consequences of the presence of a solid wall which depend on the choice of filter and Lagrangian, are discussed in section 2.3.3.

2.3.1 Wall treatment

The wall treatment proposed here, is based on the requirement that the behavior of the flow in the interior of the domain with solid boundaries, coincides with the behavior of the flow for a periodic domain. This choice complies with the physical idea that far away from a wall the influence of that wall is negligible. Mathematically, this wall treatment means that conditions have to be imposed, such that the resulting smoothed equations for the domain with solid walls coincide with the equations for a periodic domain. Such a wall treatment is adopted in the rest of this work. Boundary conditions which result from the wall treatment for any Lagrangian and filter, are presented in the next section. Conditions implied by this wall treatment, depending on the choice of filter and Lagrangian, can not be treated in general. Hence, in section 2.3.3 the approach to obtain these conditions is merely discussed. In the next chapter, the approach is illustrated for a specific Lagrangian and filter (see section 3.1.4).

2.3.2 Lagrangian and filter independent wall behavior

The Lagrangian and filter independent influence of the introduction of walls is, that boundary terms arise upon integrating by parts in deriving (2.11) from (2.10) (see Appendix B). These boundary terms and conditions which cause them to vanish are presented below. Gauss' divergence theorem (C.3) and other theory from Appendix C is applied.

The first boundary term originates from partial integration in (B.1):

$$\int_{\partial S,t} \frac{\delta \mathcal{L}}{\delta \rho} \rho \left[\left(\mathbf{J}^{-1} \right)_i \delta a^i \cdot \mathbf{n} \right] \, dsdt, \tag{2.20}$$

where ∂S denotes the boundary of the surface S, $\mathbf{n}$ the outward unit normal vector on the boundary and the vector $\left(\mathbf{J}^{-1}\right)_i = \left[\left(J^{-1}\right)^1_i, \left(J^{-1}\right)^2_i \right]^T$. This boundary term vanishes if we impose that a particle located at the boundary at $t = 0$ never moves away from it (only moves along the boundary), which means that on the boundary in Eulerian space

$$\left(J^{-1} \delta \mathbf{a} \right) \cdot \mathbf{n} = 0, \tag{2.21a}$$

or equivalently on the boundary in label space

$$\delta \mathbf{x} \cdot \mathbf{n}_a = 0. \tag{2.21b}$$

Here, $\mathbf{n}_a$ is the outward unit normal vector in label space. This equivalence becomes clear if one would transform (2.20) into label space and use the following relation between variation of $\mathbf{a}$ in Eulerian space and variation of $\mathbf{x}$ in label space

$$\delta \mathbf{a} = -J \delta \mathbf{x}. \tag{2.22}$$

The second boundary term shows up in deriving (B.5) from (B.4) and is given by

$$-\int_S \left(\frac{\delta \mathcal{L}}{\delta \overline{u}_k} \, \left(J^{-1}\right)^k_i \delta a^i \right) |^{t=t_1}_{t=t_0} d\mathbf{x}, \tag{2.23}$$

which vanishes if we impose vanishing of $\delta \mathbf{a}$ at the endpoints in time

$$\delta \mathbf{a} \left(x, t_0 \right) = \mathbf{0} \quad \text{and} \quad \delta \mathbf{a} \left(x, t_1 \right) = \mathbf{0}. \tag{2.24}$$

The third and last boundary term comes from deriving (B.7) from (B.4) and is given by

$$-\int_{\partial S,t} \frac{\delta \mathcal{L}}{\delta \overline{u}_k} \, \left(J^{-1}\right)^k_i \left(\overline{\mathbf{u}} \cdot \mathbf{n} \right) \, \delta a^i dsdt. \tag{2.25}$$

Thus if we impose no normal flow through the boundary

$$\overline{\mathbf{u}} \cdot \mathbf{n} = 0 \text{ on } \partial S, \tag{2.26}$$

the boundary term (2.25) vanishes. The first (2.21) and third (2.26) boundary condition describe the same physical behavior.

Summarizing, the wall behavior for any Lagrangian and filter is implied by the following boundary conditions:

- Variations in $\mathbf{a}$ vanish at the endpoints in time:

$$\delta \mathbf{a} \left(x, t_0 \right) = \mathbf{0} \quad \text{and} \quad \delta \mathbf{a} \left(x, t_1 \right) = \mathbf{0}. \tag{2.27}$$

- No normal flow through the boundary, (2.21) or:

$$\overline{\mathbf{u}} \cdot \mathbf{n} = 0 \text{ on } \partial S. \tag{2.28}$$

The first condition is inherent to the type of variational principles our general variational principle (2.8 and 2.9) belongs to, i.e., Hamilton's principle [10]. The second condition is a natural physical constraint.

2.3.3 Lagrangian and filter specific wall behavior

Introduction of solid boundaries implies a reconsideration of resolving $\mathbf{A}$ and B from (2.16). This derivation of $\mathbf{A}$ and B is different for differential filters compared to convolution filters. Therefore, a separate kind of wall modeling depending on the choice of Lagrangian and filter, is implied for the two types of filters.

As mentioned in section 2.2, determining $\mathbf{A}$ and B for convolution filters involves exchanging integrals, and possibly solving extra integral equations. Adding a solid wall hence requires a reconsideration of these applied techniques.

In contrast, in the same section it was described that resolving $\mathbf{A}$ and B from (2.16) for differential filters involves straightforward integrating by parts, in which boundary terms arise. Obtaining the same LES equations for a domain with solid walls than for a periodic domain, requires boundary conditions to be imposed, which cause vanishing of the boundary terms. As mentioned before, this is illustrated for an example Lagrangian and filter in section 3.1.4.

3 LES equations

The variational approach to develop subgrid models for large eddy simulation, as presented in the previous chapter, is illustrated here. Therefore, we consider the Euler equations of motion for an ideal, incompressible fluid and incompressibility constraint[3],

$$(\partial_t + \mathbf{u}\cdot\nabla)\,\mathbf{u} + \nabla p = 0, \tag{3.1a}$$

$$\nabla\cdot\mathbf{u} = 0. \tag{3.1b}$$

Recall that the variational approach consists of three successive parts, which are in a nutshell, selection of the Lagrangian and filter, derivation of regularized equations from this Lagrangian and filter by means of the variational framework, and modeling of the wall. To select example LES Lagrangians, we adopt the method proposed in section 2.1. The variational framework and wall modeling is considered for a reduced LES variational principle like (2.3) and different kinds of filters in section 3.1. Then, in section 3.2, the variational framework and wall modeling for a fundamental LES variational principle like (2.1) and different types of filters is presented. Both example LES Lagrangians are deduced from the following Lagrangian for the Euler equations [9]:

$$\mathcal{L}_E = \int_S \left(\tfrac{1}{2}\rho\,|\mathbf{u}|^2 - p\,(\rho - 1)\right) d\mathbf{x}; \tag{3.2}$$

here ρ and u are expressed in the fluid parcel labels of the *full* velocity field and p is the pressure of the full velocity field.

Besides the illustrative aspect of these example Lagrangians and filters, two of them are worthwhile mentioning here. Firstly, in section 3.1.5 we derive Camassa-Holm like equations for an adjusted Helmholtz filter, $L^{-1} = (1 - \alpha^2\partial_{jj})$, in which α is not a constant, but a general function of space and time. In this way, one could enforce a more intensive filtering in regions where the flow is relatively smooth, and a reduced filtering in regions with more detailed structures, e.g., near a wall. How to make a suitable choice for $\alpha(\mathbf{x}, t)$ is not discussed here and left for future research. Secondly, as far as we know, the *full energy Lagrangian* presented in section 3.2 represents a new class of Lagrangians for which a new class of LES equations of motion can be derived. This class is both physically and mathematically more appealing, as it takes into account the energy of the full velocity field (hence its name) instead of only parts of it and hence does not involve the additional second modeling step. Future research is required to validate this class of LES equations numerically.

3.1 Reduced energy Lagrangian

In this section, the variational framework is applied to a reduced variational principle like (2.3) and several filters, and the wall treatment proposed in section 2.3.1 is adopted. First, the selected Lagrangian is presented and discussed in section 3.1.1. Subsequently, the unknowns in the resulting equations of motion (2.18) and constraint (2.19) , which result from the variational framework, are determined. Recall that these unknowns can be divided in two types: the functional derivatives and the expressions $\mathbf{A}$ and B. In section 3.1.2 is shown how to obtain the functional derivatives. Substituting the results yields regularized equations of motion and a constraint for an

[3] A reader familiar with Euler equations might notice that the continuity and energy equations are lacking. However, as they are not deduced directly from the variational principle (3.2), they are immaterial for our computations and hence left out in (3.1). If one likes, they can be deduced as follows. The continuity equation (A.10) can easily be obtained by taking the partial time derivative of the definition of ρ, (A.1), as shown in Appendix (A). Deducing an energy equation is less straightforward. It can be shown [1] that the terms $\lambda\,(\rho-1) + \rho U\,(\rho, s)$ together with the first law of thermodynamics and its variations, $\delta U = T\delta s + p/\rho^2\delta\rho$, yield the same terms in the resulting equations as the term $p\,(\rho - 1)$ in (3.3) . Here λ is a Lagrange multiplier, $U\,(\rho, s)$ the internal energy and $s\,(\mathbf{a})$ the entropy of the system, and p is a modified pressure related to the effective pressure P by $p = P + \lambda$. For ease, we might therefore as well use $p\,(\rho - 1)$ in our variational principle (3.3). Using $\partial_t s = (\partial_{a^i} s)\,(\partial_t a^i)$ an entropy equation can be deduced as the closing Euler equation. If one likes to have an energy equation instead, one can deduce it from taking the partial time derivative of $U\,(\rho, s)$ and using the continuity and entropy equation.

arbitrary filter. Next, in sections 3.1.3-3.1.5 the filter dependent expressions $\mathbf{A}$ and B are resolved from (2.16) for different kinds of filters, and the resulting regularized equations are presented. Moreover, in sections 3.1.2-3.1.5 the conditions implied by the wall treatment for any choice of filter and Lagrangian are repeated. In addition, in section 3.1.4 conditions implied by the wall treatment, which depend on the choice of filter and Lagrangian, are deduced. Finally, in section 3.1.6 we discuss how the formulation (2.18) enables a systematic investigation of the influence of choices on the resulting equations of motion.

3.1.1 Selection Lagrangian

The Lagrangian considered reads

$$\mathcal{L} = \int_S \left(\tfrac{1}{2}\rho\overline{\mathbf{u}}\cdot\mathbf{u} - p\left(\rho - 1\right)\right) d\mathbf{x}. \tag{3.3}$$

Instead of taking into account the kinetic energy of the full velocity field, $\frac{1}{2}\rho\mathbf{u}\cdot\mathbf{u}$, this Lagrangian only allows for a reduced energy, $\frac{1}{2}\rho\overline{\mathbf{u}}\cdot\mathbf{u}$, hence the name *reduced energy Lagrangian*. In addition to the fundamental modeling step, expressing the DNS Lagrangian in the labels of the filtered instead of the full velocity field (item 1 in section 2.1), this Lagrangian thus involves an extra modeling step (item 2). This step consists of neglecting the contributions to the energy of the cross term $\frac{1}{2}\rho\overline{\mathbf{u}}\cdot\mathbf{u}'$, and the subgrid scale term $\frac{1}{2}\rho\mathbf{u}'\cdot\mathbf{u}'$, where $\mathbf{u}'$ is the unresolved part of the velocity field.

The reduced energy Langrangian coincides for suitable choices of filters with a Lagrangian known in the literature [8]. Suitable choices of filters are for example differential filters which imply positivity of the Lagrangian (see section 3.1.4). This is a favorable property, as negativity of the Lagrangian might introduce additional, undesired instabilities. It can be shown that positivity of the reduced energy, $\frac{1}{2}\rho\overline{\mathbf{u}}\cdot\mathbf{u}$, also implies positivity of the neglected part of the energy, $\frac{1}{2}\rho\mathbf{u}'\cdot\mathbf{u}$. Hence, a *reduced energy Lagrangian* also literally refers to a decreased value of the considered energy.

3.1.2 General filter

In this section, the functional derivatives in (2.18) and (2.19) are determined from (2.15) and substituted, which yields the smoothed equations of motion and constraint for any filter. Performing variations for the variational principle (2.15a) with the reduced energy Lagrangian (3.3) and any filter, and rearranging terms gives

$$0 = \int_{S,t} \left(\tfrac{1}{2}\rho u_i \delta\overline{u}^i + \tfrac{1}{2}\rho\overline{u}_i\delta u^i + \left(\tfrac{1}{2}\overline{u}_i u^i - p\right)\delta\rho - \left(\rho - 1\right)\delta p\right) d\mathbf{x}dt. \tag{3.4}$$

Comparison of this expression with (2.15b) and (2.18) yields the resulting LES-equations for Lagrangian (3.3) and arbitrary filter

$$D_t\left(\tfrac{1}{2}u_i + \frac{A_i}{\rho}\right) + \left(\tfrac{1}{2}u_i + \frac{A_i}{\rho}\right)\partial_k\overline{u}^j - \partial_k\left(\tfrac{1}{2}\overline{u}_i u^i - p\right) - \partial_k B = 0. \tag{3.5}$$

Moreover, comparison of (3.4) with (2.19) results in incompressibility of the filtered velocity field[4]

$$\rho = 1, \ \text{ or, with } (2.6)\,, \ \nabla\cdot\overline{\mathbf{u}} = 0. \tag{3.6}$$

These smoothed equations apply for a periodic domain, or, with boundary conditions (2.27) and (2.28) for a domain with solid boundaries as well.

[4]One might wonder why the seemingly cumbersome approach is used, of formulating the variational principle in compressible description and introducing the Lagrange multiplier p to enforce incompressibility only at the end. Instead, one could consider to take the incompressible version of the variational principle straight from the beginning. However, as the fluid labels cannot be expressed explicitly into eachother (see (2.4), (2.5) and (2.6)), the incompressible version cannot be obtained.

In the following three sections, (classes of) filters are presented for which $\mathbf{A}/\rho = \frac{1}{2}\mathbf{u}$, such that the resulting smoothed equations remain simple. In fact, substituting $\mathbf{A}/\rho = \frac{1}{2}\mathbf{u}$ in (3.5) yields

$$D_t u_i + u_i \partial_k \overline{u}^j - \partial_k \left(\tfrac{1}{2} \overline{u}_i u^i - p + B \right) = 0. \tag{3.7}$$

3.1.3 Convolution filters

In the previous section, the functional derivatives in (2.18) and (2.19) were determined for the reduced energy Lagrangian (3.3) and any filter. This resulted in the smoothed equations of motion and constraint, valid for any filter, given by (3.5) and (3.6) respectively. In this section, the remaining unknowns, the expressions $\mathbf{A}$ and B, are resolved from (2.16) for linear symmetric (spatial) convolution filters. The resulting smoothed equations are presented.

For linear symmetric (spatial) convolution filters, the relation between the filtered and unfiltered velocity is given by

$$\overline{\mathbf{u}}(\mathbf{x}, t) = \int_S G(\mathbf{x} - \mathbf{y})\, \mathbf{u}(\mathbf{y}, t)\, d\mathbf{y}. \tag{3.8}$$

Here, the filter-kernel G is a normalized, i.e., for any constant solution $\mathbf{u} = \mathbf{c}$ we have $\overline{\mathbf{c}} = \mathbf{c}$, and symmetric in its argument, i.e., $G(\mathbf{z}) = G(-\mathbf{z})$, and integration is over a periodic domain. Moreover, the space convolution kernel $G(\mathbf{x} - \mathbf{y})$ in $\mathbb{R}^2$ is assumed to be obtained by multiplying two one-dimensional filter-kernels:

$$G(\mathbf{z}) = \Pi_{i=1,2} G_i(z_i). \tag{3.9}$$

Three classical convolution filters for LES which satisfy these properties are the box or top-hat filter, the Gaussian filter and the spectral or sharp cutoff filter [12]. To give an idea of what these filter-kernels look like, the top-hat filter is

$$G(z_i) = \begin{cases} \frac{1}{\Delta_i} & \text{if } |z_i| \leq \frac{\Delta_i}{2}, \\ 0 & \text{otherwise.} \end{cases} \tag{3.10}$$

As it is quite cumbersome to perform calculations in the reduced energy variational principle (3.3) on linear convolution filters (3.8) themselves, these convolution filters are adjusted to a more convenient, compressible convolution filter as follows

$$\overline{\mathbf{u}}(\mathbf{x}, t) = \frac{1}{\rho} \int_S G(\mathbf{x} - \mathbf{y})\, \mathbf{u}(\mathbf{y}, t)\, d\mathbf{y}. \tag{3.11}$$

As for any Lagrangian and filter incompressibility, (2.14), is obtained in the end, the original incompressible filters are recovered.

Performing variations on the variational principle with the reduced energy Lagrangian (3.3), we find $\delta \mathcal{L}_{\mathbf{u}} / \delta u^i = \frac{1}{2}\rho \overline{u}_i$. Substituting this expression in the lhs of (2.16), substituting the filter relation between $\overline{\mathbf{u}}$ and $\mathbf{u}$, (3.11), and rearranging integrals gives successively

$$\begin{aligned} \int_{S,t} \frac{\delta \mathcal{L}_{\mathbf{u}}}{\delta u^i} \delta u^i \; d\mathbf{x}dt &= \int_{S,t} \tfrac{1}{2} \rho \overline{u}_i \delta u^i \; d\mathbf{x}dt = \int_t \int_{\mathbf{x} \in S} \tfrac{1}{2} \int_{\mathbf{y} \in S} G(\mathbf{x} - \mathbf{y})\, \delta u^i(\mathbf{x}, t)\, u_i(\mathbf{y}, t) \; d\mathbf{y} \; d\mathbf{x}dt \\ &= \int_t \int_{\mathbf{y} \in S} \tfrac{1}{2} u_i(\mathbf{y}, t) \int_{\mathbf{x} \in S} G(\mathbf{y} - \mathbf{x})\, \delta u^i(\mathbf{x}, t) \; d\mathbf{x} \; d\mathbf{y}dt = \int_{S,t} \tfrac{1}{2} \rho u_i \overline{\delta u^i} \; d\mathbf{x}dt. \end{aligned} \tag{3.12}$$

Next, $\overline{\delta \mathbf{u}}$ needs to be expressed in terms of $\delta \overline{\mathbf{u}}$ and $\delta \rho$. Therefore, variations of the filter relation (3.11) are taken, which yields successively,

$$\delta \overline{\mathbf{u}} = \frac{1}{\rho} \int_S G(\mathbf{x} - \mathbf{y})\, \delta \mathbf{u}(\mathbf{y}, t)\, d\mathbf{y} + \delta \left(\frac{1}{\rho} \right) \int_S G(\mathbf{x} - \mathbf{y})\, \mathbf{u}(y, t)\, d\mathbf{y} = \overline{\delta \mathbf{u}} - \frac{\overline{\mathbf{u}}}{\rho} \delta \rho, \tag{3.13}$$

such that

$$\overline{\delta \mathbf{u}} = \delta \overline{\mathbf{u}} + \frac{\overline{\mathbf{u}}}{\rho} \delta \rho. \tag{3.14}$$

Substituting (3.14) in (3.12) yields

$$\int_{S,t} \frac{\delta \mathcal{L}_{\mathbf{u}}}{\delta u^i} \delta u^i \; d\mathbf{x}dt = \int_{S,t} \left(\tfrac{1}{2}\rho u_i \delta \overline{u}^i + \tfrac{1}{2} u_i \overline{u}^i \delta\rho \right) \; d\mathbf{x}dt. \tag{3.15}$$

Comparison of (3.15) with (2.16) shows that $\mathbf{A} = \frac{1}{2}\rho\mathbf{u}$ and $B = \frac{1}{2}u_i\overline{u}^i$. Substituting these expressions for $\mathbf{A}$ and B in (3.5) and rearranging terms, results in the equations of motion for any normalized and symmetric linear convolution filter,

$$\left(\partial_t + \overline{\mathbf{u}} \cdot \nabla\right) \mathbf{u} + \nabla p = \overline{u}_i \nabla u^i. \tag{3.16}$$

Moreover, if the boundary conditions (2.27) and (2.28) are imposed, these equations hold for a domain with solid boundaries as well.
The lhs of (3.16) conveys Leray regularization [6] of the Euler equations of motion (3.1a).

3.1.4 Homogeneous diffential filters

Similar to the previous section, the remaining unknowns $\mathbf{A}$ and B in (3.5) are determined, but this time for a subset of symmetric differential filters. The resulting regularized equations of motion are presented as well. For the well known Helmholtz filter higher dimensional incompressible Camassa-Holm equations are obtained. Finally, a wall behavior which depends on the choice of filter and Lagrangian, is deduced.

Symmetric differential filters are differential filters of the form $\mathbf{u} = p\left(\partial_{jj}\right)\overline{\mathbf{u}}$, where we denote summation over j by subscript double j and $p\left(\partial_{jj}\right) = 1 + c_1\partial_{jj} + c_2\left(\partial_{jj}\right)^2 + ...,\; c_i \in \mathbb{R}$. As explained in section 3.1.2, we restrict to filters, for which a compressible extension exists with $\mathbf{A}/\rho = \frac{1}{2}\mathbf{u}$. Therefore, the subset of symmetric differential filters we consider here is

$$\mathbf{u} = \sum_{n=0}^{k} \left(-1\right)^n \alpha^{2n} \left(\partial_{jj}\right)^n \overline{\mathbf{u}}, \quad k \in \{1, 2, ...\}. \tag{3.17}$$

From dimensional analysis, α is a length scale. Moreover, this α determines the extend of the filter [5]. In this section, α is a constant. In the following section, it will be considered as a function of space and time. The compressible version of these differential filters we consider ensures $\mathbf{A}/\rho = \frac{1}{2}\mathbf{u}$ and positivity of the Lagrangian[5],

$$\mathbf{u} = \sum_{n=0}^{k} \left(-1\right)^n \frac{\alpha^{2n}}{\rho} \left(\partial_j\right)^n \left(\rho \left(\partial^j\right)^n \overline{\mathbf{u}}\right), \quad k \in \{1, 2, ...\}. \tag{3.18}$$

For sake of clarity, we present the determination of the unknowns $\mathbf{A}$ and B for the simplest case, $k = 1$. However, for $k > 1$ the analysis is similar. For $k = 1$, (3.17) yields the well known Helmholtz filter,

$$\mathbf{u} = He\left(\overline{\mathbf{u}}\right) \equiv \left(1 - \alpha^2\partial_{jj}\right)\overline{\mathbf{u}}. \tag{3.19}$$

From (3.18) and $k = 1$, we find the desired compressible version of this Helmholtz filter,

$$\mathbf{u} = \overline{\mathbf{u}} - \alpha^2 \frac{1}{\rho} \partial_j \left(\rho \partial^j \overline{\mathbf{u}}\right). \tag{3.20}$$

To determine $\mathbf{A}$ and B from (2.16), we first substitute $\delta\mathcal{L}/\delta u^i = \frac{1}{2}\rho\overline{u}_i$ (see section 3.1.2) and (3.20) in the lhs of (2.16) and some straightforward calculations with the δ-symbol yields

$$\int \frac{1}{2}\rho\overline{u}_i \left[\delta\overline{u}^i - \alpha^2\partial_j\left(\rho\partial^j\overline{u}^i\right)\delta\left(\frac{1}{\rho}\right) - \frac{\alpha^2}{\rho}\partial_j\left(\partial^j\overline{u}^i\delta\rho\right) - \frac{\alpha^2}{\rho}\partial_j\left(\rho\left(\partial^j\delta\overline{u}^i\right)\right)\right] \; d\mathbf{x}dt. \tag{3.21}$$

[5] Positivity of the reduced energy Lagrangian (3.3) for a filter of the form (3.18) follows from substitution of (3.18) in (3.3) and n times integrating by parts of the n^{th}-term, which results in a Lagrangian *in energy form* $\mathcal{L} = \int_S \left(\frac{1}{2}\rho\left[\overline{u}_i\overline{u}^i + \alpha^2\left(\partial_j\overline{u}_i\right)\left(\partial^j\overline{u}^i\right) + \alpha^4\left(\partial_{jj}\overline{u}_i\right)\left(\partial^{jj}\overline{u}^i\right) + ...\right] - p\left(\rho - 1\right)\right) d\mathbf{x}$. It is obvious that this Lagrangian is positive. Moreover, taking variations of this Lagrangian and integrating by parts n times for a term containing an n^{th}-derivative of $\delta\overline{u}^i$ and comparing with (2.16) then shows that $A = \frac{1}{2}\rho u_i$.

Then, the third term of (3.21) is integrated by parts, which results in

$$\frac{\alpha^2}{2}\int (\partial_j \overline{u}_i)\left(\partial^j \overline{u}^i\right)\delta\rho \; d\mathbf{x}dt. \tag{3.22}$$

Next, the fourth term of (3.21) is integrated by parts, which yields

$$\frac{\alpha^2}{2}\int \rho\,(\partial_j \overline{u}_i)\left(\partial^j \delta\overline{u}^i\right) d\mathbf{x}dt, \tag{3.23a}$$

and after integrating the result once more we find

$$-\frac{\alpha^2}{2}\int \partial^j\left(\rho\partial_j \overline{u}_i\right)\; \delta\overline{u}^i d\mathbf{x}dt. \tag{3.23b}$$

Substituting (3.22), (3.23b) and $\delta\left(1/\rho\right) = -\delta\rho/\rho^2$ in (3.21), using (3.20) and rearranging terms gives

$$\int \frac{\delta\mathcal{L}}{\delta u^i}\delta u^i d\mathbf{x}dt = \int \left[\tfrac{1}{2}\rho u_i\right]\delta\overline{u}^i + \tfrac{1}{2}\alpha^2\left[\frac{\overline{u}_i}{\rho}\partial_j\left(\rho\partial^j\overline{u}^i\right) + (\partial_j\overline{u}_i)\left(\partial^j\overline{u}^i\right)\right]\delta\rho \; d\mathbf{x}dt. \tag{3.24}$$

Comparison of (3.24) with (2.16) yields the desired expressions for $\mathbf{A}$ and B,

$$\mathbf{A}/\rho = \frac{1}{2}\mathbf{u} \quad \text{and} \quad B = \tfrac{1}{2}\alpha^2\left[\frac{\overline{u}_i}{\rho}\partial_j\left(\rho\partial^j\overline{u}_i\right) + (\partial_j\overline{u}_i)\left(\partial^j\overline{u}^i\right)\right]. \tag{3.25}$$

For the reduced energy Lagrangian (3.3) and any filter, incompressibility, (3.6), holds, such that the ordinary Helmholtz filter (3.19) is recovered. Finally, the resulting smoothed equations for the reduced energy Lagrangian (3.3) and compressible Helmholtz filter (3.20) are obtained, by substituting $\rho = 1$ and (3.25) in (3.5) and reordering terms,

$$\begin{aligned}\partial_t u_k + \overline{u}^i\partial_i u_k + \partial_k p &= \left(\overline{u}_i - u_i\right)\partial_k\overline{u}^i + \tfrac{1}{2}\alpha^2\partial_k\left((\partial_j\overline{u}_i)\left(\partial^j\overline{u}^i\right)\right)\\ &= \alpha^2\left[(\partial_{jj}\overline{u}_i)\left(\partial_k\overline{u}^i\right) + \tfrac{1}{2}\partial_k\left((\partial_j\overline{u}_i)\left(\partial^j\overline{u}^i\right)\right)\right],\end{aligned} \tag{3.26}$$

where the relation between the filtered and unfiltered velocity field is defined by the Helmholtz filter (3.19). In vector notation these equations read

$$\left(\partial_t + \overline{\mathbf{u}}\cdot\nabla\right)\mathbf{u} + \nabla p = -u_i\nabla\overline{u}^i + \tfrac{1}{2}\nabla\left(\left|\overline{\mathbf{u}}\right|^2 + \alpha^2\left|\nabla\overline{\mathbf{u}}\right|^2\right), \tag{3.27}$$

where $\left|\nabla\mathbf{u}\right|^2 \equiv (\partial_j\overline{u}_i)\left(\partial^j\overline{u}^i\right)$. This is a higher-dimensional incompressible *Camassa-Holm equation* [8]. If, in addition, the boundary conditions (2.27) and (2.28) are imposed, these equations hold for a domain with solid boundaries as well.

Wall modelling First, the boundary terms are presented that arise upon integrating by parts in resolving $\mathbf{A}$ and B from (2.16), for the reduced energy Lagrangian (3.3), and the compressible Helmholtz filter (3.20). Next, boundary conditions are given, which imply vanishing of these boundary terms. In this way, the resulting smoothed equations for a domain with solid walls coincide with those for a periodic domain, as proposed in section 2.3.1. Gauss' divergence theorem (C.3) and other theory from Appendix C is applied without further notification.

The first boundary term which arises in deriving (3.22) from (3.21) reads

$$-\tfrac{1}{2}\alpha^2\int_{\partial S,t}\overline{u}_i\;\left(\nabla\overline{u}^i\cdot\mathbf{n}\right)\;\delta\left(\frac{1}{\rho}\right)\; d\mathbf{x}dt. \tag{3.28}$$

The second boundary term shows up in integrating by parts in deriving (3.23a) from (3.22),

$$-\tfrac{1}{2}\alpha^2\int_{\partial S,t}\rho\overline{u}_i\;\left(\nabla\delta\overline{u}^i\cdot\mathbf{n}\right)\; d\mathbf{x}dt. \tag{3.29}$$

Finally, a boundary term arises in deriving (3.23b) from (3.23a),

$$\tfrac{1}{2}\alpha^2 \int_{\partial S,t} \rho \left(\nabla \overline{u}_i \cdot \mathbf{n}\right) \; \delta \overline{u}^i \; d\mathbf{x}dt. \tag{3.30}$$

Boundary conditions which imply vanishing of these boundary terms are

- no gradients normal to the boundary,

$$\nabla \overline{u}^i \cdot \mathbf{n} = 0, \tag{3.31}$$

- and no gradients in the variation of u^i normal to the boundary

$$\nabla \delta \overline{u}^i \cdot \mathbf{n} = 0. \tag{3.32}$$

As taking variations and differentiating commute, the second condition is automatically fulfilled if the first one is imposed. Hence, for the reduced energy Lagrangian (3.3) and the compressible Helmholtz filter (3.20), (3.31) is the only boundary condition required for coinciding of the smoothed equations for a domain with solid walls, with those without walls.

In the next section, the variational framework is applied to the same Lagrangian, but a modified version of the filter under consideration in this section.

3.1.5 Inhomogeneous diffential filters

In this section, the filters (3.17) and their compressible extensions (3.18) are considered, but with α a different type of length scale. In the previous section, the length scale was taken constant. However, here α is considered as a general function of space and time. This enables space (and time) dependent filtering and hence a modelling of the flow near a solid wall. Appropriate choices of $\alpha(x,t)$ are not discussed here and left for future research.

Similar to the previous section, for sake of clarity computations are shown for $k = 1$. Substituting α by $\alpha(x,t)$ in (3.19) gives the inhomogeneous Helmholtz filter considered here,

$$\mathbf{u} = \overline{\mathbf{u}} - \partial_j \left(\alpha(x,t)^2 \left(\partial^j \overline{\mathbf{u}}\right)\right). \tag{3.33}$$

The considered compressible version emerges after substituting $\alpha(x,t)$ for α in (3.20),

$$\mathbf{u} = \overline{\mathbf{u}} - \frac{1}{\rho}\partial_j \left(\rho\alpha(x,t)^2 \, \partial^j \overline{\mathbf{u}}\right). \tag{3.34}$$

Almost similar to the computations in section 3.1.4, one can show that the resulting smoothed equations of motion are

$$\partial_t u_k + \overline{u}^i \partial_i u_k + \partial_k p = \left(\overline{u}_i - u_i\right) \partial_k \overline{u}^i + \frac{1}{2}\partial_k \left(\alpha^2 \left(\partial_j \overline{u}_i\right)\left(\partial^j \overline{u}^i\right)\right), \tag{3.35}$$

or, in vector notation,

$$\left(\partial_t + \overline{\mathbf{u}} \cdot \nabla\right) \mathbf{u} + \nabla p = -u_i \nabla \overline{u}^i + \nabla \left(\frac{1}{2}\left|\overline{\mathbf{u}}\right|^2 + \frac{1}{2}\left|\alpha \nabla \overline{\mathbf{u}}\right|^2\right). \tag{3.36}$$

3.1.6 Analyzing tool

Comparison of the regularized equations (3.5), which result from the reduced energy Lagrangian (3.3) and any filter, with the smoothed equations (3.39), which result from the second example Lagrangian (3.37) and any filter, gives insight in the consequences of these choices of Lagrangians. Likewise, comparison of the smoothed equations in sections 3.1.3-3.1.5, which result from the same Lagrangian (3.3), but different kinds of filters, would illustrate the systematic investigation of the influences of the choice of filters on the resulting equations of motion.

3.2 Full energy Lagrangian

Correspondingly to the previous section, the variational framework is applied here to another example LES Lagrangian and several filters. The example Lagrangian considered is a fundamental LES variational principle like (2.2). The exact variational principle is presented and discussed in section 3.2.1. Then, the first type of unknowns in the resulting equations of motion (2.18) and constraint (2.19), the functional derivatives, are determined in section 3.2.2. This yields the smoothed equations of motion and constraint for any filter. Then, the remaining type of unknowns, $\mathbf{A}$ and B, are resolved from (2.16), and the resulting smoothed equations are presented. First, this is done for linear convolution filters in section 3.2.3 and subsequently for the Helmholtz filter, as an example of differential filters, in section 3.2.4.

3.2.1 Selection Lagrangian

The fundamental LES Lagrangian (see item 1 in section 2.1) derived from the DNS Lagrangian for the Euler equations, (3.2), is given by

$$\mathcal{L} = \int_S \left(\frac{1}{2} \rho \left| \mathbf{u} \right|^2 - p \left(\rho - 1 \right) \right) d\mathbf{x}. \tag{3.37}$$

This Lagrangian has two advantages over the reduced energy Lagrangian from the previous section. First, no additional modelling step is involved in deriving this LES Lagrangian from the DNS Lagrangian. This Langrangian thus takes into account the energy of the full velocity field, hence the name *full energy Lagrangian*. Second, this Lagrangian is positive for any filter. As far as we know, this choice of Lagrangian is new and results in a new class of LES models. Disadvantage is, that the resulting equations might contain too much details and hence simulations might become unstable. Therefore, future research is required to validate subgrid models emerging from fundamental LES Lagrangians.

3.2.2 General filter

The regularized equations for an arbitrary filter are obtained by determining the functional derivatives in (2.18) and (2.19) for (2.15), and substituting the results. Variations are taken of the variational principle for the full energy Lagrangian (3.37), and terms are rearranged, which yields

$$0 = \int_{S,t} \left[\rho u_i \delta u^i + \left(\frac{1}{2} u_i u^i - p \right) \delta \rho - \left(\rho - 1 \right) \delta p \right] \, d\mathbf{x} dt. \tag{3.38}$$

Comparison of (3.38) with (2.18) gives the desired expressions for $\mathbf{A}$ and B. Substituting these expressions in (2.15*b*) yields that the resulting LES-equations for the full energy Lagrangian and arbitrary filter,

$$D_t \left(\frac{A_k}{\rho} \right) + \left(\frac{A_j}{\rho} \right) \partial_k \overline{u}^j - \partial_k \left(\frac{1}{2} u_i u^i - p \right) - \partial_k B = 0, \tag{3.39}$$

with the incompressibility constraint

$$\rho = 1. \tag{3.40}$$

Again, these equations apply for a periodic domain, or with the boundary conditions (2.27) and (2.28) for a domain with solid boundaries.

3.2.3 Convolution filters

In this section is indicated how to resolve the remaining unknowns in (3.39), $\mathbf{A}$ and B, from (2.16) for the compressible extension of linear symmetric convolution filters, defined by (3.11).

In the previous section we obtained $\delta \mathcal{L}_{\mathbf{u}} / \delta u^i = \rho u_i$ for any filter. Hence, (2.16) becomes

$$\int_{S,t} \rho u_i \delta u^i d\mathbf{x} dt \equiv \int_{S,t} A_i \delta \overline{u}^i + B \delta \rho \; d\mathbf{x} dt. \tag{3.41}$$

To resolve $\mathbf{A}$ and B from this expression, (3.14) is substituted in (3.41), which yields after reordering of terms,

$$\int_{S,t} \rho u_i \delta u^i d\mathbf{x}dt \equiv \int_{S,t} A_i \overline{\delta u}^i + \left(B - A_i \frac{\overline{u}^i}{\rho} \right) \delta\rho \; d\mathbf{x}dt. \tag{3.42}$$

Subsequently, $\overline{\delta u}^i$ is expressed in of $\delta \overline{u}^i$ and $\delta\rho$ by using the filter relation (3.11), and the first term of the rhs of (3.42) becomes successively

$$\int_{S,t} A_i \overline{\delta u}^i \; d\mathbf{x}dt = \int_t \int_{\mathbf{x}\in S} \frac{A_i(\mathbf{x},t)}{\rho(\mathbf{x},t)} \int_{\mathbf{y}\in S} G(\mathbf{x}-\mathbf{y}) \, \delta u^i(\mathbf{y},t) \, d\mathbf{y} \; d\mathbf{x}dt$$

$$= \int_t \int_{\mathbf{y}\in S} \delta u^i(\mathbf{y},t) \int_{\mathbf{x}\in S} G(\mathbf{y}-\mathbf{x}) \frac{A_i(\mathbf{x},t)}{\rho(\mathbf{x},t)} d\mathbf{x} \; d\mathbf{y}dt = \int_{S,t} \rho \overline{\left(\frac{A_i}{\rho} \right)} \delta u^i \; d\mathbf{x}dt. \tag{3.43}$$

Here the second step follows from exchanging intergrals and moving terms into or out of integrals like in (3.12). Substituting the result in (3.42) yields

$$\int_{S,t} \rho u_i \delta u^i d\mathbf{x}dt \equiv \int_{S,t} \rho \overline{\left(\frac{A_i}{\rho} \right)} \delta u^i + \left(B - A_i \frac{\overline{u}^i}{\rho} \right) \delta\rho \; d\mathbf{x}dt. \tag{3.44}$$

Finally, $\mathbf{A}$ and B can be resolved from (3.44). The second term in the rhs of (3.44) vanishes for $B = A_i \overline{u}^i / \rho$. Moreover, $\mathbf{A}$ has to satisfy

$$\overline{\left(\frac{A_i}{\rho} \right)} = u_i, \tag{3.45a}$$

or, substituting the filter relation (3.11),

$$\frac{1}{\rho} \int_S G(\mathbf{x}-\mathbf{y}) \frac{A_i(\mathbf{y},t)}{\rho(\mathbf{y},t)} d\mathbf{y} = u_i. \tag{3.45b}$$

Resolving $\mathbf{A}$ from these equations (3.45) constitutes the well known problem of finding the inverse filter relation [6]. $\mathbf{A}$ and B can now be substituted in (3.39) to yield the smoothed equations of motion for the full energy Lagrangian, (3.37), and any linear symmetric convolution filter, (3.8). These equations apply for a periodic domain, or, if the boundary conditions (2.27) and (2.28) are imposed, for a domain with solid walls as well.

In the following section, the variational framework is applied to the same Lagrangian, but a different kind of filter.

3.2.4 Differential filters

In this section, $\mathbf{A}$ and B, the remaining unknowns in (3.39), are resolved from (2.16) for the Helmholtz filter, (3.19). Recall that the fundamental distinction between differential filters and the remaining convolution filters is, that for differential filters the inverse filter, L^{-1}, is known as well. In this section, the associated technical advantage becomes clear once more, as we are able to explicitly write down the resulting smoothed equations of motion for the Helmholtz filter, which was not possible for the remaining convolution filters, as was shown in the previous section.

In the previous section is shown that (2.16) becomes (3.41) for the full energy Lagrangian. To resolve $\mathbf{A}$ and B from (3.41), the adjusted compressible inverse filter relation, (3.20), is substituted in δu^i in the lhs of (3.41), which yields

$$\int_{S,t} \rho u_i \delta \left(L^{-1} \overline{u}^i \right) d\mathbf{x}dt = \int_{S,t} \rho u_i \delta \left(\overline{u}^i - \alpha^2 \frac{1}{\rho} \partial_j \left(\rho \partial^j \overline{u}^i \right) \right) d\mathbf{x}dt. \tag{3.46}$$

Further computations yields

$$\int_{S,t} \left[\rho L^{-1}(u_i) \right] \delta \overline{u}^i + \left[\frac{\alpha^2}{\rho} u_i \partial_j \left(\frac{1}{\rho} \partial^j \overline{u}^i \right) - \frac{\alpha^2}{\rho^2} (\partial_j u_i) \left(\partial^j \overline{u}^i \right) + \frac{1}{2} u_i u^i - p \right] \delta\rho \; d\mathbf{x}dt, \tag{3.47}$$

where L^{-1} is the compressible Helmholtz filter, (3.20). Comparing with (3.41) yields the desired expressions for $\mathbf{A}$ and B. Substituting the obtained expressions and $\rho = 1$, in (2.13), yields the resulting smoothed equations of motion

$$D_t He\left(u_i\right) + \partial_k p = -He\left(u_i\right)\left(\partial_k \overline{u}^j\right) + \partial_k \left[\alpha^2 u_i \partial_{jj} \overline{u}^i - \alpha^2 \left(\partial_j u_i\right)\left(\partial^j \overline{u}^i\right) + \frac{1}{2} u_i u^i\right], \qquad (3.48)$$

where $He\left(\overline{\mathbf{u}}\right) \equiv \left(1 - \alpha^2 \partial_{jj}\right) \overline{\mathbf{u}}$ is the ordinary Helmholtz filter.

4 Conclusions and discussion

In this work, the design of subgrid models in large eddy simulation is structured by means of a variational approach. Moreover, a treatment of the flow near a wall is proposed.

The variational approach basically consists of three parts:

In the first part, a filter and a variational principle suitable to derive an LES equation is selected. In theory, the variational approach allows any variational principle consisting of the full and filtered velocity field, expressed in the fluid parcel labels of this filtered velocity field, and the density and pressure of the filtered velocity field. Expectation is that a suitable LES variational principle roughly resembles a variational principle from which the considered DNS equation can be derived. Based on this, a method to derive an LES variational principle from a DNS variational principle can be proposed. Moreover, the modeling steps involved in this derivation are presented. Appropriate choices of filters are not discussed. We simply refer to the available literature, e.g. [12].

The second part of the variational approach consists of the so-called variational framework. This variational framework gives the resulting regularized equations of motion, (2.18), and constraint, (2.19), for an arbitrary Lagrangian and filter. The framework applies to a periodic domain and is developed for two spatial dimensions. The formulation (2.18) consist of two different kinds of unknown terms: the functional derivatives, which depend on the choice of Lagrangian but are independent of the choice of filter, and the expressions $\mathbf{A}$ and B, which depend on both the choice of Lagrangian and filter. The framework instructs how to resolve these unknowns. In fact, the functional derivatives can be derived straightforwardly from the LES variational principle by (2.15), whereas $\mathbf{A}$ and B can be resolved from (2.16), which typically requires more effort. Besides, by means of (2.18) the variational framework enables a systematic investigation of the consequences of the choice of filter and Lagrangian. Moreover, an alternative formulation of the regularized equations is given by (2.13), which applies mainly to differential filters and does not enable the systematic investigation of the consequences of choices. However, if it is the goal to derive the resulting regularized equations straightforwardly, formulation (2.13) is advisable over (2.19). Finally, we want to stress that adopting the variational framework saves time and effort, as calculations which hold for an arbitrary variational principle and filter are processed in the formulations (2.13) and (2.18).

The third and final part of the variational approach addresses one of the major challenges in present-day large eddy simulation: appropriate modeling of the flow near a solid wall. A treatment of the flow near a wall is proposed, which is based on the requirement that the equations for a domain with solid boundaries coincide with the equations for the periodic domain. The underlying physical consideration is that the influence of a wall is negligible far from the wall. Mathematically, this treatment avoids complicated equations. For any Lagrangian and filter, the proposed wall treatment implies no normal flow through the boundary. Obviously, this is the natural constraint. Moreover, the wall treatment yields boundary conditions which depend on the choice of Lagrangian and filter. Obviously, these conditions can not be treated in general. An illustrating example is provided to facilitate the reader.

Summarizing, deriving a subgrid model by means of the variational approach requires subsequently the selection of an LES Lagrangian and filter, and determination of the unknowns in the regularized equations and constraint. Moreover, modeling of the flow near a wall by means of the variational approach requires derivation of constraints in addition to the natural boundary condition.

To illustrate the variational approach, subgrid models and a wall treatment are derived for the incompressible Euler equations of motion. As the emphasis in this work lies on outlining and illustrating the variational approach, only two results of this illustration are mentioned:

First, for an adjusted Helmholtz filter whose filter width depends on space and time, regularized equations of motion are obtained which resemble the higher-dimensional incompressible Camassa-Holm equations. This space dependency of the filter enables a treatment of the wall, as the filter width can for example be reduced near a wall and enlarged far from the wall. The exact way in which the filter depends on space and time is left for future research.

Second, as far as we know, the introduction of the fundamental Lagrangian (2.2) constitutes a new class of variational principles and hence regularized equations. This Lagrangian emerges from a Lagrangian for the considered DNS equation when the Lagrangian is expressed in the fluid parcel labels of the filtered instead of the full velocity field. The latter modeling step imitates the fundamental idea behind the well-known Leray-regularization. However, future research is required to validate the regularized equations resulting from the fundamental Lagrangian numerically.

In this report, much attention has been paid to detailed calculations. In doing so, we want to enable the reader to apply the variational framework and wall treatment for other Lagrangians and filters without much effort. Hence, extensions of the variational approach presented in this work should now be straightforward. For example, the variational approach presented in this work is developed for variational principles in an Eulerian frame of reference. However, an alternative method would be to consider variational principles formulated in a Lagrangian frame of reference which moves with the fluid parcel labels of the filtered velocity field. Some preliminary investigations indicated that deriving subgrid models from the Lagrangian frame of reference is technically much easier. However, the interpretation of the filters arising from this approach becomes more complex. At this moment, we are not able to predict the consequences of this increased complexity.

A Preliminary calculations

In this appendix, preliminary calculations are shown, which result in the various expressions used. Moreover, this section might serve as framework to extend the results to three dimensions, for example. The main results are the expressions for $\delta\rho$ in $(A.2)$, and $\delta\overline{u}^j$ in $(A.8)$ in terms of $\delta\mathbf{a}$ and an evolution equation for $\rho\left(J^{-1}\right)_i^j$ in $(A.15)$. The remaining expressions and equations are used in the derivations. (see [9])

We repeat the definitions

$$\rho \equiv \det\left(J\right), \tag{2.4}$$

$$\left(J\right)_j^i \equiv \partial_j a^i, \tag{2.5}$$

$$\partial_t a^i + \overline{u}^p \partial_p a^i = 0. \tag{2.6}$$

1. The density ρ, defined by (2.4) and (2.5), can be expressed in various ways:

$$\rho = \left(\partial_i a^1\right)\left(\partial_j a^2\right)\varepsilon^{ij}, \tag{A.1a}$$

$$\rho = \left(\partial_1 a^k\right)\left(\partial_2 a^l\right)\varepsilon_{kl} \quad \text{and} \tag{A.1b}$$

$$\rho = \tfrac{1}{2}\left(\partial_i a^k\right)\left(\partial_j a^l\right)\varepsilon^{ij}\varepsilon_{kl}. \tag{A.1c}$$

   Here ε_{ij} is the two dimensional alternating symbol, specified by $\varepsilon_{12} = 1$, $\varepsilon_{21} = -1$ and $\varepsilon_{11} = \varepsilon_{22} = 0$. These expressions for ρ can be found from expanding the determinant of the Jabobi matrix (2.4) and introducing the alternating symbol.

2. Variations in the density, $\delta\rho$, can be expressed in the variations in the fluid parcel label, $\delta\mathbf{a}$, by

$$\delta\rho = \rho\left(J^{-1}\right)_n^p \partial_p \delta a^n. \tag{A.2}$$

   This expression is obtained when taking variations of $(A.1c)$ and after exchanging i with j and k with l and twice applying the relation

$$\varepsilon^{ji} = -\varepsilon^{ij}, \tag{A.3}$$

   the result is

$$\boxed{\delta\rho = \left(\partial_i \delta a^k\right)\left(\partial_j a^l\right)\varepsilon^{ij}\varepsilon_{kl}}. \tag{A.4}$$

   Next, substitute $\left(\partial_i \delta a^k\right) = \left(\partial_p \delta a^k\right)\delta_i^p$, where δ_i^p is the Kronecker delta, and subsequently

$$\delta_i^p = \left(J^{-1}\right)_n^p \left(J\right)_i^n \tag{A.5}$$

$$= \left(\partial_i a^n\right)\left(J^{-1}\right)_n^p. \tag{A.6}$$

   Here, $(A.5)$ reflects that a matrix element of the identity, $Id = J^{-1}J$, is either one on the diagonal or zero otherwise, and (2.5) is substituted in the last step. Then, write out ε_{kl} and realize that $\left(\partial_i a^n\right)\left(\partial_j a^l\right)\varepsilon^{ij} = 0$ for $l = n$. Finally, substitution of $(A.1a)$ yields $(A.2)$.

3. A different formulation of the convection equation (2.6), is obtained by multiplying it by $\left(J^{-1}\right)_i^j$, using $(A.6)$, working out δ_p^j, and reordering:

$$\overline{u}^j = -\left(J^{-1}\right)_i^j \partial_t a^i, \;\; j = 1, 2. \tag{A.7}$$

4. Variations in the filtered velocity, $\delta\overline{\mathbf{u}}$, can be expressed in variations in the fluid particle label, $\delta\mathbf{a}$, by

$$\boxed{\delta\overline{u}^j = -\left(J^{-1}\right)_i^j \left(\partial_t \delta a^i + \overline{u}^p\, \partial_p \delta a^i\right)}. \tag{A.8}$$

This expression follows from taking variations of $(A.7)$, using the product rule and substituting

$$\delta\left(J^{-1}\right)_i^j = -\left(J^{-1}\right)_n^j \left(J^{-1}\right)_i^p \left(\partial_p \delta a^n\right) \tag{A.9}$$

and subsequently $(A.7)$ in the result, and some reordering of terms. The expression $(A.9)$ can be obtained from $0 = \delta\left(\delta_i^n\right)$, using a relation similar to $(A.5)$, $\delta_i^n = \left(J^{-1}\right)_i^p (J)_p^n$, using the product rule for δ, multiplying the obtained by $\left(J^{-1}\right)_n^j$, using $(A.5)$ and working out the Kronecker delta.

5. The continuity equation,

$$\partial_t \rho + \partial_k \left(\rho \overline{u}^k\right) = 0 \tag{A.10}$$

is implied by the definition of the density. Hence mass conservation holds for a general variational principle. It can be derived by taking the partial time derivative of $(A.1c)$. Similar to $(A.4)$ this can be rewritten into $\partial_t \rho = \left(\partial_i\left(\partial_t a^k\right)\right)\left(\partial_j a^l\right) \varepsilon^{ij} \varepsilon_{kl}$. Substituting (2.6) and applying the product rule of ordinary differentiation for ∂_i yields

$$\partial_t \rho = -\left(\partial_i \overline{u}^p\right)\left(\partial_p a^k\right)\left(\partial_j a^l\right) \varepsilon^{ij} \varepsilon_{kl} - \overline{u}^p \left(\partial_p\left(\partial_i a^k\right)\right)\left(\partial_j a^l\right) \varepsilon^{ij} \varepsilon_{kl}. \tag{A.11}$$

The first term of $(A.11)$ vanishes for $p = j$, as then $\left(\partial_p a^k\right)\left(\partial_j a^l\right) \varepsilon_{kl} = 0$. The remaining part of this term can be rewritten into $-\left(\partial_i \overline{u}^i\right) \rho$, by writing out ε^{ij}, exchanging k and l and applying $(A.3)$ and substituting $(A.1b)$. The second term of $(A.11)$ equals $-\overline{u}^p \partial_p \rho$, which follows from an expression like $(A.4)$, but with δ replaced by ∂_p. Combining the results gives $(A.10)$.

6. The partial time derivative of J^{-1} can be expressed as follows

$$\partial_t \left(J^{-1}\right)_i^j = \left(J^{-1}\right)_i^q \partial_q \overline{u}^j - \overline{u}^p \partial_p \left(J^{-1}\right)_i^j . \tag{A.12}$$

To obtain this expression, we need two equations similar to $(A.9)$, which read

$$\partial_t \left(J^{-1}\right)_i^j = -\left(J^{-1}\right)_n^j \left(J^{-1}\right)_i^q \left(\partial_q \left(\partial_t a^n\right)\right) \quad \text{and} \tag{A.13}$$

$$\partial_p \left(J^{-1}\right)_i^j = -\left(J^{-1}\right)_n^j \left(J^{-1}\right)_i^q \left(\partial_q \left(\partial_p a^n\right)\right). \tag{A.14}$$

Next, substitute (2.6) in $(A.13)$, apply the product rule and substitute (2.5). Then, substitute $(A.5)$ and work out the delta function. Finally, substitute $(A.14)$ to obtain $(A.12)$.

7. Finally, to obtain the expression,

$$\boxed{\partial_t \left(\rho \left(J^{-1}\right)_i^j\right) + \partial_p \left(\rho \overline{u}^p \left(J^{-1}\right)_i^j\right) = \rho \left(J^{-1}\right)_i^q \partial_q \overline{u}^j}, \tag{A.15}$$

substitute $(A.10)$ and $(A.12)$ in $\partial_t \left(\rho \left(J^{-1}\right)_i^j\right) = \left(\partial_t \rho\right) \left(J^{-1}\right)_i^j + \rho \left(\partial_t \left(J^{-1}\right)_i^j\right)$, which yields

$$\partial_t \left(\rho \left(J^{-1}\right)_i^j\right) = -\partial_n \left(\rho \overline{u}^n\right) \left(J^{-1}\right)_i^j + \rho \left(J^{-1}\right)_i^p \partial_p \overline{u}^j - \rho \overline{u}^q \partial_q \left(J^{-1}\right)_i^j . \tag{A.16}$$

Next, the first and third term of the rhs of $(A.16)$ can be combined into $-\partial_p \left(\rho \overline{u}^p \left(J^{-1}\right)_i^j\right)$, such that $(A.16)$ becomes $(A.15)$.

B Variational framework

This appendix is an addition to the presentation of the variational framework in section 2.2. It contains calculations performed to derive the smoothed equations of motion (2.11) from (2.10). All integrals are over space S and time t, unless explicitly stated otherwise. As periodicity is assumed, all boundary terms arising upon integration by parts vanish. (see also [7])

First one needs to express $\delta\rho$ and $\delta\overline{u}^k$ in terms of δa, which is done in appendix A. Substituting the expression for $\delta\rho$, $(A.2)$, in the first term of (2.10), and integrating by parts yields

$$\int \frac{\delta\mathcal{L}}{\delta\rho}\delta\rho \; d\mathbf{x}dt = -\int \partial_k \left(\frac{\delta\mathcal{L}}{\delta\rho}\rho\left(J^{-1}\right)^k_i\right)\delta a^i \; d\mathbf{x}dt = -\int \rho\left(J^{-1}\right)^k_i \partial_k \frac{\delta\mathcal{L}}{\delta\rho}\delta a^i \; d\mathbf{x}dt, \tag{B.1}$$

where the last step follows from ordinary differentiation and

$$-\int \frac{\delta\mathcal{L}}{\delta\rho}\partial_k \left(\rho\left(J^{-1}\right)^k_i\right)\delta a^i \; d\mathbf{x}dt = \int \frac{\delta\mathcal{L}}{\delta\rho} \; \left[\left(\partial_{xy}b - \partial_{yx}b\right)\delta a - \left(\partial_{xy}a - \partial_{yx}a\right)\delta b\right] \; d\mathbf{x}dt = 0. \tag{B.2}$$

To express $\rho\left(J^{-1}\right)$ in terms of J^j_i the standard relation between a 2×2-matrix and its inverse is applied,

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}^{-1} = \frac{1}{\det(A)}\begin{pmatrix} d & -b \\ -c & a \end{pmatrix}. \tag{B.3}$$

Substituting $(A.8)$ for $\delta\overline{u}^k$ in the second term of (2.10) yields

$$\int \frac{\delta\mathcal{L}}{\delta\overline{u}^k}\delta\overline{u}^k \; d\mathbf{x}dt = -\int \frac{\delta\mathcal{L}}{\delta\overline{u}^k}\left(J^{-1}\right)^k_i \left(\partial_t\delta a^i + \overline{u}^q \; \partial_q\delta a^i\right) \; d\mathbf{x}dt. \tag{B.4}$$

Integrating by parts the first term of $(B.4)$ gives

$$\int \partial_t \left(\frac{\delta\mathcal{L}}{\delta\overline{u}^k}\left(J^{-1}\right)^k_i\right)\delta a^i \; d\mathbf{x}dt = \tag{B.5}$$

$$\int \rho\left(J^{-1}\right)^k_i \; \partial_t\left(\frac{1}{\rho}\frac{\delta\mathcal{L}}{\delta\overline{u}^k}\right)\delta a^i + \frac{1}{\rho}\frac{\delta\mathcal{L}}{\delta\overline{u}^k}\partial_t\left(\rho\left(J^{-1}\right)^k_i\right)\delta a^i \; d\mathbf{x}dt, \tag{B.6}$$

and partial integration of the second term of $(B.4)$ yields

$$\int \partial_q\left(\frac{\delta\mathcal{L}}{\delta\overline{u}^k}\frac{\rho}{\rho}\left(J^{-1}\right)^k_i \; \overline{u}^q\right) \; \delta a^i \; d\mathbf{x}dt = \tag{B.7}$$

$$\int \rho\left(J^{-1}\right)^k_i \; \overline{u}^q\partial_q\left(\frac{1}{\rho}\frac{\delta\mathcal{L}}{\delta\overline{u}^k}\right) \; \delta a^i + \frac{1}{\rho}\frac{\delta\mathcal{L}}{\delta\overline{u}^k}\partial_q\left(\rho\left(J^{-1}\right)^k_i\overline{u}^q\right) \; \delta a^i \; d\mathbf{x}dt. \tag{B.8}$$

The second terms of the rhs of $(B.6)$ and $(B.8)$ can be combined using $(A.15)$ into

$$\int \rho\left(J^{-1}\right)^k_i \; \frac{1}{\rho}\frac{\delta\mathcal{L}}{\delta\overline{u}^j}\partial_k\overline{u}^j \; \delta a^i \; d\mathbf{x}dt. \tag{B.9}$$

Putting all results together and introducing the material derivative (2.12) leads to the smoothed equations of motion for any Lagrangian and filter (2.11).

C Integration by parts

To facilitate the reader, this appendix provides straightforward formulas regarding integration by parts.

Partial integration applied on an integral of two scalars simply reads

$$\begin{aligned} \int_{t_0}^{t_1} (\partial_t r_1)\, r_2 \; dt &= \int_{t_0}^{t_1} (\partial_t r_1 r_2) \; dt - \int_{t_0}^{t_1} r_1\, (\partial_t r_2) \; dt \\ &= r_1 r_2|_{t=t_0}^{t=t_1} - \int_{t_0}^{t_1} r_1\, (\partial_t r_2) \; dt. \end{aligned} \tag{C.1}$$

Integrating an integral over surface S of the gradient of an arbitrary scalar r multiplied by a vector v reads

$$\begin{aligned} \int_S v \cdot \nabla r \; d\mathbf{x} &= \int_S \nabla \cdot (vr) \; d\mathbf{x} - \int_S (\nabla \cdot v)\, r \; d\mathbf{x} \\ &= \int_{\partial S} (v \cdot \mathbf{n})\, r \; ds - \int_S (\nabla \cdot v)\, r \; d\mathbf{x}, \end{aligned} \tag{C.2}$$

where ∂S denotes the boundary of the surface S and $\mathbf{n}$ the outward unit normal vector on the boundary, and Gauss is applied,

$$\int_S (\nabla \cdot F) \; dA = \int_{\partial S} F \cdot \mathbf{n} \; ds. \tag{C.3}$$

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