Convection in a Single Column
– Modelling, Algorithm and Analysis

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The group focused on a model problem of idealised moist air convection in a single column of atmosphere. Height, temperature and moisture variables were chosen to simplify the mathematical representation (along the lines of the Boussinesq approximation in a height variable defined in terms of pressure). This allowed exact simple solutions of the numerical and partial differential equation problems to be found. By examining these, we identify column behaviour, stability issues and explore the feasibility of a more general solution process.
1. Introduction

Atmospheric models used for weather and climate prediction use the classical compressible Navier-Stokes equations, laws of thermodynamics, and laws governing phase changes, radiation and surface fluxes. However, the exact solution of these equations is not computationally feasible, and the equations have to be averaged in space and time before being solved. It is then necessary to design sub-grid models which represent the averaged effects of the unresolved small scales on the resolved solution.

A particularly difficult situation arises with cumulus convection. This is responsible for much of the severe weather outside the tropics, and is the main driver of the tropical circulation which is a fundamental part of the climate system. Cumulus convection can only be directly represented in models with a horizontal grid of at most one or two kilometres. This is not affordable in global climate models at present. The sub-grid modelling of convection is very difficult because of the jump-like nonlinearity of the moisture-heat exchange processes involved. Such a model has to build in the effects of the large-scale solution on the convection.

In order to understand these effective large-scale constraints, and thus improve the sub-grid models, it is useful to consider the evolution of a single column of moist air. It is well-known by practising weather forecasters that the occurrence and intensity of convection can be predicted by studying the temperature and moisture profiles in such a column together with knowledge of the external forcing, e.g. see [5], chapter 4. The challenge set for the study group was to make a mathematically rigorous version of a single column model which behaved in a way that agreed with the observed behaviour. Such a model can then be used to validate the sub-grid models in daily forecasts, and potentially to improve them. The existence of a rigorous model which describes at least the most important part of the convective process would also indicate high potential deterministic predictability in a situation where deterministic predictions are not yet consistently successful.

We therefore study the stability of a moist vertical column of air in the presence of external forcing, such as the bodily lifting of the column. Stability requires that the potential temperature $\theta$ must increase as a function of the height $z$ (in suitably scaled pressure units). But the physics also requires a constraint holds that the water vapour $q$, i.e. the moisture carried by the air, must be less than a critical level denoted by $Q_{\text{sat}}(\theta, z)$. If not, the excess vapour in an air parcel then condenses and releases heat to the air parcel, thus increasing the potential temperature, and hence possibly changing the stability of the parcel. For simplicity, we treat all condensation as vapour to rain, ignoring things like ice/snow mixtures, and allow the rain to fall out of the column.

2. Physical constraints in convection modelling

Some key features of the local convection problem are as follows.
Convective processes happen in a shorter time-scale than that of the horizontal dynamics, and are usually localized in the horizontal scale.

Given a parcel, there are three constraints for potential temperature $\theta$, humidity $q$ and air mass, as the parcel moves vertically.

(i) If the parcel stays unsaturated, then $\theta, q$ and its air mass are conserved respectively.

(ii) If the parcel stays saturated, then its air mass is conserved. The second constraint simply is $q = Q_{\text{sat}}(\theta, z)$. The third constraint is that the “moist potential temperature”

$$\theta^M := \theta + Lq$$

is conserved. Here, $L$ is a physical constant which gives the latent heat of conversion released to the air parcel when some of the water vapour condenses to precipitation (cloud, rain, ice or some mixture), and $Q_{\text{sat}}(\theta, z)$ is a given function of $\theta, z$ determined by the physical properties of the air and its water vapour.

The conditions (i), (ii) arise from conservation in both the physical and mathematical senses of moist thermal energy (measured by the suitably defined potential temperature which is related to the entropy), of moisture as either water vapour or cloud/rain, and of air mass, all defined on the air parcels as they move.

**Definition 1.** Given the saturation specific humidity $Q_{\text{sat}}(\theta, z) : \mathbb{R}^2 \mapsto \mathbb{R}$ as a smoothly differentiable function of $\theta, z$ satisfying

\begin{equation}
\frac{\partial Q_{\text{sat}}}{\partial \theta} > 0 \quad \text{and} \quad \frac{\partial Q_{\text{sat}}}{\partial z} < 0,
\end{equation}

the “moist adiabat” is a formula associated with a given parcel (with saturated status) and represented by a curve in the $(\theta, z)$ plane, which obeys the above constraint (ii), i.e.

\begin{equation}
\theta^M = \text{constant} = \theta + Lq = \theta + LQ_{\text{sat}}(\theta, z).
\end{equation}

The monotonicity conditions (2.1) guarantee that there exist two smoothly differentiable functions $Z_{\text{ad}}(\cdot, \cdot), \Theta_{\text{ad}}(\cdot, \cdot)$ so that the above moist adiabat formula is equivalent to

$$z = Z_{\text{ad}}(\theta, \theta^M) \iff \theta = \Theta_{\text{ad}}(z, \theta^M).$$

In other words, a moist adiabat curve is the level set curve of function $\theta + LQ_{\text{sat}}(\theta, z) = \theta^M = \text{constant}$ in the $(\theta, z)$ plane, which is identical to the graph of $z = Z_{\text{ad}}(\theta, \theta^M)$, and of $\theta = \Theta_{\text{ad}}(z, \theta^M)$, with constant $\theta^M$.

Following this definition and applying the chain rule, we obtain:

**Proposition 2.** On the moist adiabat with a constant $\theta^M$,

$$\frac{\partial Z_{\text{ad}}}{\partial \theta} = 1 + L \frac{\partial Q_{\text{sat}}}{\partial \theta} \quad \text{and} \quad \frac{\partial Z_{\text{ad}}}{\partial \theta} \frac{\partial \Theta_{\text{ad}}}{\partial z} = 1.$$
We can combine this with (2.1) to immediately have, with a constant $\theta^M$,

\[
\frac{\partial \Theta_{\text{ad}}}{\partial z} > 0 \quad \text{and} \quad \frac{\partial Z_{\text{ad}}}{\partial \theta} > 0.
\]

Now, consider that $\theta^M$ is defined by the parcel’s initial configuration and remains constant during the convection process, for both unsaturated and saturated parcels. Then, we can unify these two cases to give a relation between the initial (subscript “in”) and final (subscript “fi”) configurations of a given dry/wet parcel experiencing a rising/lowering displacement from $z_{in}$ to $z_{fi}$,

\[
\theta_{fi} = \Theta_{\text{disp}}(\theta_{in}, q_{in}, z_{fi}) := \max \{ \theta_{in}, \Theta_{\text{ad}}(z_{fi}, \theta_{in} + Lq_{in}) \},
\]

\[
Lq_{fi} = \theta_{in} + Lq_{in} - \theta_{fi}.
\]

The definition of $\Theta_{\text{disp}}$ is regardless of the stability of these configurations, and can be used to describe virtual displacement in the variational formulation. Several remarks are in order.

1. The use of moist adiabat implies $\theta^M = \theta_{in} + Lq_{in} = \theta_{fi} + Lq_{fi}$ for both wet/dry cases.

2. We impose the maximum since by (2.1) and (2.2), having $\theta_{fi} < \Theta_{\text{ad}}(z_{fi}, \theta^M)$ would mean

\[
\theta_{fi} < \Theta_{\text{ad}}(z_{fi}, \theta^M) \implies LQ_{\text{sat}}(\theta_{fi}, z_{fi}) < LQ_{\text{sat}}(\Theta_{\text{ad}}(z_{fi}, \theta^M), z_{fi}) = \theta^M - \Theta_{\text{ad}}(z_{fi}, \theta^M) < \theta^M - \theta_{fi} = Lq_{fi}
\]

i.e. $Q_{\text{sat}}(\theta_{fi}, z_{fi}) < q_{fi}$ which would be unphysical. Interestingly, if we replace all occurrences of $<$ with $=$ above, the calculation still holds; and likewise if we replace all occurrences of $<$ with $>$ above. Thus, we obtain an equivalent saturation condition,

\[
\text{sign} \left( q - Q_{\text{sat}}(\theta, z) \right) = \text{sign} \left( \Theta_{\text{ad}}(z, \theta^M) - \theta \right) \quad \text{where} \quad \theta^M = \theta + Lq.
\]

3. The use of maximum above also means $\theta_{fi} \geq \theta_{in}$, namely, only a rising parcel can possibly increase temperature upon condensation of some of its water vapour. Re-evaporation is neglected, and its modelling is possible only if cloud information is included. Our model is time irreversible.

**Convective instability and monotonicity of $Q_{\text{sat}}$.** Convective instability is tied to the key properties that $Q_{\text{sat}}$ increases with $\theta$ and decreases with height $z$ (c.f. (2.1)). First, the column is unstable whenever $\theta$ is not monotonically increasing in $z$. Further, even the monotonicity holds, we still need to check the saturation condition. When the actual humidity of a parcel reaches the saturation level $q = Q_{\text{sat}}$, condensation takes place and latent heat is released, resulting in increase in $\theta$. In turn, the parcel is lifted up by buoyancy. Then, one can use the monotonicity of $Q_{\text{sat}}$ in (2.1) and Proposition 2 to show that following any rising, saturated parcel, the Lagrangian derivative $\frac{DQ_{\text{sat}}}{Dt} < 0$. This decrease in $Q_{\text{sat}}$ will encourage more condensation and thus release of more latent heat, resulting in a positive feedback mechanism for a saturated parcel to rise.
For the parcel to *continue* rising (i.e. convective instability) however, we need more. If \( \theta \) is differentiable in \( z \), we propose two conditions related to convective instability,

(2.7) \( \text{“triggering condition”:} \quad \frac{\partial \Theta_{\text{ad}}}{\partial z}(z, \theta^M) \geq \frac{\partial \theta}{\partial z}(z, \theta^M) \) and \( q = Q_{\text{sat}}(\theta, z) \),

(2.8) \( \text{“stopping condition”:} \quad \frac{\partial \Theta_{\text{ad}}}{\partial z}(z, \theta^M) < \frac{\partial \theta}{\partial z}(z, \theta^M) \),

the latter of which defines the bottom of an “inversion layer” or is near the tropopause. Note that the inversion layer can be dynamically changing with time and actually dependent on the \( \theta^M \) of each parcel.

These two conditions are consistent with the maximisation of \( \int z \theta \, dz \) over all rearrangements of the parcels, i.e. measure-preserving maps, which is carried out in the algorithm below. The conditions can be shown using a variational argument with the perturbation being swapping of two small measures/blocks of parcels. In the general situation where \( \theta \) is not necessarily differentiable, the conditions (2.7), (2.8) are applied on small blocks of air at different heights (locally or globally) by comparing their temperatures.

### 3. Settings of the model problem

Consider a single vertical column that is horizontally uniform. It is being uniformly lifted on a longer timescale than that of the convective adjustment.

**Assumption 1.** The column responds/makes adjustment, according to the physical environment’s thermodynamic change, but any feedback to the environment is neglected.

**Assumption 2.** For simplicity, physical processes such as background thermal radiation and ice/water re-evaporation are neglected so that a given parcel’s humidity \( q \) never increases, and so here its \( \theta \) never decreases.

**Assumption 3.** There are no mass/heat/water vapor fluxes at the top and bottom boundaries.

The column may be rising as a whole at a given speed and still satisfying the no flux boundary conditions. This is a simplified model for a cold front wedging at a constant rate under a column of moist air. The wedging is at a slower rate than the convective adjustment.

By using a co-moving frame, the spatial domain is fixed as \( z \in [0, 1] \). Then, the term \( (-\alpha t) \) in (3.9) accounts for the column’s actual upward motion.

Under the hydrostatic assumption, for the single column model, the actual height and pressure are monotonically linked. Then, we use Hoskins’ pseudo-height \( z \),

\[
z := \left\{ 1 - \left( \frac{p}{p_0} \right)^{R/c_p} \right\} z_a
\]

so that the (environmental) pressure variable becomes implicit. The constant \( z_a > 1 \).

For simplicity and to provide explicit examples, we adopt an accurate approximation ([4])

(3.9) \( Q_{\text{sat}}(\theta, z) = A_0 \exp \left( r \left[ \theta - \beta z - \theta_{\text{PBL}} - \alpha t \right] \right) \),
where $A_0$, $r$, $\beta$, $\theta_{\text{PBL}}$ and $\alpha$ are constants. The $Z_{\text{ad}}$ function of Definition 1 is then explicitly given as

$$Z_{\text{ad}}(\theta, \theta^M) = \frac{1}{\beta} \left[ \theta - \frac{1}{r} \ln \frac{\theta^M - \theta}{L A_0} - \theta_{\text{PBL}} - \alpha t \right].$$

(3.10)

In light of Proposition 2, we have that on the moist adiabat with constant $\theta^M$,

$$\frac{\partial Z_{\text{ad}}}{\partial \theta} = \frac{1}{\beta} \left[ 1 + \frac{1}{r (\theta^M - \theta)} \right] = \frac{1}{\beta} \left[ 1 + \frac{1}{r L Q_{\text{sat}}} \right].$$

(3.11)

Therefore, the threshold used in instability/stability conditions (2.7), (2.8) is explicitly

$$\frac{\partial \Theta_{\text{ad}}}{\partial z}(z, \theta^M) = \beta \left[ 1 + \frac{1}{r L Q_{\text{sat}}} \right]^{-1}.$$

(3.12)

Rearrangement/adjustment problem. Based on Lock and Norbury [4] and Goldman’s MSc thesis [2], we make

Assumption 4. The column responds/makes adjustment at a much shorter time scale compared to the environment’s thermodynamic change. So we do not model the actual dynamics, i.e. the acceleration and deceleration of a saturated parcel rising due to buoyancy. Mathematically, the response time is infinitesimal.

Main idea: the potential energy $\int z \theta \, dz$ is maximised in a way consistent with the moist adiabat. See the next two sections.

Remark 3. The PDEs (7), (8) in Goldman’s thesis [2] are basically the same as Definition 1 of “moist adiabat”. That result was regarding the existence of weak solutions to (7), (8) in [2] under some stability condition – no uniqueness was proven. The maximisation of $\int z \theta \, dz$ was not explicitly stated in the theorems there, but in the construction of weak solutions, the proof of [2] uses a rearrangement strategy to enforce a certain monotonicity condition which, combined with his stability condition, may just maximize $\int z \theta \, dz$. Goldman claims his version of the stability condition is consistent with that of Cullen & Purser [1].

4. Sorting algorithm

Recall constraints (i), (ii) and Definition 1 of “moist adiabat”.

Dependent variables are $\theta_P$, $q_P$, $z_P$ with subscript P indicating they are Lagrangian variables on a parcel. These variables are subject to either the unsaturated constraint, i.e. $\theta_P, q_P$ remain constant, or the saturated constraint, i.e. $q_P = Q_{\text{sat}}(\theta_P, z_P)$ and $\theta_P = \Theta_{\text{ad}}(z_P, \theta^M_P)$. Mass is conserved due to the fact that the algorithm simply rearranges the discrete blocks of parcels.

The saturation function $Q_{\text{sat}}$ is given by (3.9). For now consider $t = 0$.

The numerical sorting algorithm assumes that the atmosphere is divided into $N$ parcels with initial temperatures $\theta^0_1, \theta^0_2, ..., \theta^0_N$ and moistures $q^0_1, q^0_2, ..., q^0_N$ (some of which are at saturation) at the heights $z_1, z_2, ..., z_N$. For each parcel the combination $\theta^M_i = \tilde{\theta}_i + L \tilde{q}_i =$
\( \theta_i^0 + Lq_i^0 \) is conserved during the rearrangement. Here the hat on the variables denotes the value of \( \theta_p, q_p \) and \( z_p \) during the sort. Thus if the moisture level changes due to condensation, then the temperature increases. With the function defined in (2.4) that unifies the dry and wet cases, we can write

\[
\hat{\theta}_i = \Theta_{\text{disp}}(\theta_i^0, q_i^0, \hat{z}_i) \quad \text{and} \quad \hat{q}_i = (\theta_i^0 + Lq_i^0 - \hat{\theta}_i)/L.
\]

The algorithm works by starting at height \( z_N \). It then temporarily lifts every parcel below this height up to \( z = z_N \) with the would-be \( \hat{\theta}_i \) determined by the above formula. Once this is done for all parcels below \( z_N \), the parcel with the largest temperature (e.g. labelled \( m \)) is chosen to be at height \( z_N \). Parcel \( m \) is then eliminated from the sort. Parcels previously labelled \((m + 1)\) to \( N \) have their heights lowered by one grid.

The code then moves to \( z_{N-1} \) and repeats until it reaches \( z_1 \).

Results of this code are presented in Figure 1 for the initial configuration and in Figure 2 for the final configuration. We choose the following parameters

\[
z_i = \frac{i - 0.5}{N}, \quad i = 1, ..., N,
\]

and initial temperature configuration

\[
\theta_i^0 = 300 \exp\left(\frac{z_i}{6}\right),
\]

where

\[
A_0 = 0.025, \quad r = 0.09, \quad \beta = 120, \quad \theta_{\text{PBL}} = 300,
\]

in \( Q_{\text{sat}} \). The value of \( L = 2400 \). The initial moisture levels are taken to be

\[
q_i^0 = \min\left\{1, \frac{5}{4} + \frac{1}{2} \sin(8\pi z_i)\right\} Q_{\text{sat}}(\theta_i^0, z_i).
\]

The results in Figure 2 show that the numerical sorting algorithm appears to converge as \( N \) is increased. At this stage the visual convergence is sufficient, but more detailed numerical analysis is required to confirm this. As \( N \) increases the system moves towards that of unsaturated air for \( z \lesssim 0.4 \) and approximately a region of saturated air parcels above this. The highly oscillatory behaviour of moisture in Plot (f) may suggest that as \( N \to \infty \), the algorithm converges to some kind of transport plan rather than a transport map. Also note that the final temperature distribution contains step jumps in the temperature for \( N = 50 \) and 500, but these get smoothed out as the number of parcels increases to \( N = 5000 \). However, the final temperature distribution and its smoothness depend on the given initial data.

5. Theory of optimal transport

For SG motion in the \( x - z \) plane ([3]), a saturated parcel moves along an adiabatic surface and conserves the \( x \)-momentum (since there is no movement in the \( y \)-direction). If the energy minimisation property in the dry case also applies here, then the total energy
\(- \int z \theta \, dz + \text{kinetic energy}\) is minimised. But since the kinetic energy is constant, we must have that \(\int z \theta \, dz\) is maximized.

Back to the column problem. For the transport map, it is represented by a function \(\sigma : [0, 1] \mapsto [0, 1]\) which preserves the Lebesgue measure, i.e., for any \(0 \leq a \leq b \leq 1\),

\[
\int_a^b \sigma(z) \, dz = b - a.
\]

Let \(\mathcal{M}\) be the collection of all such measure preserving maps. Recall \(\Theta_{\text{disp}}\) defined in (2.4). Then we look for (maybe more than one) maximizer

\[
\sigma^* = \arg \max_{\sigma \in \mathcal{M}} \left\{ \int_0^1 \sigma(z) \Theta_{\text{disp}}(\theta(z), q(z), \sigma(z)) \, dz \right\}.
\]

For the transport plan, it is represented by a (generalized) nonnegative function \(K(z, z')\) defined on \([0, 1] \times [0, 1]\). It quantifies the percentage of parcels moved from \(z\) to \(z'\). It preserves things in the sense of marginal probability measures,

\[
\int_0^1 K(z, z') \, dz = \int_0^1 K(z', z) \, dz' = 1.
\]

The transport map \(\sigma(z)\) is a special case \(K(z, z') = \delta(z' - \sigma(z))\). So, in general, \(K(\cdot, \cdot)\) is a measure (nonnegative distribution) defined on \([0, 1] \times [0, 1]\).

Let \(\mathcal{P}\) be the collection of all such measure preserving plans. Then we look for (maybe more than one) maximizer

\[
K^* = \arg \max_{K \in \mathcal{P}} \left\{ \int_0^1 \int_0^1 z' K(z, z') \Theta_{\text{disp}}(\theta(z), q(z), z') \, dz \, dz' \right\}.
\]

6. Conclusion

We constructed a numerical algorithm whose solutions converged to exact solutions that we found for some idealised test cases. But we also found that the numerical solutions for certain initial moisture and temperature data appeared to converge to “new” types of solutions which correspond to transport plans (rather than maps) for the variational problems. These new solutions are extremely challenging for conventional fluid dynamics codes because they are highly, and discontinuously, oscillatory and vary rapidly from wetter to drier layers. The sorting algorithm appeared to find that different solutions may exist for the same initial data and this suggests further work in how to devise computer code in practical forecasting.
REFERENCES

[1] Cullen, M. J. P., and R. J. Purser. “An extended Lagrangian theory of semi-geostrophic frontogenesis.” Journal of the atmospheric sciences 41, no. 9 (1984): 1477-1497.

[2] Goldman, Dorian. “Weak Lagrangian Solutions to a One Dimensional Model of the Moist Semi-geostrophic Equations.” M.Sc. diss., University of Toronto, 2008.

[3] Holt, M. W. “Semigeostrophic moist frontogenesis in a Lagrangian model.” Dynamics of Atmospheres and Oceans 14 (1989): 463-481.

[4] Lock, A. M., and J. Norbury. “A column model of moist convection: some exact equilibrium solutions.” Quarterly Journal of the Royal Meteorological Society 137, no. 657 (2011): 979-991.

[5] Met Office “Forecaster’s Reference Book”, 2nd ed. Met O. 1012 (1993).
Figure 1. Plot (a0) is the initial temperature distribution $\theta^0_i(z_i)$ and (b0) is the initial moisture distribution $q^0_i(z_i)$ (blue line) for $N = 5000$ parcels. In Plot (b0) the red line denotes $Q_{sat}(\theta^0_i, z_i)$.

Figure 2. Plots of (a), (c), (e) are the final temperature distribution $\theta_i(z_i)$ and (b), (d), (f) are the final moisture distribution $q_i(z_i)$ where the red curves denote the new $Q_{sat}$. The number of parcels is: $N = 50$ in (a), (b); $N = 500$ in (c), (d); and $N = 5000$ in (e), (f).