Around the 3D diffusion: stability and testing

WG2/CELO-meeting at the COSMO User Seminar
5 March 2015, Offenbach

Michael Baldauf (DWD)

many thanks for discussions with Slavko Brdar and Günther Zängl

3D diffusion in spherical and terrain-following coordinates

scalar flux divergence

$$\rho \frac{\partial s}{\partial t} = -\nabla_j H^j = -\frac{\partial}{\partial x^j} H^j - \Gamma^j_{jk} H^k$$

vectorial flux divergence

$$\frac{\partial v^i}{\partial t} = -\frac{1}{\rho} \nabla_j T^{ij} = -\frac{1}{\rho} \left(\frac{\partial}{\partial x^j} T^{ij} + \Gamma^i_{jk} T^{kj} + \Gamma^j_{jk} T^{ik} \right)$$

with gradient expressions for scalar diffusion flux $\boldsymbol{H}$ and momentum flux tensor $\boldsymbol{T}$

$$H^i = -\rho K_s \, g^{ij} \nabla_j s$$

$$T^{ij} = -\rho K \left(g^{il} \nabla_l v^j + g^{jl} \nabla_l v^i \right)$$

These formulae cannot be used directly since many meteorological models use *spherical* (i.e. *non-terrain-following*) and *normalized* base vectors →

Metric terms of 3D-diffusion

scalar flux divergence:

terrain following coordinates — vertical

$$\rho \frac{\partial s}{\partial t} = -\frac{1}{r\cos\phi}\frac{\partial H^{*1}}{\partial \lambda} - \frac{J_\lambda}{\sqrt{G}}\frac{1}{r\cos\phi}\frac{\partial H^{*1}}{\partial \zeta} - \frac{1}{r}\frac{\partial H^{*2}}{\partial \phi} - \frac{J_\phi}{\sqrt{G}}\frac{1}{r}\frac{\partial H^{*2}}{\partial \zeta} + \frac{1}{\sqrt{G}}\frac{\partial H^{*3}}{\partial \zeta}$$
$$-\frac{2}{r}H^{*3} + \frac{\tan\phi}{r}H^{*2}.$$

horizontal (cartesian)

earth curvature

scalar fluxes:

$$H^{*1} = -\rho K_s \frac{1}{r\cos\phi}\left(\frac{\partial s}{\partial \lambda} + \frac{J_\lambda}{\sqrt{G}}\frac{\partial s}{\partial \zeta}\right),$$
$$H^{*2} = -\rho K_s \frac{1}{r}\left(\frac{\partial s}{\partial \phi} + \frac{J_\phi}{\sqrt{G}}\frac{\partial s}{\partial \zeta}\right),$$
$$H^{*3} = +\rho K_s \frac{1}{\sqrt{G}}\frac{\partial s}{\partial \zeta},$$

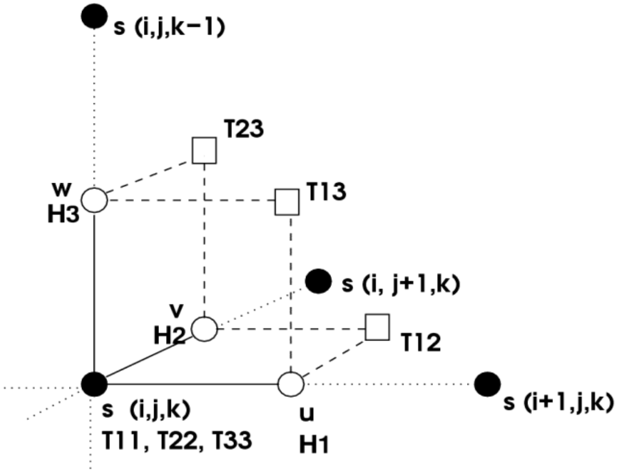
analogous:
‚vectorial‘ diffusion of *u*, *v*, *w*

Baldauf (2005), COSMO-Newsl. Nr. 5

Current implementation, Numerics

- all metric terms are treated explicitly ->
  implemented in Subr. `explicit_horizontal_diffusion`
- This is done in a two-step approach:
  1. discretize the fluxes at their ‚own' positions
  2. discretize the divergence of these fluxes
- PHYCTL-namelist-parameter `l3dturb, l3dturb_metr`

Positions of turbulent fluxes in staggered grid:



Disadvantages of the current implementation in COSMO

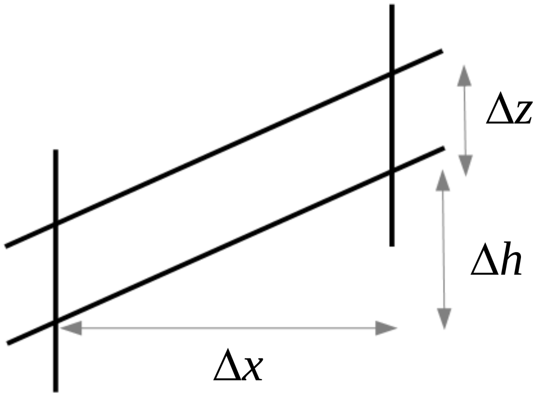
- due to the above mentioned ‚two-step' approach, some terms use a wider stencil than necessary
  solution: analytically insert fluxes i.e. boil down the formulae to derivatives of the prognostic variables and discretize afterwards (results in a huge amount of terms!)
- the scalar diffusion has been tested (*Baldauf (2005) COSMO-Newsl. No 6*) but not the vector diffusion!
- though spherical metric terms are contained, only shallow atmosph. approx is used (i.e. $1/r \cdot \ldots \rightarrow 1/a \cdot \ldots$). However, this is less important.
- the current implementation is not stable in steep terrain (*Langhans …*)

→ new implementation of subroutines `explicit_horiz_diffusion` and `implicit_vert_diff_uvwt`

Stability

Linear von-Neumann stability analysis of 2D (i.e. x-z-diffusion) in tilted terrain

consider diffusion with
constant diffusion coeff. K and
constant steepness



$$\frac{\Delta h}{\Delta z} = m \cdot M_z$$

<u>dimensionless variables:</u>

diffusion-Courant number

$$C_{diff} := K \frac{\Delta t}{\Delta x^2}$$

steepness

$$m := \left. \frac{\partial z}{\partial x} \right|_{\zeta} = \frac{\Delta h}{\Delta x}$$

grid anisotropy

$$M_z := \frac{\Delta x}{\Delta z}$$

Linear von-Neumann stability analysis of 2D (i.e. x-z-diffusion) in tilted terrain

scalar flux divergence:

vertical

$$\rho \frac{\partial s}{\partial t} = -\frac{1}{r\cos\phi}\frac{\partial H^{*1}}{\partial \lambda} - \frac{J_\lambda}{\sqrt{G}}\frac{1}{r\cos\phi}\frac{\partial H^{*1}}{\partial \zeta} - \frac{1}{r}\frac{\partial H^{*2}}{\partial \phi} - \frac{J_\phi}{\sqrt{G}}\frac{1}{r}\frac{\partial H^{*2}}{\partial \zeta} + \boxed{\frac{1}{\sqrt{G}}\frac{\partial H^{*3}}{\partial \zeta}} - \frac{2}{r}H^{*3} + \frac{\tan\phi}{r}H^{*2}.$$

scalar fluxes:

$$H^{*1} = -\rho K_s \frac{1}{r\cos\phi}\left(\frac{\partial s}{\partial \lambda} + \frac{J_\lambda}{\sqrt{G}}\frac{\partial s}{\partial \zeta}\right),$$

$$H^{*2} = -\rho K_s \frac{1}{r}\left(\frac{\partial s}{\partial \phi} + \frac{J_\phi}{\sqrt{G}}\frac{\partial s}{\partial \zeta}\right),$$

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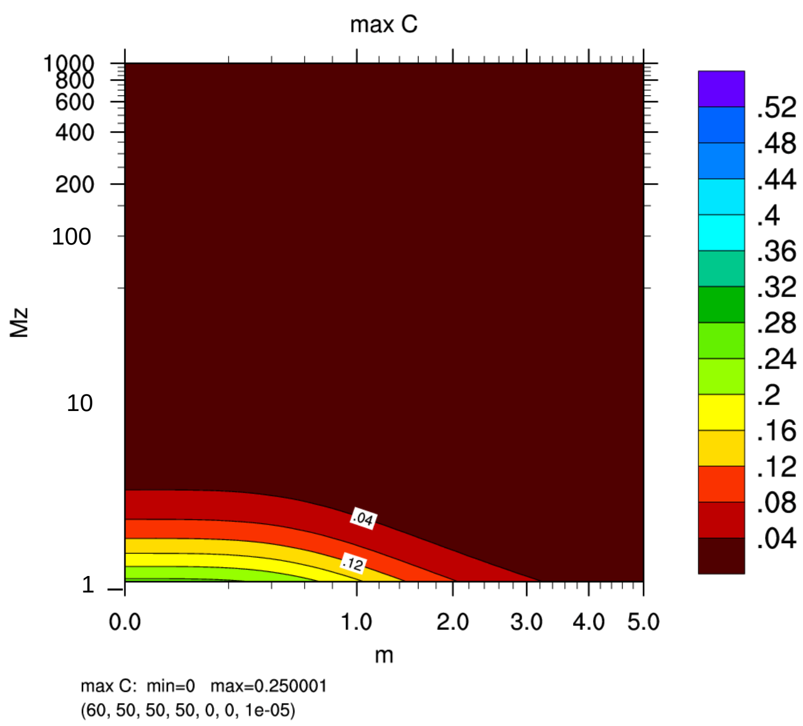
analogous:
‚vectorial' diffusion of *u*, *v*, *w*

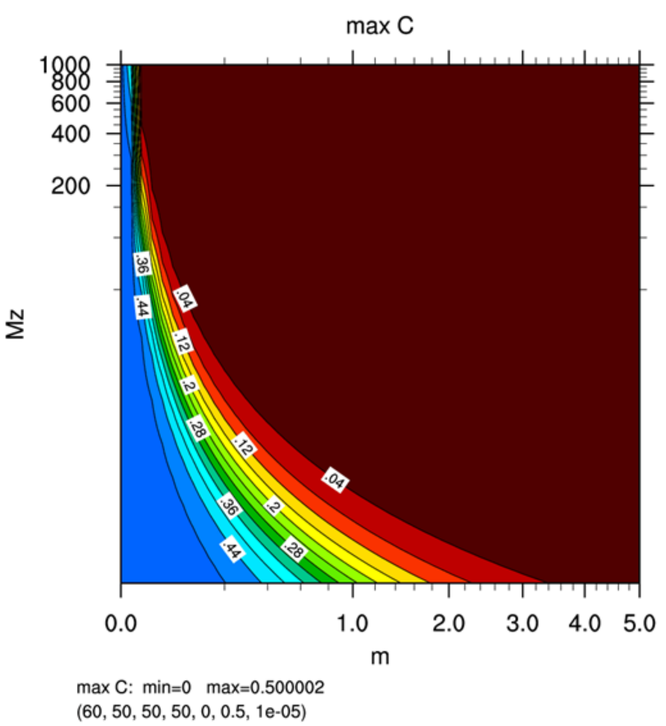
Baldauf (2005), COSMO-Newsl. Nr. 5

Stability of 3D scalar diffusion in tilted terrain: max C_{Diff}

purely explicit

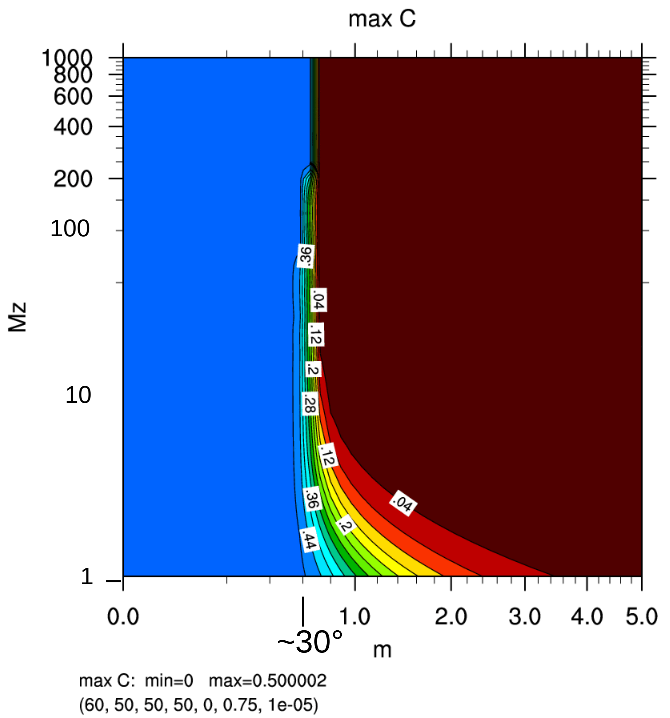


vertically implicit, only ‚pure' z-deriv
no off-centering (0.5)



Stability of 3D scalar diffusion in tilted terrain: max C_{Diff}

vertically implicit, only ‚pure' z-deriv
off-centering 0.75
(=current COSMO-version)



Linear von-Neumann stability analysis of 2D (i.e. x-z-diffusion) in tilted terrain

scalar flux divergence:

terrain following coordinates

vertical

$$\rho \frac{\partial s}{\partial t} = -\frac{1}{r\cos\phi}\frac{\partial H^{*1}}{\partial \lambda} - \frac{J_\lambda}{\sqrt{G}}\frac{1}{r\cos\phi}\frac{\partial H^{*1}}{\partial \zeta} - \frac{1}{r}\frac{\partial H^{*2}}{\partial \phi} - \frac{J_\phi}{\sqrt{G}}\frac{1}{r}\frac{\partial H^{*2}}{\partial \zeta} + \frac{1}{\sqrt{G}}\frac{\partial H^{*3}}{\partial \zeta} - \frac{2}{r}H^{*3} + \frac{\tan\phi}{r}H^{*2}.$$

scalar fluxes:

$$H^{*1} = -\rho K_s \frac{1}{r\cos\phi}\left(\frac{\partial s}{\partial \lambda} + \frac{J_\lambda}{\sqrt{G}}\frac{\partial s}{\partial \zeta}\right),$$

$$H^{*2} = -\rho K_s \frac{1}{r}\left(\frac{\partial s}{\partial \phi} + \frac{J_\phi}{\sqrt{G}}\frac{\partial s}{\partial \zeta}\right),$$

$$H^{*3} = +\rho K_s \frac{1}{\sqrt{G}}\frac{\partial s}{\partial \zeta},$$

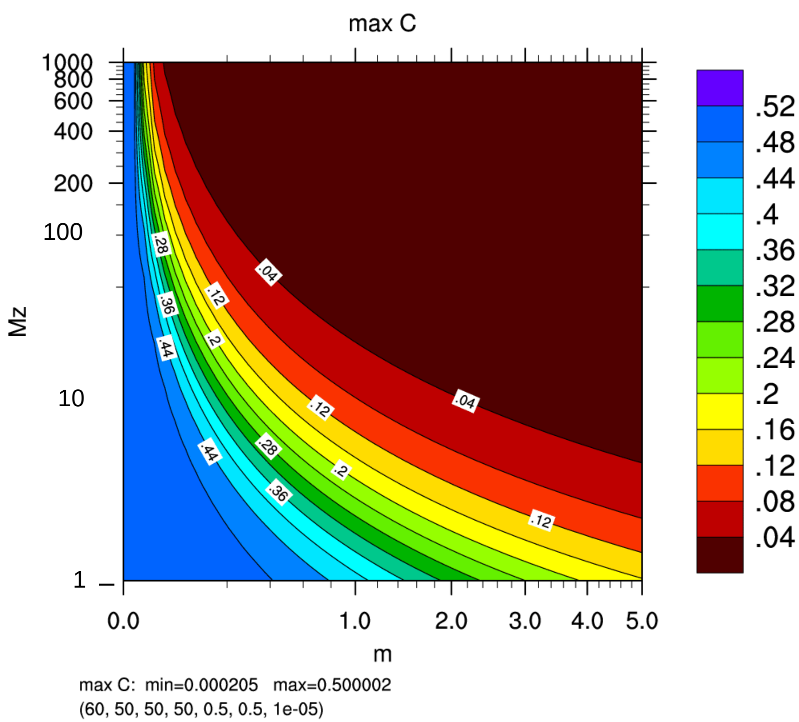
analogous:
‚vectorial' diffusion of *u*, *v*, *w*

Baldauf (2005), COSMO-Newsl. Nr. 5

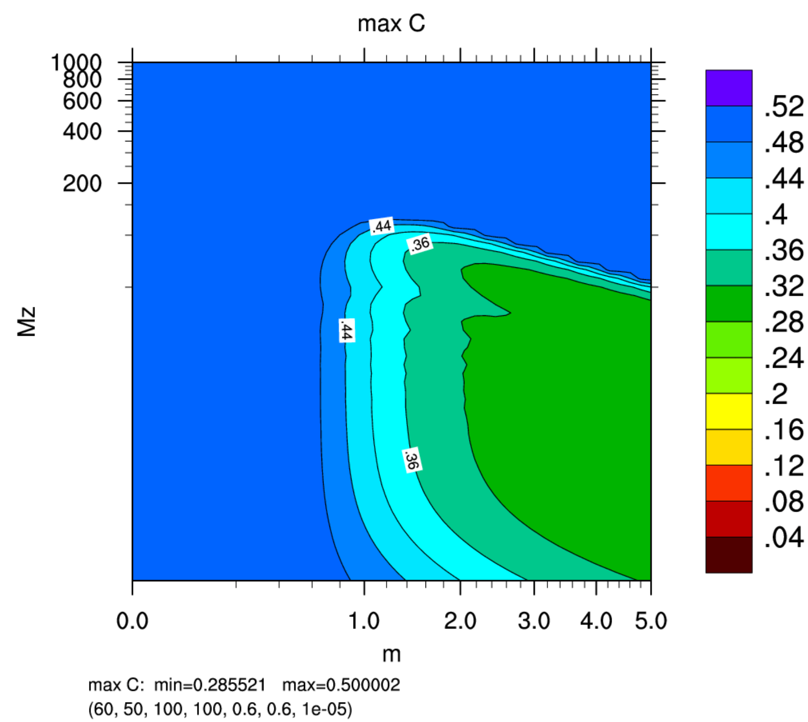
Stability of 3D <u>scalar</u> diffusion in tilted terrain: max C_{Diff}

now: all vertical terms implicit !

0.5 (=no off-centering)



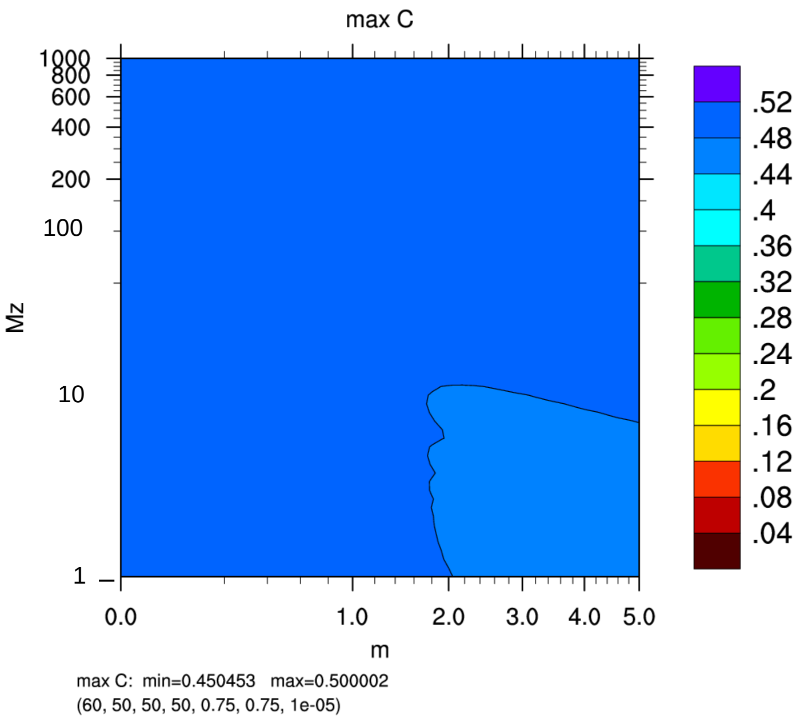
off-centering 0.6



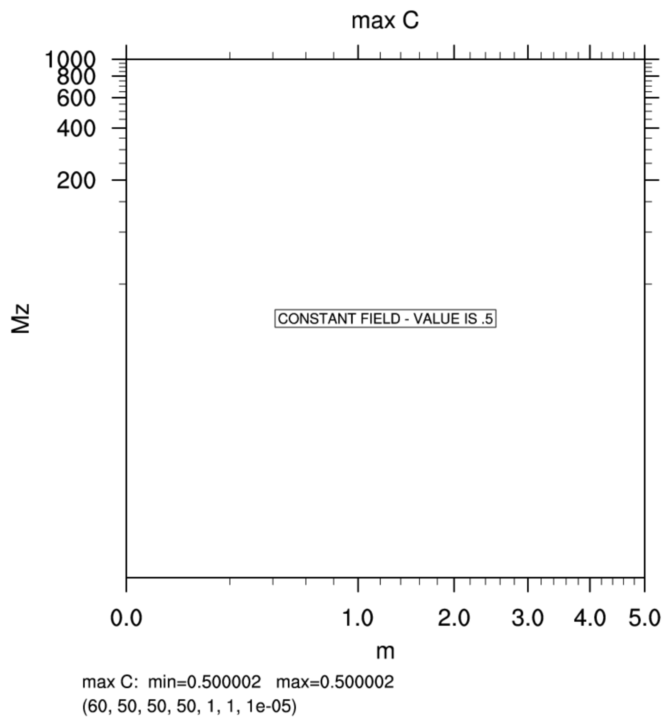
Stability of 3D scalar diffusion in tilted terrain: max C_{Diff}

now: all vertical terms implicit !

off-centering 0.75



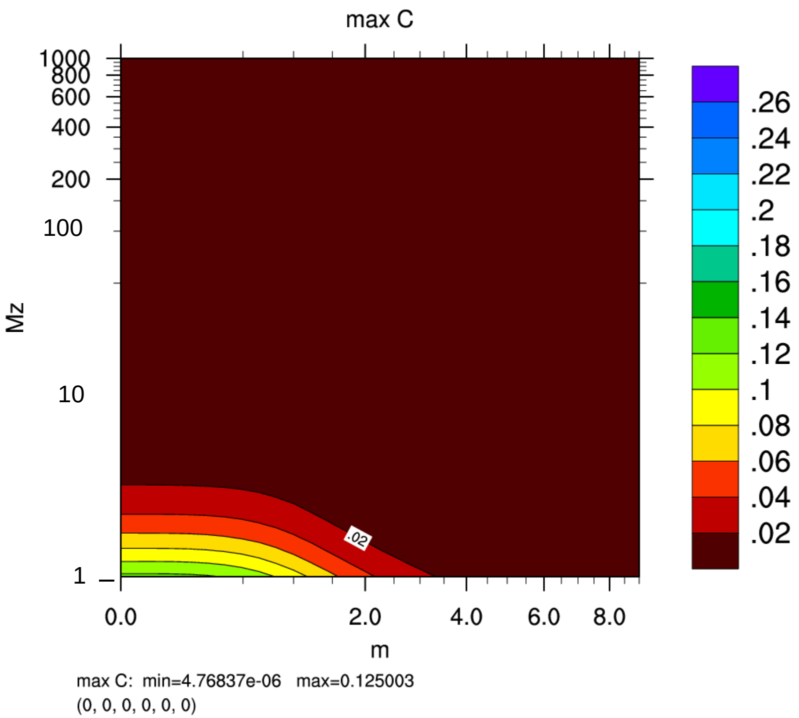
1.0 (=fully vertical implicit)



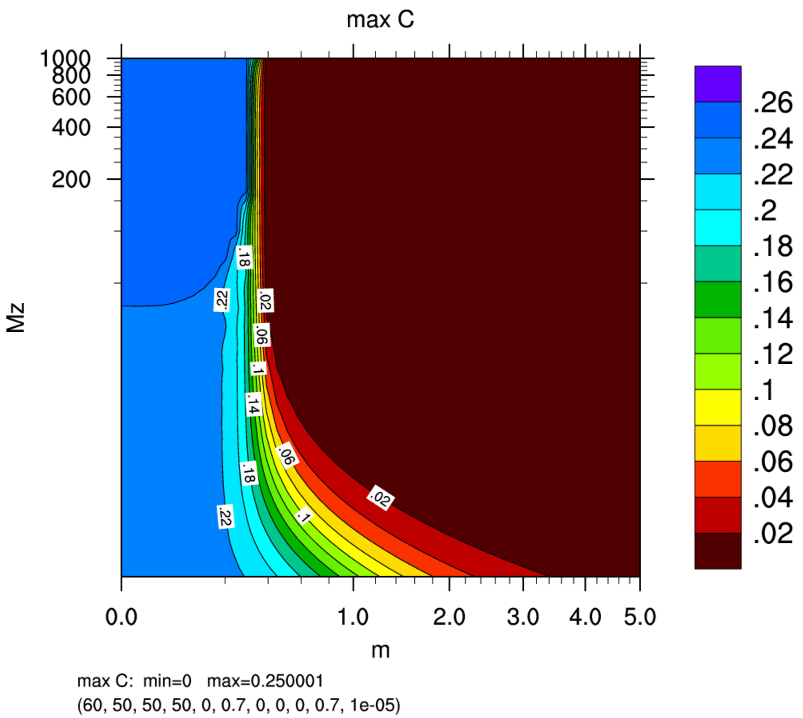
Vector diffusion

Stability of 3D vector diffusion in tilted terrain: max C_{Diff}

purely explicit



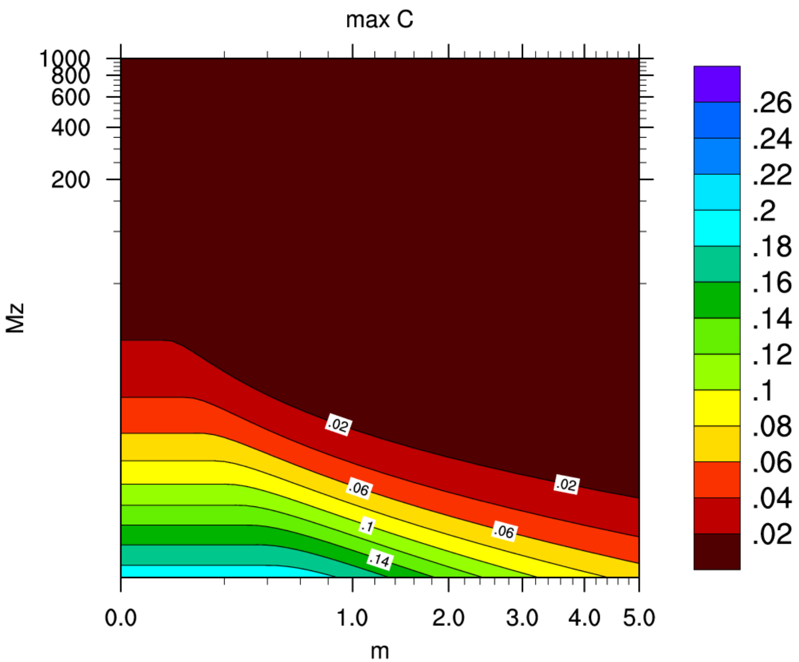
vertically implicit, only ‚pure' z-deriv
off-centering=0.7 (=current COSMO)



Stability of 3D vector diffusion in tilted terrain: max C_{Diff}

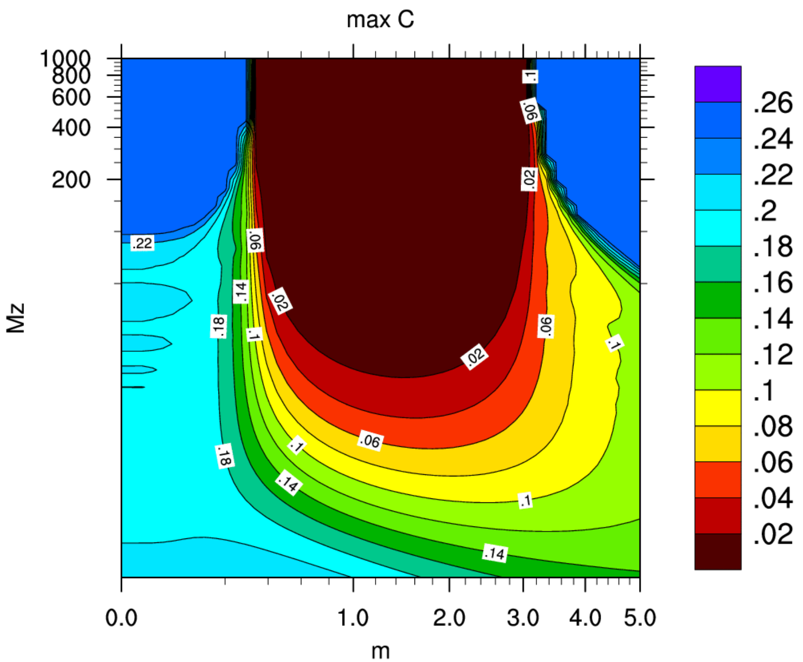
now: vertically implicit treatment of all possible terms

no off-centering (0.5)



max C: min=0 max=0.190985
(60, 50, 50, 50, 0.5, 0.5, 0, 0, 0.5, 0.5, 1e-05)

off-centering (0.6)

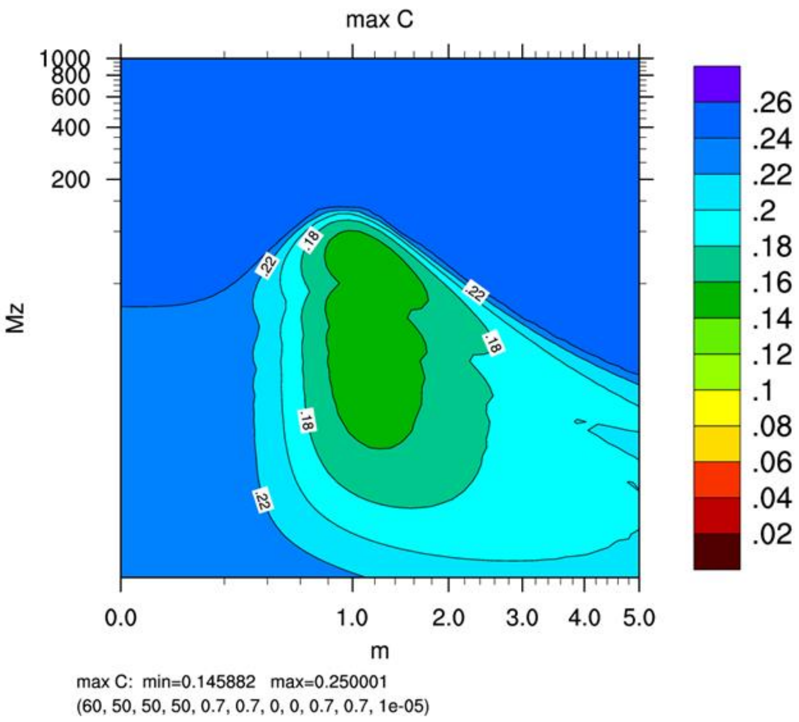


max C: min=6e-06 max=0.250001
(60, 50, 50, 50, 0.6, 0.6, 0, 0, 0.6, 0.6, 1e-05)

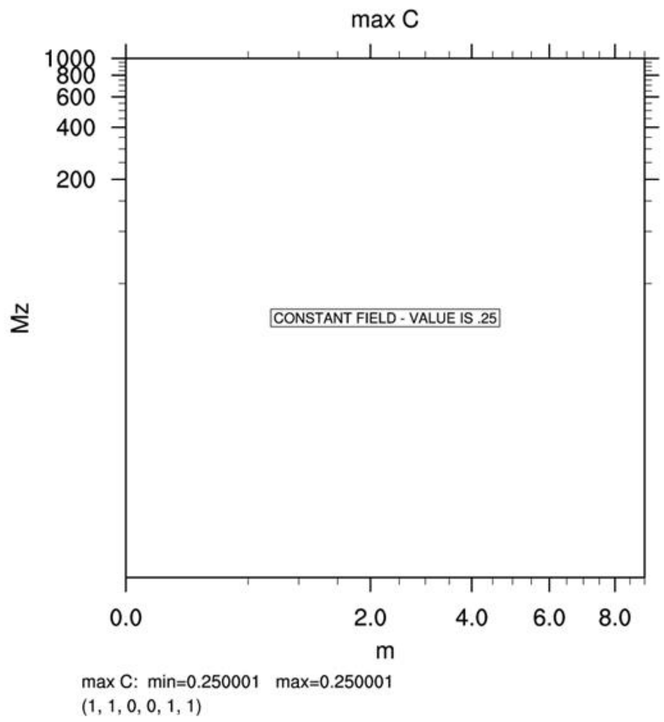
Stability of 3D vector diffusion in tilted terrain: max C_{Diff}

vertically implicit treatment of all possible terms

off-centering (0.7)



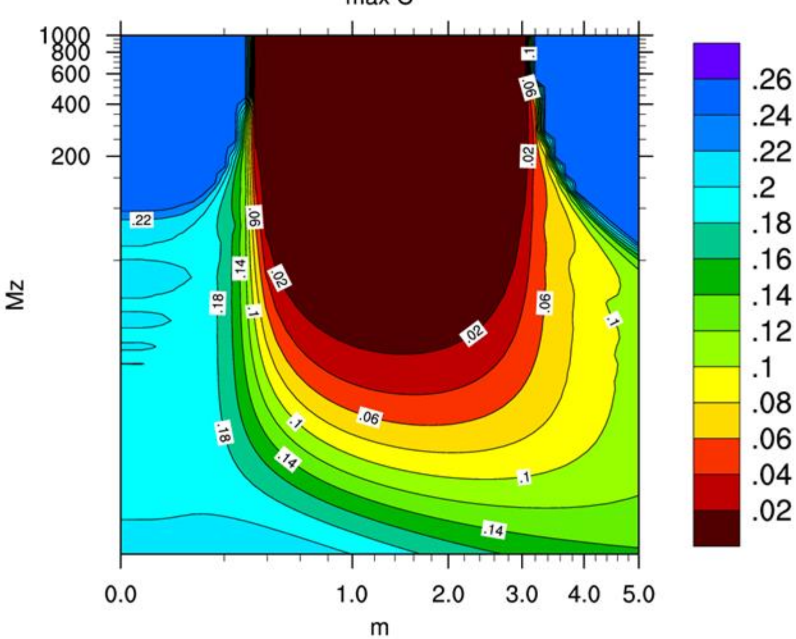
vericall fully implicit (1.0)



Stability of 3D vector diffusion in tilted terrain: max C_{Diff}

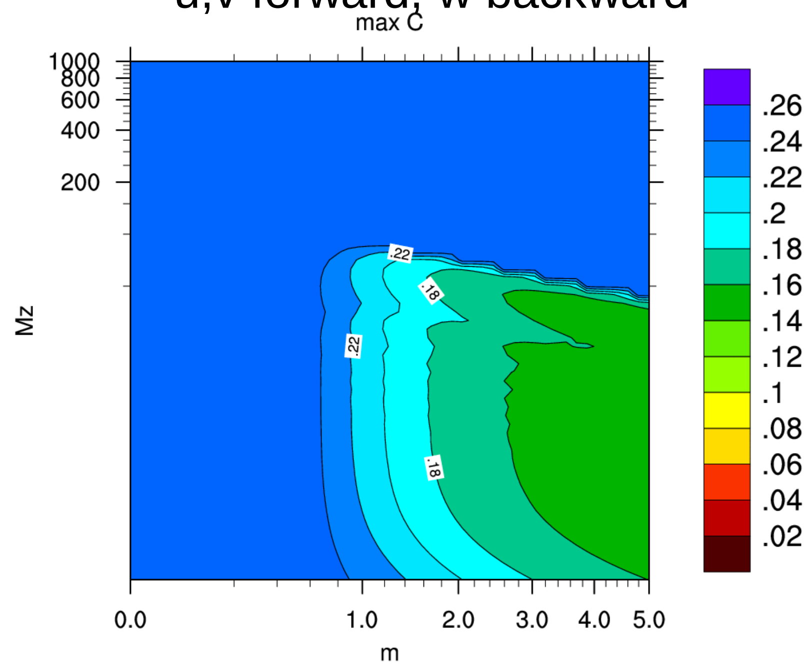
vertically implicit treatment of all possible terms, off-centering 0.6

‚normal'



max C: min=6e-06 max=0.250001
(60, 50, 50, 50, 0.6, 0.6, 0, 0, 0.6, 0.6, 1e-05)

u,v forward, w backward



max C: min=0.145677 max=0.250001
(60, 50, 100, 100, 0.6, 0.6, 0, 0.6, 0.6, 0.6, 1e-05)

Testing

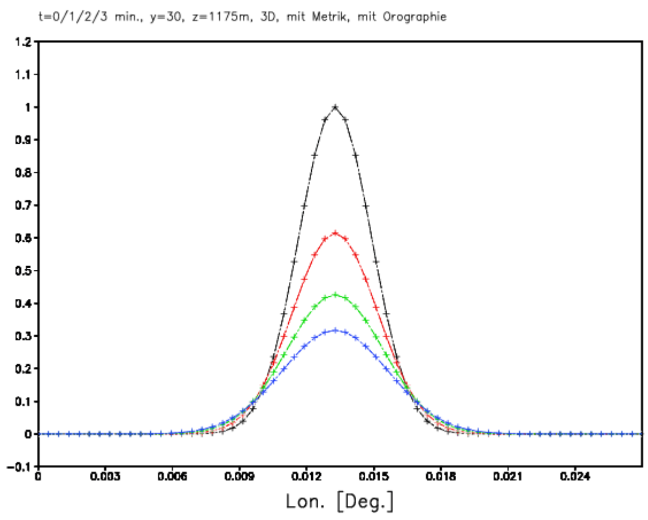
Test of scalar diffusion:
3-dim. isotropic gaussian tracer distribution

3D diffusion equation:

$$\frac{\partial \phi}{\partial t} = K \Delta \phi$$

analytic Gaussian solution for K=const.:

$$\begin{aligned}\phi(r,t) &= \frac{\Phi_0}{\sqrt{4\pi K (t+t_0)^3}} \exp\left(-\frac{r^2}{4K(t+t_0)}\right), \\ r &:= \sqrt{x^2+y^2+z^2}\end{aligned}$$

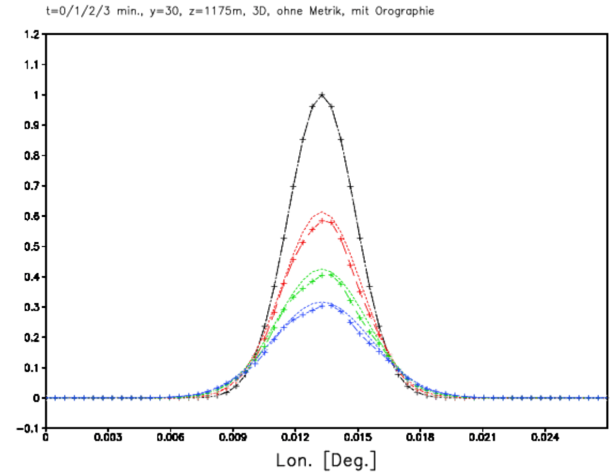


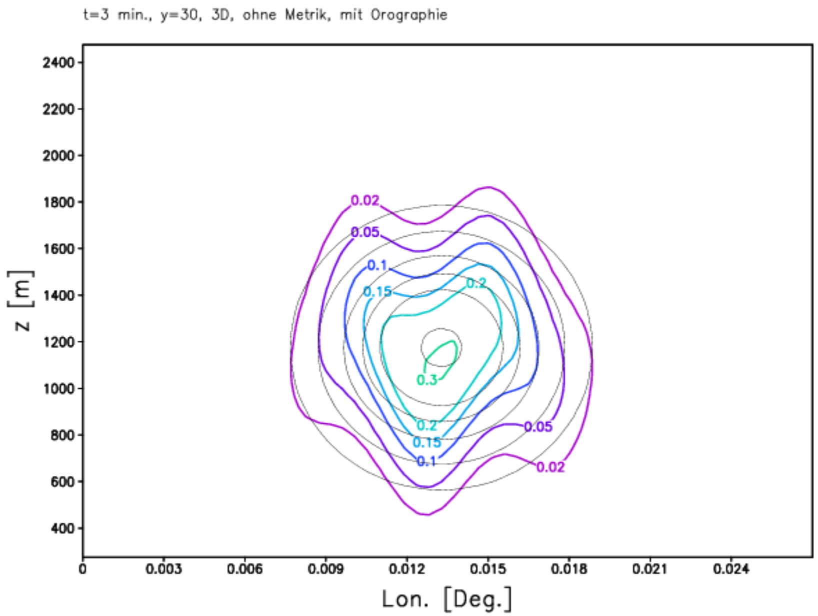
Baldauf (2005) COSMO-Newsl. no. 6

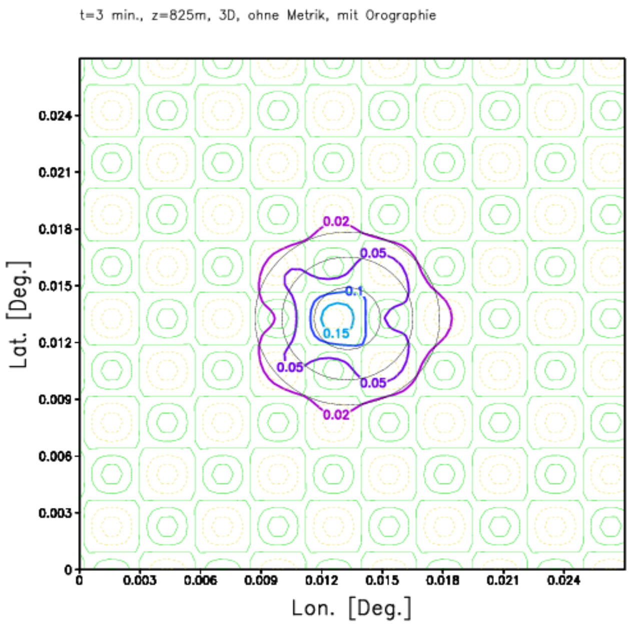
Case 3: 3D-diffusion, without metric terms, with orography

nearly isotropic grid

goal: show false diffusion in the presence of orography



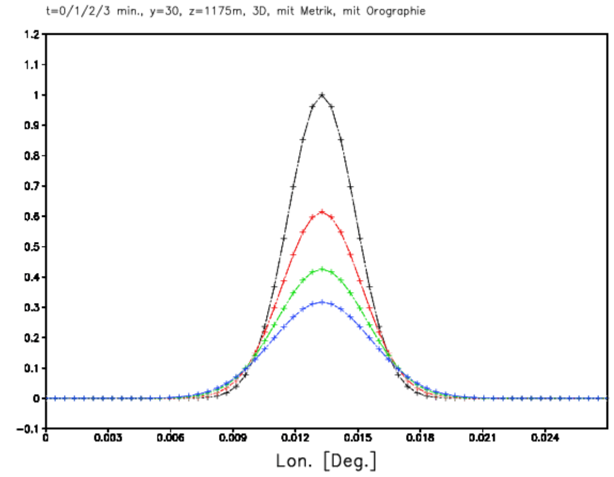


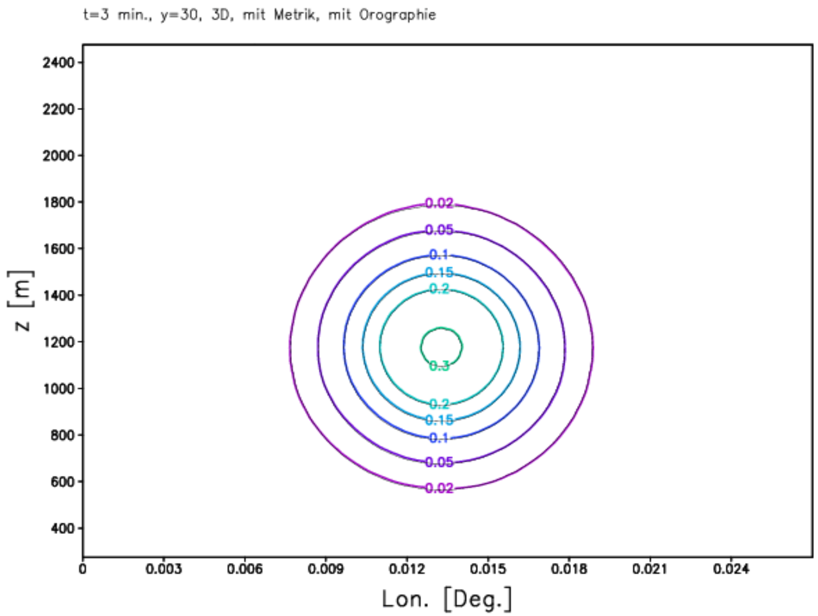


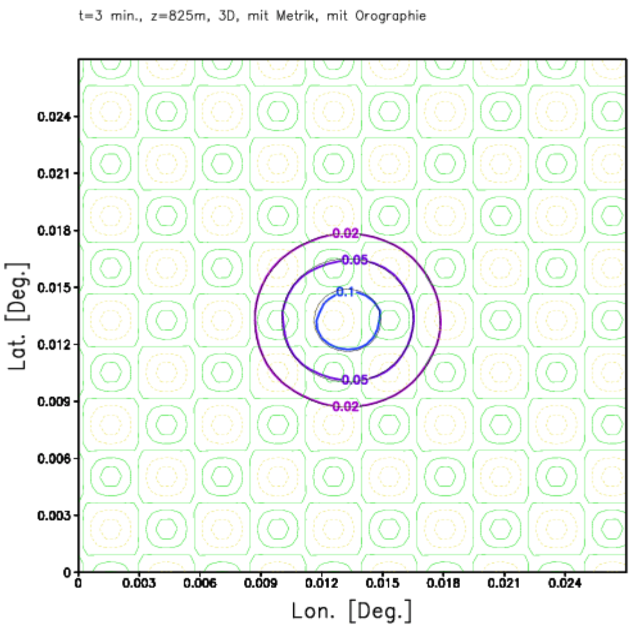
Case 4: 3D-diffusion, with metric terms, with orography

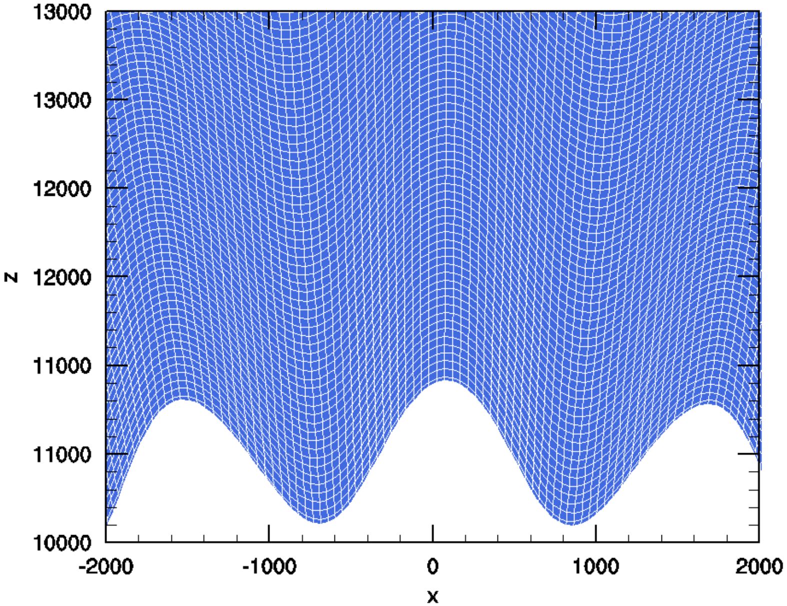
nearly isotropic grid

goal: show correct implementation of the new metric terms

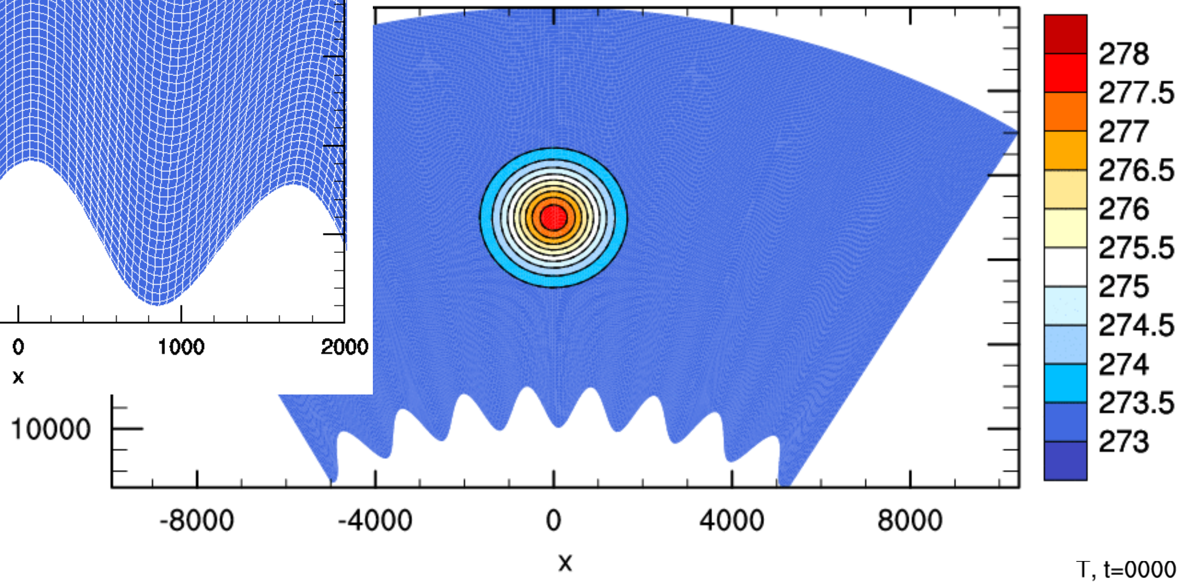








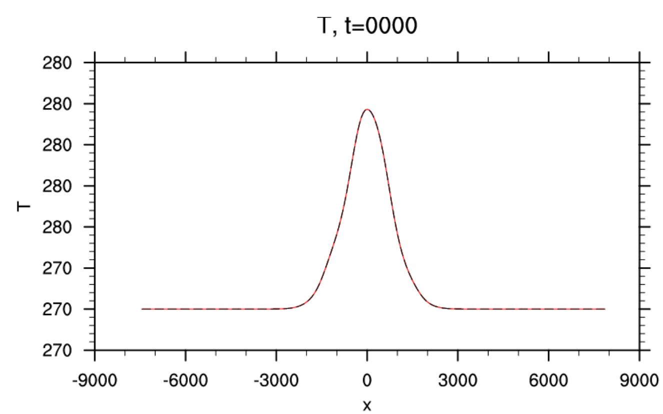
T, t=0000 timesteps



T,analy: min=273 max=277.864
T,simul: min=273 max=277.864

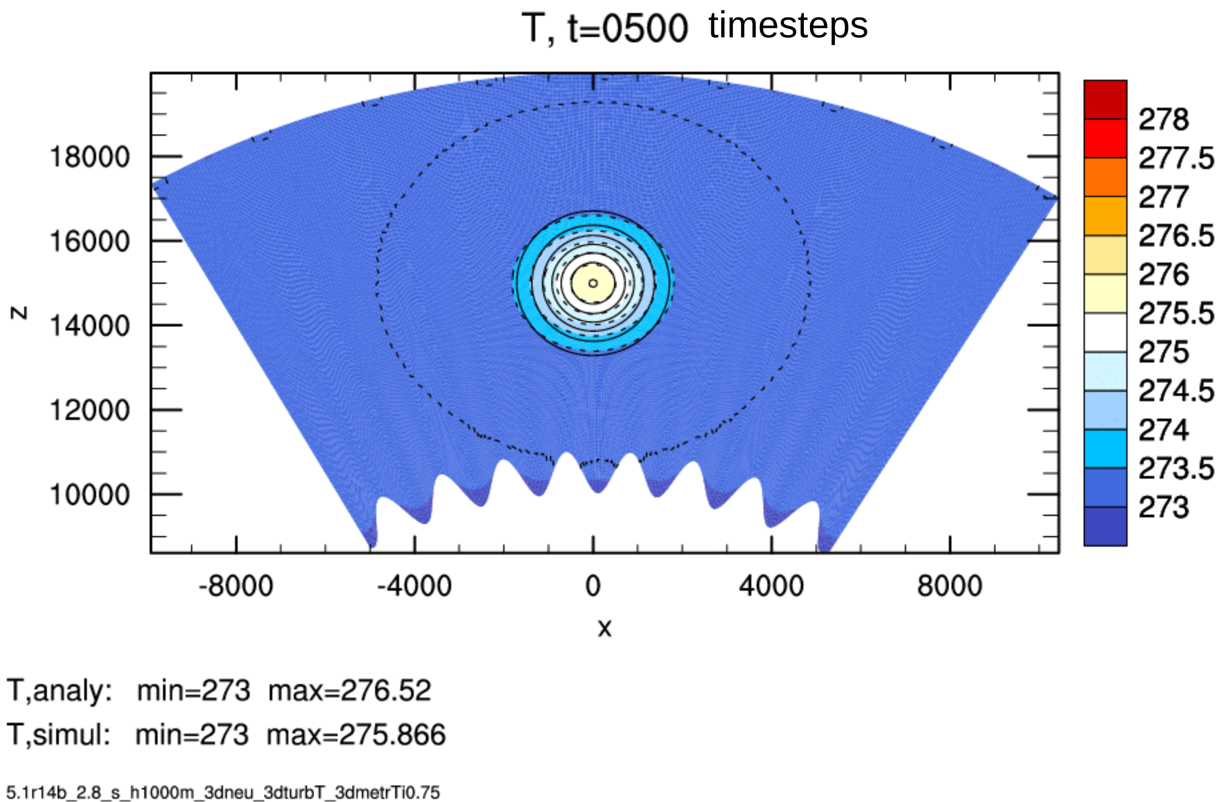
5.1r14b_2.8_s_h1000m_3dneu_3dturbT_3dmetrTi0.75

analytic solution: solid lines
COSMO solution: colors, dashed lines



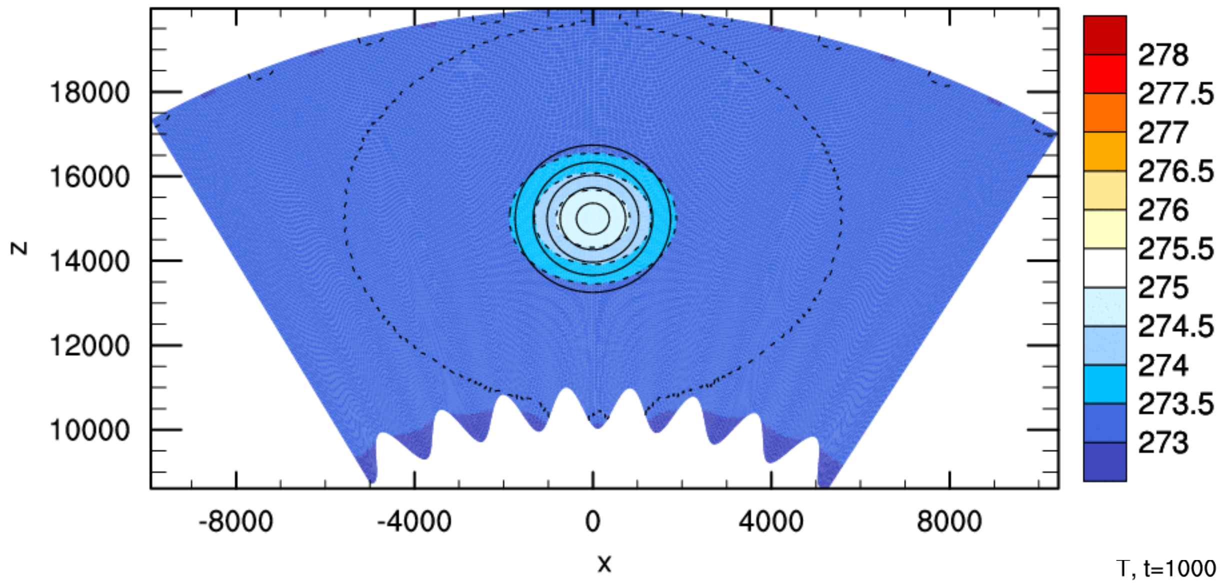
T,analy: min=273 max=277.864
T,simul: min=273 max=277.864

5.1r14b_2.8_s_h1000m_3dneu_3dturbT_3dmetrTi0.75



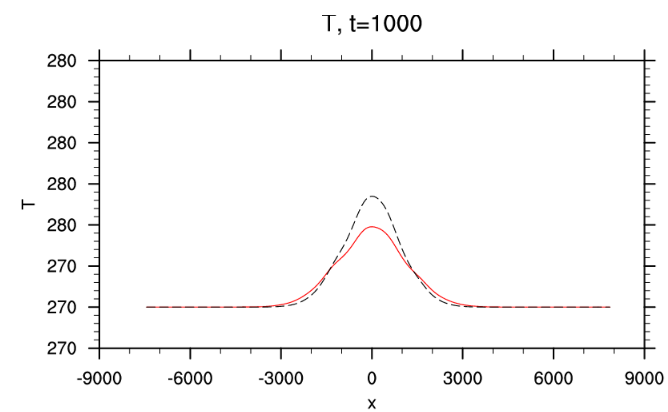
analytic solution: solid lines
COSMO solution: colors, dashed lines

T, t=1000 timesteps



T,analy: min=273 max=275.699
T,simul: min=273 max=274.956

5.1r14b_2.8_s_h1000m_3dneu_3dturbT_3dmetrTi0.75

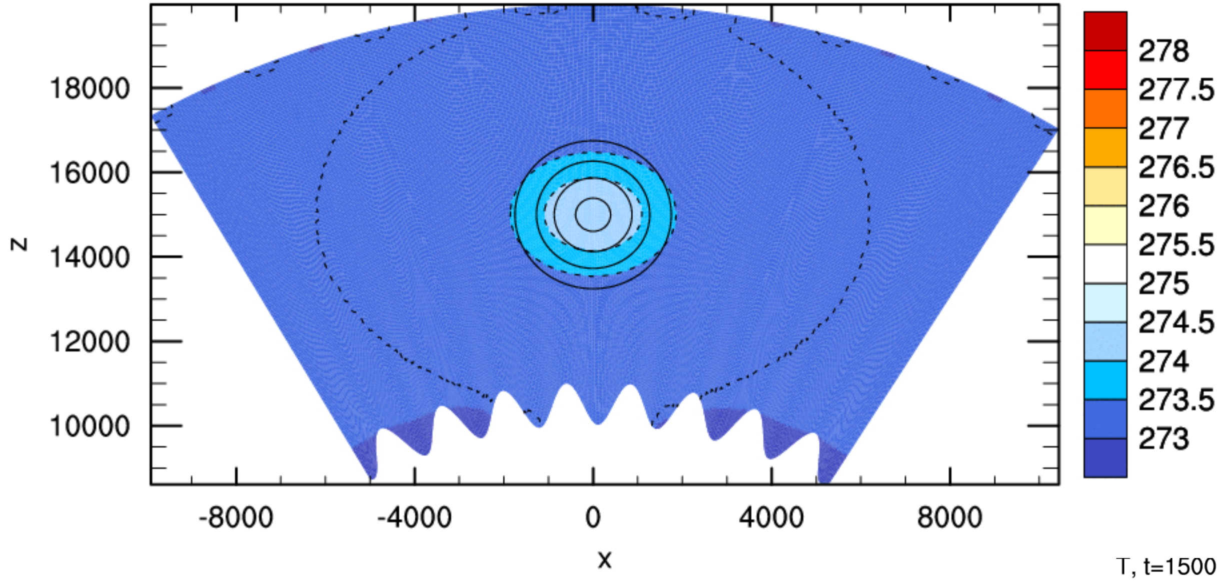


T,analy: min=273 max=275.699
T,simul: min=273 max=274.956

5.1r14b_2.8_s_h1000m_3dneu_3dturbT_3dmetrTi0.75

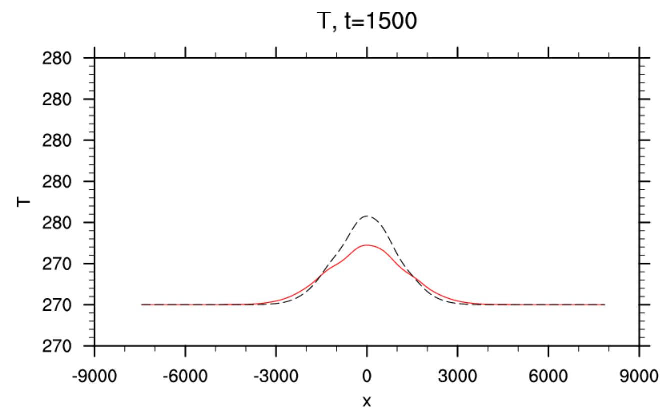
analytic solution: solid lines
COSMO solution: colors, dashed lines

T, t=1500 timesteps

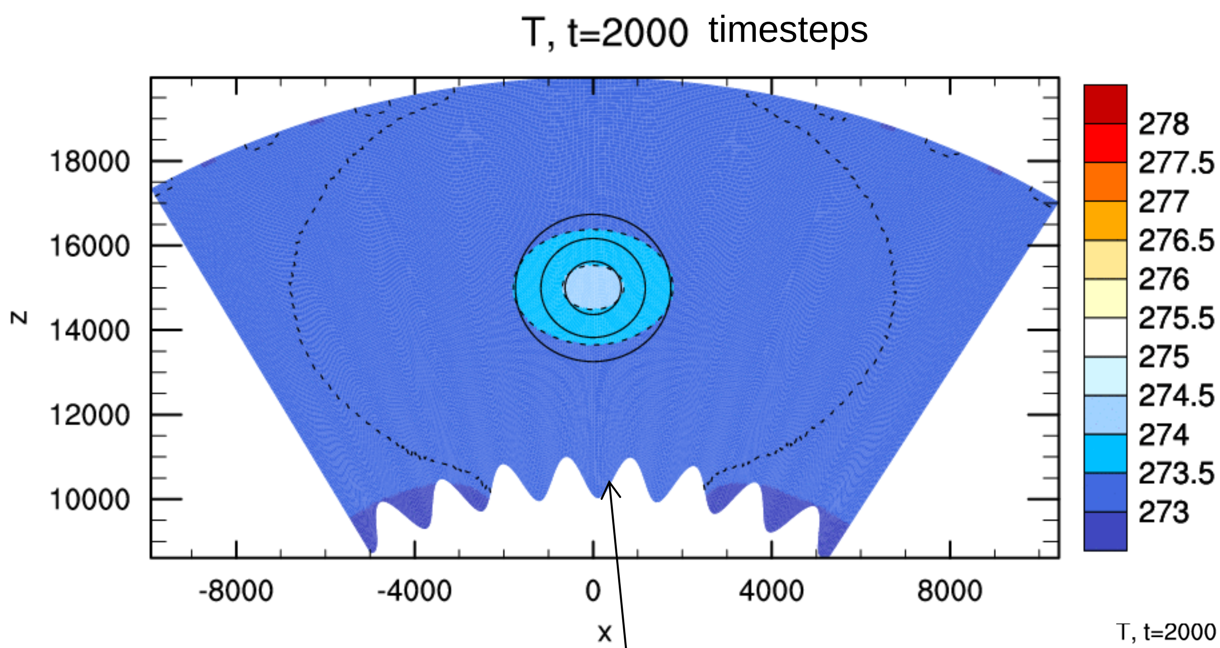


T,analy: min=273 max=275.153
T,simul: min=273 max=274.447

5.1r14b_2.8_s_h1000m_3dneu_3dturbT_3dmetrTi0.75



analytic solution: solid lines
COSMO solution: colors, dashed lines

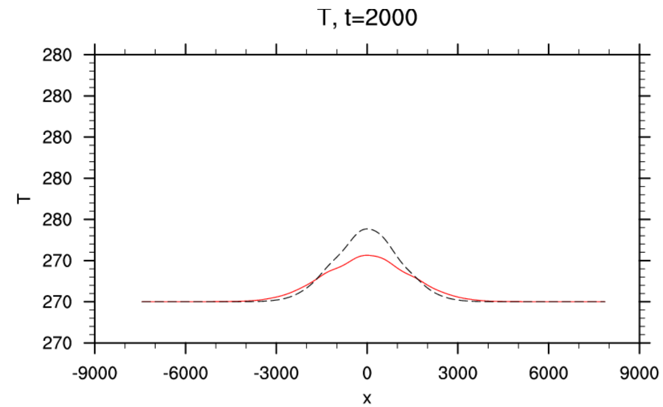


T,analy: min=273 max=274.77
T,simul: min=273 max=274.127

5.1r14b_2.8_s_h1000m_3dneu_3dturbT_3dmetrTi0.75

max slope ~ 2.3 ~ 67°

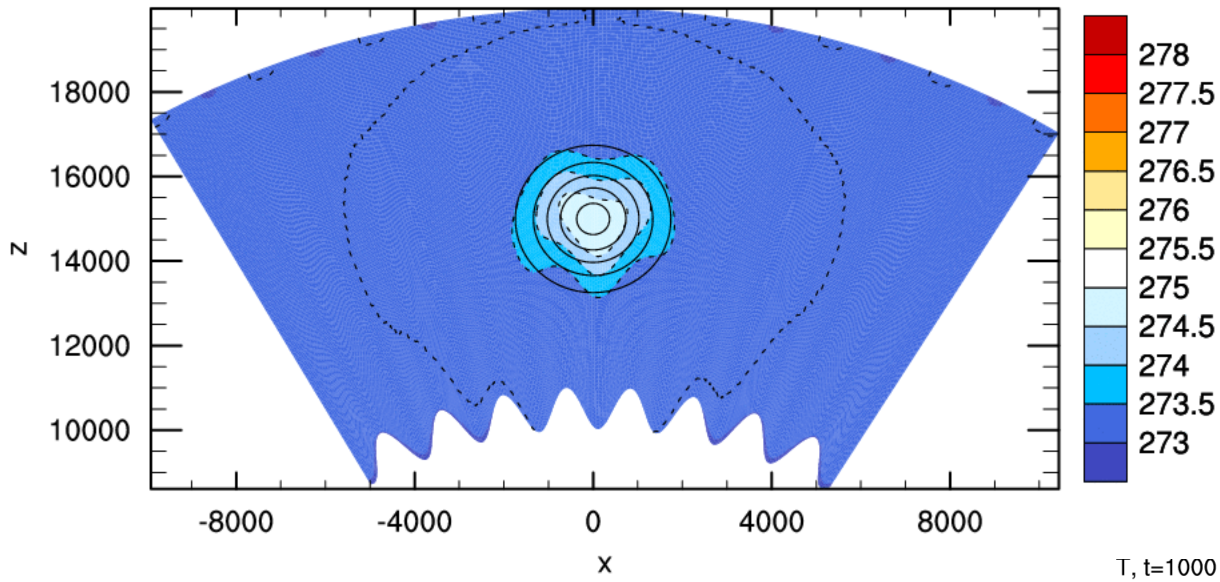
the run with only one vertical implicit term
(=current COSMO version) became unstable!



T,analy: min=273 max=274.77
T,simul: min=273 max=274.127

5.1r14b_2.8_s_h1000m_3dneu_3dturbT_3dmetrTi0.75

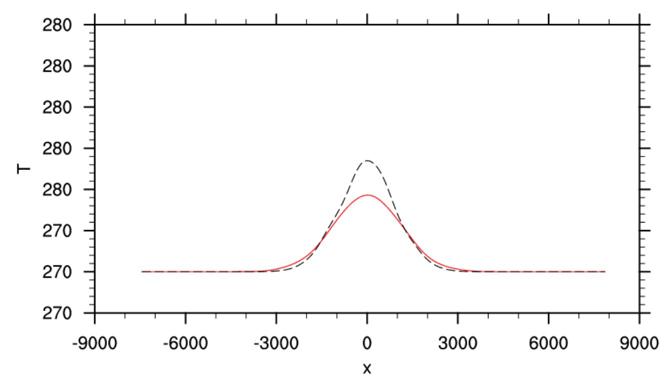
T, t=1000 timesteps



T,analy: min=273 max=275.699
T,simul: min=273 max=274.894

5.1r14b_2.8_s_h1000m_3dneu_3dturbT_3dmetrFi0.75

T, t=1000

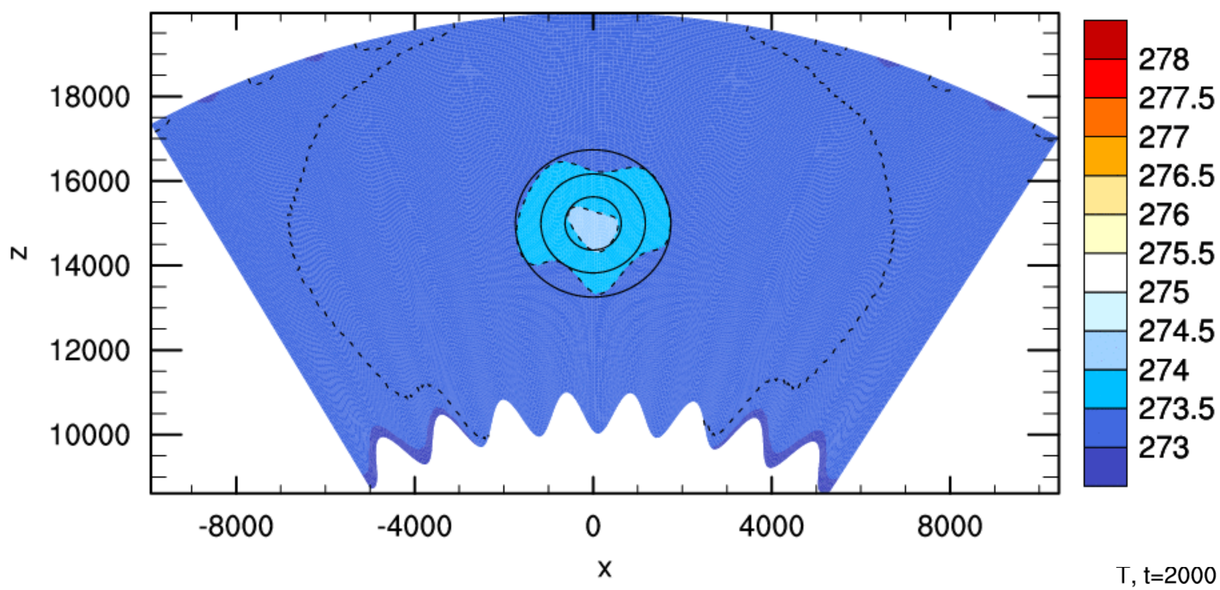


T,analy: min=273 max=275.699
T,simul: min=273 max=274.861

5.1r14b_2.8_s_h1000m_3dneu_3dturbT_3dmetrFi0.75

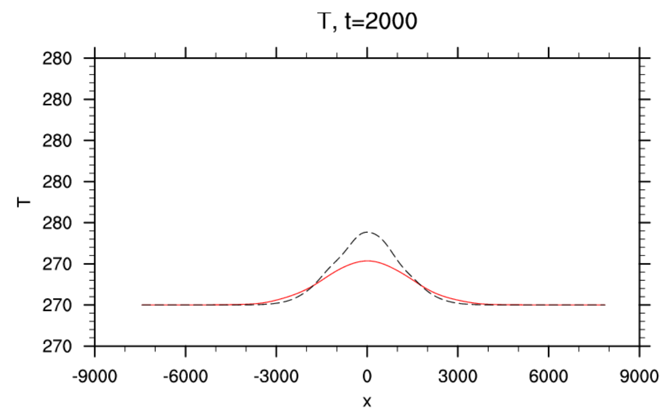
without metric terms

T, t=2000 timesteps



T,analy: min=273 max=274.77
T,simul: min=273 max=274.087

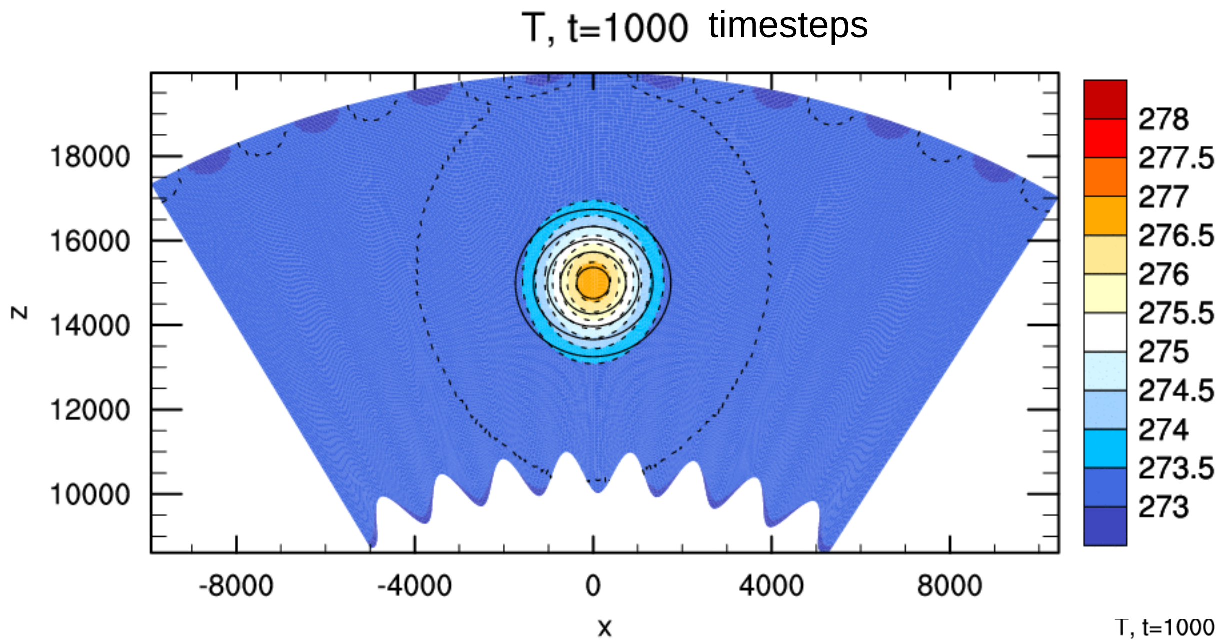
5.1r14b_2.8_s_h1000m_3dneu_3dturbT_3dmetrFi0.75



T,analy: min=273 max=274.77
T,simul: min=273 max=274.071

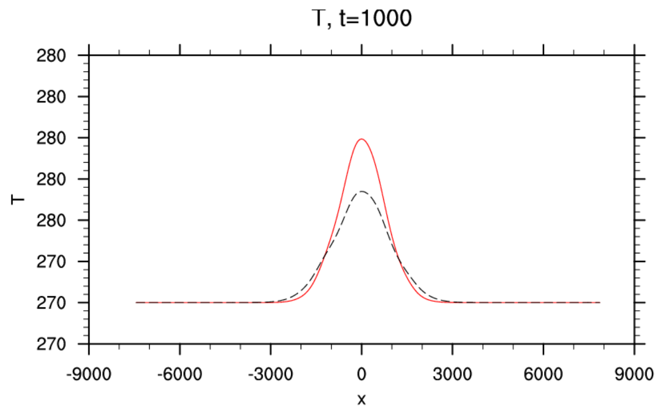
5.1r14b_2.8_s_h1000m_3dneu_3dturbT_3dmetrFi0.75

without metric terms



T,analy: min=273 max=275.699
T,simul: min=273 max=276.97

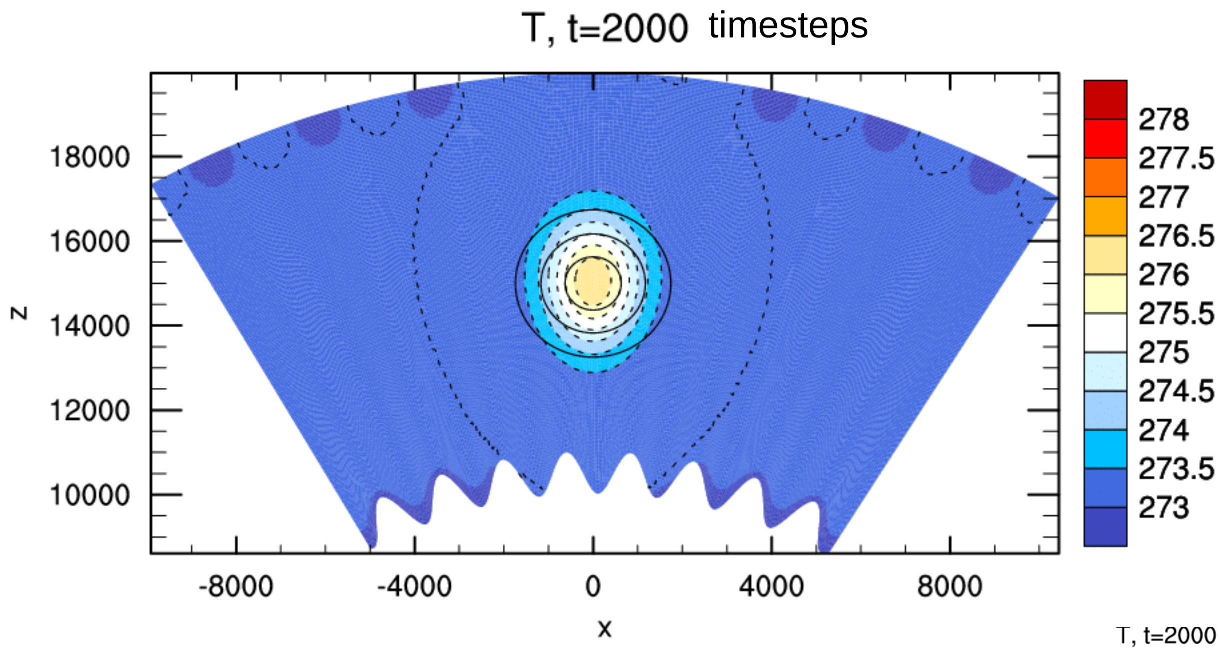
5.1r14b_2.8_s_h1000m_3dneu_3dturbF_3dmetrFi0.75



T,analy: min=273 max=275.699
T,simul: min=273 max=276.97

5.1r14b_2.8_s_h1000m_3dneu_3dturbF_3dmetrFi0.75

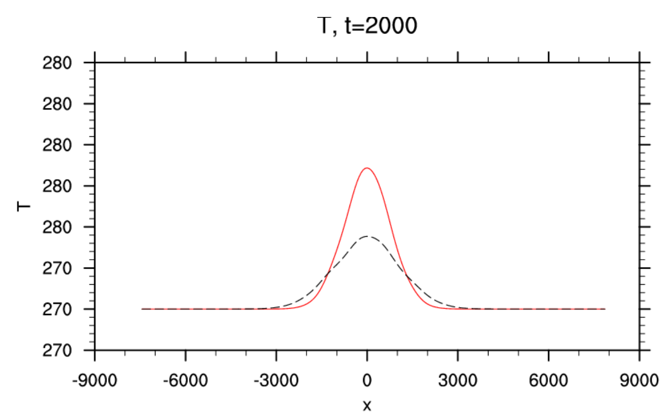
only 1D (vertical) diffusion



T,analy: min=273 max=274.77

T,simul: min=273 max=276.436

5.1r14b_2.8_s_h1000m_3dneu_3dturbF_3dmetrFi0.75



T,analy: min=273 max=274.77

T,simul: min=273 max=276.436

5.1r14b_2.8_s_h1000m_3dneu_3dturbF_3dmetrFi0.75

only 1D (vertical) diffusion

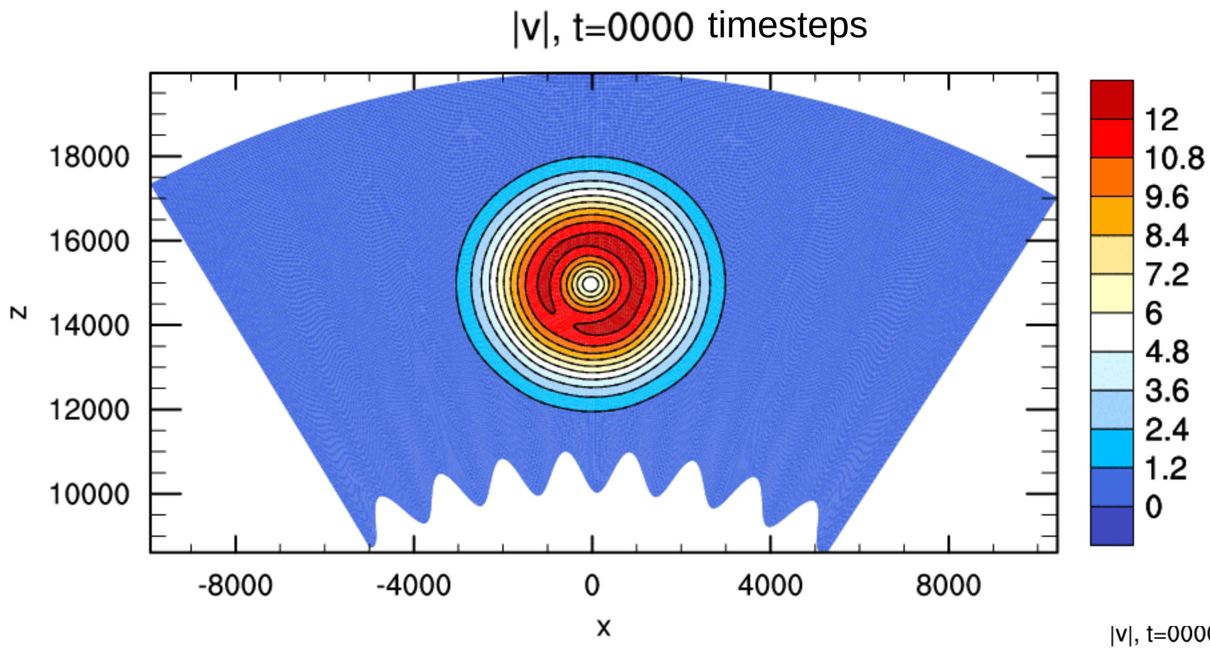
A proposal for an analogous test case for 3D vector diffusion:

isotropic, purely radial vector field:

$$\mathbf{v}(\mathbf{r},t) = v_r(r,t)\hat{\mathbf{e}}_r$$

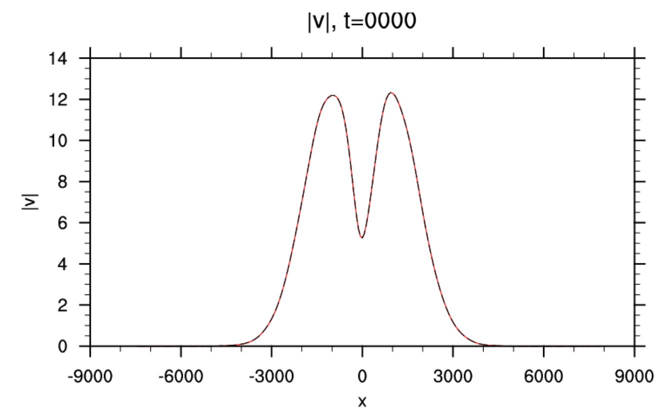
with

$$v_r(r,t) = const.\frac{r}{\sqrt{K}(t+t_0)^{5/2}} \cdot e^{-\frac{r^2}{8K(t+t_0)}}$$



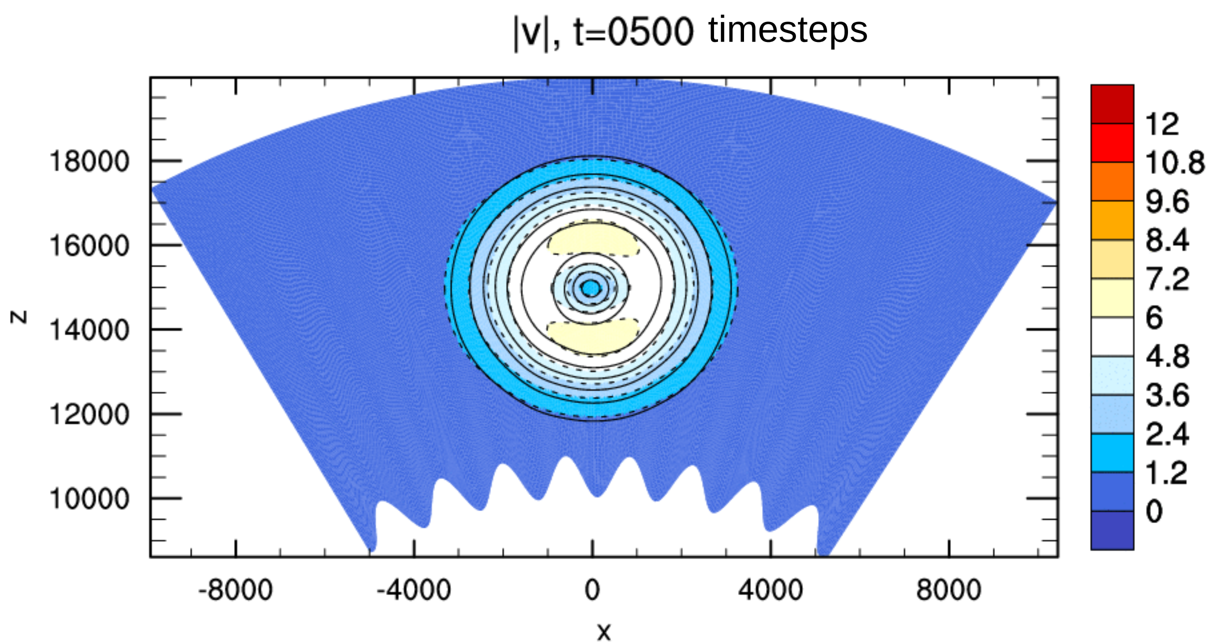
v,analy: min=5.27626e-19 max=12.3702
v,simul: min=2.81965e-18 max=12.3702

5.1r14b_2.8_v_h1000m_3dneu_3dturbT_3dmetrTi0.75



v,analy: min=1.16256e-10 max=12.3223
v,simul: min=4.30403e-10 max=12.3223

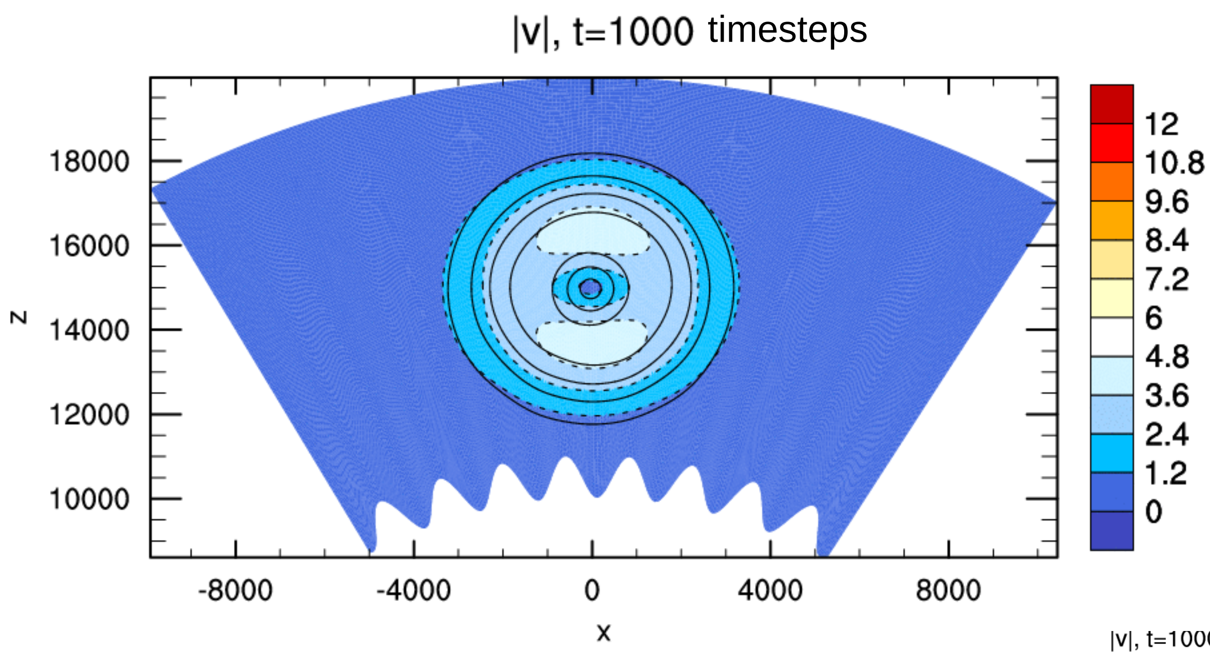
5.1r14b_2.8_v_h1000m_3dneu_3dturbT_3dmetrTi0.75



v,analy: min=3.9194e-15 max=7.8975

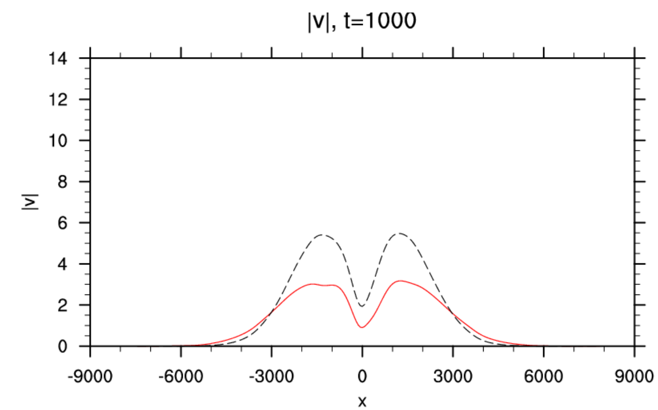
v,simul: min=2.71722e-11 max=6.67046

5.1r14b_2.8_v_h1000m_3dneu_3dturbT_3dmetrTi0.75



v,analy: min=1.37236e-12 max=5.4797
v,simul: min=1.42489e-08 max=4.28371

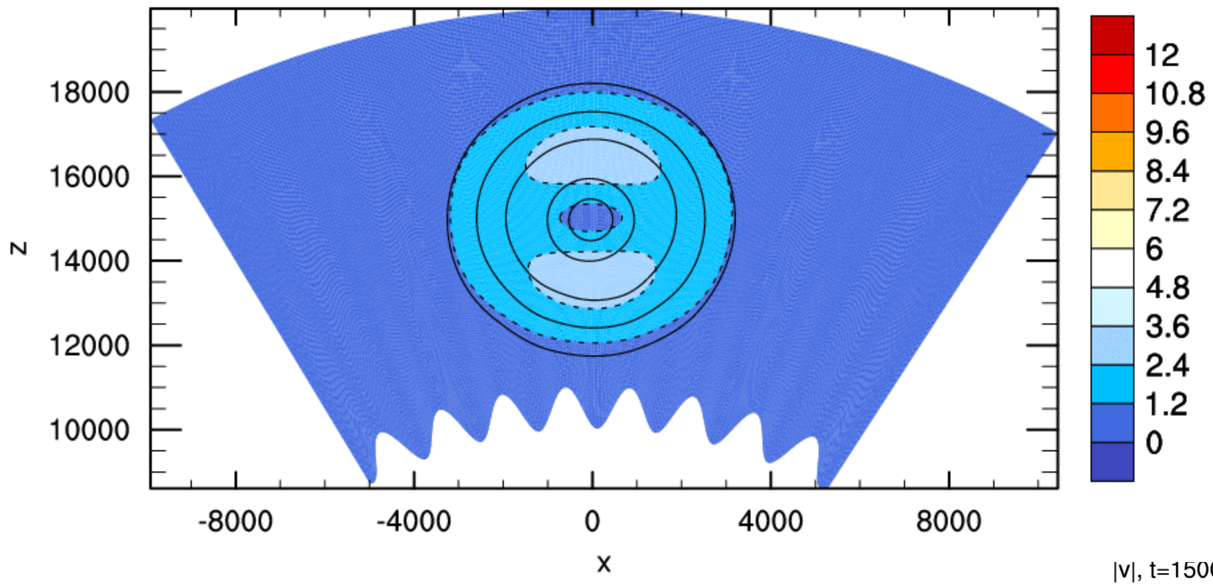
5.1r14b_2.8_v_h1000m_3dneu_3dturbT_3dmetrTi0.75



v,analy: min=4.58721e-07 max=5.4752
v,simul: min=3.90949e-05 max=3.17098

5.1r14b_2.8_v_h1000m_3dneu_3dturbT_3dmetrTi0.75

|v|, t=1500 timesteps

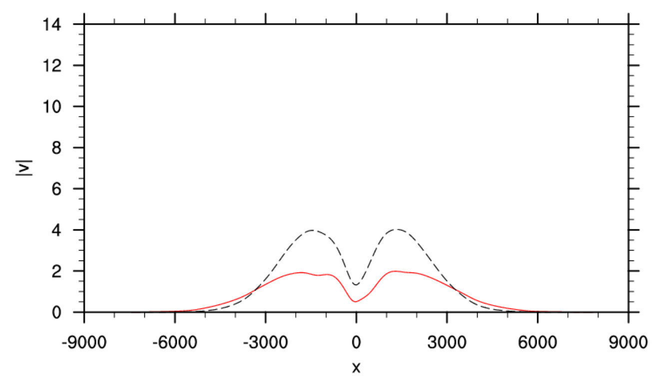


v,analy: min=8.48909e-11 max=4.02671

v,simul: min=4.2466e-07 max=3.0124

5.1r14b_2.8_v_h1000m_3dneu_3dturbT_3dmetrTi0.75

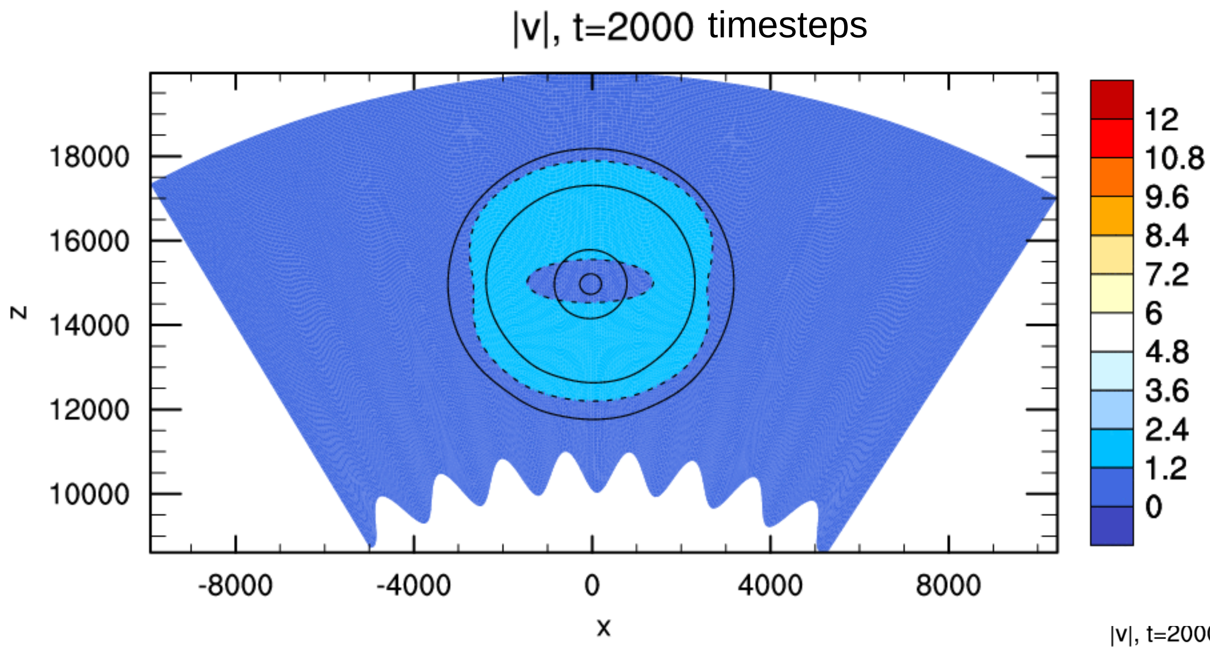
|v|, t=1500



v,analy: min=4.44067e-06 max=4.01978

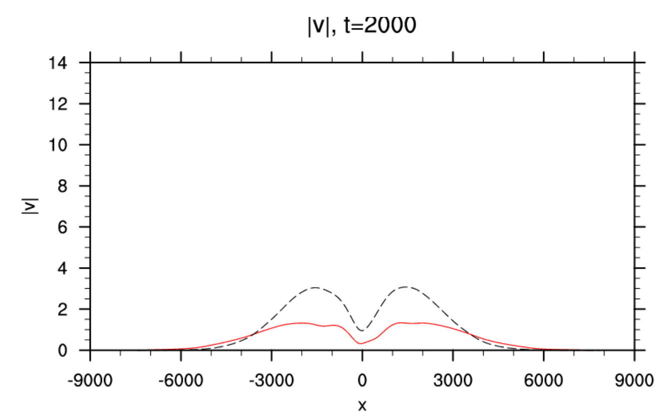
v,simul: min=0.000218621 max=1.9863

5.1r14b_2.8_v_h1000m_3dneu_3dturbT_3dmetrTi0.75



v,analy: min=1.79051e-09 max=3.08313
v,simul: min=3.54149e-06 max=2.24209

5.1r14b_2.8_v_h1000m_3dneu_3dturbT_3dmetrTi0.75



v,analy: min=2.33037e-05 max=3.07233
v,simul: min=0.000605022 max=1.33161

5.1r14b_2.8_v_h1000m_3dneu_3dturbT_3dmetrTi0.75

Summary

- The current version of 3D-diffusion is not stable in steep terrain (finding by MeteoCH) ← instability of metric terms
- A new stability analysis indicates how to cure the problem:
  - treat **all** of the possible vertical terms in the tridiagonal solver
  - some off-centering (~0.7) is necessary and leads to

$$K \Delta t \left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} \right) \leq$$ 0.45 (scalar case) / 0.146 (vector case)

  - in the v-equations additional forward-backward even slightly increases stability (not planned yet)
- new subroutines `explicit_horiz_diffusion` (replaces the old one) and `implicit_vert_diff_uvwT_3D`
- A new test case for vector diffusion has been proposed

Outlook

- Resharp the test case definition a bit (less time steps, perhaps numerical diffusivity of the diffusion is too prominent?)
- or still bugs in implementation?
- proper lower and upper boundary treatment
- implement also *spherical* metric terms into `explicit_horiz_diffusion`
- deliver a version of `explicit_horiz_diffusion` without shallow approx. i.e. using the *deep* form ($1/a \rightarrow 1/r$)
- possibly available in COSMO 5.2
(volunteers for 4-eyes principle?)