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Equation of state of a compressible fluid

Commonly encountered approach (ideal perfect gas) :

- equation of state relates pressure, density and temperature
- specific heat defines internal energy
- potential temperature used to characterize adiabatic transforms
- complemented by a bunch of other relationships

$$
\begin{aligned}
p &= \rho R T \\
e &= c_v T \\
\theta &= T \left(\frac{p}{p_0} \right)^{-R/c_p} \\
c_p - c_v &= R
\end{aligned}
$$

Pro :

- simple
- avoids reviving bad memories about entropy, second law, Maxwell relationships, ...

$$
\begin{aligned}
\pi &= c_p \left(\frac{p}{p_0} \right)^{R/c_p} \\
e + \frac{p}{\rho} &= c_p T = \theta \pi \\
\frac{1}{\rho} \mathrm{d}p &= \theta \mathrm{d}\pi
\end{aligned}
$$

Con :

- « accidental » relationships
- cumbersome for non-ideal gases (variable cp)
- cumbersome for mixtures (moist air, salty water)
- overall *energetic consistency*

Thermodynamics of a compressible fluid

Systematic approach (Ooyama, 1990 ; Bannon, 2003 ; Feistel, 2008)

- state variables :
  - specific volume/pressure
  - specific entropy / temperature
  - mixing ratio / chemical potential (mixtures)
- All relations follow from the expression of a single thermodynamic potential

$$\begin{aligned} \mathrm{d}e(s,\alpha,r) &= T\mathrm{d}s - p\mathrm{d}\alpha + \mu\mathrm{d}r \\ \mathrm{d}\left(e+\alpha p\right) = \mathrm{d}h(s,p,r) &= T\mathrm{d}s + \alpha\mathrm{d}p + \mu\mathrm{d}r \\ \mathrm{d}\left(h - Ts\right) = \mathrm{d}g(T,p,r) &= -s\mathrm{d}T + \alpha\mathrm{d}p + \mu\mathrm{d}r \end{aligned}$$

Pro :

- always energetically consistent
- general : variable cp, mixtures

Con :

- none
- unless you *really* hate thermodynamics

$$\begin{aligned} e(\alpha,\, s) &= c_v T_r \left(\frac{\alpha}{\alpha_r}\right)^{-R/C_v} \exp\frac{s}{C_v} \\ T(\alpha,\, s) &= \frac{\partial e}{\partial s} = \frac{e}{C_v} \\ p(\alpha,s) &= -\frac{\partial e}{\partial \alpha} = \frac{R}{C_v}\frac{e}{\alpha} \\ \alpha p &= RT \\ s &= C_p \log\frac{T}{T_r} - R\log\frac{p}{p_r} = C_p\log\frac{\theta}{T_r} \end{aligned}$$

Gibbs function for CAM-SE

See Lauritzen et al., JAMES 2017

- Dry air, water vapor and condensates : cloud liquid, cloud ice, rain, snow
- Gaseous phase (d,wv) is a perfect mixture of ideal perfect gases
- Condensates (cl, ci, rn, sn) have constant heat capacity and specific volume.

$$G(T,p) = \sum_{l=d,wv} N^{(l)} \left(c_p^{(l)} \left(1 - \log \frac{T}{T_0} \right) + r \log \frac{p}{p_0} \right) T - T S_{mix}(N^{(d)}, N^{(wv)})$$

$$+ \sum_{l=cl,ci,rn,sn} m^{(l)} \left(c^{(l)} \left(1 - \log \frac{T}{T_0} \right) T + \alpha^{(l)} p \right)$$

$$V(T,p) = \frac{\partial G}{\partial p} = \frac{rT}{p} \sum_l N^{(l)} + \sum_l V^{(l)}$$

$$S(T,p) = -\frac{\partial G}{\partial T} = \sum_l N^{(l)} \left(c_p^{(l)} \log \frac{T}{T_0} - r \log \frac{p}{p_0} \right) + S_{mix}(N^{(d)}, N^{(wv)})$$

$$+ \sum_l m^{(l)} c^{(l)} \log \frac{T}{T_0}$$

$$H(T,p) = G + TS = \left(\sum_l N^{(l)} c_p^{(l)} + \sum_l m^{(l)} c^{(l)} \right) T + \sum_l V^{(l)} p$$

Basic idea of Boussinesq approximations :
pressure remains close to a fixed reference profile

$$p = \overline{p}(\Phi) + p'$$

$$\overline{\rho}(\Phi) \equiv -\frac{\partial \overline{p}}{\partial \Phi}$$

$$\overline{\rho} = \rho(\overline{p}, \overline{s})$$

$$\frac{D\dot{\mathbf{x}}}{Dt} + \mathrm{curl}\mathbf{R} \times \dot{\mathbf{x}} + \frac{1}{\rho}\nabla p' = \underbrace{-\left(\frac{\overline{\rho}}{\rho} - 1\right)\mathbf{g}}$$

Inertia *Buoyancy*

$$\rho(\overline{p}+p', s) = \underbrace{\rho(\overline{p}, \overline{s})}_{\overline{\rho}(\Phi)} + \underbrace{\rho(\overline{p}, s)}_{\rho^*(\Phi, s)} - \rho(\overline{p}, \overline{s}) + \underbrace{\rho(\overline{p}+p', s) - \rho(\overline{p}, s)}_{\simeq \rho' = c^{-2}p'}$$

Reference density varies with altitude / depth

Warmer air rises, colder water sinks

Density fluctuates due to pressure variations caused by flow (dynamic pressure)

$$\boxed{\frac{D\dot{\mathbf{x}}}{Dt} + \mathrm{curl}\mathbf{R} \times \dot{\mathbf{x}} + \frac{1}{\rho}\nabla p' = -b\mathbf{g}}$$

- Exact : $\rho = \rho(p, s)$ $\qquad$ $b = \dfrac{\overline{\rho}}{\rho} - 1$

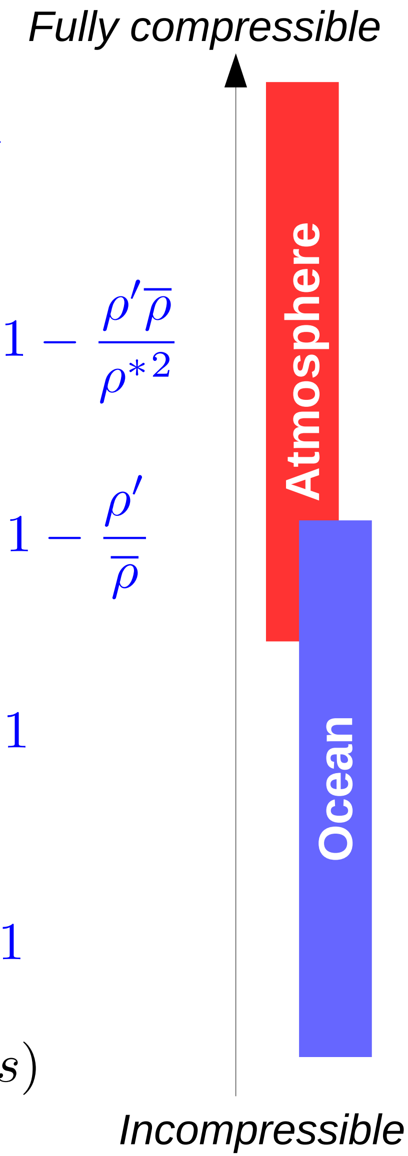
- Pseudo-incompressible : $\rho = \rho^*(\Phi, s)$ $\qquad$ $b = \dfrac{\overline{\rho}}{\rho^*} - 1 - \dfrac{\rho'\overline{\rho}}{\rho^{*2}}$

- Anelastic : $\rho = \overline{\rho}(\Phi)$ $\qquad$ $b = \dfrac{\overline{\rho}}{\rho^*} - 1 - \dfrac{\rho'}{\overline{\rho}}$

- Depth-dependent Boussinesq : $\rho = \rho_0 = cst$ $\qquad$ $b = \dfrac{\overline{\rho}}{\rho^*} - 1$

- Simple Boussinesq : $\rho = \rho_0 = cst$ $\qquad$ $b = \dfrac{\overline{\rho}}{\rho_0^*} - 1$

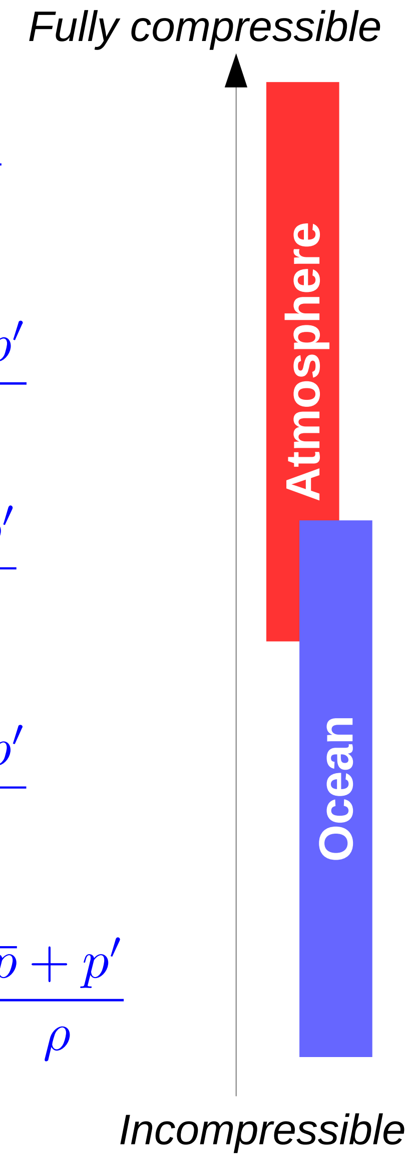
$$\rho_0^*(s) \equiv \rho(p_0, s)$$



All the above combinations conserve energy/momentum/potential vorticity.

$$\boxed{\frac{D}{Dt}\frac{\partial L}{\partial \dot{\mathbf{x}}} - \frac{\partial L}{\partial \mathbf{x}} - \frac{1}{\rho}\nabla\left(\rho^2\frac{\partial L}{\partial \rho}\right) = 0 \qquad \frac{\partial L}{\partial p'} = 0 \qquad L = K(\mathbf{x}, \dot{\mathbf{x}}) - E(\mathbf{x}, \rho, s, p')}$$

- Exact : $E = \Phi + h(\overline{p} + p', s) - \dfrac{\overline{p} + p'}{\rho}$
- Pseudo-incompressible : $E = \Phi + h(\overline{p}, s) + \dfrac{p'}{\rho^*} - \dfrac{\overline{p} + p'}{\rho}$
- Anelastic : $E = \Phi + h(\overline{p}, s) + \dfrac{p'}{\overline{\rho}} - \dfrac{\overline{p} + p'}{\rho}$
- Depth-dependent Boussinesq : $E = \Phi + h(\overline{p}, s) + \dfrac{p'}{\rho_0} - \dfrac{\overline{p} + p'}{\rho}$
- Simple Boussinesq : $E = \Phi\left(1 - \dfrac{\rho_0}{\rho_0^*(s)}\right) + \dfrac{p'}{\rho_0} - \dfrac{\overline{p} + p'}{\rho}$



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Possible moist energies
and implications for phys/dyn coupling

$$\overset{\text{water}}{\rho_w} = \overset{\text{vapor}}{\rho_v} + \overset{\text{liquid}}{\rho_l} + \overset{\text{ice}}{\rho_s} \qquad \rho = \rho_d + \rho_w \qquad \mathcal{H} = \int \left(\overset{\text{Kinetic}}{K} + \overset{\text{Potential}}{P} + \overset{\text{Internal}}{U} \right) \mathrm{d}^3 x$$

1) Thermodynamic equilibrium $\quad S, \rho_d, \rho_w \mapsto \rho_v, \rho_l, \rho_s$

e.g. *Bannon (2003)* $\quad P + U = \rho\Phi + U(S, \rho_d, \rho_w)$

2) Out-of-equilibrium $\quad P + U = \rho\Phi + \overbrace{U(S, \rho_d, \rho_v, \rho_l, \rho_s)}^{\textit{Per unit volume}}$

+ return to thermodynamic equilibrium

3) Box-averaged $\quad P + U = \rho\Phi + \langle U(S, \rho_d, \rho_v, \rho_l, \rho_s) \rangle$

4) Constant latent heat (~CAM) $\quad P + U = \rho\Phi + U(S, \rho_d, \rho_v) - L_{vap}\rho_l - L_{sub}\rho_s$

5) Passive water (LMDZ) $\quad P + U = \rho_d\Phi + U(S, \rho_d) - L_{vap}\rho_l - L_{sub}\rho_s$

Possible moist energies
and implications for phys/dyn coupling

1) $P+U=\rho\Phi+U(S,\rho_d,\rho_w)$

2) $P+U=\rho\Phi+U(S,\rho_d,\rho_v,\rho_l,\rho_s)$

3) $P+U=\rho\Phi+\langle U(S,\rho_d,\rho_v,\rho_l,\rho_s)\rangle$

4) $P+U=\rho\Phi+U(S,\rho_d,\rho_v)-L_{vap}\rho_l-L_{sub}\rho_s$

5) $P+U=\rho_d\Phi+U(S,\rho_d)-L_{vap}\rho_l-L_{sub}\rho_s$

1-2 : neglects subgrid variability => CRM

3 : blurs the frontier between dynamics and physics

1-4 : precipitation changes hydrostatic surface pressure

1-4 : kinetic + potential energy lost through precipitation should be converted into heat (atmosphere); convert lost internal energy into heat (ocean) ?

4-5 : Kirchoff's law imposes $C_{pv}=C_l \quad \Leftarrow \quad \mathrm{d}L_{vap}=(C_{pv}-C_l)\mathrm{d}T$

5 : Evaporation/precipitation changes ocean pressure
less accurate, good enough until … ?

Tendencies vs sources, fluxes

$$\rho C_p \left(\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T \right) = \frac{Dp}{Dt} + \dot{Q} + \nabla \cdot \mathbf{F} \quad \Rightarrow \quad \begin{cases} \dfrac{\partial T}{\partial t} = -\mathbf{u} \cdot \nabla T + \dfrac{1}{\rho C_p} \dfrac{Dp}{Dt} \\ \dfrac{\partial T}{\partial t} = \dfrac{\dot{Q} + \nabla \cdot \mathbf{F}}{\rho C_p} \end{cases}$$

Dynamics Physics

- This splitting of roles is typically associated with some kind of time splitting
- Makes sense from a purely mathematical point of view
- However we are not just solving equations ; these terms come with « meta-data » :
    - Fast / slow
    - Reversible / irreversible
    - Sources / fluxes
- We should use that information when designing physics/dynamics coupling

- Some physical processes perform an instantenous reorganization of the atmospheric column : *dry static adjustment, deep/shallow convection.*
- Such processes are not described by sources/fluxes/tendencies. Can sometimes be described by other concepts : deep convection => map describing how mass of each layer gets redistributed into other layers.

Tendencies vs sources, fluxes

$$\rho C_p \left(\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T \right) = \frac{Dp}{Dt} + \dot{Q} + \nabla \cdot \mathbf{F} \quad \Rightarrow \quad \left\{ \begin{aligned} \frac{\partial T}{\partial t} &= -\mathbf{u} \cdot \nabla T + \frac{1}{\rho C_p} \frac{Dp}{Dt} \\ \frac{\partial T}{\partial t} &= \frac{\dot{Q} + \nabla \cdot \mathbf{F}}{\rho C_p} \end{aligned} \right.$$

Dynamics Physics

To compute physics tendencies from sources/fluxes, one needs to make **assumptions** on **thermodynamics** (perfect gas, Cp), **geometry** (deep atm / shallow atm), choice of **prognostic variable.**

$$\rho \pi \left(\frac{\partial \theta}{\partial t} + \mathbf{u} \cdot \nabla \theta \right) = \dot{Q} + \nabla \cdot \mathbf{F} \qquad \rho T \left(\frac{\partial s}{\partial t} + \mathbf{u} \cdot \nabla s \right) = \dot{Q} + \nabla \cdot \mathbf{F}$$

- Sources/fluxes are objective : observable / unambiguously defined independently from implementation choices

  caveat : proper conventions still required, e.g. flux per unit surface / angle

- Source terms in **flux-form** have implications in terms of **total energy budget**, computing their divergence consistently would better be done by dynamics or physics-dynamics interface
- Even more the case if physics is a black-box (e.g. neural network)

The above may not be relevant for processes which quickly reorganize the atmospheric column.

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