Entropy production as a constraint to subgrid-scale modeling: role of subgrid scales for the simulation of breaking gravity waves

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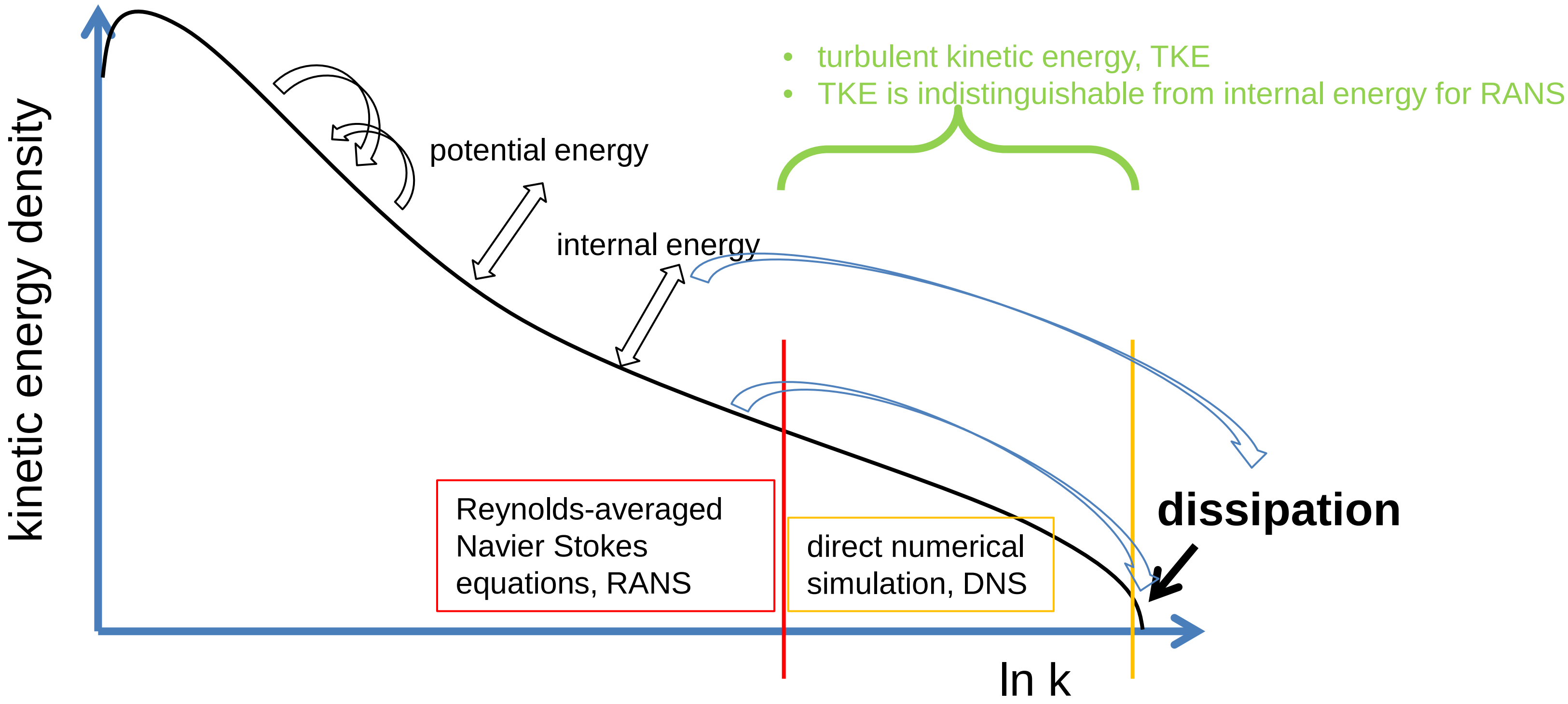
dissipation in nature ↔ dissipation in modeling



dissipation = temperature * internal entropy production

resolved scales = reversible energy transformations, forth and back

unresolved scales = resolved kinetic or internal energies are irreversibly converted into internal energy (=dissipation)

work and heat

$$d\,U = \delta A + \delta Q$$

makrocopically visible

macroscopically invisible

$$d\,U = -pdV + TdS$$

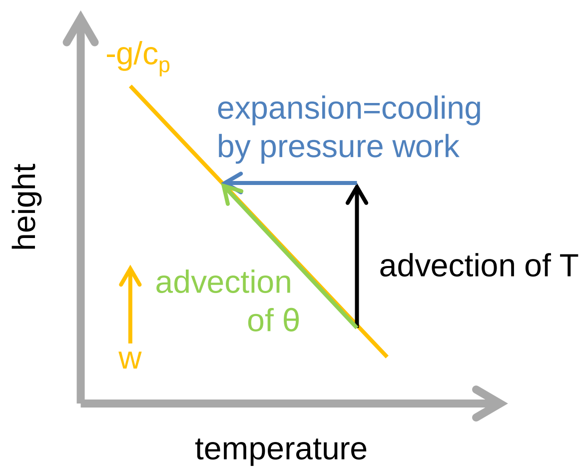
nature, DNS: $\rho \frac{d}{dt} c_v T = -p\nabla \cdot \boldsymbol{v} + \nabla \cdot \boldsymbol{W} + \varepsilon_{vfr}$

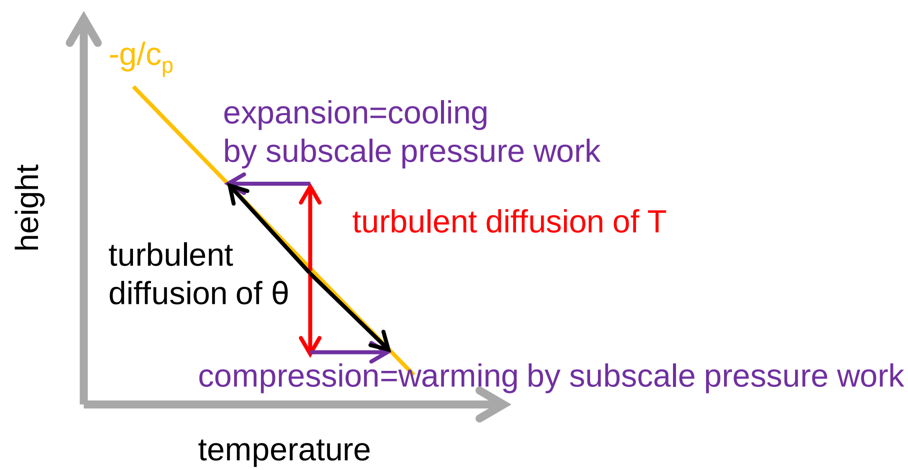
model, RANS: $\overline{\rho \frac{d}{dt} c_v T} = \overline{-p\nabla \cdot \boldsymbol{v}} + \overline{\nabla \cdot \boldsymbol{W}} + \overline{\varepsilon_{vfr}}$

$$\bar{\rho} \frac{\hat{d}}{dt} c_v \hat{T} = -\bar{p}\,\nabla \cdot \hat{\boldsymbol{v}} \underbrace{- \nabla \cdot \left(\overline{c_v \rho \boldsymbol{v}''T''}\right) \boxed{- \left(\overline{p\nabla \cdot \boldsymbol{v}} - \bar{p}\,\nabla \cdot \hat{\boldsymbol{v}}\right)} + \varepsilon_{tfr}}_{\bar{\rho}\hat{T} \frac{\hat{d}}{dt} \hat{s}}$$

Consequences of turbulence averaging

$$\frac{\partial}{\partial t}\bar{\rho}c_v\hat{T} = -\nabla\cdot(c_v\bar{\rho}\hat{\boldsymbol{v}}\hat{T}) - \bar{p}\,\nabla\cdot\hat{\boldsymbol{v}} - \nabla\cdot\left(\overline{c_v\rho\boldsymbol{v}''T''}\right) - \left(\overline{p\nabla\cdot\boldsymbol{v}} - \bar{p}\,\nabla\cdot\hat{\boldsymbol{v}}\right) + \varepsilon_{tfr}$$





$$\frac{\partial}{\partial t}\bar{\rho}c_v\hat{T} = -c_p\bar{\Pi}\nabla\cdot\left(\bar{\rho}\hat{\boldsymbol{v}}\hat{\theta}\right) - \nabla\cdot\left(\overline{c_v\rho\boldsymbol{v}''T''}\right) + \nabla\cdot\left(\overline{c_v\rho\boldsymbol{v}''T''}\right) - c_p\bar{\Pi}\nabla\cdot\left(\overline{\rho\boldsymbol{v}''\theta''}\right) + \varepsilon_{tfr}$$

Sole approximation: $\Pi'/\bar{\Pi} \ll 1$
This approximation is common.

$\Pi = (\frac{p}{p_0})^{R/c_p}$ $\quad T = \Pi\theta$

θ is diffused: internal entropy production positive

$$\frac{\partial}{\partial t}\,\bar{\rho}c_v\hat{T} = -c_p\overline{\Pi}\nabla\cdot\left(\bar{\rho}\hat{\boldsymbol{v}}\hat{\theta}\right) \underbrace{- c_p\overline{\Pi}\nabla\cdot\left(\overline{\rho\boldsymbol{v}''\theta''}\right) + \varepsilon_{tfr}}_{\bar{\rho}\hat{T}\frac{\hat{d}}{dt}\hat{s}}$$

Second law of thermodynamics

$$\bar{\rho}\frac{\hat{d}}{dt}\hat{s} = \underbrace{-\nabla\cdot\left(\frac{c_p\overline{\rho\boldsymbol{v}''\theta''}}{\hat{\theta}}\right)}_{\text{export / import}} \underbrace{- \frac{c_p\overline{\rho\boldsymbol{v}''\theta''}}{\hat{\theta}^2}\cdot\nabla\hat{\theta} + \varepsilon_{tfr}/\hat{T}}_{\text{internal entropy production has to be positive for every single process}}$$

gradient approach: $\overline{\rho\boldsymbol{v}''\theta''} = -\rho\underline{\boldsymbol{K}^{\theta}}\cdot\nabla\hat{\theta}$

$$\sigma_\theta = \frac{c_p\bar{\rho}}{\hat{\theta}^2}K_{ii}^{\theta}(\partial_i\hat{\theta})^2 \geq 0$$

always positive, regardless of stratification

dissipation by θ-diffusion: $\varepsilon_\theta = \hat{T}\sigma_\theta$

BUT: Inspect energy conversions!

$$\frac{\partial}{\partial t}\bar{\rho}c_v\hat{T} = -c_p\overline{\Pi}\nabla\cdot\left(\bar{\rho}\hat{\boldsymbol{v}}\hat{\theta}\right) - c_p\overline{\Pi}\nabla\cdot\left(\overline{\rho\boldsymbol{v}"\theta"}\right) + \varepsilon_{tfr}$$

$$\psi\nabla\cdot\boldsymbol{f} + \boldsymbol{f}\cdot\nabla\psi = \nabla\cdot(\psi\boldsymbol{f})$$

$$\frac{\partial}{\partial t}\bar{\rho}c_v\hat{T} = -c_p\overline{\Pi}\nabla\cdot\left(\bar{\rho}\hat{\boldsymbol{v}}\hat{\theta}\right) - \nabla\cdot\left(c_p\overline{\Pi}\overline{\rho\boldsymbol{v}"\theta"}\right) + c_p\overline{\rho\boldsymbol{v}"\theta"}\cdot\nabla\overline{\Pi} + \varepsilon_{tfr}$$

$\bar{\rho}K^{\theta}N^2$

vertical fluxes

Energy exchange with kinetic energy has not been inspected thorougly enough!

$\bar{\rho}K^{\theta}N^2 > 0$

- gain of internal energy
- entropy production **meaningful**
- loss of resolved kinetic energy
- a force must represent this kinetic energy loss in the momentum equation

$\bar{\rho}K^{\theta}N^2 < 0$

- loss of internal energy
- entropy production **meaning less**!
- making it meaningful must prevent the gain of resolved kinetic energy
- instead, TKE is generated, but TKE is indistinguishable from internal energy
- the traditional approach (grey box) is safe

Case distinction necessary!

Case distinction: N²<0

- omit resolved energy conversion, only applicable to N²<0

$$\frac{\partial}{\partial t}\bar{\rho}c_v\hat{T} = -c_p\overline{\Pi}\nabla\cdot\left(\bar{\rho}\hat{\boldsymbol{v}}\hat{\theta}\right)\underbrace{-\nabla\cdot\left(c_p\overline{\Pi}\overline{\rho\boldsymbol{v}"\theta"}\right)+\varepsilon_{tfr}}_{\bar{\rho}\hat{T}\frac{\hat{d}}{dt}\hat{s}}$$

$$\bar{\rho}\frac{\hat{d}}{dt}\hat{s} = \underbrace{-\nabla\cdot\left(\frac{c_p\overline{\rho\boldsymbol{v}"\theta"}}{\hat{\theta}}\right)}_{\text{export / import}}\underbrace{-\frac{c_p\overline{\Pi}\overline{\rho\boldsymbol{v}"\theta"}}{\hat{T}^2}\cdot\nabla\hat{T}+\varepsilon_{tfr}/\hat{T}}_{\text{internal entropy production}}$$

gradient apporoach:

$$c_p\overline{\Pi}\overline{\rho\boldsymbol{v}"\theta"} = -c_p\bar{\rho}\underline{\boldsymbol{K}^T}\cdot\nabla\hat{T}$$

Countergradient

$$c_p\overline{\Pi}\overline{\rho w"\theta"} = -c_p\bar{\rho}\overline{\Pi}K^\theta\left(\partial_z\hat{\theta}-\gamma\right)$$

$$\sigma_T = \frac{c_p\bar{\rho}}{\hat{T}^2}K_{ii}^T\left(\partial_i\hat{T}\right)^2 \geq 0$$

$$\sigma_T = \frac{c_p\bar{\rho}}{\hat{T}^2}\overline{\Pi}K^\theta\left(\partial_z\hat{\theta}-\gamma\right)\partial_z\hat{T} \geq 0$$

Formally, this is a temperature diffusion = subscale heat flux.

For unstable stratification $\partial_z\hat{\theta}$ and $\partial_z\hat{T}$ are parallel.

Dissipation by T-diffusion: $\varepsilon_T = \hat{T}\sigma_T$

Contradiction to 2nd law, if applied in case of N²>0

Case distinction: $N^2>0$

$$\frac{\partial}{\partial t}\bar{\rho}c_v\hat{T} = -c_p\overline{\Pi}\nabla\cdot\left(\bar{\rho}\hat{\boldsymbol{v}}\hat{\theta}\right) - c_p\overline{\Pi}\nabla\cdot\left(\overline{\rho\boldsymbol{v}"\theta"}\right) + \varepsilon_{tfr}$$

$$\varepsilon_{tfr} = -\overline{\rho\boldsymbol{v}"\boldsymbol{v}"}\cdot\cdot\nabla\hat{\boldsymbol{v}} \geq 0$$

$$\psi\nabla\cdot\boldsymbol{f} + \boldsymbol{f}\cdot\nabla\psi = \nabla\cdot(\psi\boldsymbol{f})$$

$$\frac{\partial}{\partial t}\bar{\rho}\left(\frac{\hat{\boldsymbol{v}}^2}{2}+\Phi\right) = -c_p\bar{\rho}\hat{\boldsymbol{v}}\hat{\theta}\cdot\nabla\overline{\Pi} - c_p\overline{\rho\boldsymbol{v}"\theta"}\cdot\nabla\overline{\Pi} - \hat{\boldsymbol{v}}\cdot\nabla\cdot\overline{\rho\boldsymbol{v}"\boldsymbol{v}"} - \nabla\cdot\left(\bar{\rho}\hat{\boldsymbol{v}}\left(\frac{\hat{\boldsymbol{v}}^2}{2}+\Phi\right)\right)$$

Which momentum equation belongs to kinetic energy equation?

Consider only vertical direction.

$$\frac{\partial}{\partial t}\hat{w} = -g - c_p\hat{\theta}\partial_z\overline{\Pi} - c_p\frac{\overline{\rho w"\theta"}}{\bar{\rho}\hat{w}}\partial_z\overline{\Pi}$$

- **new term**
- turbulent pressure gradient term
- similarity to Rayleigh damping

$$R_w = N^2K^\theta/\hat{w}^2$$

$$\frac{\partial}{\partial t}\hat{w} = -g - c_p\hat{\theta}\partial_z\overline{\Pi} - \frac{K^\theta N^2}{\hat{w}}$$

- diffusion coefficient must prevent singularity
- new term leads to downward turbulent θ-flux.

$$\frac{\partial}{\partial t}\hat{w} = -g - c_p\hat{\theta}\partial_z\overline{\Pi} - R_w\hat{w}$$

$$-c_p\hat{\theta}\partial_z\overline{\Pi} = -\frac{1}{\bar{\rho}}\partial_z\bar{p}$$

Case distinction: $N^2>0$

$$\frac{\partial}{\partial t}\hat{w} = -g - c_p\hat{\theta}\partial_z\overline{\Pi} - R_w\hat{w}$$

$$R_w = N^2K^\theta/\hat{w}^2$$

Hypothesis: For shortest resolvable scales, the horizonal wind is damped by vertical diffusion as fast as the vertical wind is damped by Rayleigh damping.

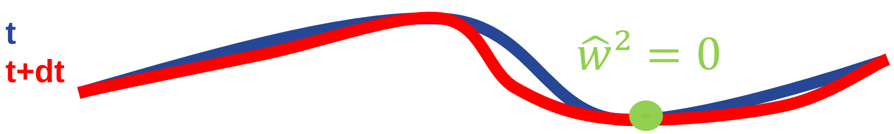
$$R_w = K^m\frac{\pi^2}{(\Delta z)^2}$$

$$K^\theta = K^m\frac{\pi^2\hat{w}^2}{(\Delta z)^2N^2}$$

There is no diffusion for $\hat{w}^2 = 0$.

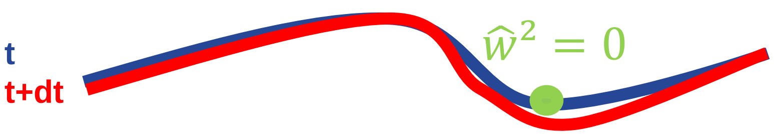
Consider isentropes of a breaking gravity wave

New procedure



wave overturns
amplitude does not grow

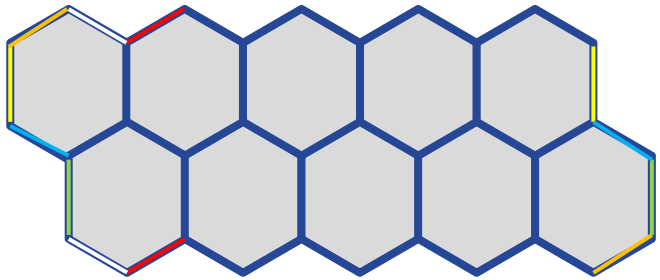
State of the art



wave overturns less
amplitude grows

Examplary 2-d modeling with ICON-IAP

ICON-IAP model with hexagonal mesh (QJRMS,2013)



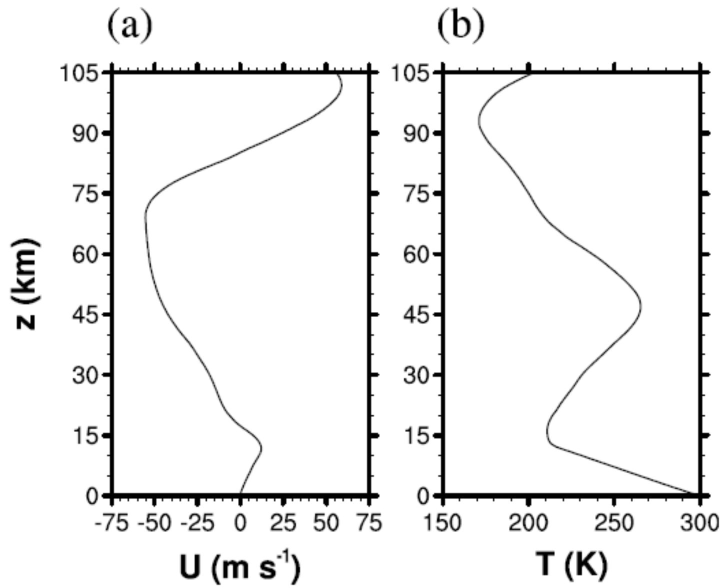


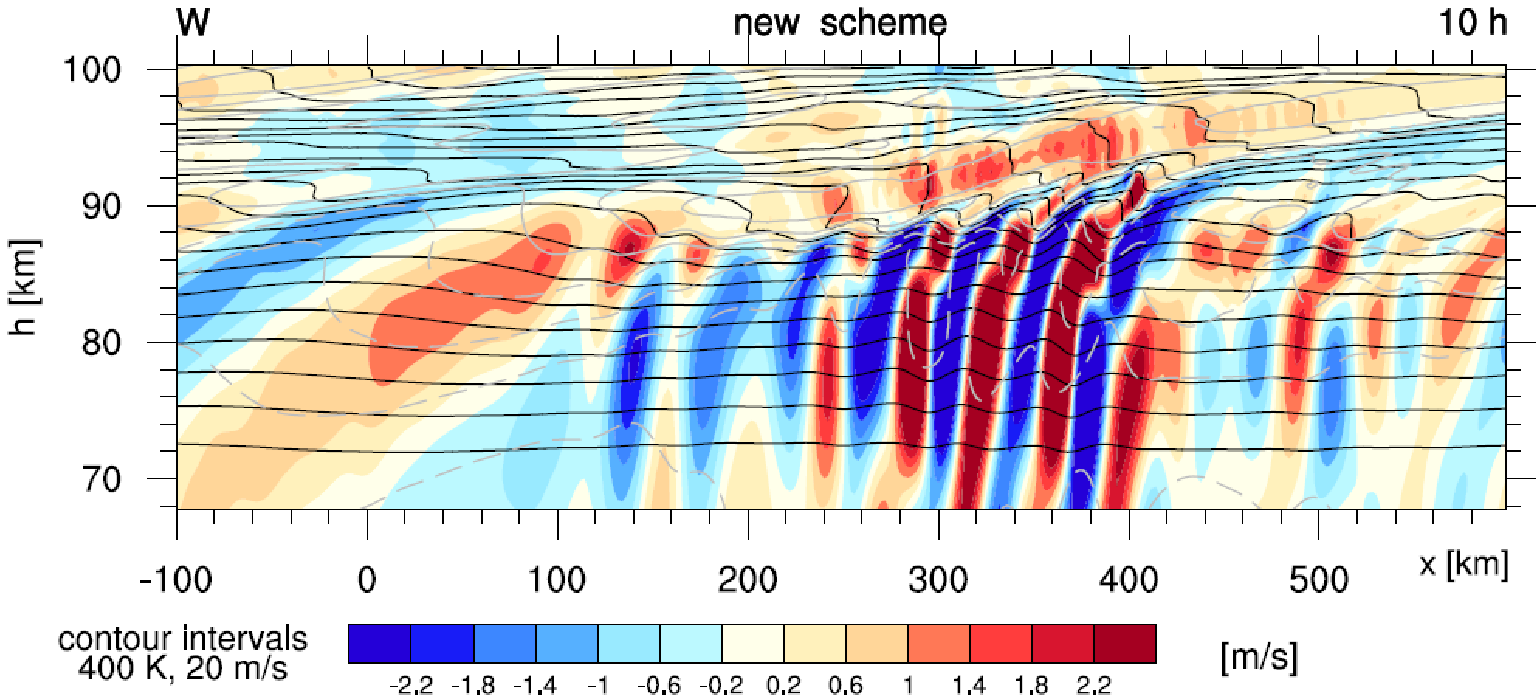
Figure 1. The basic-state (a) zonal wind and (b) temperature used for the numerical simulations. These are the July mean values at 35°N from the CIRA climate data.

Δz =250 m, Δx=2 km, Δt = 3 s,
H=120 km, L=1200 km, T=32 h

- K^m as in Holtslag und Boville (1993)
- initial profile as in Chun and Kim (2008)

- gravity wave generator as in Durran (1999), ceases after 16 hours

w, θ and u in breaking region

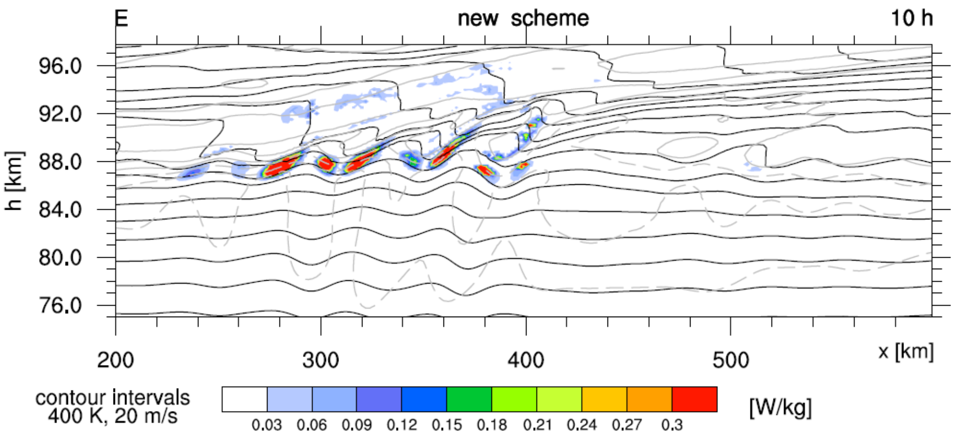


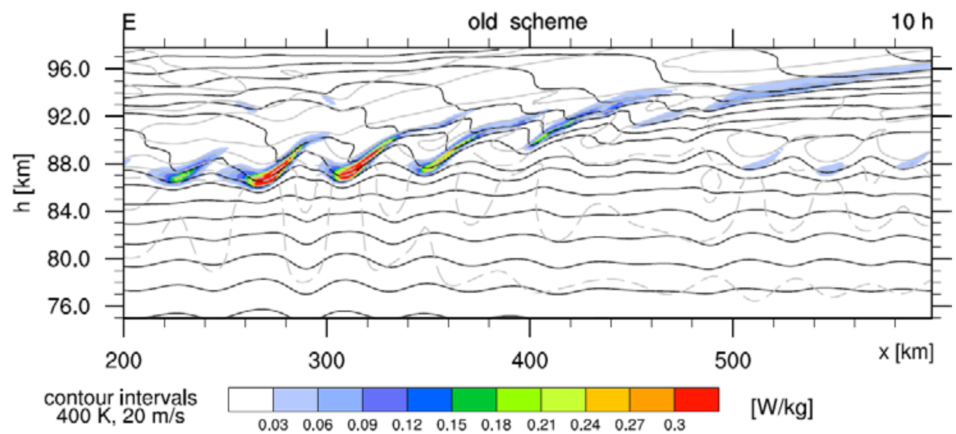
- isentropes have local minimum at $w = 0$
- gravity wave breaks near the critical level: $m^2 \rightarrow \infty$
- isentropes overturn
- vertical wind shear is large

Downward directed θ fluxes

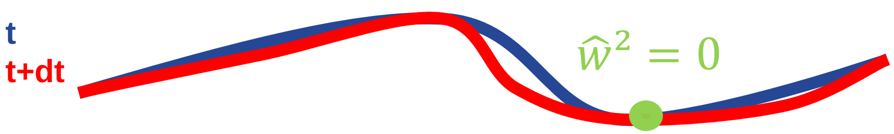
$$E_{new} = \rho K^m w^2 \pi^2 / (\Delta z)^2$$

$$E_{old} = \rho K^m N^2$$



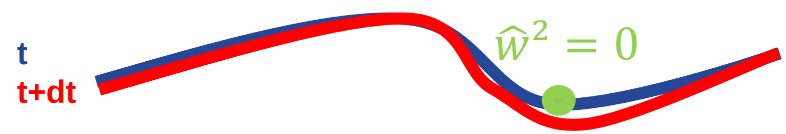


New procedure



wave overturns
amplitude does not grow

State of the art

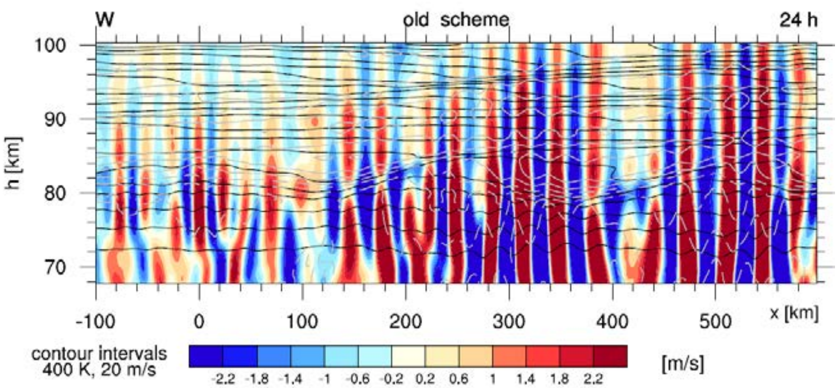


wave overturns less
amplitude grows

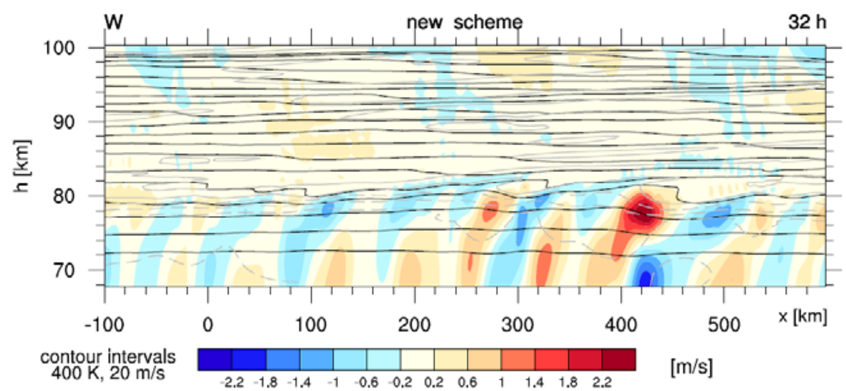
Three runs

EXP 1: state of the art, inconsistent for $N^2>0$

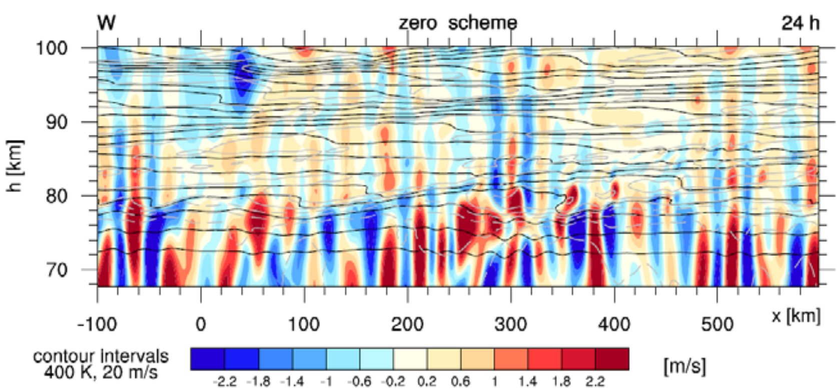
After a long time....



EXP 2: entropically consistent for $N^2>0$



EXP 4: nothing for $N^2>0$

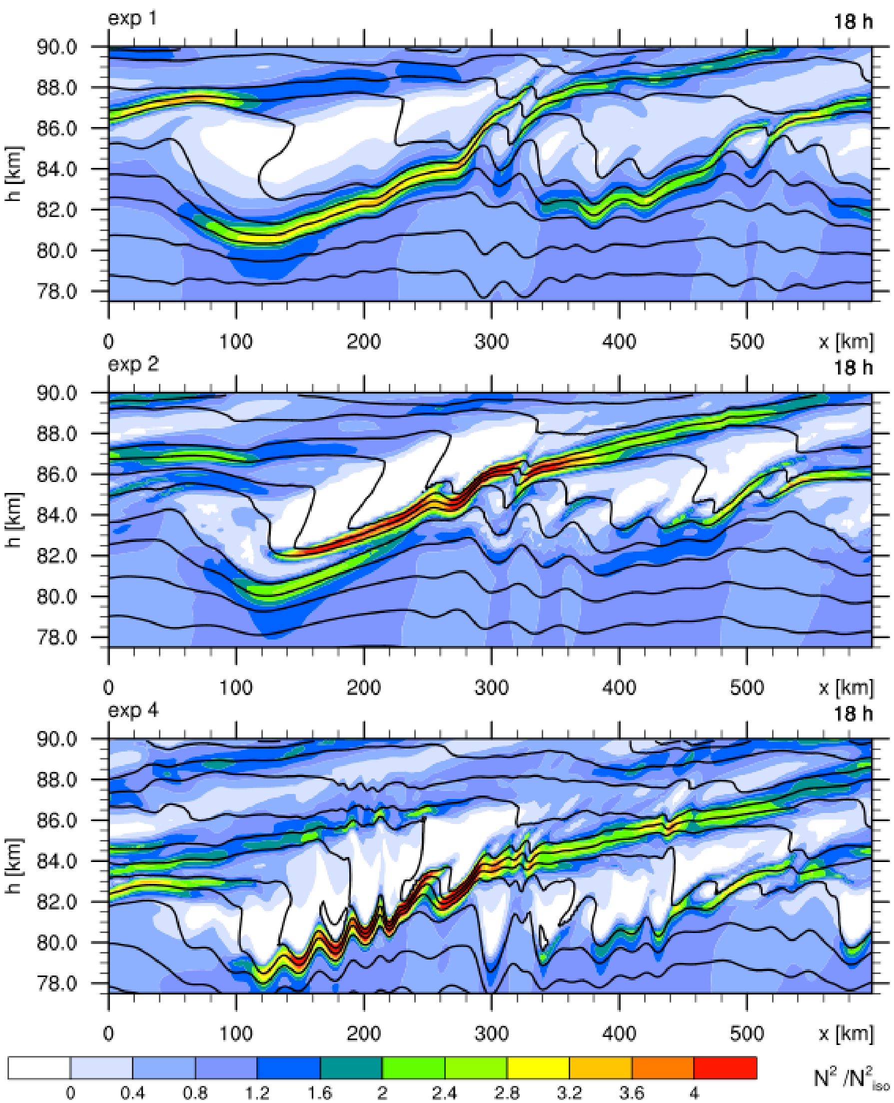


Further experiments (not shown):
If

- forcing in w-eq. is omitted, but θ-flux is retained in θ-eq,
- typical numerical off-centering in the implicit solver for w is used,

results are very similar to exp 2.

Relative static stability N^2/N^2_{iso}



EXP 1: state of the are, inconsistent for $N^2>0$

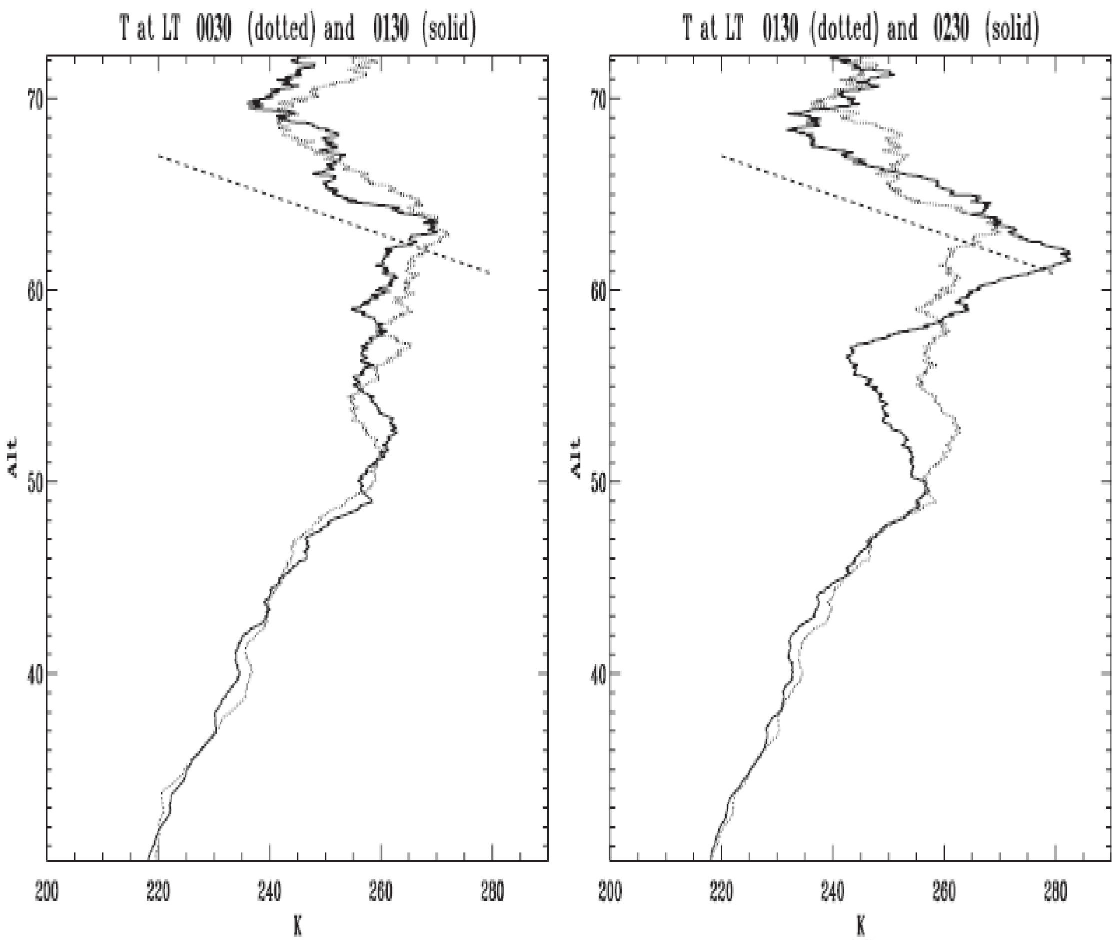
EXP 2: entropically consistent for $N^2>0$

EXP 4: nothing for $N^2>0$

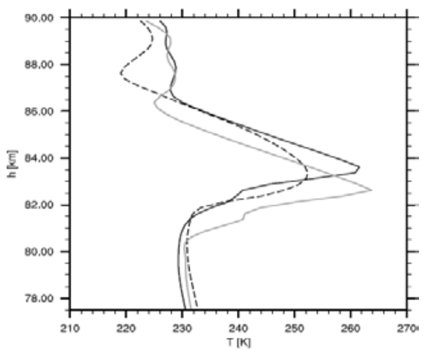
$$N^2_{iso} = g^2/(cpT)$$

N^2 for isothermal stratification

Temperature profiles



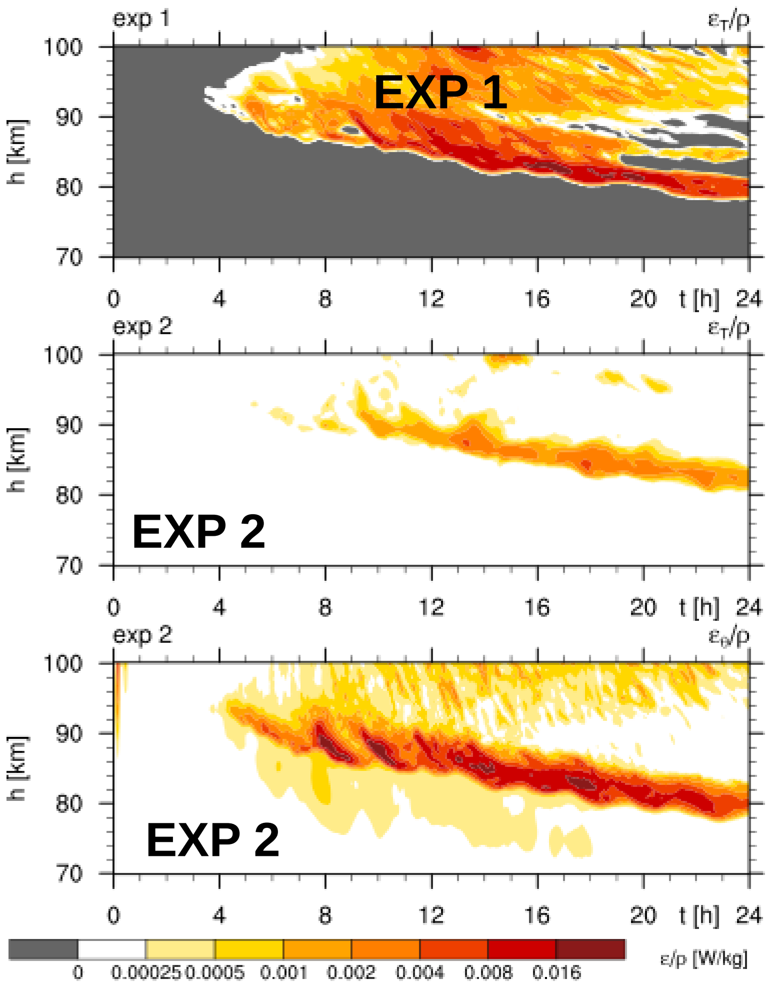
Lidar-measurements (Liu and Meriwether, 2004)

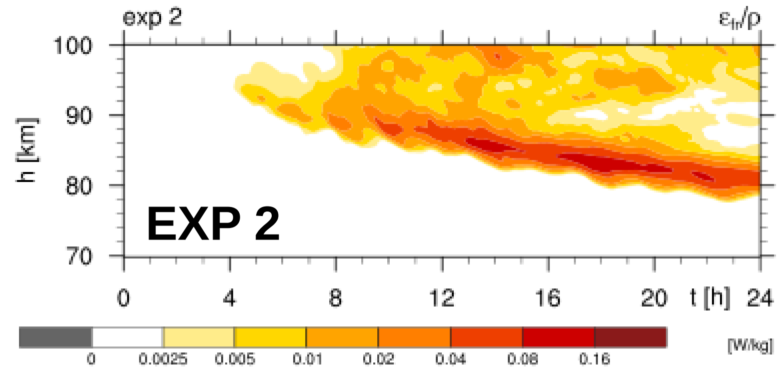


Experiments 1,2,4

- sharp maxima, peaks
- sometimes overadiabatic stratification
- no parabolic shape

Dissipations rates $\varepsilon_\theta, \varepsilon_T, \varepsilon_{tfr}$





↑ frictional dissipation is 10 times larger than thermal dissipation

← thermal dissipation

upper left picture:

- $\partial_z\theta\partial_z T$ changes sign at isothermal stratification
- inversion layer ($\partial_z T > 0$) has positive dissipation, but the physical process is wrong
- there should not be any qualitative difference between less and more stable stratification than isothermal stratification, if the stratification is stable

Other parameterizations in light of 2nd law

$$\hat{T}\sigma = \varepsilon_{\mathrm{sh}} - \mathbf{J}_{\mathrm{s}} \cdot \frac{\nabla \hat{T}}{\hat{T}} - \Sigma_i \mathbf{J}_{\mathrm{i}}^{*} \cdot \nabla \hat{\mu}_i|_{\hat{T}} - \Sigma_i I_i \hat{\mu}_i.$$

- Friction
  - symmetric diffusion tensor with shear and strain deformations
  - no hyperdiffusion
- Water vapour fluxes
  - correct: $\mathbf{J}_{\mathrm{v}}^{\mathrm{t}} = -\bar{\varrho}\mathbf{K}^{\mathrm{v}} \cdot \left(\frac{\hat{q}_{\mathrm{d}} \nabla \bar{p}_{\mathrm{v}} - \hat{q}_{\mathrm{v}} \nabla \bar{p}_{\mathrm{d}}}{\bar{p}} \right)$
  - state of the art, but incorrect $\mathbf{J}_{\mathrm{vK}}^{\mathrm{t}} = -\bar{\varrho}\mathbf{K}_{\mathrm{K}}^{\mathrm{v}} \cdot \nabla \hat{q}_{\mathrm{v}}$
- Precipitation fluxes
  - Sum of all subscale fluxes = 0
  - interpretation: mixing process
  - misconception: frictional process
  - Not: „Frictional dissipation: Blame it to the rain“

Conclusion

Case distinction for subscale parameterization:

stable N²>0 and **unstable N²<0**

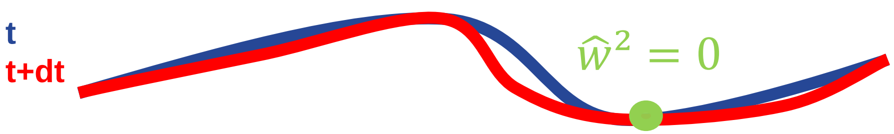
Energy conversion between resolved kinetic and internal energy is necessary for N²>0.

This requires a new term in the vertical momentum equation.

The friction term converts likewise kinetic energy into internal energy.

But this process is described by tensor fluxes and not by vector fluxes.

New procedure



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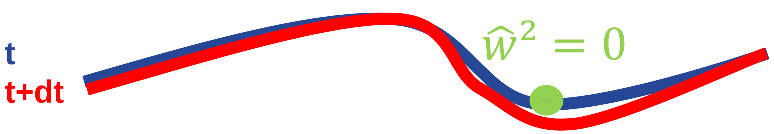
State of the art



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