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A framework for convection and boundary layer parameterization derived from conditional filtering

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ABSTRACT

A new theoretical framework is derived for parameterization of subgrid physical processes in atmospheric models; the application to parameterization of convection and boundary layer fluxes is a particular focus. The derivation is based on conditional filtering, which uses a set of quasi-Lagrangian labels to pick out different regions of the fluid, such as convective updrafts and environment, before applying a spatial filter. This results in a set of coupled prognostic equations for the different fluid components, including subfilter-scale flux terms and entrainment/detrainment terms. The framework can accommodate different types of approaches to parameterization, such as local turbulence approaches and mass-flux approaches. It provides a natural way to distinguish between local and nonlocal transport processes, and makes a clearer conceptual link to schemes based on coherent structures such as convective plumes or thermals than the straightforward application of a filter without the quasi-Lagrangian labels. The framework should facilitate the unification of different approaches to parameterization by highlighting the different approximations made, and by helping to ensure that budgets of energy, entropy, and momentum are handled consistently and without double counting. The framework also points to various ways in which traditional parameterizations might be extended, for example by including additional prognostic variables. One possibility is to allow the large-scale dynamics of all the fluid components to be handled by the dynamical core. This has the potential to improve several aspects of convection-dynamics coupling, such as dynamical memory, the location of compensating subsidence, and the propagation of convection to neighboring grid columns.

1. Introduction

In weather and climate models a range of important processes occur on scales that are too fine to be resolved. These processes must therefore be represented by subgrid models or 'parameterizations'; for an introduction and overview see, e.g., Mote and O'Neill (2000); Randall (2000); Kalnay (2003). A formal theoretical framework on which to build a subgrid model can be obtained by applying a spatial filter to the governing equations (e.g. Leonard 1975; Germano 1992; Pope 2000); this leads to equations for the filtered variables that resemble the original equations for the unfiltered variables, supplemented by terms representing the filter-scale effects of subfilter-scale variability. This formal approach is widely used in the development of numerical models for large eddy simulation (LES), but tends to be applied less systematically in the development of weather and climate models.

In weather and climate models a great variety of processes need to be parameterized; these include unresolved waves, local turbulence, and coherent structures such as convective thermals or plumes. These physical processes are qualitatively quite different from each other, and lead to subgrid models that are structurally quite different, for example eddy diffusivity schemes for local turbulence compared with mass flux schemes for cumulus convection. The usual LES filtering approach does not, itself, make any distinction between these different types of subgrid process.

Recent developments have suggested a requirement to be able to combine and extend these structurally different types of subgrid model (e.g. Lappen and Randall 2001; Arakawa 2004; Siebesma et al. 2007; Gerard et al. 2009; Grandpeix and Lafore 2010; Arakawa and Wu 2013; Storer et al. 2015). For example, a convective boundary layer involves turbulent eddies on a range of length scales up to the depth of the boundary layer, implying that the turbulent vertical transport has both local and nonlocal contributions. This has motivated the inclusion of 'countergradient' transport terms in boundary layer parameterizations (e.g. Holtslag and Boville 1993), as well as the development of the Eddy Diffusivity Mass Flux (EDMF) scheme (Soares et al. 2004; Siebesma et al. 2007) which, as its name implies, combines the eddy diffusivity and mass flux approaches within a single scheme.

A number of authors have argued for greater unification of parameterization schemes (e.g. Lappen and Randall 2001; Jakob and Siebesma 2003; Arakawa 2004; Siebesma et al. 2007), pointing out that the real atmosphere does not switch discontinuously for example between a dry boundary layer and a shallow-cumulus-topped boundary layer or between shallow convection and deep convection, and that such switching behavior in numerical models is unrealistic and undesirable. A concrete step in this direction is the scheme of Neggers et al. (2009) (see also Soares et al. 2004), which extends the EDMF approach by including moist processes and by allowing the thermals in the mass flux part of the scheme to penetrate above the top of the well-mixed boundary layer. The scheme is thus able to smoothly model transitions, in space and time, between a stratocumulus-topped boundary layer, a shallow cumulus regime, and a dry convective boundary layer.

Finally, there is a need for parameterization schemes to take into account the grid resolution of the parent model, i.e. to be ‘scale aware’. The issue is particularly acute at resolutions that partly resolve the process in question: the so-called ‘gray zone’. Approaches to handling the convective gray zone have considered not only relaxing the assumption of small convective area fraction, traditionally employed in mass flux schemes (Arakawa and Wu 2013; Grell and Freitas 2014), but also broadening the structure of the scheme to include a stochastic element to account for local departures from statistical equilibrium (Keane and Plant 2012), to include additional prognostic quantities to carry some dynamical memory (e.g. Gerard et al. 2009; Grandpeix and Lafore 2010; Park 2014), or by using a higher-order turbulence model rather than an entraining plume model to calculate convective transports (e.g. Bogenschutz et al. 2013; Storer et al. 2015). It should also be noted that the deep convective gray zone merges gradually into the shallow convective gray zone and then the boundary layer gray zone as horizontal resolution is refined. In other words, there is a rather broad range of model resolutions across which the challenges of representing gray zone processes must be addressed.

These considerations point to the need for a theoretical framework that can accommodate these multiple approaches to parameterization, both individually and in combination. Such a framework would facilitate the unification of different parameterizations, or the coupling of different parameterizations to each other and to the dynamical core. For example, it could help ensure that any dynamical or thermodynamic approximations are made consistently throughout a model. It could also help to prevent 'double counting' in which some contribution to a flux is computed in two different ways by two different parts of the model and counted twice in the total flux. It should be possible to derive specific parameterization schemes from the general framework via a set of clearly identifiable assumptions or approximations; this should enable the assumptions behind different parameterizations to be compared more easily. The framework should also be useful in interpreting observational data or LES data to underpin the development of parameterization schemes.

In this paper a new theoretical framework is derived and proposed for developing, coupling, and unifying subgrid parameterizations. We particularly have in mind the application of this framework to the parameterization of convection and its coupling to the boundary layer and to the larger scale dynamics, motivated by current challenges in this area (e.g. Holloway et al. 2014; Gross et al. 2017). However, the derivation is quite general.

The derivation (sections 2 and 3) is based on the idea of conditional filtering. It is closely related to the idea of conditional averaging, which has been proposed, for example, by Dopazo (1977) for the study of intermittent turbulent flows. Here, however, we use a spatial filter rather than an ensemble average, and we extend the approach to the fully compressible Euler equations. The spatial filter is analogous to that used in LES. However, in the conditional filtering approach the fluid is first partitioned into a number of regions identified by a set of quasi-Lagrangian labels that each take only the values 0 or 1. Multiplying the governing equations by one of the labels before applying the spatial filter effectively picks out only the fluid identified by that label. The process is repeated for each label in turn. For example, in the simplest version, one label might pick out cumulus updrafts while a second label picks out the rest of the fluid. In this way, with very few approximations, one obtains separate (but coupled) prognostic equations for each fluid component, each with corresponding subfilter-scale terms. The resulting equations resemble those used in modeling multiphase flow for engineering applications (e.g. Städtke 2006), though our derivation is somewhat simpler.

A critical element of any application of the proposed framework is to ensure that fluid parcels are appropriately labelled, which will require fluid parcels to be relabelled as the flow evolves. For example, if different labels are used for updraft fluid and environmental fluid then fluid parcels must be relabelled as they are entrained into the updraft and relabelled again when they are detrained. Section 4 discusses how relabelling may be included in the framework, and briefly discusses the relationship between relabelling and physical processes such as mixing and source terms.

Section 5 outlines how local turbulence closures and mass flux schemes are both accommodated in the proposed framework. It is instructive to see how a typical simple mass flux scheme is obtained by making certain approximations within the framework; this example is discussed in some detail.

An attractive feature of the proposed framework is that it suggests how one might extend traditional mass flux schemes for convection to include a prognostic treatment of the convective dynamics, allowing some aspects of dynamical memory to be captured. One could, moreover, allow the dynamical core to handle the convective as well as non-convective (or mean) dynamics. Such a treatment would allow convective systems to be advected to neighboring grid cells (e.g. Grandpeix and Lafore 2010). It would also allow the resolved dynamics to control the horizontal distribution of the compensating subsidence rather than the parameterized contribution being imposed in the convecting grid column (e.g. Krueger 2001; Kuell and Bott 2008). It would thus have the potential to overcome some significant limitations of most current convection schemes, especially at high horizontal resolution. This possibility is discussed briefly in section 6. Progress in analysing and implementing this approach will be reported elsewhere.

2. Conditionaly filtered compressible Euler equations

The derivation begins with the fully compressible Euler equations:

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

$$\frac{D\eta}{Dt} = 0, \tag{2}$$

$$\frac{Dq}{Dt} = 0, \tag{3}$$

$$\frac{D\mathbf{u}}{Dt} + \frac{1}{\rho}\nabla p + \nabla \Phi = 0, \tag{4}$$

$$p = P(\rho, \eta, q). \tag{5}$$

Here, ρ is the total fluid density, $\mathbf{u} = (u, v, w)$ is the fluid velocity, p is pressure, and Φ is geopotential. For simplicity the governing equations have been expressed in terms of ‘conservative’ variables η the specific entropy and q the total specific water content, and sources and sinks have been neglected. In reality source and sink terms are often important (e.g. Bannon 2002; Raymond 2013), and it is straightforward to include them (section 3). It may be convenient to replace η by some function of η; see section 4. Similarly, Coriolis terms have also been omitted, but it is straightforward to include them. The equation of state has been written in the generic form (5);

this form assumes thermodynamic equilibrium so that knowledge of ρ, η and q is enough to determine the mass fractions of water in vapor, liquid and frozen form, and hence determine p. This assumption is not critical to the derivation below and can be relaxed.

The derivation also applies to simplified equation sets such as hydrostatic, anelastic, or Boussinesq. However, an increasing number of weather and climate models are now based on the non-hydrostatic compressible Euler equations in order to be accurate across a wide range of scales (Davies et al. 2003). In order to be applicable to such models, we retain the compressible Euler equations here. Moreover, we do not wish to encourage the introduction of inconsistencies that might result from the use of different underlying equation sets in the parameterizations and the dynamical core.

In order to carry out conditional filtering a set of n Lagrangian labels I_i, $i = 1, \ldots, n$ is introduced. At any point in the fluid one of the I_i is equal to 1 while the others are equal to 0. We will refer to the fluid with $I_i = 1$ as the i^{th} fluid component. Eventually we envisage that the different fluid components might correspond to environment, updraft, and possibly downdraft, cold pool, near environment, further updrafts, etc. (Fig. 1). However, for the moment the I_i are just arbitrary Lagrangian labels.

Because the I_i are Lagrangian labels, we can write

$$\frac{DI_i}{Dt} = 0. \tag{6}$$

This equation will be used in the form

$$\frac{\partial I_i}{\partial t} + \mathbf{u} \cdot \nabla I_i = 0. \tag{7}$$

In this form there are time and space derivatives of discontinuous functions; these must be interpreted as Dirac δ-functions, and they will only make sense when integrated. However, the derivation below avoids explicit consideration of these δ-functions. Also, the derivation avoids the need to explicitly consider a surface integral over the boundary of any fluid component (though such consideration might be needed to formulate a specific parameterization of some terms).

Now consider a formal spatial filtering of the governing equations. This is analogous to the derivation of the filtered equations used in LES, with the key difference that the filter is restricted to each fluid component in turn with the aid of the labels I_i. Let $G(\boldsymbol{\xi},\Delta)$ be a kernel for the filter, where Δ is the filter width and $\int_D G(\boldsymbol{\xi},\Delta)\,d\boldsymbol{\xi} = 1$. Then a filtered variable, indicated by an overbar, is defined as a convolution of the unfiltered variable with the kernel:

$$\overline{X}(\mathbf{x}) = \int_D G(\mathbf{x}-\mathbf{x}',\Delta)X(\mathbf{x}')\,d\mathbf{x}', \tag{8}$$

where the integration is over the domain D of interest. (A density-weighted filter $\overline{X}^*$ may also be defined; see (A1).) It will be assumed below that the filter commutes with space and time derivatives: [1]

$$\overline{\frac{\partial X}{\partial t}} = \frac{\partial \overline{X}}{\partial t}; \qquad \overline{\nabla X} = \nabla \overline{X}; \qquad \text{etc.} \tag{9}$$

Now define σ_i to be the volume fraction of the i^{th} fluid component on the filter scale:

$$\sigma_i = \overline{I_i}. \tag{10}$$

Then, since $\sum_i I_i = 1$, it follows that $\sum_i \sigma_i = 1$. Also define the average density of the i^{th} fluid component on the filter scale ρ_i by

$$\sigma_i \rho_i = \overline{I_i \rho}. \tag{11}$$

To derive an evolution equation for $\sigma_i\rho_i$, multiply (1) by I_i and add to ρ times (7) to obtain

$$\frac{\partial}{\partial t}(I_i\rho) + \nabla\cdot(I_i\rho\mathbf{u}) = 0. \tag{12}$$

[1]This assumption will not be valid if the filter scale Δ varies in space or time. It will also break down near boundaries (such as the Earth's surface). The additional terms that arise from variations in Δ and from the presence of boundaries can be formally included at the expense of some additional complexity (e.g. Fureby and Tabor 1997; Chaouat and Schiestel 2013), and may be estimated numerically with the aid of a second filter scale $\tilde{\Delta} = 2\Delta$ (Chaouat and Schiestel 2013).

Apply the filter to this equation and use (9) to obtain

$$\frac{\partial}{\partial t}(\sigma_i\rho_i)+\nabla\cdot(\overline{I_i\rho\mathbf{u}})=0. \tag{13}$$

If we now define $\mathbf{u}_i$ to be the density-weighted velocity of the i^{th} fluid component on the scale of the filter

$$\mathbf{u}_i=\overline{I_i\rho\mathbf{u}}/\overline{I_i\rho}, \tag{14}$$

i.e.

$$\sigma_i\rho_i\mathbf{u}_i=\overline{I_i\rho\mathbf{u}}, \tag{15}$$

then (13) becomes

$$\frac{\partial}{\partial t}(\sigma_i\rho_i)+\nabla\cdot(\sigma_i\rho_i\mathbf{u}_i)=0. \tag{16}$$

Next we derive an evolution equation for the entropy of the i^{th} fluid component. Start by combining (2) with (1) to obtain the conservative form

$$\frac{\partial}{\partial t}(\rho\eta)+\nabla\cdot(\rho\mathbf{u}\eta)=0. \tag{17}$$

Take I_i times (17) plus $\rho\eta$ times (7) to obtain

$$\frac{\partial}{\partial t}(I_i\rho\eta)+\nabla\cdot(I_i\rho\mathbf{u}\eta)=0. \tag{18}$$

Now apply the filter and use (9) to obtain

$$\frac{\partial}{\partial t}(\overline{I_i\rho\eta})+\nabla\cdot(\overline{I_i\rho\mathbf{u}\eta})=0. \tag{19}$$

By analogy with (15), define η_i to be the density-weighted entropy of the i^{th} fluid:

$$\sigma_i\rho_i\eta_i=\overline{I_i\rho\eta}. \tag{20}$$

Now write

$$\begin{aligned}\overline{I_i\rho\mathbf{u}\eta} &= \overline{I_i\rho\mathbf{u}}\,\eta_i+(\overline{I_i\rho\mathbf{u}\eta}-\overline{I_i\rho\mathbf{u}}\,\eta_i)\\ &= \sigma_i\rho_i\mathbf{u}_i\eta_i+\mathbf{F}_{\text{SF}}^{\eta_i},\end{aligned} \tag{21}$$

where $\mathbf{F}_{\mathrm{SF}}^{\eta_i}$ is the subfilter-scale flux of η_i. Thus, (19) becomes

$$\frac{\partial}{\partial t}(\sigma_i \rho_i \eta_i) + \nabla \cdot (\sigma_i \rho_i \mathbf{u}_i \eta_i) = -\nabla.\mathbf{F}_{\mathrm{SF}}^{\eta_i}. \tag{22}$$

Subtracting η_i times (16) gives

$$\frac{\partial \eta_i}{\partial t} + \mathbf{u}_i \cdot \nabla \eta_i = -\frac{1}{\sigma_i \rho_i} \nabla.\mathbf{F}_{\mathrm{SF}}^{\eta_i}, \tag{23}$$

or, defining

$$\frac{D_i}{Dt} \equiv \frac{\partial}{\partial t} + \mathbf{u}_i \cdot \nabla \tag{24}$$

to be the 'material' derivative following the i^{th} fluid component,

$$\frac{D_i \eta_i}{Dt} = -\frac{1}{\sigma_i \rho_i} \nabla.\mathbf{F}_{\mathrm{SF}}^{\eta_i}. \tag{25}$$

In an analogous way, one may define the average density-weighted water content of the i^{th} fluid q_i and obtain its evolution equation

$$\frac{D_i q_i}{Dt} = -\frac{1}{\sigma_i \rho_i} \nabla.\mathbf{F}_{\mathrm{SF}}^{q_i}. \tag{26}$$

The subfilter-scale fluxes $\mathbf{F}_{\mathrm{SF}}^{\eta_i}$ and $\mathbf{F}_{\mathrm{SF}}^{q_i}$ are completely analogous to those obtained in the standard approach to filtering, in which there is only a single fluid component. But note that these are fluxes *within* fluid component i and involve contributions only from fluid component i; any fluxes *between* fluid components must occur through relabelling terms—see section 4.

Next consider the momentum equation. A key feature of this derivation is that we wish to end up with the same pressure gradient term appearing in the momentum equations for each of the labelled fluid components; see section 6 for a brief discussion. Taking ρ times (4) plus $\mathbf{u}$ times (1) gives the flux form of the momentum equation

$$\frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) + \nabla p + \rho \nabla \Phi = 0. \tag{27}$$

Then I_i times (27) plus $\rho\mathbf{u}$ times (7) gives

$$\frac{\partial}{\partial t}(I_i\rho\mathbf{u}) + \nabla\cdot(I_i\rho\mathbf{u}\mathbf{u}) + I_i\nabla p + I_i\rho\nabla\Phi = 0. \tag{28}$$

Now apply the filter to (28) and consider each term in turn. To an excellent approximation $\nabla\Phi$ will be constant over the filter scale, so

$$\overline{I_i\rho\nabla\Phi} = \overline{I_i\rho}\nabla\Phi = \sigma_i\rho_i\nabla\Phi. \tag{29}$$

The pressure gradient term is

$$\begin{aligned}\overline{I_i\nabla p} &= \sigma_i\nabla\overline{p} + \left(\overline{I_i\nabla p} - \sigma_i\nabla\overline{p}\right) \\ &= \sigma_i\nabla\overline{p} + \left(\overline{\nabla(I_i p)} - \sigma_i\nabla\overline{p}\right) - \overline{p\nabla I_i}.\end{aligned} \tag{30}$$

The term $\overline{p\nabla I_i}$ involves δ-functions at the boundary of the regions containing the i^{th} fluid component, and it represents the net pressure force (per unit volume) exerted upon fluid i by the other components. It may be decomposed into contributions from the boundary between fluid component i and each other fluid component j:

$$\overline{p\nabla I_i} = -\sum_j \mathbf{d}_{ij}, \tag{31}$$

where $\mathbf{d}_{ij}$ is minus the pressure force (i.e. the 'drag') exerted by fluid j on fluid i on the scale of the filter. It can be seen that $\mathbf{d}_{ij} = -\mathbf{d}_{ji}$, as required for conservation of momentum. (The case $j = i$ can be included by defining $\mathbf{d}_{ii} = 0$.) The term

$$\mathbf{b}_i = \left(\overline{\nabla(I_i p)} - \sigma_i\nabla\overline{p}\right) \tag{32}$$

accounts for the fact that the remaining filter-scale pressure gradient force is not given exactly by $\sigma_i\nabla\overline{p}$. By summing over i and using (10) it can be seen that

$$\sum_i \mathbf{b}_i = 0. \tag{33}$$

Now consider the time derivative term in (28). In (15) we have already defined $\mathbf{u}_i$ to be the density-weighted $\mathbf{u}$ of the i^{th} fluid, so

$$\frac{\partial}{\partial t}\overline{I_i \rho \mathbf{u}} = \frac{\partial}{\partial t}\left(\sigma_i \rho_i \mathbf{u}_i\right). \tag{34}$$

Finally, consider the momentum flux due to advection and write

$$\begin{aligned} \overline{I_i \rho \mathbf{u}\mathbf{u}} &= \overline{I_i \rho \mathbf{u}}\,\mathbf{u}_i + \left(\overline{I_i \rho \mathbf{u}\mathbf{u}} - \overline{I_i \rho \mathbf{u}}\,\mathbf{u}_i\right) \\ &= \sigma_i \rho_i \mathbf{u}_i \mathbf{u}_i + \mathsf{F}_{\text{SF}}^{\mathbf{u}_i}, \end{aligned} \tag{35}$$

where $\mathsf{F}_{\text{SF}}^{\mathbf{u}_i}$ is the subfilter-scale momentum flux tensor.

Combining these results gives

$$\begin{aligned} & \frac{\partial}{\partial t}(\sigma_i \rho_i \mathbf{u}_i) + \nabla \cdot (\sigma_i \rho_i \mathbf{u}_i \mathbf{u}_i) + \sigma_i \nabla \overline{p} + \sigma_i \rho_i \nabla \Phi \\ = \; & -\left\{ \nabla \cdot \mathsf{F}_{\text{SF}}^{\mathbf{u}_i} + \mathbf{b}_i + \sum_j \mathbf{d}_{ij} \right\}. \end{aligned} \tag{36}$$

Then, subtracting $\mathbf{u}_i$ times (16) and dividing through by $\sigma_i \rho_i$ gives

$$\frac{D_i \mathbf{u}_i}{Dt} + \frac{1}{\rho_i}\nabla \overline{p} + \nabla \Phi = -\frac{1}{\sigma_i \rho_i}\left\{ \nabla \cdot \mathsf{F}_{\text{SF}}^{\mathbf{u}_i} + \mathbf{b}_i + \sum_j \mathbf{d}_{ij} \right\}. \tag{37}$$

It is easily verified that including a Coriolis term $2\boldsymbol{\Omega} \times \mathbf{u}$ on the left hand side of (4) leads to the appearance of a term $2\boldsymbol{\Omega} \times \mathbf{u}_i$ on the left hand side of (37).

For completeness a filtered version of the equation of state is also needed.

$$\overline{p} = P(\rho_i, \eta_i, q_i) + P_{\text{SF}}^i, \tag{38}$$

where $P_{\text{SF}}^i = \overline{P(\rho, \eta, q)} - P(\rho_i, \eta_i, q_i)$ represents subfilter-scale contributions to the equation of state. Because of the short time needed for acoustic waves to propagate across a grid cell and equilibrate the pressure field, it will often be justifiable to neglect P_{SF}^i. A variety of alternative forms can be obtained by rearranging (5) before apply the filter. In making a specific choice, the points discussed in section 4 should be noted.

So far, the only approximations made in going from (1)-(5) to the conditionally filtered equations (16), (25), (26), (37) and (38) is that $\nabla\Phi$ is constant on the filter scale, and that the filter commutes with space and time derivatives.

3. Inclusion of source terms

Up to this point, to simplify the presentation, source and sink terms for entropy and total water have been neglected. In realistic flows such sources are important. This section shows that the inclusion of source terms in the framework is straightforward.

For illustration, consider the budget of liquid water (superscript (l)), but neglect precipitation as well as freezing and thawing. The analogue of (3) for liquid water is then

$$\frac{Dq^{(l)}}{Dt} = C - E, \tag{39}$$

where C and E are the rates of condensation and evaporation, respectively. Combining with (1) to obtain the flux form of the equation, and then with (7) gives

$$\frac{\partial}{\partial t}(I_i \rho q^{(l)}) + \nabla \cdot (I_i \rho \mathbf{u} q^{(l)}) = I_i \rho (C - E). \tag{40}$$

Application of the filter then leads to

$$\frac{\partial}{\partial t}(\sigma_i \rho_i q_i^{(l)}) + \nabla \cdot (\sigma_i \rho_i \mathbf{u}_i q_i^{(l)}) = \sigma_i \rho_i C_i - \sigma_i \rho_i E_i - \nabla . \mathbf{F}_{\mathrm{SF}}^{q_i^{(l)}}, \tag{41}$$

where $q_i^{(l)}$ is the mass-weighted filter-scale mean $q^{(l)}$ in fluid component i, $\mathbf{F}_{\mathrm{SF}}^{q_i^{(l)}}$ is the subfilter-scale flux of $q^{(l)}$ in fluid i, and C_i and E_i are the mass-weighted filter-scale condensation and evaporation rates in fluid i, defined by

$$\sigma_i \rho_i C_i = \overline{I_i \rho_i C}; \qquad \sigma_i \rho_i E_i = \overline{I_i \rho_i E}. \tag{42}$$

The final result can be converted back to advective form by subtracting $q_i^{(l)}$ times (16):

$$\frac{D_i q_i^{(l)}}{Dt} = C_i - E_i - \frac{1}{\sigma_i \rho_i} \nabla . \mathbf{F}_{\mathrm{SF}}^{q_i^{(l)}}. \tag{43}$$

Thus the source and sink terms are carried through the conditional filtering operation in a straightforward way. (Note, however, that care may be required if a source term is to be expressed as a nonlinear function of other variables. For example, if condensation rate is a function of water vapor $q^{(v)}$ and temperature T then $\sigma_i\rho_i C_i = \overline{I_i\rho_i C(q^{(v)},T)} \neq \sigma_i\rho_i C(q_i^{(v)},T_i)$ if there are subfilter-scale variations in $q^{(v)}$ or T within fluid i. However, such differences are commonly neglected.) Other source terms can be included in an analogous way. This particular example will be used to discuss the link between sources and relabelling in the next section.

4. Relabelling

A crucial aspect of any practical application of the proposed framework will be the relabelling of fluid parcels. In the above derivation the I_i are simply arbitrary Lagrangian labels. It is envisaged that the framework might be exploited by using the labels to pick out subsets of fluid parcels with certain properties. For example, fluid 2 might represent convective clouds or updrafts, as identified, for example, by the fluid's vertical velocity, buoyancy, or liquid water content, while fluid 1 represents the updraft environment. It would then be necessary to allow fluid parcels to be relabelled as their properties change. For example, relabelling some of fluid 1 as fluid 2 would correspond to entrainment while relabelling some of fluid 2 as fluid 1 would correspond to detrainment. Specifying cloud base mass fluxes, for example, would also involve relabelling.

Even when there is such a clear conceptual link between fluid parcel labels and their physical properties, defining a suitable relabelling scheme is a difficult and far from fully solved research problem (e.g. de Rooy et al. 2013). Moreover, there are situations where it is not at all clear how best to assign parcel labels. For example, in the dry convective boundary layer there are local and nonlocal contributions to the vertical transport, and some success has been achieved in modeling these with the EDMF approach (Siebesma et al. 2007). However, joint probability density functions (pdfs) of vertical velocity and temperature from LES (e.g. Wyngaard and Moeng 1992) do not suggest any clear criterion for labelling the fluid as updraft and environment. Again, the best choice of relabelling scheme is an open research question. In this section we first note how relabelling can be included in the conditionally filtered equations. We then briefly discuss how the mathematical operation of relabelling may be linked to physical processes such as mixing and source terms.

a. Inclusion of relabelling terms

One way to bring relabelling into the framework would be to introduce source terms for the Lagrangian labels I_i. However, such source terms would necessarily have δ-function structure, making the subsequent mathematics cumbersome. Instead we choose to introduce the relabelling terms directly in the filtered equations (16), (25), (26), (37).

Let $\mathscr{M}_{ij}$ be the rate per unit volume at which mass is converted from component j to component i. Then (16) becomes

$$\frac{\partial}{\partial t}(\sigma_i\rho_i) + \nabla\cdot(\sigma_i\rho_i\mathbf{u}_i) = \sum_{j\neq i}\left(\mathscr{M}_{ij} - \mathscr{M}_{ji}\right). \tag{44}$$

(If we define $\mathscr{M}_{ii} = 0$ then we can include $j = i$ in the sum too.) This formulation clearly introduces no net source to the total density $\overline{\rho} = \sum_i \sigma_i\rho_i$.

Next, let $\hat{q}_{ij}$ be a representative value of q for the fluid that is converted from component j to component i. The flux form of the q_i equation becomes

$$\frac{\partial}{\partial t}(\sigma_i\rho_i q_i) + \nabla\cdot(\sigma_i\rho_i\mathbf{u}_i q_i) = \sum_{j\neq i}\left(\mathscr{M}_{ij}\hat{q}_{ij} - \mathscr{M}_{ji}\hat{q}_{ji}\right) - \nabla\cdot\mathbf{F}^{q_i}_{\mathrm{SF}}. \tag{45}$$

Subtracting q_i times (44) then leads to

$$\frac{D_i q_i}{Dt} = \frac{1}{\sigma_i\rho_i}\left[\sum_{j\neq i}\left\{\mathscr{M}_{ij}(\hat{q}_{ij} - q_i) - \mathscr{M}_{ji}(\hat{q}_{ji} - q_i)\right\} - \nabla.\mathbf{F}^{q_i}_{\mathrm{SF}}\right]. \tag{46}$$

This formulation clearly introduces no net source to the total density of water $\overline{\rho q} = \sum_i \sigma_i \rho_i q_i$. A simple choice would be to set $\hat{q}_{ji} = q_i$, in which case the right hand side of (46) simplifies. However, we are not restricted to this choice, and a more accurate scheme might be obtained by making a different choice. For example, the air detrained from a cumulus updraft might typically be less moist than the average air in the updraft (e.g. de Rooy et al. 2013). There is an analogy here with flux-form advection schemes, as noted by Yano (2014), with $\hat{q}_{ij}$ analogous to the moisture mixing ratio at a cell edge used in computing a moisture flux. The choice $\hat{q}_{ji} = q_i$ corresponds to a first order upwind scheme, but other choices might give more accurate schemes.

A similar argument allows the inclusion of relabelling terms in the entropy equation

$$\frac{D_i \eta_i}{Dt} = \frac{1}{\sigma_i \rho_i} \left[\sum_{j \neq i} \left\{ \mathscr{M}_{ij} (\hat{\eta}_{ij} - \eta_i) - \mathscr{M}_{ji} (\hat{\eta}_{ji} - \eta_i) \right\} - \nabla . \mathbf{F}_{\mathrm{SF}}^{\eta_i} \right]. \tag{47}$$

This formulation clearly conserves the total entropy. The simple choice $\hat{\eta}_{ji} = \eta_i$ is possible, leading to some simplification, but other choices might give more accurate results.

As noted in section 2, it is possible to work with some function of entropy rather than entropy itself. If the fluid is a perfect gas and moisture can be neglected then there are two advantages to working with potential temperature θ rather than η. First note that the conditionally filtered potential temperature equation, including relabelling terms, would be

$$\frac{D_i \theta_i}{Dt} = \frac{1}{\sigma_i \rho_i} \left[\sum_{j \neq i} \left\{ \mathscr{M}_{ij} (\hat{\theta}_{ij} - \theta_i) - \mathscr{M}_{ji} (\hat{\theta}_{ji} - \theta_i) \right\} - \nabla . \mathbf{F}_{\mathrm{SF}}^{\theta_i} \right]. \tag{48}$$

This formulation would conserve the density-weighted potential temperature, rather than entropy. In this case it is appealing to write the equation of state in the form

$$\left(\frac{p}{p_0} \right)^{(1-\kappa)} = \frac{R}{p_0} \rho \theta, \tag{49}$$

where p_0 is a constant reference pressure, R is the gas constant for dry air, and $\kappa = R/C_p$ with C_p the specific heat capacity at constant pressure. Multiplying by I_i and applying the filter then gives

$$\left(\frac{\overline{p}}{p_0}\right)^{(1-\kappa)} = \frac{R}{p_0}\rho_i\theta_i + P^i_{\mathrm{SF}}. \tag{50}$$

If the subfilter-scale terms are negligible then multiplying by σ_i and summing over fluid components gives

$$\left(\frac{\overline{p}}{p_0}\right)^{(1-\kappa)} = \frac{R}{p_0}\sum_i \sigma_i\rho_i\theta_i = \frac{R}{p_0}\overline{\rho\theta}. \tag{51}$$

Since the relabelling terms in (48) would preserve the right hand side of (51), they would therefore preserve $\overline{p}$. Thus, relabelling terms should not introduce any pressure fluctuations that could generate acoustic waves and cause numerical problems.

A closely related point is that the internal energy density of the i^{th} fluid component (neglecting subfilter-scale contributions) $C_v\rho_i T_i = (C_v/R)\overline{p}$ (where $C_v = C_p - R$ is the specific heat capacity at constant volume) is a function only of $\overline{p}$, and so would also be preserved by the relabelling terms in (48). Thus the total internal energy density $\sum_i C_v\sigma_i\rho_i T_i$ would also be preserved by the relabelling terms.

Finally, relabelling terms can be included in the momentum equation in an analogous way

$$\begin{aligned} &\frac{D_i\mathbf{u}_i}{Dt} + \frac{1}{\rho_i}\nabla\overline{p} + \nabla\Phi = \\ &\frac{1}{\sigma_i\rho_i}\left[\sum_{j\neq i}\left\{\mathscr{M}_{ij}(\hat{\mathbf{u}}_{ij}-\mathbf{u}_i) - \mathscr{M}_{ji}(\hat{\mathbf{u}}_{ji}-\mathbf{u}_i)\right\}\right. \\ &\qquad\qquad \left. -\nabla\cdot\mathsf{F}^{\mathbf{u}_i}_{\mathrm{SF}} - \mathbf{b}_i - \sum_j \mathbf{d}_{ij}\right]. \end{aligned} \tag{52}$$

In this formulation the relabelling terms conserve momentum. On the other hand, they do not generally conserve the filter-scale kinetic energy; instead they imply a transfer of kinetic energy to (or from) the subfilter-scale. This transfer could, in principle, be diagnosed and used as a source for subfilter-scale kinetic energy or as a term in a diagnostic budget.

b. The relation between relabelling and physical processes

In the discussion so far we have identified entrainment and detrainment with relabelling. Now, in the continuous equations (1)-(6), before filtering, the labels are completely passive; i.e. the values of I_i do not affect the solution for the other variables in any way. The labelling is purely a *mathematical device* for picking out certain regions of the fluid. On the other hand, it is normal to regard entrainment and detrainment as closely associated with *physical processes* such as mixing, condensation, and evaporation. The key to reconciling these two viewpoints is to recognize that, in order to be most useful, the choice of labelling should reflect the physical properties of the fluid. For example, in diagnosing entrainment rates from high-resolution simulations a critical step is how one defines, i.e. labels, updrafts (Couvreux et al. 2010; Yeo and Romps 2013). Consequently, relabelling should reflect changes in the physical properties of the fluid, which in turn will often be associated with source and sink terms. These ideas are explored a little more in this subsection.

First note that there is a close relationship between relabelling and mixing. As a simple illustrative thought experiment, consider a situation in which q is uniform in fluid 1 and also in fluid 2, but with different values in each. Now consider relabelling some of fluid 1 as fluid 2. As a result the mean mixing ratio in fluid 2 q_2 will change. Also, there will now be some subfilter-scale variability of q in fluid 2; previously it was zero. In principle, if we were to keep track of the subfilter-scale variability, for example through budgets of variance and higher order moments, then the relabelling could be reversed; after all, the physical state of the system has not changed. However, if no attempt is made to keep track of the subfilter-scale variability then this information is lost; as far as a numerical model is concerned, the relabelled fluid 1 has effectively been mixed into fluid 2. Because of this implied mixing, in practice we will want to relabel in situations where it is reasonable to assume that mixing occurs. This is exactly what is done in typical mass flux convection schemes for entrainment and detrainment.

Next consider the link between source terms and relabelling. To illustrate the idea, consider the equation for liquid water mixing ratio (43), which includes condensation and evaporation terms. Introduce relabelling terms, by analogy with (46), but for simplicity neglect the subfilter-scale flux term, to leave

$$\begin{aligned} \frac{D_i q_i^{(l)}}{Dt} &= C_i - E_i \\ + \quad & \frac{1}{\sigma_i \rho_i} \left[\sum_{j \neq i} \left\{ \mathcal{M}_{ij} (\hat{q}_{ij}^{(l)} - q_i^{(l)}) - \mathcal{M}_{ji} (\hat{q}_{ji}^{(l)} - q_i^{(l)}) \right\} \right] . \end{aligned} \tag{53}$$

At this point the mathematical operation of relabelling and the physical sources are conceptually distinct and correspond to different terms in the equation.

Now suppose there are just two fluid components, and we wish to label air containing liquid water as fluid 2 and air without liquid water as fluid 1. In this way we impose a link between the mathematical labels and the physical state of the system. Since we now impose $q_1^{(l)} = 0$, the equation for $q_1^{(l)}$ becomes

$$0 = C_1 - E_1 + \frac{1}{\sigma_1 \rho_1} \left[\mathcal{M}_{12} \hat{q}_{12}^{(l)} - \mathcal{M}_{21} \hat{q}_{21}^{(l)} \right] . \tag{54}$$

Thus we have a constraint relating the relabelling terms to the source terms. It would be natural to require that any condensation that occurs in fluid 1 will immediately result in relabelling (entrainment) into fluid 2, while any relabelling of fluid containing liquid water from fluid 2 to fluid 1 would immediately result in evaporation. In that case (54) breaks into two separate constraints:

$$\sigma_1 \rho_1 C_1 \quad = \quad \mathcal{M}_{21} \hat{q}_{21}^{(l)} , \tag{55}$$

$$\sigma_1 \rho_1 E_1 \quad = \quad \mathcal{M}_{12} \hat{q}_{12}^{(l)} . \tag{56}$$

These constraints ensure that the proposed labelling scheme remains consistent with the source and sink terms.

5. Relation to existing approaches

It will be useful to note how existing approaches to parameterizing the boundary layer and convection fit into the proposed framework. Many such schemes fit broadly into two types: local turbulence closures, and mass flux schemes. The example of a mass flux scheme for convection is perhaps the most instructive, and is discussed in some detail in section 5b. The local turbulence closure approach is mentioned briefly first. The EDMF approach may be considered a hybrid of the two, and is discussed briefly at the end of this section.

An important detail is that atmospheric models are generally formulated to predict the evolution of filter-scale mean variables $\overline{\rho}$, $\overline{\eta}^*$, $\overline{q}^*$, $\overline{\mathbf{u}}^*$, with the dynamical core handling transport by $\overline{\mathbf{u}}^*$. Appendix A obtains the equations for these mean variables in the conditionally filtered framework.

a. Local turbulence closures

In terms of the conditionally filtered framework, local turbulence closures amount to considering a single fluid component, and modeling all of the boundary layer and convective fluxes through the subfilter-scale terms $\mathbf{F}^{\eta}_{\mathrm{SF}}$, $\mathbf{F}^{q}_{\mathrm{SF}}$, and $\mathsf{F}^{\mathbf{u}}_{\mathrm{SF}}$. In this approach the calculation of the fluxes is *essentially local*, that is, the parameterized flux at a given point depends only on prognostic fields and quantities constructed from them, and their derivatives, at that point.

The simplest such schemes include diagnostic eddy diffusivity schemes, usually applied to the boundary layer, in one dimension (e.g. Louis 1979) or three dimensions (e.g. Smagorinsky 1963; Germano et al. 1991). More sophisticated schemes attempt to diagnose or predict some higher order moments of the turbulent flow (e.g. Mellor and Yamada 1982). By assuming a particular functional form for the subfilter-scale joint pdf of w, θ and q, for example, and predicting enough moments in order to fix the free parameters describing the pdf, it is possible to reconstruct all the other desired moments. This approach has been applied to unifying the treatment of the boundary layer, shallow convection, and even deep convection (Lappen and Randall 2001; Golaz 2002; Storer et al. 2015). All of these approaches correspond to making particular choices and approximations within the proposed framework. Although the framework does not explicitly include the additional prognostic equations that might be needed for some higher-order turbulence closure, there is no barrier to including them.

b. Reduction to a mass flux scheme

It is instructive to see how a typical mass flux scheme can be obtained by making systematic approximations within the conditional filtering framework. The approximations are all familiar from the literature on convection parameterization. Since the purpose here is to illustrate how the argument goes, we neglect sources of entropy and water and consider only a very simple mass flux scheme.

We begin by noting that mass flux schemes are often based on budgets of moist static energy rather than entropy. The moist static energy budget in turn is often broken down into separate budgets for dry static energy and for water vapor and condensed water with corresponding source and sink terms (e.g. Arakawa and Schubert 1974; Tiedtke 1989). Moist static energy is only approximately conserved, both materially and in an integral sense (e.g. Romps 2015), so an approximation is involved in using its budget. Other mass flux schemes work in terms of entropy or related quantities, and the budget may be broken down into separate budgets for potential temperature and moisture quantities (e.g. Gregory and Rowntree 1990; Siebesma et al. 2007). In this section we will use the entropy budget as it is the simplest for the purpose of illustration. The formulation in terms of conserved moist static energy is analgous.

A typical mass flux scheme comprises three components: (i) convective source terms for the large-scale budget equations, which depend on the vertical profiles of properties within the cloud; (ii) a cloud model that determines the vertical profiles of cloud properties such as mass flux, entropy, and water content, given their values at cloud base; (iii) some trigger and closure assumptions that determine whether convection occurs and the cloud base properties if it does. In this section we note how the large-scale budgets and cloud model for a typical mass flux scheme can be systematically derived from the conditionally filtered equations by making certain approximations. Triggering and closure will not be discussed; as noted above, these remain difficult open research questions. We will consider the simplest possible situation with just two fluid components, $i = 2$ being the convecting fluid and $i = 1$ being the environment.

The budgets for the filter-scale mean entropy and total moisture are given by (A8), (A6). We neglect the $\mathbf{F}_{\mathrm{SF}}^{\eta_i}$ and $\mathbf{F}_{\mathrm{SF}}^{q_i}$ terms. Such terms are not usually included in mass flux convection schemes. They are typically accounted for by other parameterizations such as the boundary layer scheme, or by a combined scheme such as EDMF (e.g. Siebesma et al. 2007). Also, horizontal contributions to the flux divergence on the right hand side of (A8) and (A6) are neglected. This leaves

$$\overline{\rho}\frac{\overline{D}\overline{\eta}^*}{Dt} = -\frac{\partial}{\partial z}F_{\mathrm{CF}}^{\eta}, \tag{57}$$

$$\overline{\rho}\frac{\overline{D}\overline{q}^*}{Dt} = -\frac{\partial}{\partial z}F_{\mathrm{CF}}^{q}, \tag{58}$$

where

$$F_{\mathrm{CF}}^{\eta} = \sigma_1\rho_1 w_1\eta_1 + \sigma_2\rho_2 w_2\eta_2 - \overline{\rho}\overline{w}^*\overline{\eta}^* \tag{59}$$

and

$$F^q_{\mathrm{CF}} = \sigma_1\rho_1 w_1 q_1 + \sigma_2\rho_2 w_2 q_2 - \overline{\rho}\overline{w}^*\overline{q}^*. \tag{60}$$

Next, if we assume that $\sigma_2 \ll 1$ then $\eta_1 \approx \overline{\eta}^*$ and $q_1 \approx \overline{q}^*$. Then, using (A2), (59) and (60) simplify to

$$F^\eta_{\mathrm{CF}} = \sigma_2\rho_2 w_2(\eta_2 - \overline{\eta}^*) = M(\eta_2 - \overline{\eta}^*) \tag{61}$$

and

$$F^q_{\mathrm{CF}} = \sigma_2\rho_2 w_2(q_2 - \overline{q}^*) = M(q_2 - \overline{q}^*), \tag{62}$$

where $M = \sigma_2\rho_2 w_2$ is the vertical mass flux in the convecting fluid.

Equations (57) and (58), together with (61) and (62), specify the convective source terms for the large-scale thermodynamic variables in terms of the profiles of M, η_2, and q_2. The simplest convection schemes neglect the effect of convection on the large-scale momentum budget, and for simplicity we will do the same here.

The cloud model is obtained by approximating the conditionally filtered equations for fluid 2. First Consider the mass budget (44). Assume that $\sigma_2\rho_2$ is steady and neglect horizontal transport in fluid 2 to obtain

$$\frac{\partial M}{\partial z} = E - D, \tag{63}$$

where $E = \mathscr{M}_{21}$ is the entrainment rate, and $D = \mathscr{M}_{12}$ is the detrainment rate. If desired, the entrainment and detrainment may be expressed as fractional entrainment rates per unit height: $E = \varepsilon M, D = \delta M$.

For the cloud water budget, in (45) assume that $\sigma_2\rho_2 q_2$ is steady, i.e. neglect storage of water in the cloud. Also neglect horizontal transport of water by the cloud, and neglect the $\mathbf{F}^{q_i}_{\mathrm{SF}}$ term, which represents transport of water by sub-cloud variability. The water budget then reduces to

$$\frac{\partial}{\partial z}(Mq_2) = E\hat{q}_{21} - D\hat{q}_{12}. \tag{64}$$

Next assume that the specific humidity in entrained air is equal to the mean environmental value $\hat{q}_{21} = q_1$, while the specific humidity in detrained air is equal to the mean cloud value $\hat{q}_{12} = q_2$, so that (64) simplifies to

$$\frac{\partial}{\partial z}(Mq_2) = Eq_1 - Dq_2. \tag{65}$$

An alternative form is obtained by subtracting q_2 times (63):

$$M\frac{\partial q_2}{\partial z} = E(q_1 - q_2). \tag{66}$$

In a similar way, by making analogous approximations, the cloud entropy budget may be written

$$\frac{\partial}{\partial z}(M\eta_2) = E\eta_1 - D\eta_2 \tag{67}$$

or

$$M\frac{\partial \eta_2}{\partial z} = E(\eta_1 - \eta_2). \tag{68}$$

Given cloud base values of M, q_2, and η_2, and vertical profiles of E and D (or ε and δ), equations (63), (65), and (67) may be integrated to obtain vertical profiles of M, q_2, and η_2.

Values of cloud buoyancy will be needed to determine whether convection occurs. They will also be needed if a zero buoyancy condition is used to determine cloud top, if entrainment or detrainment are assumed to depend on buoyancy, or if an equation for cloud vertical velocity is to be solved. Consider the vertical momentum budget for fluid 2, i.e. the vertical component of (52):

$$\begin{aligned} \frac{D_2 w_2}{Dt} + \frac{1}{\rho_2}\frac{\partial \overline{p}}{\partial z} + \frac{\partial \Phi}{\partial z} = \\ \frac{1}{\sigma_2 \rho_2}\Bigg[\mathscr{M}_{21}(\hat{w}_{21} - w_2) - \mathscr{M}_{12}(\hat{w}_{12} - w_2) \\ - \frac{\partial}{\partial z}F^{w_2}_{\mathrm{SF}} - b_2 - d_{21}\Bigg]. \end{aligned} \tag{69}$$

Here b_2 and d_{21} are the vertical components of $\mathbf{b}_2$ and $\mathbf{d}_{21}$. The second and third terms on the left hand side together represent the negative of the buoyancy. They may be written in a more familiar form by assuming that the filter-scale mean state is in hydrostatic balance

$$\frac{1}{\overline{\rho}}\frac{\partial \overline{p}}{\partial z} + \frac{\partial \Phi}{\partial z} = 0, \tag{70}$$

so that

$$B = -\frac{1}{\rho_2}\frac{\partial \overline{p}}{\partial z} - \frac{\partial \Phi}{\partial z} = -\frac{\partial \Phi}{\partial z}\left(\frac{\rho_2 - \overline{\rho}}{\rho_2}\right). \tag{71}$$

In a typical mass flux scheme ρ_2 is not calculated directly. However, B can be diagnosed from the vertical profiles of thermodynamic properties of the cloud and its environment, together with the usual parcel assumption that the pressures in the cloud and the environment are equal.

Some mass flux schemes solve an equation for vertical velocity in the updraft. This is useful, for example, if the vanishing of the vertical velocity is used to define the top of the updraft (e.g. Siebesma et al. 2007), or E and D are assumed to depend on updraft vertical velocity (e.g. Rio et al. 2010). Assuming w_2 to be steady and neglecting horizontal transport of w_2 and transport by subfilter-scale variations, (69) becomes

$$\begin{aligned} w_2\frac{\partial w_2}{\partial z} &= B + \frac{1}{\sigma_2\rho_2}\left[E(\hat{w}_{21} - w_2) - D(\hat{w}_{12} - w_2)\right. \\ &\qquad \left. - b_2 - d_{21}\right]. \end{aligned} \tag{72}$$

This is typically simplified further by assuming $\hat{w}_{21} = w_1 \approx 0$ and $\hat{w}_{12} = w_2$ to give

$$\frac{\partial}{\partial z}\left(\frac{w_2^2}{2}\right) = B - \frac{1}{\sigma_2\rho_2}\left[E w_2 + b_2 + d_{21}\right]. \tag{73}$$

However, there is evidence that this assumption is a not a good approximation (e.g. Sherwood et al. 2013), and some schemes account for other values of $\hat{w}_{21}$ and $\hat{w}_{12}$ by using (73) with a modified value of E for the entrainment of w (e.g. Siebesma et al. 2007). A variety of schemes have been proposed for parameterizing the pressure drag terms $b_2 + d_{21}$.

All of the assumptions and approximations made above are standard ones that can be found in the literature on parameterization of convection. Recent develpments have attemped to relax some of these approximations. For example, Gerard et al. (2009); Arakawa and Wu (2013); Grell and Freitas (2014) attempt to remove the assumption that the volume fraction of convecting fluid is small. Kain (2004); Plant and Craig (2008); Gerard et al. (2009); Grandpeix and Lafore (2010) include some elements of memory about the state of convection or boundary layer cold pools resulting from convective downdrafts, thereby relaxing the steadiness assumption. Vertical transport of horizontal momentum, both by advection and via pressure fluctuations (the $\mathbf{b}_i$ and $\mathbf{d}_{ij}$ terms), may be taken into account (e.g. Kim et al. 2008), representing 'cumulus friction'.

c. Eddy Diffusivity Mass Flux schemes

EDMF schemes have been proposed to parameterize the local and nonlocal transports in the convective boundary layer, as well as transitions between the shallow cumulus, stratocumulus, and dry convective boundary layer. The net transport is decomposed into a local turbulent contribution modelled as an eddy diffusivity and a nonlocal contribution modelled using the mass flux approach. Thus, it combines the approaches discussed in sections 5a and 5b above, and it nicely illustrates how such hybrid approaches can be accommodated in the proposed framework. The dry convective boundary layer scheme of Siebesma et al. (2007) would correspond to using two fluid components, one to represent updraft and one to represent the rest of the fluid. The extended scheme of Neggers et al. (2009) would correspond to using three fluid components, one for dry updrafts, one for moist updrafts, and one for the rest of the fluid. In both cases subfilter-scale flux terms $\mathbf{F}_{\mathrm{SF}}^{\theta_i}$, $\mathbf{F}_{\mathrm{SF}}^{q_i}$, etc., could be included in one or more components to represent the eddy diffusive fluxes.

6. Multi-fluid schemes

One of our motivations for introducing the above framework is to provide a derivation of the multi-fluid equations (44), (46), (47), (52), along with (38), in preparation for exploring their potential for representing convection in atmospheric models. The multi-fluid approach, like mass flux schemes, represents environment, updrafts, downdrafts, etc., by different fluid components. It could be simplified by neglecting the subfilter-scale fluxes $\mathbf{F}_{\mathrm{SF}}^{\eta_i}$ and $\mathsf{F}_{\mathrm{SF}}^{\mathbf{u}_i}$ and the pressure terms $\mathbf{b}_i$ and $\mathbf{d}_{ij}$. But crucially, unlike traditional mass flux schemes, it retains the full material derivative D_i/Dt for all fluid components. Hence it provides a natural and physically sound basis for representing some dynamical memory about the state of convection.

A particularly attractive possibility for solving the multi-fluid equations in a numerical model is to allow the dynamical core to represent the filter-scale terms (i.e. the left hand sides) in the equations for *all* fluid components. Parameterizations of entrainment/detrainment terms $\mathscr{M}_{ij}$ and subfilter-scale fluxes $\mathbf{F}_{\mathrm{SF}}$ would still be needed; these could be based on exisiting approaches to modeling these terms. However, the main burden of handling the convective dynamics would be shifted to the dynamical core.[2] We believe this approach has the potential to improve the model representation of the coupling between convection and the larger-scale circulation. First, it would help to ensure the consistency of the governing equations used throughout the model. Second, it would allow the dynamical core to control the location of the subsidence compensating convective mass flux, rather than a parameterized contribution being imposed in the convecting grid column. Third, it would allow information about the state of convection to be transported by the dynamical core to neighboring grid columns. Finally, with a suitably scale aware formulation of the parameterized terms, such an approach should work both at grid resolutions where convection

[2]On a philosophical note, this would shift the established—but artificial—boundary between ‘dynamics’ and ‘physics’.

is usually parameterized and at convection-resolving resolutions, and may even be able to work at intermediate gray zone resolutions.

The difficulty of parameterizing convection, and the potential benefits of using a more fundamental equation set with fewer approximations, has been used as a justification for the 'superparameterization' approach to convection (Grabowski and Smolarkiewicz 1999; Randall et al. 2003), and is summarized in the epithet 'the equations know more about convection than we do'. The epithet might also be applied to the multi-fluid approach, since it attempts to solve a more complete and fundamental equation set than is usually done in conventional parameterizations.

The derivation of section 2 was constructed in such a way that the same mean pressure gradient $\nabla\overline{p}$ appears in the momentum equations for all fluid components. This feature becomes important when considering the multi-fluid equations, and particularly their numerical solution. If different fluid components were permitted to have different pressures p_i then this would permit the equations to support subfilter-scale acoustic modes with the entire cloud field in synchronized oscillation. Besides being manifestly unphysical, such modes would likely be difficult to handle numerically. The use of a single pressure field in all the component momentum equations can be considered a type of filter that removes such acoustic modes. Note, however, that the different fluid components are not required to have the same density. Since buoyancy can be expressed entirely in terms of the densities of a fluid parcel and its environment together with gravity (e.g. Holton 2004; Vallis 2017, see also equation (71) above), the use of a single pressure field does not prevent buoyancy effects from being explicitly represented. On the other hand, rising thermals do not in general experience the same pressure gradient as their environment. For example, pressure perturbations above and below a thermal can provide an effective drag (e.g. Romps and Charn 2015). Such small-scale pressure perturbations are included in the conditional filtering framework, but appear in the $\mathbf{b}_i$ and $\mathbf{d}_{ij}$ terms, which must be parameterized.

Another advantage of using a single mean pressure field arises when considering numerical solutions. For example, a semi-implicit semi-Lagrangian solution scheme for the multi-fluid equations may be written down, by analogy with the ENDGame scheme used operationally at the Met Office (Wood et al. 2014). Seeking an iterative solution method and eliminating unknowns leads to a Helmholtz problem for (increments to) the single pressure field that has the same form as that in ENDGame itself. Such a straightforward scheme would not be expected if different p_i were allowed.

It is important to check that the derivation in section 2 provides the right number of equations to determine all the unknowns; in particular we need to be able to determine both σ_i and ρ_i even though there is a prognostic equation only for the combined quantity $\sigma_i\rho_i$. Counting the velocity vector as three components, we have $7n+1$ unknown fields: σ_i, ρ_i, η_i, q_i, $\mathbf{u}_i$, and $\overline{p}$. We also have $7n+1$ equations: (16), (25), (26), (37), (5), and $\sum_i \sigma_i = 1$. How the equations determine σ_i and ρ_i is most transparent for a perfect gas equation of state. The middle expression in (51) may be evaluated from directly predicted quantities $\sigma_i\rho_i$ and θ_i, giving $\overline{p}$. Then (50) determines ρ_i, and finally $\sigma_i = \sigma_i\rho_i/\rho_i$. It is noteworthy that the different fluid components are coupled by the $\nabla\overline{p}$ term even in the case $\mathscr{M}_{ij} = 0$.

One variant of the multi-fluid scheme makes the approximation that the horizontal velocities $\mathbf{v}_i$ of all fluid components are equal. This amounts to assuming that the horizontal components of $\mathbf{d}_{ij}$ are just what is required to maintain that equality of the $\mathbf{v}_i$. Since the $\mathbf{v}_i$ are equal, $\mathbf{v}_i = \left(\sum_i \sigma_i\rho_i\mathbf{v}_i\right)/\overline{\rho} = \overline{\mathbf{v}}^*$. The prognostic equation for $\mathbf{v}_i$ is then just the horizontal component of (A9):

$$\overline{\rho}\frac{\overline{D}\overline{\mathbf{v}}^*}{Dt} + \nabla_H\overline{p} + \overline{\rho}\nabla_H\Phi = -\sum_i \nabla\cdot\mathsf{F}^{\mathbf{v}_i}_{\mathrm{SF}}, \tag{74}$$

where ∇_H is the horizontal gradient operator, $\mathsf{F}^{\mathbf{v}_i}_{\mathrm{SF}}$ are the subfilter-scale fluxes of horizontal momentum, and the $\mathsf{F}^{\mathbf{v}}_{\mathrm{CF}}$ contribution vanishes because of the equality of the $\mathbf{v}_i$. There might be some computational benefit from making this approximation. On the other hand, there might be some benefit in modeling the vertical flux of horizontal momentum by retaining separate $\mathbf{v}_i$ for each component, for example near squall lines or frontal convection. It would be valuable to explore this trade-off.

We have begun to explore the potential of the multi-fluid approach theoretically and numerically. In the absence of entrainment/detrainment terms and subfilter-scale terms we have shown that the multi-fluid equations have a Hamiltonian formulation, and that the two-fluid system has a physically reasonable set of linear normal modes, providing some confidence in their physical soundness. We also have some preliminary results from a Boussinesq two-fluid model and from a single-column two-fluid model of the dry convective boundary layer, confirming that the system is amenable to numerical solution. These developments will be reported elsewhere.

Ideas closely related to the multi-fluid approach have appeared previously several times in the literature. Libby (1975) and Dopazo (1977) derived conditionally averaged equations for incompressible flow, using labels to pick out turbulent and non-turbulent regions of the fluid. Equations closely resembling the multi-fluid equations are used in engineering applications to model two-phase flows such as particle-laden flow, bubbly liquids, and combustion of fuel droplets (e.g. Weller 2005; Städtke 2006). The applications include disperse flows, in which the changes of phase occur on unresolved scales (e.g. Drew 1983; Lance and Bataille 1991; Jackson 1997; Zhang and Prosperetti 1997; Rafique et al. 2004), and flows in which the interface between two phases is resolved but modeled as a thin region of mixed phase (e.g. Abgrall and Karni 2001; Allaire et al. 2002; Garrick et al. 2017). These two regimes are analogous to the regimes of subfilter-scale convection and resolved convection, which our proposed approach is intended to represent.

Application of similar ideas to convective flows go back at least as far as Cushman-Roisin (1982), who proposed to describe dry convection in terms of 'thermals' and 'antithermals' with separate dynamical equations for each. In relation to the meteorological literature, there are a number of similarities between our proposed framework and the work of Yano et al. (2010); Yano (2012, 2014, 2016). He too proposes to decompose the flow into a number of components each occupying distinct regions, with separate dynamical equations for each component. However, there are some important differences too. Yano (2012) restricts attention to the hydrostatic primitive equations. He makes the segmentally constant approximation in which fluid properties within each component are assumed constant within a grid cell; he thus omits terms corresponding to our subfilter-scale fluxes. As a result of other approximations, the equations for the different fluid components fully decouple from each other in the absence of entrainment and detrainment; this is in contrast to (37) above, in which the fluid components remain coupled through the common $\nabla\overline{p}$ term and the requirement for $\sum_i \sigma_i = 1$. Yano et al. (2010); Yano (2014, 2016) also make the segmentally constant approximation, but now the underlying equation set is the nonhydrostatic anelastic equations. Again the flow is decomposed into a number of components with the aid of labels analogous to our I_i. Yano (2014) and Yano (2016) focus on the transport equation and on the conceptual aspects of the approach. Yano et al. (2010) develop the approach into a two-dimensional vertical slice model and apply it to simulation of dry convection. To do this they must numerically solve a Poisson equation for the pressure at each time step. Thus their implementation resembles an adaptive mesh refinement method rather than a typical parameterization.

Finally, the work of Kuell et al. (2007); Kuell and Bott (2008) should be mentioned. They allow the dynamical core to handle the environmental subsidence that compensates the net convective mass flux due to updrafts and downdrafts. The parameterization itself handles the convective updrafts and downdrafts and hence determines mass sink and source terms for the dynamical core. These mass source and sink terms correspond to the $\mathscr{M}_{ij}$ terms discussed in section 4 above.

7. Summary and discussion

We have derived conditionally filtered versions of the compressible Euler equations. The conditionally filtered equations provide a framework for the parameterization of subgrid-scale processes such as convection and boundary layer fluxes in atmospheric models. We have shown how several existing approaches to parameterization fit within the framework. It has the benefit of accommodating both local turbulence approaches and mass-flux approaches in a very natural way. It provides a natural way to distinguish between local and nonlocal transport processes, and makes a clearer conceptual link to schemes based on coherent structures such as convective plumes or thermals than the traditional unconditional filtering approach. It is hoped that the framework will facilitate the unification of different approaches to parameterization by highlighting the different approximations made, and helping to ensure consistency such as the avoidance of double counting.

A major motivation for developing this framework is that it can accommodate various extensions to current approaches to parameterization, such as the inclusion of additional prognostic variables. In particular, it indicates how one could allow the dynamical core to handle the dynamics of convection; this multi-fluid approach has the potential to improve coupling between convection and large-scale dynamics in several ways (section 6), and we have begun to explore this possibility.

A closely related point is that, in the proposed framework, the dynamics is expressed through a set of partial differential equations, to which standard numerical methods can be applied, supplemented by some subfilter-scale fluxes and relabelling terms that must be parameterized. In contrast, most convection parameterization schemes are not expressed as partial differential equations (Cullen et al. 2001; Arakawa and Wu 2013), and they typically involve a variety of ad hoc switches to which the model behaviour may be very sensitive (Jakob and Siebesma 2003). Thus, for a typical climate model, convergence with increasing resolution (if obtained at all) must be interpreted with considerable caution (Williamson 2008).

Finally it should be emphasized that what we have derived is no more than a framework. It does not specify how the subfilter-scale fluxes or the relabelling terms are to be modeled. These remain very challenging problems in atmospheric modeling, though existing approaches will provide a very useful starting point. Moreover, the framework does not specify how many fluid components are to be used or how they are to be chosen. More components will lead to greater computational cost, particularly if the dynamics of all components is to be handled by the dynamical core, as suggested in section 6. There is clearly great scope for optimizing this choice, and again existing approaches should provide a useful starting point.

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APPENDIX

Atmospheric models are generally formulated such that the dynamical core integrates prognostic equations for unconditionally filtered variables. It will therefore be useful to note how these prognostic equations arise in the proposed framework. First define a density-weighted filter operation by

$$\overline{\rho}\overline{X}^{*} \equiv \overline{\rho X}, \tag{A1}$$

and note a useful identity

$$\overline{\rho}\overline{X}^{*} = \overline{\rho X} = \overline{\sum_i I_i \rho X} = \sum_i \sigma_i \rho_i X_i. \tag{A2}$$

Summing (44) over i and noting the cancellation of the $\mathscr{M}_{ij}$ gives

$$\frac{\partial \overline{\rho}}{\partial t} + \nabla \cdot (\overline{\rho}\,\overline{\mathbf{u}}^*) = 0. \tag{A3}$$

This is exactly what we would obtain by directly applying the filter to the original density equation (1).

Summing (45) over i and again noting the cancellation of the $\mathscr{M}_{ij}$ gives

$$\frac{\partial}{\partial t}(\overline{\rho}\overline{q}^*) + \nabla \cdot (\overline{\rho}\,\overline{\mathbf{u}}^*\overline{q}^*) = -\nabla \cdot \left(\sum_i \mathbf{F}_{\mathrm{SF}}^{q_i} + \mathbf{F}_{\mathrm{CF}}^{q} \right), \tag{A4}$$

where

$$\mathbf{F}_{\mathrm{CF}}^{q} = \sum_i \sigma_i \rho_i \mathbf{u}_i q_i - \overline{\rho}\,\overline{\mathbf{u}}^*\overline{q}^*. \tag{A5}$$

The advective form of the moisture equation is then obtained by subtracting $\overline{q}^*$ times (A3) to obtain

$$\frac{\overline{D}\overline{q}^*}{Dt} = -\frac{1}{\overline{\rho}}\nabla \cdot \left(\sum_i \mathbf{F}_{\mathrm{SF}}^{q_i} + \mathbf{F}_{\mathrm{CF}}^{q} \right), \tag{A6}$$

where

$$\frac{\overline{D}}{Dt} \equiv \frac{\partial}{\partial t} + \overline{\mathbf{u}}^* \cdot \nabla \tag{A7}$$

is the 'material' derivative following the density-weighted mean flow. This equation agrees with what we would obtain by directly applying the filter to the flux form of the original moisture equation (3), but note how the subfilter-scale flux has been decomposed into contributions from the variations of properties within each fluid component $\mathbf{F}_{\mathrm{SF}}^{q_i}$ plus a contribution from the variations of properties between fluid components picked out by the conditional filtering $\mathbf{F}_{\mathrm{CF}}^{q}$.

In an exactly analogous way we obtain an evolution equation for the filter-scale mean entropy

$$\frac{\overline{D}\overline{\eta}^*}{Dt} = -\frac{1}{\overline{\rho}}\nabla \cdot \left(\sum_i \mathbf{F}_{\mathrm{SF}}^{\eta_i} + \mathbf{F}_{\mathrm{CF}}^{\eta} \right), \tag{A8}$$

An evolution equation for the filter-scale mean velocity is obtained by converting the fluid component momentum equation (52) to flux form, summing over i, and converting back to advective form:

$$\frac{\overline{D}\overline{\mathbf{u}}^*}{Dt} + \frac{1}{\overline{\rho}}\nabla\overline{p} + \nabla\Phi = -\frac{1}{\overline{\rho}}\nabla\cdot\left(\sum_i \mathsf{F}^{\mathbf{u}_i}_{\mathrm{SF}} + \mathsf{F}^{\mathbf{u}}_{\mathrm{CF}}\right). \tag{A9}$$

Here we have used the antisymmetry of $\mathbf{d}_{ij}$ and the fact that $\sum_i \mathbf{b}_i = 0$.

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LIST OF FIGURES

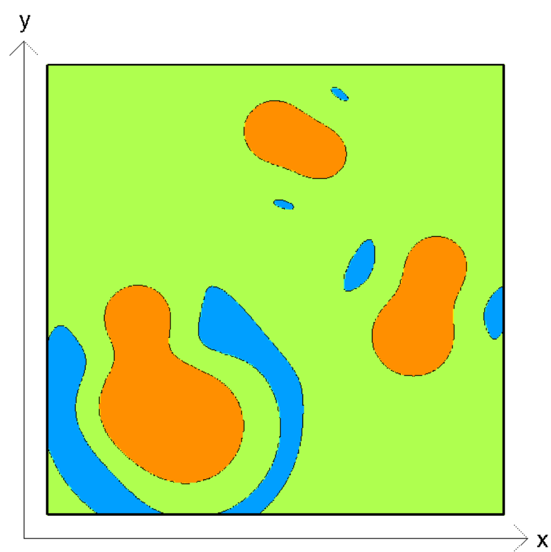

FIG. 1. Schematic horizontal section showing a decomposition of the fluid into multiple components, for example updrafts (orange), downdrafts (blue), and environment (green). In each component one of the I_i is equal to 1 and the others are equal to 0.