Interest of doing clean thermodynamics in models: rules, conditions of their application and a few (present and anticipated) examples

Jean-François GELEYN

CNRM, Météo-France, Toulouse

(many thanks to P. Marquet, B. Catry, R. Brožková, I. Bašták-Ďurán and M. Van Ginderachter)

COST ES0905 WG1+2 meeting Reading, 14/01/2013



Introduction

- Lead idea of the talk: clean thermodynamics does not need to be too complicated ... and it has nice practical applications.
- But reaching this advantageous situation requires a good deal of consistency.
- This does not mean that there should be no simplifications with respect to the full complexity of the system ... but that they should be decided as a whole and ab-initio!
- But sometimes practical implementation decisions do have some level of arbitrariness (type of adjustment; reversible or irreversible adiabatic ascent conditions; case of simultaneous presence of the three phases of water; etc.) => the transversal issues, like global conservation properties, must be treated through global constraints.
- But the devil is sometimes still in the details!

Split of the presentation

- <u>Rules</u>:
 - Additivity
 - Conservation of theoretical invariants
 - Consistency
- <u>Conditions of application</u>:
 - Simplifying (and structuring) hypotheses
 - Global ⇔ local interplay (under an 'inter-parameterisation consistency' condition)
 - Algorithmic hurdles
- <u>Examples</u>:
 - Discretisation issues
 - Consequences of the 'specific view for entropy' (role of *qt*, see PM's talk) for moist turbulence's parameterisation

Additivity rule

- When having a complete system of parameterisation algorithms, one must know how to combine the outputs of individual computations in terms of evolutions of the main-model's prognostic variables.
- In the case of water species (or any 'passive tracer' of course) things are simple thanks to the intrinsic linearity of the tendency equations.
- But for energy linked quantities (cpT+Φ, (u²+v²)/2, ...), this is not anymore true.
- On must then realise that tendencies (which do have a lot of conditional aspects in their definition) ARE NOT ADDITIVE: $d(cpT) \neq cpdT + \sum (\partial cp/\partial qx) dqx$!
- Only fluxes (which have an intrinsic physical meaning) ARE ADDITIVE.

This gives a central role to the Green-Ostrogradsky theorem

Transversal conservation issue

Taking the 'heat part' of the 'specific moist enthalpy + geopotential' defines S'li as the exact counterpart of cpd. $T+\Phi$ for the fully dry case. It corresponds to the dry static energy in the unsaturated case got after evaporation (interpretation of Betts'

system Moreover, in the general case, local conservation of S'li is equivalent to conservation of the quantity (cp. T+Φ-Lv(0).ql-Ls(0).qi), with Lv/s(0) the temperature-independent extrapolations of Lv/s at 0 K. The linearity of the last two terms allows to develop in function of the various transport fluxes of the water species (diffusion & precipitation) and to so obtain a Green-Ostrogradsky-type

 $\frac{\partial}{\partial t}(c_{p}T) = -g\frac{\partial}{\partial p}\left[(c_{l} - c_{pd})P_{l}T + (c_{i} - c_{pd})P_{i}T - (\hat{c} - c_{pd})(P_{l} + P_{i})T + J_{s} + J_{rad}\right]$ Catry et al., Catry et al., 2007, Tellus A $S'_{li} = \left[c_{pd} + (c_{pv} - c_{pd})q_{l}\right]T + gz$ $-L_{v}(T)q_{l} - L_{s}(T)q_{i}$ $\theta_{li} = \theta \cdot \exp\left(-\frac{L_{vap}q_{l} + L_{sub}q_{i}}{c_{pd}T}\right) \Leftrightarrow S'_{li}$ $q_{l} = q_{v} \oplus q_{l} + q_{i}$

Basic assumptions for consistency

- Two types of consistency ought to be sought when designing a parameterisation set:
 - Between the 'dynamical' and 'physical' parts of the model. Here the Green-Ostrogradsky approach is the easiest one (using θs as synthetic variable would be equivalent, but the way-backcomputations are very complex; neither θ , nor θli nor $(\theta s)1$ can help if one wants an exact solution). In the non-hydrostatic case, the issue about projecting the energy tendencies on the temperature and pressure prognostic variables also appear, but it exists in all solutions, albeit under differing shapes.
 - Between the individual parameterisation computations. There, if a policy for global conservation of the invariants exists (see just above), the issue is shifted to the one of having the same basic hypotheses on all sides. This requires a clear, compact and purposeful definition of so-called 'simplifying hypotheses' which become de-facto 'structuring constraints'.
- All this appears simple and logical. Yet it is very hard to be enforced in models' design ... 6

'Simplifying' assumptions and/or 'structuring' constraints

- **Barycentric system** (condensates are an integral part of the parcel)
- Hydrostatism (for the vertical gradient aspects in 'physics')
- Zero assumed volume for condensates
- Gases obey Boyle-Mariotte's and Dalton's laws (together with the previous one => p/(ρ.T)=Rd.qd+Rv.qv=R)
- Homogeneity of temperature across species (even for falling condensates)
- Constant values of specific heats across the atmospheric temperature range (a bit problematic for *ci*)
- Linear variations of latent heats with temperature
- In presence of condensates, water vapour partial pressure around them depends only on temperature (no treble phase situation, though in practice many results may be robust to that ...)
- Clausius-Clapeyron relationship

... and then nice analytical results (including the one about G-O-type conservation of 'cp.T') become possible!

Global vs. local interplay (in the physics time-step)

- The main difficulty appears here when one wants the results of one parameterisation computation to influence the prognostic type variables used in input to a subsequent one (sequential view). In the other case (parallel view) there is no new problem.
- For the sequential case, short of an expensive incremental solving of the physics ⇔ dynamics system after each new contribution, the trick is to say that the output => input computations may be approximated (via *cp*, *R*, *Lv/s* values kept unchanged during the physics time-step), provided:
 - 1. The underlying communication is done via fluxes (or their linear divergences expressed in quantities having the physical dimension of tendencies => pseudo-fluxes).
 - 2. The final summation is done on the fluxes and/or pseudo-fluxes.
 - 3. The basic hypotheses are still transversal to all processes.
- Then additivity, conservation and consistency are still ensured!

Algorithmic hurdles (i.e. devils in the details) (1/2)

- There are several types of them: linked to the (vertical) space discretisation, linked to the time discretisation (degree of implicitness), combination of both (fight against linear and non-linear instability), basic decisions about the considered process' behaviour.
- The latter are the most interesting ones from the purely thermodynamics point of view. The decisions are about:
 - Reversible or irreversible character (for instance condensation is reversible and precipitation irreversible; and yet microphysical packages sometimes mix them without caution).
 - Local adjustment or transport-type process (nature does not make such a distinction, but in models we need it most of the time, for the sake of simplicity).
 - How to deal with the treble phase problem (even if the final computations may be solved by linear combination tricks, this contradicts the way in which we obtained, in the case of to phases only, the simple formulae allowing this strategy).

Algorithmic hurdles (i.e. practical consequences) (2/2)

- Reversible or irreversible character:
 - $\circ~$ for irreversible saturation conditions (precipitation) we have

 $q_{sat}(T,p) = (R_d/R_v) [e_{sat}(T)/(p - e_{sat}(T)(1 - R_d/R_v))]$

• for reversible saturation conditions (no precipitation) we have

 $r_{sat}(T,p) = (R_d/R_v)[e_{sat}(T)/(p-e_{sat}(T))]$

- Local adjustment or transport-type process. The issue is here:
 - whether to use (q/r)sat as implicit target for a return to saturation (in the transport case where one cannot anticipate the change of [T,p] characteristics along the vertical displacements;
 - Or to use (q/r)w (wet-bulb value) as explicit target for a return to saturation (in order to implicitly couple the temperature and humidity evolutions in the local case)
- The treble phase problem: there is no ideal solution; probably an additional prognostic quantity ought to be defined and added in order to keep both consistency and physical realism!

Practical examples, first part: importance of discretisation details. Slides extracted from a talk at the ECMWF 2010 Workshop on 'Non-Hydrostatic modelling'

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(Φ)* 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 *qv* is treated spectrally) the computation is approximated by using *R=Rd+qv(Rv-Rd)*
- But, if we use the exact equations, in the vertical we get d(Φ)=-[Rd(1-qv-ql-qi-qr-qs)+Rv.qv].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 *qv* in grid-point or *qv* spectral. 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



Wrong

Correct

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)

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

- This following will have to do with the intra-time-step variations of *Cp*, *Cv* and hence *R*, following the phase changes of a barycentric multi-phasic system (here *qv/l/i/r/s*)
- Using *Cp=Cv+R* and the first Law of thermodynamics, one gets a Green-Ostrogradsky form for the evolution of enthalpy (with *δm* a tag for conservation or not of the total mass and with *P'* & *P'''* the mass-weighted integrals of phase changes with respect to vapour):

$$\begin{aligned} \frac{d}{dt}(c_p T) &= g \frac{\partial}{\partial p} \left[L_l(T=0)(P_l' - P_l''') - (c_l - c_{pd})P_l T + L_i(T=0)(P_i' - P_i''') - (c_i - c_{pd})P_l T + \delta_m (\hat{c} - c_{pd})(P_l + P_i)T) \right] \\ &- (c_i - c_{pd})P_i T + \delta_m (\hat{c} - c_{pd})(P_l + P_i)T] \\ &\hat{c} &= \frac{c_{pd}q_a + c_{pv}q_v + c_lq_l + c_iq_i}{1 - a_l - a_l} \end{aligned}$$

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

- The previous equation must be complemented by the radiative and 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(Cp.T)*' by '*Cp.dT*' !

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 qr/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 *qr/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 also felt in the whole atmospheric column</u>.

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 *qr/s*) it is correct to assume that *dp=-p.dΦ* must be computed with *p* 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=ρgasRgasT= ρRT* (with *R* and *ρ* from all species).
- When going to the non-barycentric system, the filtering disappears for *qr/s* and one should in principle account for their acceleration phase as well as for their return to vapour!

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



without enthalpy conservation with enthalpy conservation

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

Courtesy of R. Brožková

Practical examples, second part: (moist) turbulence

Excursion towards turbulence: so-called 'moist conservative' transforms

- When trying to compute turbulent fluxes in a situation where cloudiness is different from 0 or 1, or simply changes along the vertical, one is facing two delicate issues:
 - (1) The calculation of the buoyancy flux <w'.ρ'> becomes extremely nonlinear and complex (we shall come back to this issue later);
 - (2) The interaction between phase changes and transport of heat, water vapour and condensate(s) during the 'physics time-step' is not tractable.
- Concerning the issue N°2, Betts (1973) proposed to use two socalled 'moist conservative' variables, namely the total water amount *qt* and the liquid water potential temperature *θl* (no consideration of the ice phase in those early years!).
- While the conservative character is only approximate and the advocated link with entropy wrong, what remains from Betts' idea is the 'transform' method: (i) evaporate (with temperature change), (ii) transport both variables and (iii) condense back.
- The last step needs additional hypotheses, linked to the issue N°1!

And observations tell us about the 'target' of mixing



Transport problems: which fluxes and variables?

Transport problems: additional remarks

Originally
Practical evolution
$$MSE = c_{pd} T + L_v q_v + g z$$
Neither Ls counterpart, nor
even any appearance of ql ??Stevens et al. (2003) $S_l = c_{pd} T + g z - \overline{L_v} q_l$ $\frac{c_{pd}}{\overline{(\theta_l)}} \overline{w'\theta_l'} \approx \frac{1}{\overline{(T)}} \overline{w'S_l'}$ Asymmetric (MSE inheritance), no qt=1-qd related
part

In p-type coordinates, the new quantity S'li is the exact counterpart of cpd. $T+\Phi$ for the fully dry case. It also has a strong similarity with SI and this will be useful to understand the link of Shm with moist static energy (MSE)

$$S'_{li} = \left(c_{pd} + (c_{pv} - c_{pd})q_{t}\right)T + g z - L_{v}(T)q_{l} - L_{s}(T)q_{i}$$

$$\theta_{li} = \theta \cdot \exp\left(-\frac{L_{vap} q_{l} + L_{sub} q_{i}}{c_{pd} T}\right) \Leftrightarrow S_{hm} - c_{pd} T_{Y}q_{t}$$

$$q_{t} = q_{v} \oplus q_{l} + q_{i}$$

$$q_{t} = q_{v} \oplus q_{l} + q_{i}$$

$$24$$

Why has MSE a 'quasi-conservative' reputation?

Originally S'l adaptation

$$MSE = c_{pd} T + L_{v} q_{v} + g z$$
$$MSE' = c_{p}'T + L_{v}(T) q_{v} + g z$$

$$MSE' = (c_{pd} + (c_{pv} - c_{pd})(q_v + q_l)) + g z - L_v(T) q_l + L_v(T)(q_v + q_l))$$

So, if qi=0, MSE' and Shm <u>differ only by the last term</u> But TY = 2362 K & Lv(T0)/cpd=2489 K !!! (while AT0=1603 K)

The close match between the two values <i>is a coincidence. *It explains why MSE' (or its MSE approximation) is nearly conservative (5% difference), <i>in the 'warm' case.*

But, as soon as we have ice phase, it collapses $(Ls(T0)/cpd=2821 \ K) \Rightarrow$ Use Shm: $S'_{li} = (c_{pd} + (c_{pv} - c_{pd})q_{t})T$ $+ g z - L_{v}(T)q_{l} - L_{s}(T)q_{i}$ $S_{hm} = S'_{li} \oplus c_{pd} T_{Y} q_{t}$ $S_{hm} = S'_{li} \oplus c_{pd} T_{Y} q_{t}$

May we use M11's findings in moist turbulence (apart from upgrading Betts' transforms & better measuring stability)?

- The relevant issues are:
 - Finding a way to express how nature seems to tend to full mixing of θs (i.e. maximising turbulent energy conversion via the transport of qt).
 - Going around the fact that θs is a very bad tracer of cloudiness (not addressed here).
 - Doing both steps while remaining close to the present formalism for the computation of the buoyancy flux (the development of a formulation for the Brunt-Väisälä-Frequency (BVF) is an interesting intermediate step for that).
 - Finding a way to introduce the fact that there is a part of the heat and moisture transports which is realised through the asymmetry between the situations inside and outside the clouds (*not addressed here*).

'Classical turbulence' interpretations (i.e. fully dry ones)

The prognostic TKE equation

$$\frac{\partial E}{\partial t} = A_{dv}(E) + \frac{1}{\rho} \frac{\partial}{\partial z} \rho K_E \frac{\partial E}{\partial z} + K_m \left[\left(\frac{\partial u}{\partial z} \right)^2 + \left(\frac{\partial v}{\partial z} \right)^2 \right] - \frac{g}{\theta} K_h \frac{\partial \theta}{\partial z} - \frac{C_E E^{3/2}}{L}$$
Development of the terms of shear production and of
production/destruction by buoyancy ('conversion term')
$$K_m \left[\left(\frac{\partial u}{\partial z} \right)^2 + \left(\frac{\partial v}{\partial z} \right)^2 \right] - \frac{g}{\theta} K_h \frac{\partial \theta}{\partial z} \approx K_m S^2 \left[1 - \frac{K_h}{K_m} \frac{g}{\theta} \frac{\partial \theta}{\partial z} / S^2 \right]$$

$$= K_m S^2 \left[1 - \frac{K_h}{K_m} (N^2 / S^2) \right] = K_m S^2 \left[1 - \frac{K_h}{K_m} R_i \right] = K_m S^2 (1 - R_{if})$$

One thus establishes a direct link between the Richardson number, the Richardson-flux number, the conversion term ($\langle w'. \rho' \rangle$) and the static stability (i.e. the squared BVF N²). Should all this be reproduced identically in the 'moist' case? One has to realise that the above fully relies on a dual role of θ : conserved quantity AND stability parameter.

The moist entropic potential temperature θs within its related Brunt-Väisälä Frequency expansion (1/2)

- For homogenous (non-saturated and fully-saturated) situations, one can compute the squared BVF by noticing that density is function of moist entropy 's', total water content 'qt' and pressure 'p' only.
- Let us suppose that we know a 'transition parameter' ('*C*', which can be identified to a cloudiness or to a cloud efficiency) and let us define:

$$F(C) = 1 + C \left[\frac{L_{v}(T)}{C_{p}T} \frac{R}{R_{v}} - 1 \right] \qquad M(C) = \frac{1 + D_{C}}{1 + D_{C}F(C)} \quad D_{C} = \frac{T}{p - e_{s}(T)} \frac{de_{s}(T)}{dT}$$

- F(C) ensures the transition between the non-saturated case (C=0) where moisture acts only through expansion (Rv/R) and the fully-saturated one (C=1) where it acts only through latent heat release (Lv(T)/(Cp.T)).
- M(C) cares for the linked change of adiabatic gradient, without any need for a second transition variable.
- Remarkably *DC* does not depend on moisture amounts.

A digression concerning vertical adiabatic lapse rates (1/2)

- We compare here the new formulation with the 'classical' ones of Durran and Klemp (1982) and of Emanuel (1994) by expressing the vertical adiabatic lapse rates $\Gamma = -dT/dz$.
- In the non-saturated case the correct solution is *Γns=g/cp*
 - In the case of full extinction with respect to liquid water we have: $\Gamma_{sw} = (g/c_p) \frac{1 + \left[\frac{L_v(T).r_{sw}}{R_d.T}\right]}{1 + \left(\frac{R}{c_p}\right) \left(\frac{L_v(T)}{R_v.T}\right) \left[\frac{L_v(T).r_{sw}}{R_d.T}\right]} \quad (MG13)$ (MG13) Without any doubt, the more exact the derivation, the simpler the final result! $\Gamma_{sw} = \left(g(1+r_t)/c_{pd}\right) \frac{1 + \left[\frac{L_v(T) \cdot r_{sw}}{R_d \cdot T}\right]}{1 + \frac{c_{pv} \cdot r_{sw} + c_l \cdot r_l}{C_{nd}} + \left(\frac{R(1+r_t)}{C_{nd}}\right) \left(\frac{L_v(T)}{R_w T}\right) \left[\frac{L_v(T) \cdot r_{sw}}{R_d \cdot T}\right]} \quad (DK82)$ $\Gamma_{sw} = \left(g(1+r_t) / (c_{pd} + c_{pv} \cdot r_{sw}) \right) \frac{1 + \left[\frac{L_v(T) \cdot r_{sw}}{R_d \cdot T} \right]}{1 + \frac{c_l \cdot r_l}{c_{pd} + c_{pv} \cdot r_{sw}} + \left(\frac{R(1+r_t)}{c_{pd} + c_{pv} \cdot r_{sw}} \right) \left(\frac{L_v(T)}{R_v \cdot T} \right) \left[\frac{L_v(T) \cdot r_{sw}}{R_d \cdot T} \right]}$ (E94) 29

A digression concerning vertical adiabatic lapse rates (2/2)

• But we have a similar loss of simplicity when replacing the complex θs by its simple approximation $(\theta s)1$:

$$\Gamma_{sw} = \left(g/c_p\right) \frac{1 + \left[\frac{L_v(T) \cdot r_{sw}}{R_d \cdot T}\right]}{1 + \left(\frac{R}{c_p}\right) \left(\frac{L_v(T)}{R_v \cdot T}\right) \left[\frac{L_v(T) \cdot r_{sw}}{R_d \cdot T}\right]} \qquad (MG13, \ \theta s \)$$

$$\Gamma_{sw} = \left(g/c_{pd}\right) \left(\frac{\frac{R_d}{R}}{R}\right) \frac{1 + \left(\frac{R}{R_d}\right) \left[\frac{L_v(T) \cdot r_{sw}}{R_d \cdot T}\right]}{1 + \frac{L_v(0) \cdot q_l}{c_{pd} \cdot T} + \left(\frac{R}{c_{pd}}\right) \left(\frac{L_v(T)}{R_v \cdot T}\right) \left[\frac{L_v(T) \cdot r_{sw}}{R_d \cdot T}\right]} \qquad (MG13, \ (\theta \text{s} \)1)$$

• Remark: all the relevant computations were performed for reversible adiabatic (reverse) = (Ra/Ry)[eav(T)/(R - eav(T))] :

• In the irrev $a_{sw}(T,p) = (R_a/R_v)[e_{sw}(T)/(p - e_{sw}(T)(1 - R_a/R_v))]$ and p:

The moist entropic potential temperature θs within its related Brunt-Väisälä Frequency expansion (2/2)

• Going back to *F(C)* and *M(C)*, for any atmospheric condition, one gets for the squared 'BVF' (Marquet & Geleyn, 2013, QJRMS):

$$N^{2}(C)/g = M(C)\frac{1}{C_{p}}\frac{\partial s}{\partial z} + \frac{\partial \ln(1-q_{t})}{\partial z}M(C)\left((1+r_{v})\frac{R_{v}}{R}F(C) - \frac{C_{pd}}{C_{p}}\Lambda\right)\frac{\partial q_{t}}{\partial z}$$

• Interpretation (following Pauluis and Held (2002)):

Classical' TKE ⇔ TPE conversion

Total water lifting effect (TKE ⇔PE)

 Λ -scaled differential expansion and latent heat effects (TKE \Leftrightarrow ?)

A hint for a new way of looking at the d(TKE)/dt equation in order to account for the fact that, as soon as moisture appears, the dual role of θ is split between θs (conservation) and θv (conversion term)? - They are too various and too interdependent to be listed and ranked

- One just hopes to have made more evident the need and interest of treating thermodynamics more carefully and more purposefully in future modelling endeavours
- The consequences of the M11 and MG13 papers for treatment of moist turbulence are still under investigation

- The next step would be to consider the potential of application to the deep convective situation (closure?), most probably with even more reference to PH02