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

John Thuburn*

University of Exeter, Exeter, UK

Hilary Weller

University of Reading, Reading, UK

Henry G. Weller

CFD Direct Ltd, Reading, UK

Geoffrey K. Vallis, Robert J. Beare

University of Exeter, Exeter, UK

Michael Whittall

Met Office, Exeter, UK

*Corresponding author address: Department of Mathematics, University of Exeter, North Park Road, Exeter, UK.

E-mail: j.thuburn@exeter.ac.uk

ABSTRACT

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

40 **1. Introduction**

41 In weather and climate models a range of important processes occur on scales that are too fine
42 to be resolved. These processes must therefore be represented by subgrid models or ‘parameterizations’;
43 for an introduction and overview see, e.g., Mote and O’Neill (2000); Randall (2000);
44 Kalnay (2003). A formal theoretical framework on which to build a subgrid model can be obtained
45 by applying a spatial filter to the governing equations (e.g. Leonard 1975; Germano 1992; Pope
46 2000); this leads to equations for the filtered variables that resemble the original equations for the
47 unfiltered variables, supplemented by terms representing the filter-scale effects of subfilter-scale
48 variability. This formal approach is widely used in the development of numerical models for large
49 eddy simulation (LES), but tends to be applied less systematically in the development of weather
50 and climate models.

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

57 Recent developments have suggested a requirement to be able to combine and extend these struc-
58 turally different types of subgrid model (e.g. Lappen and Randall 2001; Arakawa 2004; Siebesma
59 et al. 2007; Gerard et al. 2009; Grandpeix and Lafore 2010; Arakawa and Wu 2013; Storer et al.
60 2015). For example, a convective boundary layer involves turbulent eddies on a range of length
61 scales up to the depth of the boundary layer, implying that the turbulent vertical transport has both
62 local and nonlocal contributions. This has motivated the inclusion of ‘countergradient’ transport

63 terms in boundary layer parameterizations (e.g. Holtslag and Boville 1993), as well as the devel-
64 opment of the Eddy Diffusivity Mass Flux (EDMF) scheme (Soares et al. 2004; Siebesma et al.
65 2007) which, as its name implies, combines the eddy diffusivity and mass flux approaches within
66 a single scheme.

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

77 Finally, there is a need for parameterization schemes to take into account the grid resolution of
78 the parent model, i.e. to be ‘scale aware’. The issue is particularly acute at resolutions that partly
79 resolve the process in question: the so-called ‘gray zone’. Approaches to handling the convective
80 gray zone have considered not only relaxing the assumption of small convective area fraction,
81 traditionally employed in mass flux schemes (Arakawa and Wu 2013; Grell and Freitas 2014), but
82 also broadening the structure of the scheme to include a stochastic element to account for local
83 departures from statistical equilibrium (Keane and Plant 2012), to include additional prognostic
84 quantities to carry some dynamical memory (e.g. Gerard et al. 2009; Grandpeix and Lafore 2010;
85 Park 2014), or by using a higher-order turbulence model rather than an entraining plume model to
86 calculate convective transports (e.g. Bogenschütz et al. 2013; Storer et al. 2015). It should also be

87 noted that the deep convective gray zone merges gradually into the shallow convective gray zone
88 and then the boundary layer gray zone as horizontal resolution is refined. In other words, there is
89 a rather broad range of model resolutions across which the challenges of representing gray zone
90 processes must be addressed.

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

103 In this paper a new theoretical framework is derived and proposed for developing, coupling, and
104 unifying subgrid parameterizations. We particularly have in mind the application of this frame-
105 work to the parameterization of convection and its coupling to the boundary layer and to the larger
106 scale dynamics, motivated by current challenges in this area (e.g. Holloway et al. 2014; Gross et al.
107 2017). However, the derivation is quite general.

108 The derivation (sections 2 and 3) is based on the idea of conditional filtering. It is closely related
109 to the idea of conditional averaging, which has been proposed, for example, by Dopazo (1977)
110 for the study of intermittent turbulent flows. Here, however, we use a spatial filter rather than an

111 ensemble average, and we extend the approach to the fully compressible Euler equations. The
112 spatial filter is analogous to that used in LES. However, in the conditional filtering approach the
113 fluid is first partitioned into a number of regions identified by a set of quasi-Lagrangian labels
114 that each take only the values 0 or 1. Multiplying the governing equations by one of the labels
115 before applying the spatial filter effectively picks out only the fluid identified by that label. The
116 process is repeated for each label in turn. For example, in the simplest version, one label might
117 pick out cumulus updrafts while a second label picks out the rest of the fluid. In this way, with
118 very few approximations, one obtains separate (but coupled) prognostic equations for each fluid
119 component, each with corresponding subfilter-scale terms. The resulting equations resemble those
120 used in modeling multiphase flow for engineering applications (e.g. Stadtke 2006), though our
121 derivation is somewhat simpler.

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

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

132 An attractive feature of the proposed framework is that it suggests how one might extend tra-
133 ditional mass flux schemes for convection to include a prognostic treatment of the convective
134 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. Conditionally filtered compressible Euler equations

The derivation begins with the fully compressible Euler equations:

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

$$\frac{D\eta}{Dt} = 0, \quad (2)$$

$$\frac{Dq}{Dt} = 0, \quad (3)$$

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

$$p = P(\rho, \eta, q). \quad (5)$$

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);

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

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

166 In order to carry out conditional filtering a set of n Lagrangian labels I_i , $i = 1, \dots, n$ is introduced.
 167 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
 168 to the fluid with $I_i = 1$ as the i^{th} fluid component. Eventually we envisage that the different fluid
 169 components might correspond to environment, updraft, and possibly downdraft, cold pool, near
 170 environment, further updrafts, etc. (Fig. 1). However, for the moment the I_i are just arbitrary
 171 Lagrangian labels.

172 Because the I_i are Lagrangian labels, we can write

$$\frac{DI_i}{Dt} = 0. \quad (6)$$

173 This equation will be used in the form

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

174 In this form there are time and space derivatives of discontinuous functions; these must be inter-
 175 preted as Dirac δ -functions, and they will only make sense when integrated. However, the deriva-
 176 tion below avoids explicit consideration of these δ -functions. Also, the derivation avoids the need

177 to explicitly consider a surface integral over the boundary of any fluid component (though such
 178 consideration might be needed to formulate a specific parameterization of some terms).

179 Now consider a formal spatial filtering of the governing equations. This is analogous to the
 180 derivation of the filtered equations used in LES, with the key difference that the filter is restricted
 181 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,
 182 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,
 183 is defined as a convolution of the unfiltered variable with the kernel:

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

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

$$\overline{\frac{\partial X}{\partial t}} = \frac{\partial \bar{X}}{\partial t}; \quad \overline{\nabla X} = \nabla \bar{X}; \quad \text{etc.} \quad (9)$$

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

$$\sigma_i = \bar{I}_i. \quad (10)$$

188 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
 189 component on the filter scale ρ_i by

$$\sigma_i \rho_i = \bar{I}_i \bar{\rho}. \quad (11)$$

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

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

¹This 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).

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

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

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

$$\mathbf{u}_i = \overline{I_i \rho \mathbf{u}} / \overline{I_i \rho}, \quad (14)$$

194 i.e.

$$\sigma_i \rho_i \mathbf{u}_i = \overline{I_i \rho \mathbf{u}}, \quad (15)$$

195 then (13) becomes

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

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

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

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

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

199 Now apply the filter and use (9) to obtain

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

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

$$\sigma_i \rho_i \eta_i = \overline{I_i \rho \eta}. \quad (20)$$

201 Now write

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

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

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

203 Subtracting η_i times (16) gives

$$\frac{\partial \eta_i}{\partial t} + \mathbf{u}_i \cdot \nabla \eta_i = -\frac{1}{\sigma_i \rho_i} \nabla \cdot \mathbf{F}_{\text{SF}}^{\eta_i}, \quad (23)$$

204 or, defining

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

205 to be the ‘material’ derivative following the i^{th} fluid component,

$$\frac{D_i \eta_i}{Dt} = -\frac{1}{\sigma_i \rho_i} \nabla \cdot \mathbf{F}_{\text{SF}}^{\eta_i}. \quad (25)$$

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

$$\frac{D_i q_i}{Dt} = -\frac{1}{\sigma_i \rho_i} \nabla \cdot \mathbf{F}_{\text{SF}}^{q_i}. \quad (26)$$

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

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

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

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

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

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

$$\overline{I_i \rho \nabla \Phi} = \overline{I_i \rho} \nabla \Phi = \sigma_i \rho_i \nabla \Phi. \quad (29)$$

219 The pressure gradient term is

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

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

$$\bar{p} \nabla \overline{I_i} = - \sum_j \mathbf{d}_{ij}, \quad (31)$$

224 where \mathbf{d}_{ij} is minus the pressure force (i.e. the ‘drag’) exerted by fluid j on fluid i on the scale of
 225 the filter. It can be seen that $\mathbf{d}_{ij} = -\mathbf{d}_{ji}$, as required for conservation of momentum. (The case
 226 $j = i$ can be included by defining $\mathbf{d}_{ii} = 0$.) The term

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

227 accounts for the fact that the remaining filter-scale pressure gradient force is not given exactly by
 228 $\sigma_i \nabla \bar{p}$. By summing over i and using (10) it can be seen that

$$\sum_i \mathbf{b}_i = 0. \quad (33)$$

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

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

Finally, consider the momentum flux due to advection and write

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

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

Combining these results gives

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

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

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

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.

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

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.

243 So far, the only approximations made in going from (1)-(5) to the conditionally filtered equations
 244 (16), (25), (26), (37) and (38) is that $\nabla\Phi$ is constant on the filter scale, and that the filter commutes
 245 with space and time derivatives.

246 3. Inclusion of source terms

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

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

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

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

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

254 Application of the filter then leads to

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

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

$$\sigma_i \rho_i C_i = \overline{I_i \rho_i C}; \quad \sigma_i \rho_i E_i = \overline{I_i \rho_i E}. \quad (42)$$

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

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

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

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

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

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

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

Subtracting q_i times (44) then leads to

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

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

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

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

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

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

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

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

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

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

$$\left(\frac{\bar{p}}{p_0}\right)^{(1-\kappa)} = \frac{R}{p_0} \rho_i \theta_i + P_{\text{SF}}^i. \quad (50)$$

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

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

Since the relabelling terms in (48) would preserve the right hand side of (51), they would therefore preserve \bar{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) $C_v \rho_i T_i = (C_v/R) \bar{p}$ (where $C_v = C_p - R$ is the specific heat capacity at constant volume) is a function only of \bar{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

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

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.

334 *b. The relation between relabelling and physical processes*

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

346 First note that there is a close relationship between relabelling and mixing. As a simple illustra-
347 tive thought experiment, consider a situation in which q is uniform in fluid 1 and also in fluid 2,
348 but with different values in each. Now consider relabelling some of fluid 1 as fluid 2. As a re-
349 sult the mean mixing ratio in fluid 2 q_2 will change. Also, there will now be some subfilter-scale
350 variability of q in fluid 2; previously it was zero. In principle, if we were to keep track of the
351 subfilter-scale variability, for example through budgets of variance and higher order moments,
352 then the relabelling could be reversed; after all, the physical state of the system has not changed.
353 However, if no attempt is made to keep track of the subfilter-scale variability then this information
354 is lost; as far as a numerical model is concerned, the relabelled fluid 1 has effectively been mixed
355 into fluid 2. Because of this implied mixing, in practice we will want to relabel in situations where

356 it is reasonable to assume that mixing occurs. This is exactly what is done in typical mass flux
 357 convection schemes for entrainment and detrainment.

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

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

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

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

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

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

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

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

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

374 **5. Relation to existing approaches**

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

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

384 *a. Local turbulence closures*

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

390 The simplest such schemes include diagnostic eddy diffusivity schemes, usually applied to the
391 boundary layer, in one dimension (e.g. Louis 1979) or three dimensions (e.g. Smagorinsky 1963;
392 Germano et al. 1991). More sophisticated schemes attempt to diagnose or predict some higher
393 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 analogous.

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 $\mathbf{F}_{\text{SF}}^{\eta_i}$ and $\mathbf{F}_{\text{SF}}^{q_i}$ 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

$$\bar{\rho} \frac{D\bar{\eta}^*}{Dt} = -\frac{\partial}{\partial z} F_{\text{CF}}^{\eta}, \quad (57)$$

$$\bar{\rho} \frac{D\bar{q}^*}{Dt} = -\frac{\partial}{\partial z} F_{\text{CF}}^q, \quad (58)$$

where

$$F_{\text{CF}}^{\eta} = \sigma_1 \rho_1 w_1 \eta_1 + \sigma_2 \rho_2 w_2 \eta_2 - \bar{\rho} \bar{w}^* \bar{\eta}^* \quad (59)$$

436 and

$$F_{\text{CF}}^q = \sigma_1 \rho_1 w_1 q_1 + \sigma_2 \rho_2 w_2 q_2 - \bar{\rho} \bar{w}^* \bar{q}^*. \quad (60)$$

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

$$F_{\text{CF}}^\eta = \sigma_2 \rho_2 w_2 (\eta_2 - \bar{\eta}^*) = M(\eta_2 - \bar{\eta}^*) \quad (61)$$

439 and

$$F_{\text{CF}}^q = \sigma_2 \rho_2 w_2 (q_2 - \bar{q}^*) = M(q_2 - \bar{q}^*), \quad (62)$$

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

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

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

$$\frac{\partial M}{\partial z} = E - D, \quad (63)$$

448 where $E = \mathcal{M}_{21}$ is the entrainment rate, and $D = \mathcal{M}_{12}$ is the detrainment rate. If desired, the
 449 entrainment and detrainment may be expressed as fractional entrainment rates per unit height:
 450 $E = \varepsilon M$, $D = \delta M$.

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

$$\frac{\partial}{\partial z}(M q_2) = E \hat{q}_{21} - D \hat{q}_{12}. \quad (64)$$

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

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

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

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

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

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

or

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

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):

$$\begin{aligned} \frac{D_2 w_2}{Dt} + \frac{1}{\rho_2} \frac{\partial \bar{p}}{\partial z} + \frac{\partial \Phi}{\partial z} = \\ \frac{1}{\sigma_2 \rho_2} \left[\mathcal{M}_{21}(\hat{w}_{21} - w_2) - \mathcal{M}_{12}(\hat{w}_{12} - w_2) \right. \\ \left. - \frac{\partial}{\partial z} F_{\text{SF}}^{w_2} - b_2 - d_{21} \right]. \end{aligned} \quad (69)$$

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

468 form by assuming that the filter-scale mean state is in hydrostatic balance

$$\frac{1}{\bar{\rho}} \frac{\partial \bar{p}}{\partial z} + \frac{\partial \Phi}{\partial z} = 0, \quad (70)$$

469 so that

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

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

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

$$w_2 \frac{\partial w_2}{\partial z} = B + \frac{1}{\sigma_2 \rho_2} [E(\hat{w}_{21} - w_2) - D(\hat{w}_{12} - w_2) - b_2 - d_{21}]. \quad (72)$$

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

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

479 However, there is evidence that this assumption is a not a good approximation (e.g. Sherwood et al.
 480 2013), and some schemes account for other values of \hat{w}_{21} and \hat{w}_{12} by using (73) with a modified
 481 value of E for the entrainment of w (e.g. Siebesma et al. 2007). A variety of schemes have been
 482 proposed for parameterizing the pressure drag terms $b_2 + d_{21}$.

483 All of the assumptions and approximations made above are standard ones that can be found in
 484 the literature on parameterization of convection. Recent developments have attempted to relax some

485 of these approximations. For example, Gerard et al. (2009); Arakawa and Wu (2013); Grell and
 486 Freitas (2014) attempt to remove the assumption that the volume fraction of convecting fluid is
 487 small. Kain (2004); Plant and Craig (2008); Gerard et al. (2009); Grandpeix and Lafore (2010)
 488 include some elements of memory about the state of convection or boundary layer cold pools re-
 489 sulting from convective downdrafts, thereby relaxing the steadiness assumption. Vertical transport
 490 of horizontal momentum, both by advection and via pressure fluctuations (the \mathbf{b}_i and \mathbf{d}_{ij} terms),
 491 may be taken into account (e.g. Kim et al. 2008), representing ‘cumulus friction’.

492 *c. Eddy Diffusivity Mass Flux schemes*

493 EDMF schemes have been proposed to parameterize the local and nonlocal transports in the
 494 convective boundary layer, as well as transitions between the shallow cumulus, stratocumulus,
 495 and dry convective boundary layer. The net transport is decomposed into a local turbulent contri-
 496 bution modelled as an eddy diffusivity and a nonlocal contribution modelled using the mass flux
 497 approach. Thus, it combines the approaches discussed in sections 5a and 5b above, and it nicely
 498 illustrates how such hybrid approaches can be accommodated in the proposed framework. The
 499 dry convective boundary layer scheme of Siebesma et al. (2007) would correspond to using two
 500 fluid components, one to represent updraft and one to represent the rest of the fluid. The extended
 501 scheme of Neggers et al. (2009) would correspond to using three fluid components, one for dry
 502 updrafts, one for moist updrafts, and one for the rest of the fluid. In both cases subfilter-scale flux
 503 terms $\mathbf{F}_{\text{SF}}^{\theta_i}$, $\mathbf{F}_{\text{SF}}^{q_i}$, etc., could be included in one or more components to represent the eddy diffusive
 504 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 $\mathbf{F}_{\text{SF}}^{\eta_i}$ and $\mathbf{F}_{\text{SF}}^{\mathbf{u}_i}$ 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 \mathcal{M}_{ij} and subfilter-scale fluxes \mathbf{F}_{SF} would still be needed; these could be based on existing 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

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

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

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

535 The derivation of section 2 was constructed in such a way that the same mean pressure gra-
536 dient $\nabla \bar{p}$ appears in the momentum equations for all fluid components. This feature becomes
537 important when considering the multi-fluid equations, and particularly their numerical solution. If
538 different fluid components were permitted to have different pressures p_i then this would permit
539 the equations to support subfilter-scale acoustic modes with the entire cloud field in synchronized
540 oscillation. Besides being manifestly unphysical, such modes would likely be difficult to handle
541 numerically. The use of a single pressure field in all the component momentum equations can be
542 considered a type of filter that removes such acoustic modes. Note, however, that the different fluid
543 components are not required to have the same density. Since buoyancy can be expressed entirely
544 in terms of the densities of a fluid parcel and its environment together with gravity (e.g. Holton
545 2004; Vallis 2017, see also equation (71) above), the use of a single pressure field does not prevent
546 buoyancy effects from being explicitly represented. On the other hand, rising thermals do not in
547 general experience the same pressure gradient as their environment. For example, pressure pertur-
548 bations above and below a thermal can provide an effective drag (e.g. Romps and Charn 2015).
549 Such small-scale pressure perturbations are included in the conditional filtering framework, but
550 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 \bar{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 \bar{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 $\nabla \bar{p}$ term even in the case $\mathcal{M}_{ij} = 0$.

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, $\mathbf{v}_i = (\sum_i \sigma_i \rho_i \mathbf{v}_i) / \bar{\rho} = \bar{\mathbf{v}}^*$. The prognostic equation for \mathbf{v}_i is then just the horizontal component of (A9):

$$\bar{\rho} \frac{D\bar{\mathbf{v}}^*}{Dt} + \nabla_H \bar{p} + \bar{\rho} \nabla_H \Phi = - \sum_i \nabla \cdot \mathbf{F}_{\text{SF}}^{\mathbf{v}_i}, \quad (74)$$

where ∇_H is the horizontal gradient operator, $\mathbf{F}_{\text{SF}}^{\mathbf{v}_i}$ are the subfilter-scale fluxes of horizontal momentum, and the $\mathbf{F}_{\text{CF}}^{\mathbf{v}}$ contribution vanishes because of the equality of the \mathbf{v}_i . There might be some

573 computational benefit from making this approximation. On the other hand, there might be some
574 benefit in modeling the vertical flux of horizontal momentum by retaining separate \mathbf{v}_i for each
575 component, for example near squall lines or frontal convection. It would be valuable to explore
576 this trade-off.

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

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

595 Application of similar ideas to convective flows go back at least as far as Cushman-Roisin
596 (1982), who proposed to describe dry convection in terms of ‘thermals’ and ‘antithermals’ with

597 separate dynamical equations for each. In relation to the meteorological literature, there are a
 598 number of similarities between our proposed framework and the work of Yano et al. (2010); Yano
 599 (2012, 2014, 2016). He too proposes to decompose the flow into a number of components each oc-
 600 cupying distinct regions, with separate dynamical equations for each component. However, there
 601 are some important differences too. Yano (2012) restricts attention to the hydrostatic primitive
 602 equations. He makes the segmentally constant approximation in which fluid properties within
 603 each component are assumed constant within a grid cell; he thus omits terms corresponding to
 604 our subfilter-scale fluxes. As a result of other approximations, the equations for the different fluid
 605 components fully decouple from each other in the absence of entrainment and detrainment; this
 606 is in contrast to (37) above, in which the fluid components remain coupled through the common
 607 $\nabla \bar{p}$ term and the requirement for $\sum_i \sigma_i = 1$. Yano et al. (2010); Yano (2014, 2016) also make the
 608 segmentally constant approximation, but now the underlying equation set is the nonhydrostatic
 609 anelastic equations. Again the flow is decomposed into a number of components with the aid
 610 of labels analogous to our I_i . Yano (2014) and Yano (2016) focus on the transport equation and
 611 on the conceptual aspects of the approach. Yano et al. (2010) develop the approach into a two-
 612 dimensional vertical slice model and apply it to simulation of dry convection. To do this they must
 613 numerically solve a Poisson equation for the pressure at each time step. Thus their implementation
 614 resembles an adaptive mesh refinement method rather than a typical parameterization.

615 Finally, the work of Kuell et al. (2007); Kuell and Bott (2008) should be mentioned. They allow
 616 the dynamical core to handle the environmental subsidence that compensates the net convective
 617 mass flux due to updrafts and downdrafts. The parameterization itself handles the convective
 618 updrafts and downdrafts and hence determines mass sink and source terms for the dynamical core.
 619 These mass source and sink terms correspond to the \mathcal{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,

642 for a typical climate model, convergence with increasing resolution (if obtained at all) must be
 643 interpreted with considerable caution (Williamson 2008).

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

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 655 this paper.

656 APPENDIX

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

$$\overline{\rho X}^* \equiv \overline{\rho X}, \quad (\text{A1})$$

661 and note a useful identity

$$\overline{\rho X}^* = \overline{\rho X} = \overline{\sum_i I_i \rho X} = \sum_i \sigma_i \rho_i X_i. \quad (\text{A2})$$

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

$$\frac{\partial \bar{\rho}}{\partial t} + \nabla \cdot (\bar{\rho} \bar{\mathbf{u}}^*) = 0. \quad (\text{A3})$$

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 \mathcal{M}_{ij} gives

$$\frac{\partial}{\partial t} (\bar{\rho} \bar{q}^*) + \nabla \cdot (\bar{\rho} \bar{\mathbf{u}}^* \bar{q}^*) = -\nabla \cdot \left(\sum_i \mathbf{F}_{\text{SF}}^{qi} + \mathbf{F}_{\text{CF}}^q \right), \quad (\text{A4})$$

where

$$\mathbf{F}_{\text{CF}}^q = \sum_i \sigma_i \rho_i \mathbf{u}_i q_i - \bar{\rho} \bar{\mathbf{u}}^* \bar{q}^*. \quad (\text{A5})$$

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

$$\frac{\bar{D} \bar{q}^*}{Dt} = -\frac{1}{\bar{\rho}} \nabla \cdot \left(\sum_i \mathbf{F}_{\text{SF}}^{qi} + \mathbf{F}_{\text{CF}}^q \right), \quad (\text{A6})$$

where

$$\frac{\bar{D}}{Dt} \equiv \frac{\partial}{\partial t} + \bar{\mathbf{u}}^* \cdot \nabla \quad (\text{A7})$$

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 $\mathbf{F}_{\text{SF}}^{qi}$ plus a contribution from the variations of properties between fluid components picked out by the conditional filtering \mathbf{F}_{CF}^q .

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

$$\frac{\bar{D} \bar{\eta}^*}{Dt} = -\frac{1}{\bar{\rho}} \nabla \cdot \left(\sum_i \mathbf{F}_{\text{SF}}^{\eta i} + \mathbf{F}_{\text{CF}}^{\eta} \right), \quad (\text{A8})$$

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

677 form:

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

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

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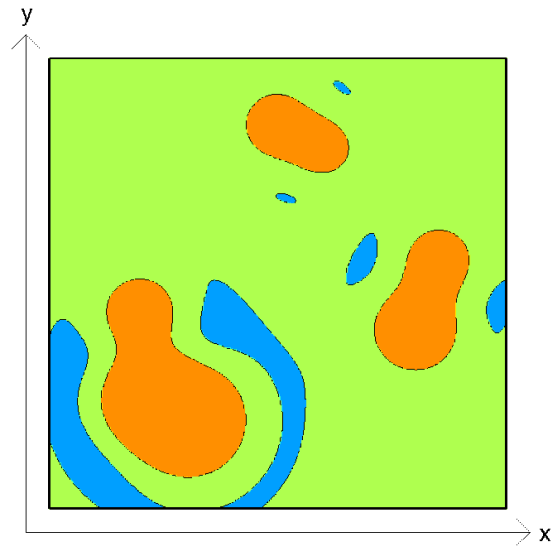
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835 **LIST OF FIGURES**

836 **Fig. 1.** Schematic horizontal section showing a decomposition of the fluid into multiple compo-
837 nents, for example updrafts (orange), downdrafts (blue), and environment (green). In each
838 component one of the I_i is equal to 1 and the others are equal to 0. 45



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