Moist thermodynamics and moist turbulence for modelling at the non-hydrostatic scales

J.-F. Geleyn and P. Marquet Météo-France, Toulouse

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Precisions

- This presentation has to do with the diabatic part of high resolution modelling (and its 'interfacing'):
 - The issue about the need (or not) of a treatment differing from the one of diabatism in the hydrostatic system is left to the next talk;
 - Hence, '*non-hydrostatic*' is here just a short-hand for 'applicable at scales where non-hydrostatism matters for reversible motions'.
- At such high (horizontal) resolutions (below $\delta x \sim 3$ km):
 - The devil is really in the detail ... (see examples later)
 - Use of quite firm modelling guidelines gets more and more crucial;
 - We need new unifying concepts and probably the revisit of some long-lasting paradigms.
- In this perspective, the key-words of this talk will be: *conservation laws*', *consistency*', *clarification of boundaries*', *entropy*', *multi-phasic systems*'.

Guidelines through the talk

- When looking at all new problems linked with reaching the 'NH scales', there are many ways to address the whole issue.
- Here we are electing to concentrate on two questions:
 - How to represent pressure gradients in multi-phasic systems (both horizontally and vertically)?
 - Which thermodynamic quantity's conservation law is most appropriate as guideline, when 'subgrid' reduces more and more to 'turbulent + cloudy vs. clear sky'?
- Our answers are (under the guideline of 'consistency'):
 - By using a barycentric framework for developping the generic equations of the 'physics-dynamics' interface;
 - **Entropy**, for several reasons.
- Let us now see why!

Simplifying hypotheses

- We first need a set of simplifying assumptions (the full problem is quasi-untractable for NWP purposes).
- Main hypotheses for the diabatic part:
 - Permanent thermodynamic equilibrium
 - Condensed phases have a zero volume
 - All gases obey Boyle-Mariotte's and Dalton's laws
 - Specific heat values are temperature-independent
 - Homogeneity of the temperature between all species
- The first four hypotheses are 'classical'. Only the last one is 'oriented' (towards the idea of a 'flux divergence' representation of conservation laws, see below).
- Note that we did these choices independently of issues that more specifically touch the dynamics (*HPE vs. NH*; *conservation of total mass or not*; *which 'atmospheric parcels' are considered?*).

'Consistency' aspects and one very synthetic consequence

$$\begin{cases} p = \rho R.T & (Perfect gas law) \\ R = R_d (1 - q_v - q_l - q_i) + R_v q_v \\ C_p = C_{pd} (1 - q_v - q_l - q_i) + C_{pv} q_v + C_l q_l + C_i q_i \\ (1 - q_v - q_l - q_i) + C_{pv} q_v + C_l q_l + C_i q_i \\ L_{v/s}(T) = L_{v/s}^{T=0} + (C_{pv} - C_{l/i}).T \\ \frac{\partial \ln(e_s(T))}{\partial T} = \frac{L_{v/s}(T)}{R_v T^2} & (Clausius - Clapeyron) \end{cases}$$

For all transformations (except 'radiation + friction => heat', but including the effect of precipitations) this leads to conservation of a given form of the 'moist' entropy, ds_m/dt=0 with:

$$s_{m} = (C_{pd} + r_{t}.C_{pv}).\ln(T) - R_{d}.\ln(p-e) - r_{t}.R_{v}.\ln(e) - \frac{L_{v}(T).r_{l} + L_{s}(T).r_{i}}{T}$$

with $r_{()} = q_{()}/(1 - q_{v} - q_{l} - q_{i})$ and $r_{t} = r_{v} + r_{l} + r_{i}$

The 'LSPRT' issue (1/3)

- The topic addressed here is specific to spectral modelling, but the 'message' is of wider interest.
- The computation of the horizontal $Grad(\Phi)$ contribution to the pressure gradient term requires to use only derivatives of the prognostic variables.
- So-called grid-point variables (hydrometeors typically) cannot enter this computation if *T* is the thermodynamic prognostic spectral variable.
- In such a case (and provided q_v is treated spectrally) the computation is approximated by using $R=R_d+q_v(R_v-R_d)$
- But, if we use the previous equations, in the vertical we get $d(\Phi) = -[R_d(1-q_v-q_l-q_i-q_s)+R_v,q_v].T.d(ln(p))$

The 'LSPRT' issue (2/3)

- Even if the order of magnitude appears small 'on the paper', the impact of the inconsistency at the 'NH scales' can be impressive (see next viewgraph).
- We know this because there exist the *LSPRT*=.*T*. option in the IFS/ARPEGE/ALADIN code, which makes *RT* the thermodynamic spectral prognostic variable, allowing the use of the 'correct' *R* value.
- And LSPRT can work either with q_v in grid-point or q_v <u>spectral</u>. The latter case allows a clean comparison with the LSPRT=.F. case, for evaluating the impact of the discrepancy between the respective vertical and horizontal gradients of geopotential.

The 'LSPRT' issue (3/3)

Grad (RT) with qv only; dx = 2.3km

Grad (RT) with all species



Associated questions:

- Any other similar '*small inconsistency*' is likely to cause similar feed-backs;

- Initialization: filtering 'RT' is detrimental (non linearity) => need for a small inconsistency between initialisation and forecast.

> Contributors: S. Malardel & Y. Bouteloup (sensitivity), R. Brožková & P. Smolíková (DFI problem)

What is behind the choice of a fully multiphasic 'R' value? (1/2)

- We have just seen the key role, at the 'NH scales', of the choice of 'R'. In the example, the falling species $q_{r/s}$ were also accounted for. This corresponds to the choice of the so-called 'barycentric' definition of the 'parcel' (precipitation becomes another sub-grid [just better organised] transport).
- The alternative is to exclude $q_{r/s}$ from what the adiabatic part of the model 'sees' and to treat these species separately.
- This is quite easy for their 'steady' regime, but what about their acceleration phase and/or the evaporation-sublimation?
- In nature, what prevents condensed species from reaching higher and higher fall-speeds is a local pressure gradient between the top and bottom of drops/crystals, <u>a gradient</u> also felt in the whole atmospheric column.

What is behind the choice of a fully multiphasic 'R' value? (2/2)

- Hence, in the case of the hydrostatic assumption (and of a prognostic treatment of $q_{r/s}$) it is correct to assume that $dp=-\rho.d\Phi$ must be computed with ρ accounting for the presence of falling species.
- In the case of barycentric equations, this choice 'filters out' the issue about local volume changes when condensed water species do appear and/or disappear.
- In the NH case, one can show that the 'filtering condition' becomes $p = \rho_{gas} R_{gas} T = \rho RT$ (with *R* and ρ from all species).
- When going to the non-barycentric system, the filtering disappears for $q_{r/s}$ and one should in principle account for their acceleration phase as well as for their return to vapour!

Green-Ostrogradsky form of the thermodynamic equation (1/3)

- This following will have to do with the intra-time-step variations of C_p , C_v and hence R, following the phase changes of a barycentric multi-phasic system (here $q_{v/l/i/r/s}$)
- Using $C_p = C_v + R$, the first principle of thermodynamics and the conservation law for moist entropy, one gets a G-O form for the evolution of enthalpy (with δ_m a tag for conservation or not of the total mass and with P' & P''' the massweighted integrals of phase changes with respect to vapour):

$$\frac{d}{dt}(c_p T) = g \frac{\partial}{\partial p} \left[L_l(T=0)(P_l' - P_l''') - (c_l - c_{pd})P_l T + L_i(T=0)(P_i' - P_i''') - (c_i - c_{pd})P_l T + \delta_m(\hat{c} - c_{pd})(P_l + P_i)T \right]$$

$$\hat{c} = \frac{c_{pd}q_a + c_{pv}q_v + c_lq_l + c_iq_i}{1 - q_r - q_s}$$

Green-Ostrogradsky form of the thermodynamic equation (2/3)

- The previous equation must be complemented by the radiative anb turbulent transport of enthalpy fluxes, but this does not change its shape or characteristics.
- It is sometimes customary to say that neglecting the time variation of *Cp* (or *Cv*, or *R*) during the 'physical time-step' (under the influence of phase changes) has little impact.
- Like in the 'LSPRT' case, we shall now see that this is not true at all at the 'NH scales'.
- The trick, given the compact shape of the previous fluxconservative form of the enthalpy equation, is just to replace on the left-hand side $(d(C_p, T))$ by (C_p, dT) !

Impact of (no) enthalpy conservation

ALARO test (with 3MT in order to make up for the difference between convection 'permitting' and convection 'resolving') on 2.3 km mesh (90s time step); 6h precipitation on 18/05/2008 (+12h to +18h)



with enthalpy conservation

without enthalpy conservation

Precipitation patterns are roughly the same, but the local intensity may be very different, nearly doubled at maximum

Courtesy of R. Brožková

Moist entropic potential temperature

- Having a 'moist potential temperature' both with good 'Lagrangian' and with good 'intensive' conservation properties is the aim of many studies. Given the nice link between 'local' moist entropy conservation and 'integral' enthalphy balanced budgets, why not trying on this track?
- Recent new proposal (submitted to QJRMS by P. Marquet):
 - Go to the most general moist entropy formulation (s_m in a previous slide) in order to implicitely define a θ_s
 - Make a few approximations to get a relatively simple equivalent named $(\theta_s)_1$
 - Find out that the new quantity is a combination of the two famous 'moist conserved quantities' of Betts, θ_l and q_t :

$$(\theta_s)_1 = \theta_l . \exp(-\Lambda . q_t)$$

Moist entropic potential temperature: verification on FIRE-I data



The 'top of PBL discontinuity' practically disappears when using the new quantity

A graphical interpretation



The (*blue*) 'state' curve (in the 3D space of Z and of the two moist-conserved variables q_t and θ_l) may be projected in tems of q_t (*red*) and θ_{I} (*green*) but also of their 'combination' $(\theta_{s})_{1}$ (brown). The 'top of PBL discontinuity', present in the first two cases, disappears in the last one!

Moist entropic potential temperature: use for turbulence at scales with cloudiness distributions tending to 0/1?

- We now have a moist potential temperature conservative for reversible and adiabatic processes, including all those linked to phase changes <u>and showing homegeneous distributions</u>.
- This may have far-reaching implications for the treatment of 'moist turbulent motions': replacing θ by (θ_s)₁ in turbulence direct-type computations, perhaps even for third order moment terms; less (or even no) need to intertwin the cloudiness and turbulence parameterisations.
- Central issue: $(\theta_s)_1$ is 'homogeneous', but may we write ?

$$w'.(\theta_s)'_1 \Leftrightarrow \overline{w'.\rho'}$$

Some thoughts about the buoyancy term (1/2)

- What is here at stake is not the fact that the new temperature may be as homogeneous in all types of clouds as in Sc (those are really the ideal case for entropy conservation). What counts is that the equilibrium position towards which 'moist turbulence' will tend is the one corresponding to this 'well mixed (θ_s)₁ case'. But what about the 'buoyancy term'?
- At first sight the asymptotic behaviours for vanishing and for total cloudiness do not correspond to the well known solutions of respectivley Lilly and Duran & Klemp.
- But in between, the 3D homogeneity of $(\theta_s)_I$ indicates that there exist some processes working to avoid discrepancies between its vertical gradients in the cloudy and clear air areas. Hence one may speculate ...

Some thoughts about the buoyancy term (2/2)

• Furthermore, numerical results indicate that the 'neutral case' is a *very* stable target for a shallow convection scheme written dirtectly in R_i from $(\theta_s)_1$. Hence why not betting on an 'entropy-based' representation of all turbulent motions?





Entropic without over-implicit scheme Oper with over-implicit scheme Courtesy of Ivan Bašták-Ďurán

Outlook

- Computing the diabatic forcing (and incorporating it correctly in the dynamical equations) undergoes a strong change of emphasis when reaching 'NH scales'. The associated NWP-type impact is perhaps even more telling than the one of the change of the dynamical equations.
- Our knowledge about what will give the forecast with most realism and reliability + least noise and costs is yet limited.
- The clearer separation between 'process description' on the one hand and 'code algorithmic superstructure' on the other hand offers a chance to see new paradigms emerging, more appropriate to the new situation.
- Selecting those which will deserve a stable role will not be easy. It has been argued here that 'consistency' and some simple 'transcription of the laws of thermodynamics' might play a key role in this selection process.