

Consistent and Flexible Thermodynamics using Thermodynamic Potentials

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Motivation I: consistency

Approximations to moist thermodynamics are often inconsistent between different components of the same model, or inconsistent with the laws of thermodynamics.

e.g.,

- effect of composition on specific heat capacity;
- $C_p^v \neq C^l$ implies $L^v \neq \text{const}$;
- use of an empirical formula for p^{sat} rather than deriving p^{sat} from the EoS etc for water.

These kinds of inconsistency can lead to errors in the global energy budget of a typical weather or climate model of order 1 Wm^{-2} (Martin Willett, pers. comm.)

Motivation II: flexibility

It may be desirable to use the same model (or dycore) with different EoS

e.g.

- Remove current approximations to quantify their effect
- More accurate EoS for air + water to improve tropical tropopause region
- Comparison with rotating annulus experiments
- Ocean and atmosphere with the same dycore!?
- Variable composition:
 - thermosphere for space weather forecasting;
 - exoplanets: non-dilute condensate; gas giant interior; ...

Typically the EoS is hard-coded into many different code segments, making it very difficult to make such changes (consistently).

Consistency via a thermodynamic potential

Recall the four standard thermodynamic potentials

Specific internal energy: $e(\alpha, \eta, q)$

Specific enthalpy: $h(p, \eta, q) = e + \alpha p$

Gibbs function: $g(p, T, q) = e + \alpha p - \eta T$

Helmholtz free energy: $f(\alpha, T, q) = e - \eta T$

where

$\alpha = 1/\rho$ is specific volume,

q is total specific humidity,

η is specific entropy.

Here (initially) we use the Gibbs function

- It is already used by oceanographers - see TEOS10;
- The conditions for equilibrium between phases are equal p , equal T , and equal g ;
if we work in terms of p and T then two conditions are satisfied more or less automatically.

E.g. Gibbs function for wet air

$$g(p, T, q) = (1 - q)g^d + (q - q^l)g^v + q^l g^l$$

where

$$g^d = -C_p^d T \ln \left(\frac{T}{T_0} \right) + R^d T \ln \left(\frac{p^d}{p_0^d} \right),$$

$$g^v = -C_p^v T \ln \left(\frac{T}{T_0} \right) + R^v T \ln \left(\frac{p^v}{p_0^v} \right) + L_0^v \left(1 - \frac{T}{T_0} \right),$$

$$g^l = -C^l \ln \left(\frac{T}{T_0} \right) + \alpha^l \left(p - p_0^{\text{sat}} \frac{T}{T_0} \right),$$

and

$$p^d = \frac{\varepsilon a p}{(1 + a(\varepsilon - 1))}, \quad p^v = \frac{(1 - a)p}{(1 + a(\varepsilon - 1))},$$

$a = (1 - q)/(1 - q^l)$ is the mass fraction of dry air in the gaseous part, and

$T_0, p_0^d, p_0^v, p_0^{\text{sat}}, L_0^v, \alpha^l$ and $\varepsilon = R^d/R^v$ are constants.

E.g. Gibbs function for wet air

To evaluate the previous expressions we must determine q^l from the condition for equilibrium between phases:

either

$$q^l > 0 \text{ and } g^v = g^l$$

or

$$q^l = 0.$$

How do we use this idea in practice?

We do not *predict* g . Rather, given p , T and q , we can use the expression for g to compute any thermodynamic quantity we like. E.g.

$$\alpha = g_p; \quad \eta = -g_T;$$

$$C_p = -Tg_{TT}; \quad C_v = \frac{T(g_{pT}^2 - g_{pp}g_{TT})}{g_{pp}};$$

$$h = g - Tg_T; \quad e = g - pg_p - Tg_T;$$

$$L^v = h^v - h^l; \quad \frac{1}{c^2} = \frac{g_{pT}^2 - g_{pp}g_{TT}}{g_p^2 g_{TT}}.$$

How do we use this idea in practice?

Because these quantities are derived from a thermodynamic potential they are guaranteed to be **consistent** with each other and with the laws of thermodynamics.

We can approximate the Gibbs function; all derived quantities inherit the approximation consistently.

Note the analogy with deriving the dynamical equations from a Lagrangian or Hamiltonian.

What if my model doesn't predict p and T ?

E.g. ENDGame predicts ρ and a quantity related to η .

Then we must solve

$$1/\rho = g_p(p, T, q), \quad \eta = -g_T(p, T, q), \quad (*)$$

for p and T .

Hmmm... 'sounds complicated?

Given a reasonable first guess for p and T , which we will usually have, one or two Newton iterations will suffice to solve (*) accurately.

Even better, for a semi-implicit dynamical core, the solution of (*) can be combined with the iterative semi-implicit solver; this leads to a familiar standard Helmholtz problem for the pressure increments! (Details in T17.)

For an incompressible fluid (*) does not determine p . However, the semi-implicit solution method still works! (The Helmholtz problem reduces to a Poisson problem because $1/c^2 = 0$.)

Implementation for flexibility

A single subroutine or set of subroutines computes the Gibbs function and its derivatives.

The rest of the code is generic.

Thus, the EoS can be modified by changing only a small number of routines (and the EoS can easily be made switchable).

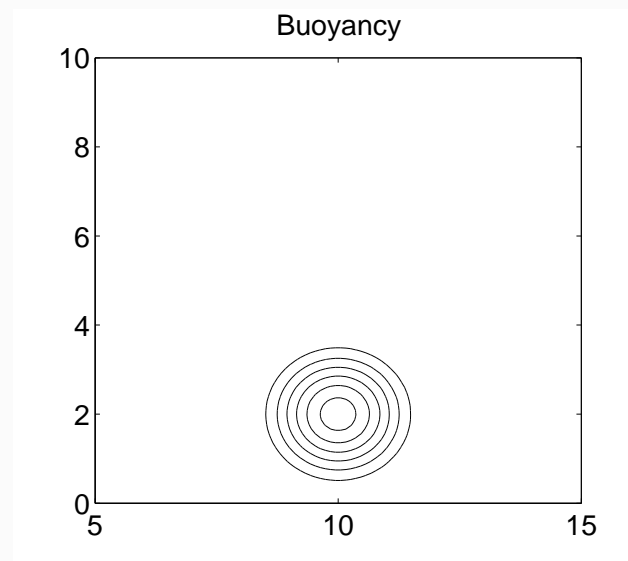
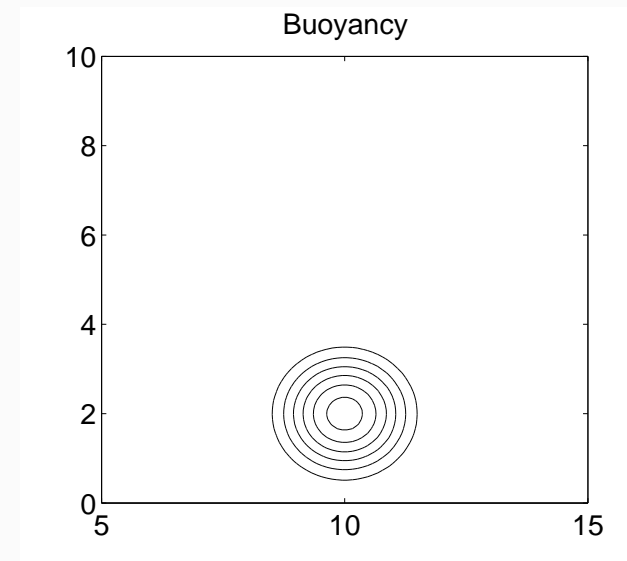
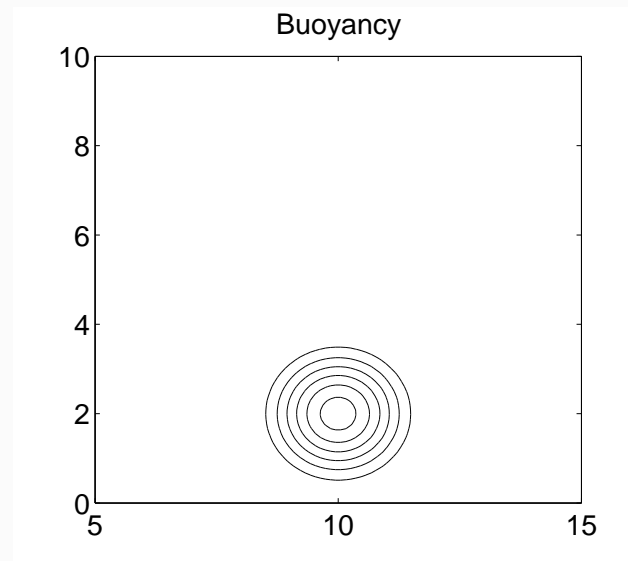
Example (T17)

BF02 2D buoyant bubble test case

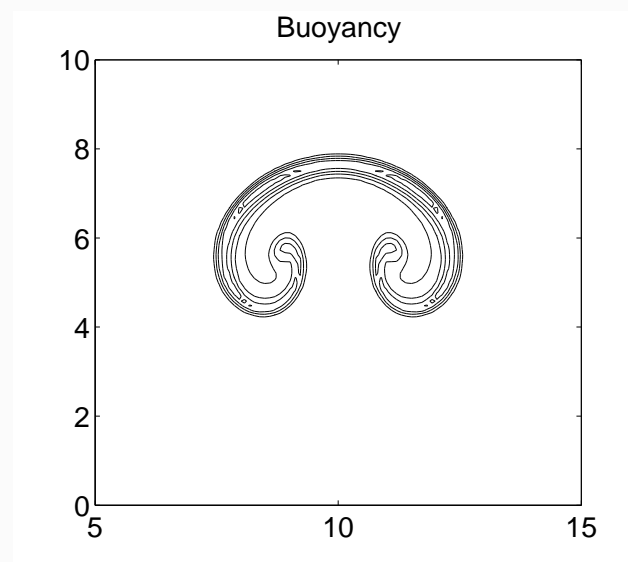
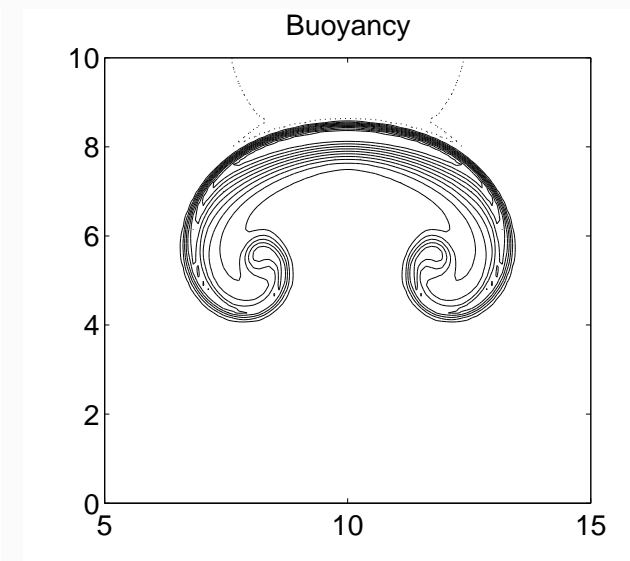
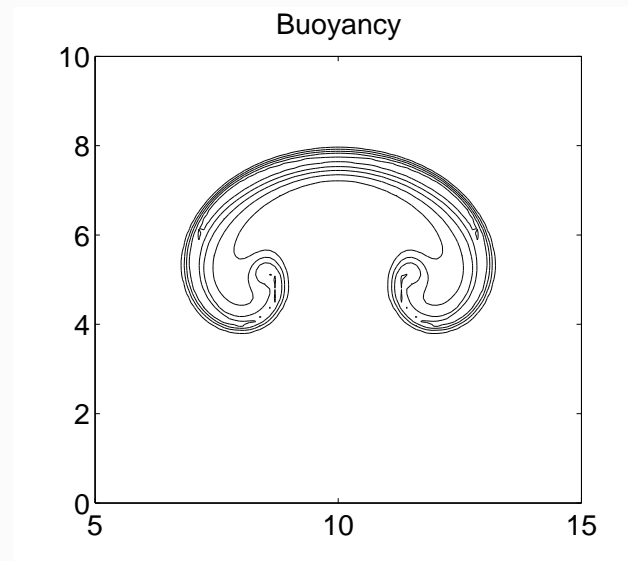
Dry
air

Saturated
air

Quasi-
incompressible



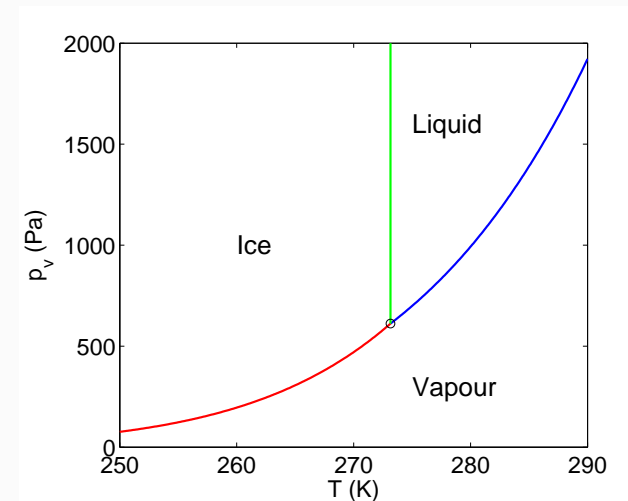
$t = 0\text{ s}$



$t = 1000 \text{ s}$

Limitations

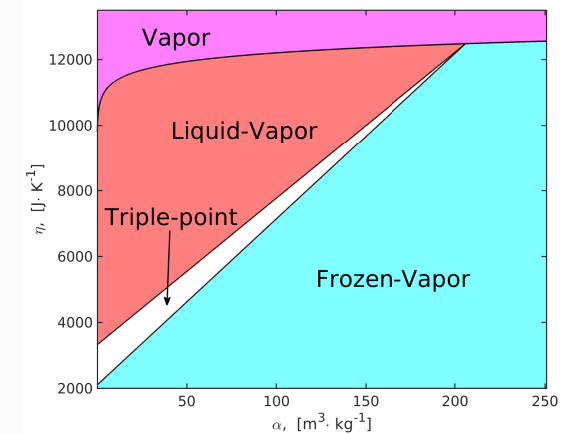
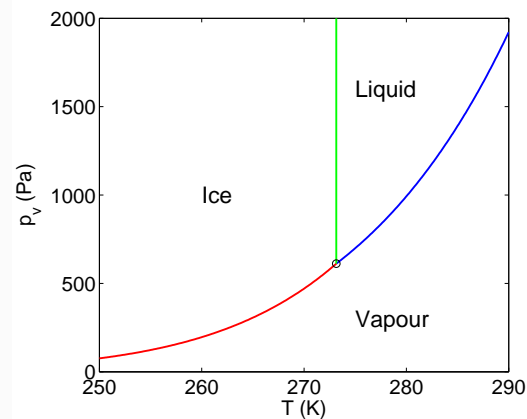
- T17 assumed equilibrium between different phases/components, but **non-equilibrium** processes are important. E.g.,
 - supercooled liquid water,
 - evaporation of rain into subsaturated air,
 - precipitation at different temperature from surrounding air, ...
- If three phases of water are present, p , T and q are **not enough to determine the fractions of each phase**.



Current work

1. Use internal energy $e(\alpha, \eta, q)$ as the thermodynamic potential.

- The triple point in (p, T) space expands to a triangle in (α, η) space.



- We want to predict (something like) α and η .
- e is more familiar to most meteorologists than g .
- However, determining equilibrium is now more complicated (7×7 system for three water phases plus dry air).

Current work

2. Want to remove the equilibrium assumption and replace it by relaxation to equilibrium on specified time scales.

It should be implemented in a way that recovers the equilibrium case as the timescales go to zero.

Entropy sources should be calculated consistently for the non-equilibrium processes.

Next steps

1. Reproduce the results of T17 using a formulation based on e instead of g .
2. Derive governing equations for the non-equilibrium case that reduce to the equilibrium case in the appropriate limit.

Summary

- Deriving all thermodynamic quantities and relations from a potential ensures **consistency** between model components and with the laws of thermodynamics.
- The idea can be implemented in a way that permits **flexibility** in the choice of EoS.
- **Feasibility** has been demonstrated using the **Gibbs function** for the case of equilibrium thermodynamics with two water phases.
- We are reformulating the approach in terms of **internal energy** in order to apply it to the case of three water phases...
- ... and extending it to handle **non-equilibrium** thermodynamic processes.

References

BF02: Bryan GH and Fritsch JM, 2002: A benchmark simulation for moist nonhydrostatic numerical models. *Mon. Wea. Rev.*, **130**, 2917-2928.

TEOS10: IOC, SCOR, and IAPSO, 2010: The international thermodynamic equation of seawater–2010: Calculation and use of thermodynamic properties. <http://www.TEOS-10.org>

T17: Thuburn J, 2017: Use of the Gibbs thermodynamic potential to express the equation of state in atmospheric models. *QJRMS*, **143**, 1185-1196.