

Energy conversions and internal entropy production in a moist atmosphere

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October 15, 2019

Outline

Continuous equ. as benchmark

Structural constraints

2nd law constraints

Interference with numerics

Mail questions

Distinctions: Physics & Dynamics

Dynamics	Physics
Grid-scale	Subgrid-scale
Energy conversions forth and back	Energy conversions end up in unavailable energy pool
Reversible processes	Irreversible processes
No internal entropy production	Positive internal entropy production

The last three lines hold for the continuous moist equations that include viscous and molecular scales (Navier Stokes eq.).

Does the distinction hold for the discretized coarse-grained equations, too?

I would wish: Yes

Modeling tradition says: No

Continuous equations as a benchmark for coarse-grained model equations?

Continuous equations

Thermal conduction
Diffusive fluxes of constituents
Viscous stresses
Phase changes
Radiation (line by line)

Known coefficients

Coarse-grained equations

Turbulent heat flux
Turbulent/sedimentation fluxes
Turbulent stresses
Subgrid phase changes, clouds
Simplified Radiation

Unknown coefficients
have to be parameterized

At the present stage: stick to continuous eq. as benchmark and highlight energy conversions and consequences of enforced positive internal entropy production for the flux formulations.

Air constituents

$$\partial_t \varrho_i = -\nabla \cdot (\mathbf{v}_i \varrho_i) + I_i = -\nabla \cdot (\mathbf{v} \varrho_i + \mathbf{J}_i) + I_i$$

- ▶ Barycentric velocity $\mathbf{v} = \sum_i \varrho_i \mathbf{v}_i / \sum_i \varrho_i$.
- ▶ Total mass $\varrho = \sum_i \varrho_i$ conservation: $\partial_t \varrho = -\nabla \cdot (\varrho \mathbf{v})$
- ▶ Diffusive flux $\mathbf{J}_i = \varrho_i (\mathbf{v}_i - \mathbf{v})$. $\sum_i \mathbf{J}_i = 0$ follows from definition. Fluxes include precipitation and turbulent fluxes.
- ▶ Surface $\mathbf{v}_{surf} \neq 0$, e.g. $\mathbf{v}_{surf} = \frac{\mathbf{J}_{precip} + \mathbf{J}_v}{\varrho - \varrho_v - \varrho_{precip}}$
- ▶ Conversion rates are mass conserving $\sum_i I_i = 0$.
- ▶ All air constituents have their thermodynamic properties $c_{pi} = c_{vi} + R_i$.
- ▶ All air constituents have the same temperature T .
- ▶ Ideal (not real) gas law : $p_d = \varrho_d R_d T$, $p_v = \varrho_v R_v T$, $p = p_d + p_v$.

Different prognostic formulations for constituents

Densities ϱ_i :

$$\partial_t \varrho_i = -\nabla \cdot (\mathbf{v} \varrho_i) + I_i - \nabla \cdot \mathbf{J}_i$$

Specific contents $q_i = \varrho_i / \varrho$:

$$\partial_t q_i = -\mathbf{v} \cdot \nabla q_i + \frac{1}{\varrho} I_i - \frac{1}{\varrho} \nabla \cdot \mathbf{J}_i$$

Mixing ratios $r_i = \varrho_i / \varrho_d$:

$$\partial_t r_i = -\mathbf{v} \cdot \nabla r_i + \frac{1}{\varrho_d} I_i - \frac{1+r_i}{\varrho_d} \nabla \cdot \mathbf{J}_i - \frac{r_i}{\varrho_d} \nabla \cdot \sum_{j \neq (i,d)} \mathbf{J}_j$$

Mechanical energy equations

Momentum equation

$$d_t \mathbf{v} = \partial_t \mathbf{v} + \nabla \frac{\mathbf{v}^2}{2} + (\nabla \times \mathbf{v}) \times \mathbf{v} = -2\boldsymbol{\Omega} \times \mathbf{v} - \frac{1}{\rho} \nabla p - \nabla \Phi - \frac{1}{\rho} \nabla \cdot \boldsymbol{\tau}$$

Dot momentum equation with $\rho \mathbf{v}$, Note: $\mathbf{v} \cdot (\mathbf{A} \times \mathbf{v}) = 0$

⇒ Kinetic energy equation, $K = \mathbf{v}^2/2$

$$\rho d_t K = \partial_t (\rho K) + \nabla \cdot (\rho \mathbf{v} K) = \underbrace{-\nabla \cdot (p \mathbf{v}) + \rho \nabla \cdot \mathbf{v}}_{=-\mathbf{v} \cdot \nabla p} - \rho \mathbf{v} \cdot \nabla \Phi - \nabla \cdot (\boldsymbol{\tau} \cdot \mathbf{v}) + \underbrace{\boldsymbol{\tau} \cdot \cdot \nabla \mathbf{v}}_{=-\varepsilon_{fric}}$$

& Potential energy ($\Phi = gz$) equation

$$\rho d_t \Phi = \partial_t (\rho \Phi) + \nabla \cdot (\rho \mathbf{v} \Phi) = +\rho \mathbf{v} \cdot \nabla \Phi$$

Internal energy equation

Repeat mechanical energy equation from last slide

$$\rho d_t(K + \Phi) = -\nabla \cdot (p\mathbf{v} + \underline{\boldsymbol{\tau}} \cdot \mathbf{v}) + p\nabla \cdot \mathbf{v} - \varepsilon_{fric}$$

Internal energy (specific symbol: u) equation is postulated from enforcing total energy conservation and allowing for further redistributions of heat

$$\rho d_t u = -p\nabla \cdot \mathbf{v} + \varepsilon_{fric} - \nabla \cdot (\mathbf{R} + \mathbf{W})$$

- ▶ $u = \sum_i u_i q_i$ and $u_i = u_{i,0} + c_{v,i}(T - T_0)$
- ▶ \mathbf{R} : radiation flux
- ▶ $\mathbf{W} = \mathbf{J}_s + \sum_i h_i \mathbf{J}_i$: total heat flux is comprised of sensible heat flux \mathbf{J}_s and the heat transported with the constituents $\sum_i h_i \mathbf{J}_i$. ▶ → Latent heat flux (?)
- ▶ $h_i = h_{i,0} + c_{p,i}(T - T_0)$ are the enthalpies of the constituents.
- ▶ Only enthalpy differences are meaningful physical quantities (→ latent heats of melting/sublimation/vaporization $L_m/L_s/L_v$).

The material entropy budget equation

Internal energy U depends on (V, S, Q_i) . Gibbs relation reads then

$$\varrho d_t u = -p \nabla \cdot \mathbf{v} + T \varrho d_t s + \sum_i \mu_i \varrho d_t q_i$$

with $\mu_i = h_i - T s_i$ the chemical potentials. Insert now internal energy equation and constituent equations. Distinguish entropy flux divergences and internal entropy production

$$\varrho d_t s = -\nabla \cdot \left(\frac{\mathbf{J}_s}{T} + \sum_i s_i \mathbf{J}_i \right) + \underbrace{\frac{\varepsilon_{\text{fric}} - \mathbf{J}_s / T \cdot \nabla T - \sum_i \mathbf{J}_i \cdot \nabla \mu_i|_T - \sum_i l_i \mu_i}{T}}_{\text{internal entropy production}}$$

Red terms are energy dissipation rates.

Consequences of the material entropy budget equation

$$\rho d_t s = -\nabla \cdot \left(\frac{\mathbf{J}_s}{T} + \sum_i s_i \mathbf{J}_i \right) + \frac{\varepsilon_{fric} - \mathbf{J}_s / T \cdot \nabla T - \sum_i \mathbf{J}_i \cdot \nabla \mu_i|_T - \sum_i l_i \mu_i}{T}$$

2nd law: Each of the dissipation terms must be positive for itself (Curie's principle: no coupling between processes of different tensor degree).

This puts constraints on the fluxes $\underline{\tau}$, \mathbf{J}_s , \mathbf{J}_i and l_i .

- ▶ $\varepsilon_{fric} = -\underline{\tau} \cdot \nabla \mathbf{v} > 0$ constraints the tensor shape of $\underline{\tau}$
- ▶ $\varepsilon_{th} = -\mathbf{J}_s / T \cdot \nabla T > 0$ constraints $\mathbf{J}_s \propto -\nabla T$ being downgradient T ,
- ▶ $\varepsilon_{mix} = -\sum_i \mathbf{J}_i \cdot \nabla \mu_i|_T > 0$ reflects the mixing of air constituents
- ▶ $\varepsilon_{pc} = -\sum_i l_i \mu_i > 0$ states the direction of phase changes

The constraints organize the direction of fluxes, but not the strengths. The task of parameterization should thus only be to tune the strengths of those fluxes.

Constraints on numerical operators(1)

In all manipulations, **for the energy and for the entropy budget equations**, the following operators are involved:

- ▶ $\mathbf{v} \cdot (\mathbf{A} \times \mathbf{v}) = 0$ This requires the Lamb transformed momentum advection term $-\mathbf{v} \cdot \nabla \mathbf{v} = -\nabla K - (\nabla \times \mathbf{v}) \times \mathbf{v}$.
- ▶ $\nabla \cdot (\psi \mathbf{w}) = \psi \nabla \cdot \mathbf{w} + \mathbf{w} \cdot \nabla \psi$. Gradient and divergence operators are not independent.
- ▶ $-\mathbf{v} \cdot \nabla \underline{\tau} = -\nabla \cdot (\underline{\tau} \cdot \mathbf{v}) + \underline{\tau} \cdot \nabla \mathbf{v}$ is a challenge to be formulated in arbitrary coordinates (on hexagonal C-grid: ref. Gassmann (2018), QJRMS).

Constraints on numerical operators(2)

Poisson brackets implicitly include $\mathbf{v} \cdot (\mathbf{A} \times \mathbf{v}) = 0$ and
 $-\psi \nabla \cdot \mathbf{w} - (-\nabla \cdot (\psi \mathbf{w}) + \mathbf{w} \cdot \nabla \psi) = 0$

$$\begin{aligned} \{\mathcal{F}, \mathcal{H}\} = & - \int_V \frac{\delta \mathcal{F}}{\delta \mathbf{v}} \cdot \left(\frac{\boldsymbol{\omega}_a}{\rho} \times \frac{\delta \mathcal{H}}{\delta \mathbf{v}} \right) dV \\ & - \int_V \left(\frac{\delta \mathcal{F}}{\delta \rho} \nabla \cdot \frac{\delta \mathcal{H}}{\delta \mathbf{v}} - \frac{\delta \mathcal{H}}{\delta \rho} \nabla \cdot \frac{\delta \mathcal{F}}{\delta \mathbf{v}} \right) dV \\ & - \int_V \left(\frac{\delta \mathcal{F}}{\delta \tilde{\theta}} \nabla \cdot \left(\theta \frac{\delta \mathcal{H}}{\delta \mathbf{v}} \right) - \frac{\delta \mathcal{H}}{\delta \tilde{\theta}} \nabla \cdot \left(\theta \frac{\delta \mathcal{F}}{\delta \mathbf{v}} \right) \right) dV, \end{aligned}$$

Main advantage: Formulate the divergence in terrain-following coords with contravariant flux components, and the respective (pressure!) gradient in terrain-following coords can be deduced.

Constraints on prognostic thermodynamic equation

The energy and the entropy budgets equation shall be derivable from the prognostic model equations. ▶

⇒ Approximations are not allowed in the prognostic equations themselves.

Temperature eq. for a height-based vertical coord. formulation:

$$\hat{c}_v \varrho dt T = -p \nabla \cdot \mathbf{v} + \varepsilon_{fric} + T \nabla \cdot \sum_i \mathbf{J}_i c_{v,i} - \sum_i (\tilde{h}_{0,i} + c_{v,i} T) l_i - \nabla \cdot (\mathbf{R} + \mathbf{J}_s + \sum_i c_{p,i} T \mathbf{J}_i)$$

Temperature eq. for a pressure-based vertical coord. formulation:

$$\hat{c}_p \varrho dt T = \omega + \varepsilon_{fric} + T \nabla \cdot \sum_i \mathbf{J}_i c_{p,i} - \sum_i (\tilde{h}_{0,i} + c_{p,i} T) l_i - \nabla \cdot (\mathbf{R} + \mathbf{J}_s + \sum_i c_{p,i} T \mathbf{J}_i)$$

$$\hat{c}_v = \sum_i c_{v,i} q_i, \hat{c}_p = \sum_i c_{p,i} q_i, \tilde{h}_{0,i} = h_{0,i} - c_{p,i} T_0, \omega = dt p$$

2nd law constraints

Repeated from a previous slide

2nd law puts constraints on the fluxes $\underline{\tau}$, \mathbf{J}_s , \mathbf{J}_i and l_i .

- ▶ $\varepsilon_{fric} = -\underline{\tau} \cdot \nabla \mathbf{v} > 0$ constraints the tensor shape of $\underline{\tau}$
- ▶ $\varepsilon_{th} = -\mathbf{J}_s / T \cdot \nabla T > 0$ constraints $\mathbf{J}_s \propto -\nabla T$ being downgradient T ,
- ▶ $\varepsilon_{mix} = -\sum_i \mathbf{J}_i \cdot \nabla \mu_i|_T > 0$ reflects the mixing of air constituents
- ▶ $\varepsilon_{pc} = -\sum_i l_i \mu_i > 0$ states the direction of phase changes

The constraints organize the direction of fluxes, but not the strengths. The task of parameterization should thus be the tuning of the strengths of those fluxes.

Momentum diffusion tensor

Constraint: $\varepsilon_{fric} = -\underline{\tau} \cdot \nabla \mathbf{v} > 0$. \Rightarrow Required tensor formulation:

$$\underline{\tau} = -\rho \begin{pmatrix} K_h(\partial_x u - \partial_y v) + K_v(\frac{1}{3}D_h - \frac{2}{3}\partial_z w) & K_h(\partial_y u + \partial_x v) & K_v(\partial_z u + \partial_x w) \\ K_h(\partial_y v - \partial_x u) + K_v(\frac{1}{3}D_h - \frac{2}{3}\partial_z w) & K_h(\partial_y v + \partial_x w) & K_v(\partial_z v + \partial_y w) \\ K_v(\partial_z u + \partial_x w) & K_v(\partial_z v + \partial_y w) & K_v(\frac{4}{3}\partial_z w - \frac{2}{3}D_h) \end{pmatrix}.$$

- ▶ Tensor is invariant to rotations of coords in the horizontal plane.
- ▶ Tensor allows for anisotropic diffusion.
- ▶ Hydrostatic model omits last column, horizontal w -derivatives in the last row, and K_v -terms on the trace.
- ▶ Optionally add a divergence damping $-\rho K_d \nabla \cdot \mathbf{v}$ on the trace.
- ▶ **Parameterization scheme must deliver positive K_v , K_h , and K_d .**

Heat flux (1)

Constraint $\varepsilon_{th} = -\mathbf{J}_s/T \cdot \nabla T > 0$. \Rightarrow Required heat flux formulation:

$$\mathbf{J}_s = -c_p \rho \underline{\mathbf{K}}_T \cdot \nabla T$$

- ▶ Compare to common practice $J_s^z = -c_p \rho K_\theta \Pi (\partial_z \theta - \gamma)$, which is not always downgradient T .
- ▶ Countergradient or EDMF-fluxes correct the direction of the downgradient θ -flux to be more compatible with the downgradient T -flux.
- ▶ Explanation: Interpret the TKE to be comprised in the internal energy reservoir (non-resolved energy!)

$$\underbrace{\partial_t(c_v \rho T)|_{sub}}_{c_p \Pi \partial_t(\rho \theta)|_{sub}} = \underbrace{-\partial_z(-c_p \Pi \rho K_\theta \partial_z \theta)}_{=-c_p \Pi \partial_z(-\rho K_\theta \partial_z \theta)} + \underbrace{\rho K_\theta N^2}_{\Delta E_{int}} - \underbrace{\rho K_\theta N^2}_{\Delta E_{kin}} - \partial_z(-\rho K_{tke} \partial_z k_e) + \varepsilon_{sh}$$

rhs of TKE-equation

Heat flux (2)

$$\underbrace{\partial_t(c_v \varrho T)|_{sub}}_{c_p \Pi \partial_t(\varrho \theta)|_{sub}} = \underbrace{-\partial_z(-c_p \Pi \varrho K_\theta \partial_z \theta)}_{=-c_p \Pi \partial_z(-\varrho K_\theta \partial_z \theta)} + \underbrace{\varrho K_\theta N^2}_{\Delta E_{int}} - \underbrace{\varrho K_\theta N^2}_{\Delta E_{kin}} - \partial_z(-\varrho K_{tke} \partial_z k_e) + \varepsilon_{sh}$$

rhs of TKE-equation

$$\partial_t(c_v \varrho T)|_{sub} = -\partial_z(-c_p \Pi \varrho K_\theta (\partial_z \theta + \frac{K_{tke} \partial_z k_e}{c_p \Pi K_\theta})) + \underbrace{\varepsilon_{sh}}_{=\varepsilon_{fric}}$$

$$\gamma = -\frac{K_{tke} \partial_z k_e}{c_p \Pi K_\theta}.$$

The inclusion of the TKE keeps the heat flux downgradient T in the upper, slightly stable, part of the boundary layer and we have

$$J_s^z = -c_p \varrho K_\theta \Pi (\partial_z \theta - \gamma) = -c_p \varrho K_T \partial_z T \text{ with } K_\theta > 0 \text{ and } K_T > 0.$$

Workshop discussion point: How can we interpret common practice in terms of a downgradient T formulation?

Heat flux (3)

- ▶ Previous slides considered the PBL in case of convective or slightly stable conditions. (buoyancy production \rightarrow TKE \rightarrow energy transport \rightarrow energy deposition at higher levels)
- ▶ What about heat flux at **stable stratification**?
- ▶ **My opinion:**
The question then is not about the heat flux, which is assumed to be tiny and downgradient T (not θ), but about the way we represent wave breaking. For this, the undulation of isentropes must be represented correctly, which requires direct access to the w -equation.

Hypothesis:

Wave breaking can be modeled with the stress tensor also present in the vertical velocity equation. (Question: What about hydrostatic models?) This allows to represent buoyancy loss (not from TKE, but from the resolved kinetic energy), i.e. kinetic energy of vertical motions gets lost and is deposited as frictional heating in the internal energy reservoir.

Turbulent water vapour and dry air fluxes

Constraint: $\varepsilon_{mix} = -\sum_i \mathbf{J}_i \cdot \nabla \mu_i|_T > 0$

▶ For ideal gases $\nabla \mu_i|_T = \frac{1}{\varrho_i} \nabla p_i = R_i T \nabla \ln \varrho_i$ (note $p_i = R_i \varrho_i T$ and $T = const$)

▶ Mixing of dry air and water vapour $\sum_i \mathbf{J}_i = 0 \rightarrow \mathbf{J}_d = -\mathbf{J}_v$

▶ $\rightarrow \mathbf{J}_v = -\varrho \underline{\mathbf{K}}_v \cdot \left(\frac{q_d \nabla p_v - q_v \nabla p_d}{p} \right) \neq -\varrho \underline{\mathbf{K}}_{v,trad,q} \cdot \nabla q^v \neq -\varrho \underline{\mathbf{K}}_{v,trad,r} \cdot \nabla r^v$

▶ compare to downgradient q_v -flux:

$$-\nabla q^v = -\frac{R_d q_d + R_v q_v}{R_v q_d + R_d q_v} \left(\frac{q_d \nabla p_v - q_v \nabla p_d}{p} \right) + \frac{(R_v - R_d) q_v q_d}{R_d q^v + R_v q^d} \nabla (\ln \varrho T)$$

▶ Entropy consistent upward directed fluxes are slightly stronger than traditional fluxes, because the water (H₂O) molecules have a lower weight than dry air (N₂ and O₂) molecules. The difference seems to be small, but this has to be checked.

Sedimentation fluxes

Constraint: $\varepsilon_{mix} = -\sum_i \mathbf{J}_i \cdot \nabla \mu_i|_T > 0$

- ▶ For precip p : $\nabla \mu_p|_T = 0$.
- ▶ The sedimentation flux is parameterized as $J_p^z = -\rho_p V_p^T$, with $V_p^T > 0$ the terminal velocity of hydrometeors.
- ▶ $\sum_i J_i^z = \sum J_p^z + J_d^z + J_v^z + \sum J_{cloud}^z = 0$
- ▶ For non-sedimenting constituents j , diffusive vertical velocities have to be assigned $w_d = w_{d,j} = \frac{\sum_p q_p V_p^T}{1 - \sum_p q_p}$, and their fluxes are $J_j^z = w_{d,j} \rho_j$.
- ▶ The dissipation is $\varepsilon_{mix} = -J_d^z \partial_z \mu_d|_T - J_v^z \partial_z \mu_v|_T = -w_d \partial_z p = w_d \rho g > 0$
- ▶ This dissipation ranks highest in magnitude under the various discussed dissipation rates. It is cleanly represented in models only if the w_d are assigned to the non-sedimenting constituents. (If this is not done explicitly, this w_d is implicitly seen for dry air if the full density is prognostic.)

Phase changes

Constraint: $\varepsilon_{pc} = -\sum_i l_i \mu_i > 0$ states the direction of phase changes.

The source terms l_i are scalar fluxes, and thus not related to accessible spatial gradients of some values. Therefore, the coarse-grained numerics is not an issue here.

$$\varepsilon_{pc} = \underbrace{-l_l(\mu_l - \mu_v)}_{\text{evaporation/condensation}} \quad \underbrace{-l_f(\mu_f - \mu_v)}_{\text{sublimation/deposition}}$$

- ▶ evaporation/condensation $\mu_l - \mu_v = -R_v T \ln \frac{p_v}{p_{v, \text{sat}, l}}$
- ▶ sublimation/deposition $\mu_f - \mu_v = -R_v T \ln \frac{p_v}{p_{v, \text{sat}, i}}$
- ▶ evaporation/sublimation in sub-saturated environment
- ▶ condensation/deposition in super-saturated environment

Reynolds averages

- ▶ Reynolds averaged fluxes like $\overline{\rho w' \psi'}$ for arbitrary scalars ψ are not needed.
- ▶ The correct variable which is diffused downgradient is determined by the second law and is not a free choice of the modeler.
- ▶ There are various moist or liquid water aware potential temperature fluxes, and to my knowledge, there is no agreement on which one is the correct one.
It is only clear that the magnitude of the diffusion coeff should depend on vertical (moisture and liquid water aware) buoyancy fluxes.
- ▶ Horizontal Reynolds-averaged momentum fluxes or heat fluxes do not necessarily lead to positive dissipation rates. (Finding of my PhD student Bastian Sommerfeld and others.)

Interference of physics and numerics

- ▶ Different computational spaces

spectral space or finite element space \Leftrightarrow grid point space

This distinction seems problematic, because it has been demonstrated that the entropy budget equation needs likewise some rules like

$$-\frac{1}{T} \nabla \cdot \mathbf{J}_s = -\nabla \cdot \left(\frac{\mathbf{J}_s}{T} \right) - \frac{1}{T^2} \mathbf{J}_s \cdot \nabla T \text{ with } \mathbf{J}_s \propto -\nabla T \text{ to be valid.}$$

Hence, physics needs the same computational space and the same numerical operators like numerics.

- ▶ Higher order or TVD advection operators

contain purely advective, purely diffusive and also anti-diffusive parts.

How do the anti-diffusive parts affect other parts of the equations?

Higher order or TVD advection operators(1)

Common advection schemes:

$$\partial_t(\varrho\psi) = -\frac{1}{\Delta x}(U_{i+1/2}\hat{\psi}_{i+1/2} - U_{i-1/2}\hat{\psi}_{i-1/2})$$

They differ in their approximation to $\hat{\psi}_{i+1/2}$.

The fluxes can be disentangled into an advective and a diffusive part

$$U_{i+1/2}\hat{\psi}_{i+1/2} = U_{i+1/2}(\bar{\psi}_{i+1/2} - K_{i+1/2}\frac{\delta_x\psi_{i+1/2}}{u_{i+1/2}\Delta x})$$

with $\bar{\psi} = (\psi_i + \psi_{i+1})/2$ and $\delta_x\psi_{i+1/2} = \psi_{i+1} - \psi_i$

Two problems: (i) Is ψ the right variable to be diffused? (ii) Is K positive?

Higher order or TVD advection operators(2)

Inspect some schemes including flux limiting schemes

Notation:

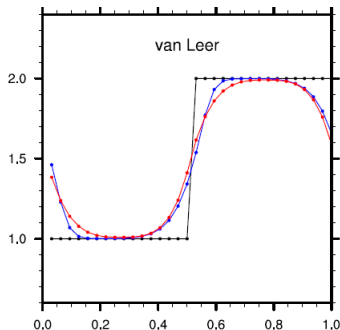
if $U_{i+1/2} \geq 0$: $r = (\psi_i - \psi_{i-1}) / (\psi_{i+1} - \psi_i)$

if $U_{i+1/2} < 0$: $r = (\psi_{i+2} - \psi_{i+1}) / (\psi_{i+1} - \psi_i)$

1st order upwind	$K = u_{i+1/2} \Delta x \frac{1}{2}$
3rd order upwind	$K = u_{i+1/2} \Delta x \frac{1-r}{6}$
van Leer scheme	$K = u_{i+1/2} \Delta x \frac{1-r}{2(1+ r)}$

Problem: K is not necessarily positive. This depends on the role of r .

Higher order or TVD advection operators (3)



analytic solution

original van Leer scheme

van Leer limiter with
 $K_{new} = \max(0, K)$

Higher order or TVD advection operators (4)

How are other dynamical fields influenced if negative diffusion coeffs are allowed for or not?

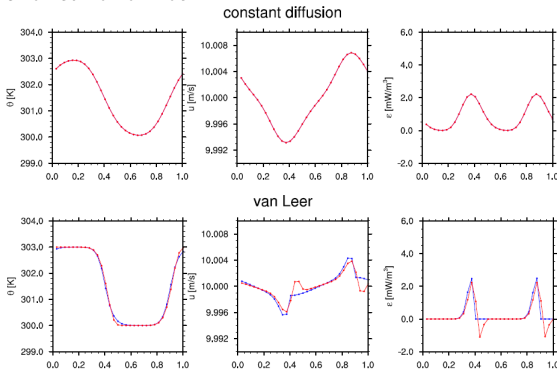


Figure below:
Entropically-corrected usage of the van Leer scheme for θ -advection.
Original van Leer scheme for θ -advection.

Selected questions raised in email (1)

What is physical understanding of the **latent heat flux**?

▸ Total heat flux $\mathbf{W} = \mathbf{J}_s + \sum_i h_i \mathbf{J}_i$ does not occur explicitly in prognostic temperature equation. ▸

Locally we have because of $\sum_i \mathbf{J}_i = 0$:

$\sum_i h_i \mathbf{J}_i = \mathbf{J}_v(h_v - h_d) + \mathbf{J}_l(h_l - h_d) + \mathbf{J}_f(h_f - h_d)$, but we do not know the enthalpy differences between dry air and any other H₂O-constituent. And this setting is physically pointless.

But in the climate mean $\bar{\mathbf{J}}_v = -\bar{\mathbf{J}}_l - \bar{\mathbf{J}}_f$ and we obtain reasonably well:

$$\sum_i h_i \bar{\mathbf{J}}_i = \bar{\mathbf{J}}_l \underbrace{(h_l - h_v)}_{-L_{\text{vap}}} + \bar{\mathbf{J}}_f \underbrace{(h_f - h_v)}_{-L_{\text{subl}}}$$

Selected questions raised in email (2)

- ▶ **Geometric structures:** Well understood for reversible dynamics. Formally less well understood for irreversible dynamics, but we know that the same gradient-divergence compatibilities must hold. → Chris Eldred
- ▶ **Structures under approximations:** For primitive equations (hydrostat. constraint), the group of Thomas Dubos has paved the path. Could be generalized...?
- ▶ **How does turbulence averaging fit into the framework?** I think that this is a matter of interpretation, if one can find a relation like $\overline{\rho \mathbf{v}'' \psi''} = -\rho \mathbf{K} \cdot \nabla \chi$ where ψ is a classical variable and χ is a 2nd law conforming variable and $K > 0$, all is fine.
- ▶ **Can we find a single set of equations that is used consistently for the entire model?** Yes, but this does not prevent us from tuning the magnitude of the coefficients according to the scales.

Thanks for your attention.