Shota Rustaveli National Science Foundation

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JÜLICH Forschungszentrum

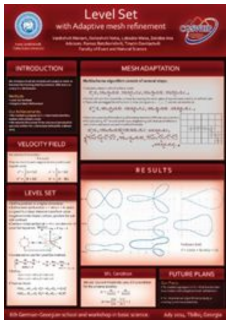
Ana Dolidze

Studying advection schemes of EURAD-IM model

Supervisors:
Ramaz Botchorishvili (TSU)
Hendrik Elbern (FZJ, Uni Köln),

23.08.2018, Tbilisi

My story

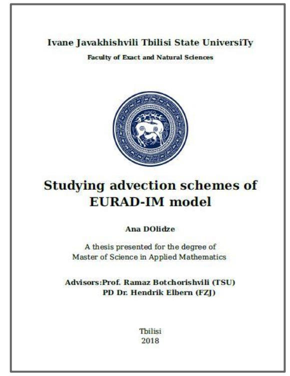


March-June 2014
Project: Level Set method
(TSU)

July 2014
Tbilisi
(6th GGSWBS)

August 2014
Jülich
(Internship)

August 2015
Jülich
(Internship)



Ivane Javakhishvili Tbilisi State UniversiTy

Faculty of Exact and Natural Sciences

Studying advection schemes of EURAD-IM model

Ana DOlidze

A thesis presented for the degree of
Master of Science in Applied Mathematics

Advisors:Prof. Ramaz Botchorishvili (TSU)
PD Dr. Hendrik Elbern (FZJ)

Tbilisi
2018

March-June 2015
Jülich
(Master's Thesis)

July 2016
Bachelor's degree in Mathematics
(TSU)

September 2016
Start of Master's studies at TSU

Oct-Nov 2017
Selection for Jülich-SRNSF Fellowship

July 2018
Master's Defense in Applied Mathematics
(TSU)

August 2018
8th GGSWBS

GEORG-AUGUST-UNIVERSITÄT GÖTTINGEN

VolkswagenStiftung

International Doctoral Program in Math

Exciting Future

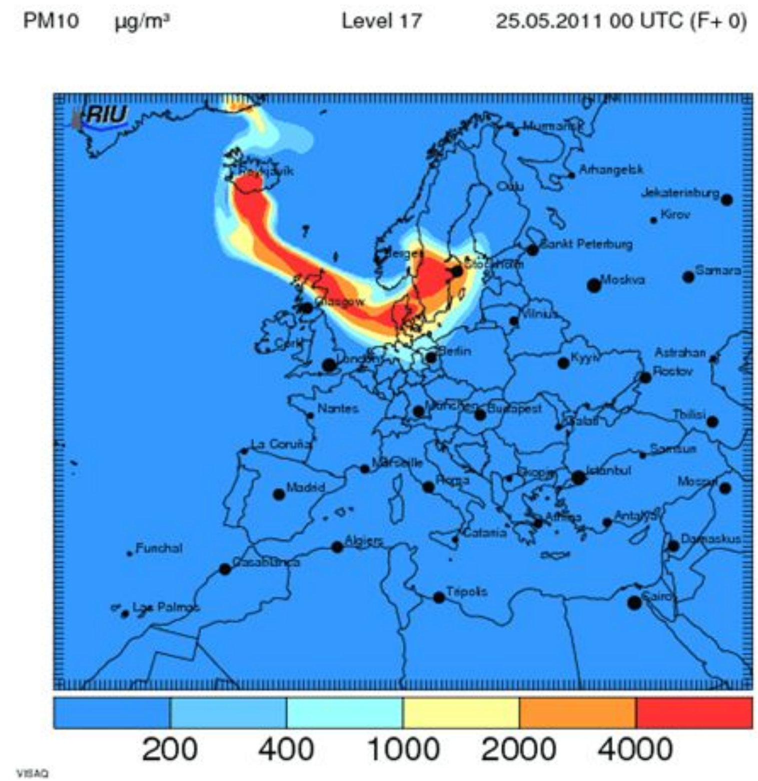
EURAD-IM model

•Developed since 1987;

•Rheinish Institute of Environmental Research at the University of Cologne (RIU);

•Based on EURAD-CTM (EURopean Air Pollution Dispersion-Chemistry Transport Model);

•It is part of European Union COPERNICUS CAMS project.



http://db.eurad.uni-koeln.de/index2_e.html?/monitoring/aqada.php

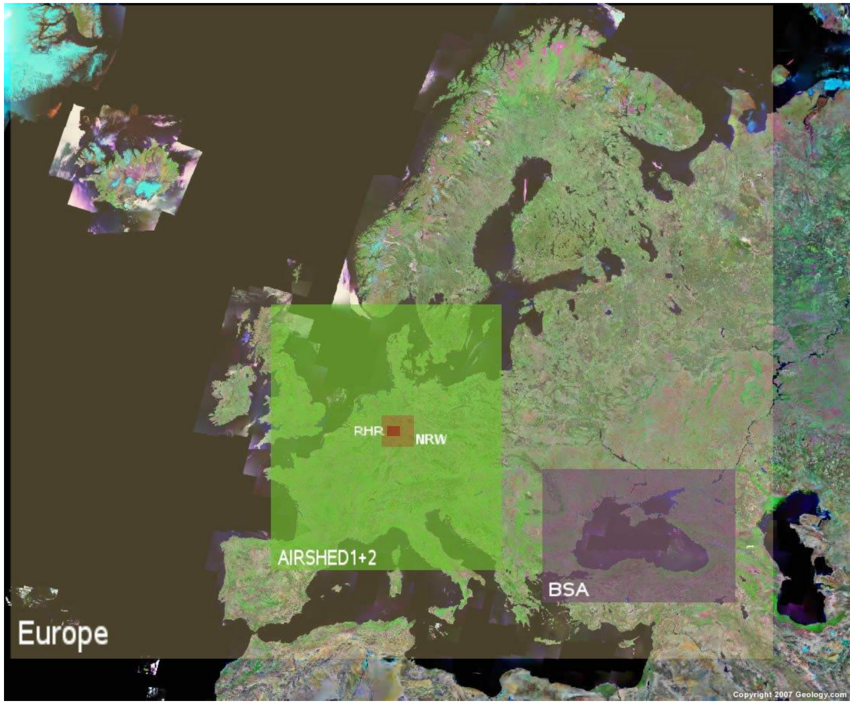
Objective of the IM group, in the frame of a large European Union Project Copernicus CAMS

- ❑ Provide **air quality forecasts** for Europe and selected regions,
- ❑ Combine models with data for **optimal analyses**

- Regional scale (15 to 1 km resolution)
  - Central Europe (5km)
  - Black Sea Area (15km)
  - NRW (5km)
  - Ruhr-Rur Area (1km)

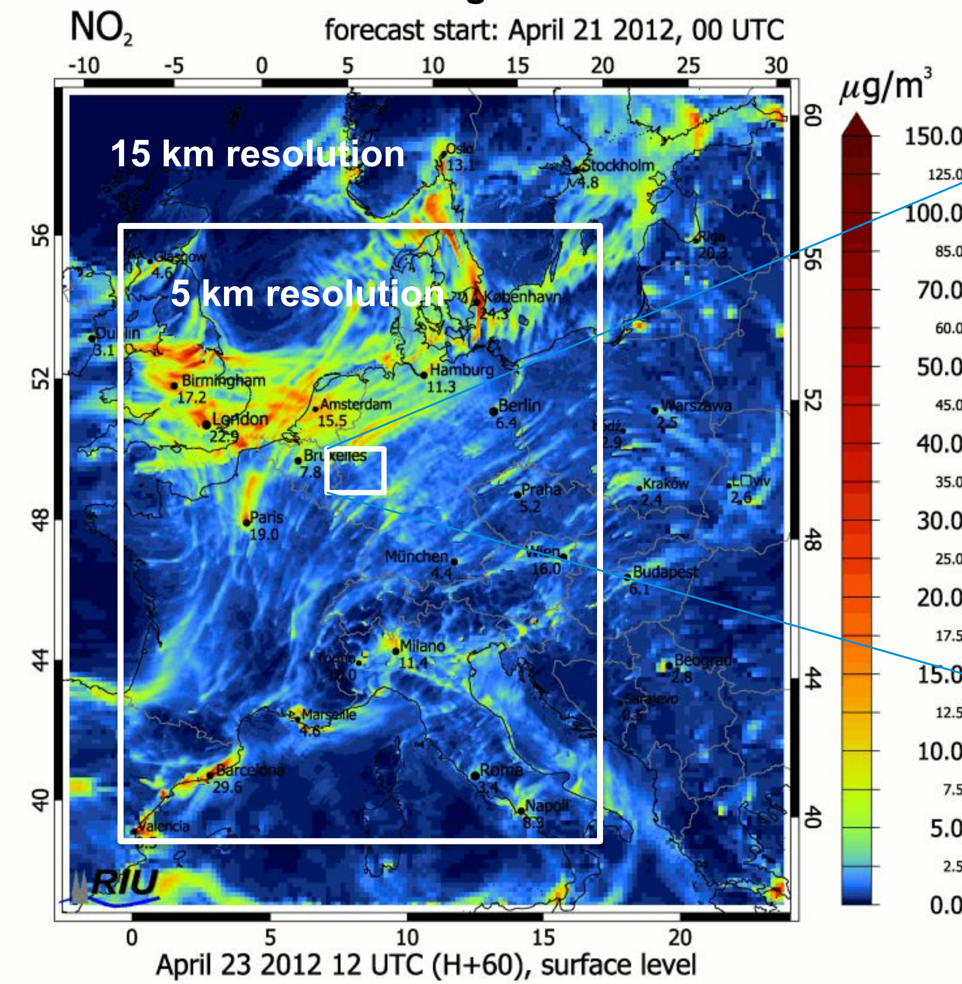
- Main institutional user:
  EPA

Landesamt für Natur, Umwelt und Verbraucherschutz Nordrhein-Westfalen

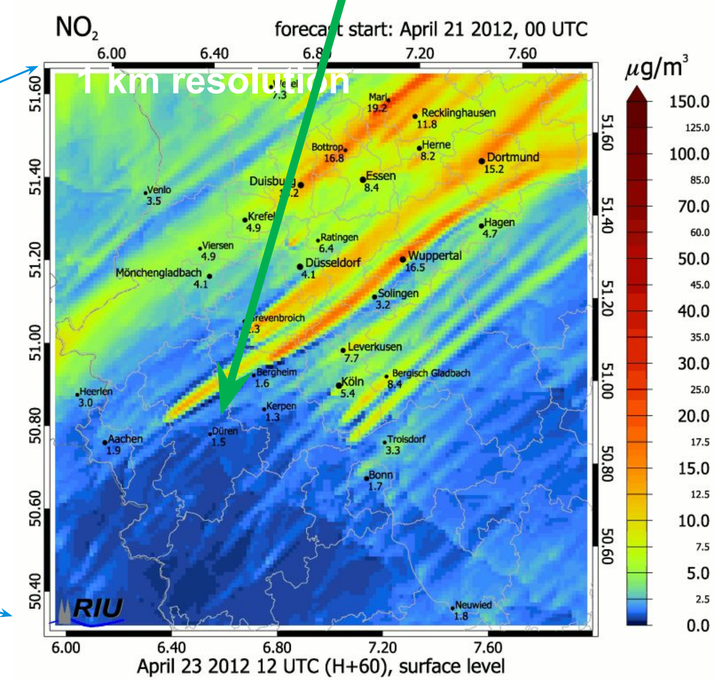


This can be transferred to Georgia

Example: Central Europe and local area with EURAD-IM nesting



EURAD-IM Ruhr-Rur Area nested into the AIRSHED domain



CAMS 50 Services

http://www.regional.atmosphere.copernicus.eu/index.php

RIU extended services incl. regional downscaling

http://db.eurad.uni-koeln.de/de/vorhersage/eurad-im.php

Research Plan

- Studying code of Eurad-IM model
  - Extracting advection numerical scheme

- Studying theoretical and numerical properties of the schemes
  - Stability analysis
  - New advection test cases
  - Numerical experiments

- Adjoint advection schemes
  - New artificial source term method for adjoint development

- Data assimilation experiments

EURAD-IM advection schemes

- Bott's area-preserving flux-form (APF) scheme
- Monotone version of APF (MAPF) scheme
- Walcek scheme
- Smolarkiewicz scheme
- Prathers scheme

EURAD-IM advection schemes

- Bott's area-preserving flux-form (APF) scheme
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Bott's area-preserving flux-form (APF) and Monotone version of APF (MAPF) schemes

Equation for transport of non-diffusivity quantity $\frac{\partial \psi}{\partial t} = -\nabla(v\psi)$

Finite-difference flux-form $\psi_j^{n+1} = \psi_j^n - \frac{\Delta t}{\Delta x}[F^n_{j+\frac{1}{2}} - F^n_{j-\frac{1}{2}}]$

> The Bott's monotonic scheme is a monotonic version of the Bott's original scheme

- Upstream method flux $F^n_{j+\frac{1}{2}} = \frac{\Delta x}{\Delta t}[c_j^+\psi_j^n - c_j^-\psi_{j+1}^n]$
- Bott's method flux $F_{j+\frac{1}{2}} = \frac{\Delta x}{\Delta t}[\frac{i_{l,j+\frac{1}{2}}}{i_{l,j}}\psi_j - \frac{i_{l,j+\frac{1}{2}}}{i_{l,j+1}}\psi_{j+1}]$

where

$$i^+_{l,j+\frac{1}{2}} = max(0, I_l^+(c_{j+\frac{1}{2}})),\ i^-_{l,j+\frac{1}{2}} = max(0, I_l^-(c_{j+\frac{1}{2}})),\ i_{l,j} = max(I_{i,j}, (i^+_{l,j+\frac{1}{2}} + i^-_{l,j+\frac{1}{2}} + \epsilon)$$

$$I_l^+(c_{j+\frac{1}{2}}) = \int_{\frac{1}{2}-c_j^+}^{\frac{1}{2}} \psi_{j,l}(x')dx' = \sum_{k=0}^{l} \frac{a_{j,k}}{(k+1)2^{k+1}}[1-(1-2c_j^+)^{k+1}]$$

$$I_l^-(c_{j+\frac{1}{2}}) = \int_{\frac{1}{2}-c_j^+}^{\frac{1}{2}} \psi_{j+1,l}(x')dx' = \sum_{k=0}^{l} \frac{a_{j+1,k}}{(k+1)2^{k+1}}(-1)^k[1-(1-2c_j^+)^{k+1}]$$

EURAD-IM advection schemes

- Bott's area-preserving flux-form (APF) scheme
- Monotone version of APF (MAPF) scheme
- **Walcek scheme**
- Smolarkiewicz scheme
- Prathers scheme

Walcek scheme

Advection equation of constituent concentration within a moving fluid

$$\frac{\partial C}{\partial t} = -\frac{\partial uC}{\partial x}$$

$C - concentration$
$u - velocity$

Numerical fluxes:

$$(\Delta t u \rho Q_f)_{i+\frac{1}{2}} = [Q_i^t D_{d-1} - Q_i^{t+\Delta t} D_d]\Delta x_i + (\Delta t u \rho Q_f)_{i-\frac{1}{2}} \quad u_{i+\frac{1}{2}} \geq 0,$$

$$(\Delta t u \rho Q_f)_{i-\frac{1}{2}} = [Q_i^{t+\Delta t} D_d - Q_i^t D_{d-1}]\Delta x_i + (\Delta t u \rho Q_f)_{i+\frac{1}{2}} \quad u_{i-\frac{1}{2}} < 0.$$

D is the fluid density:

$$D_0 = \rho_i,$$

$$D_1 = D_0 - [(\rho u)_{i+\frac{1}{2}} - (\rho u)_{i-\frac{1}{2}}]\Delta t/\Delta x_i$$

$$D_2 = D_1 - [(\rho v)_{j+\frac{1}{2}} - (\rho v)_{j-\frac{1}{2}}]\Delta t/\Delta y_j$$

$$D_3 = D_2 - [(\rho w)_{k+\frac{1}{2}} - (\rho w)_{k-\frac{1}{2}}]\Delta t/\Delta z_k$$

EURAD-IM advection schemes

- Bott's area-preserving flux-form (APF) scheme
- Monotone version of APF (MAPF) scheme
- Walcek scheme
- Smolarkiewicz scheme
- Prathers scheme

Smolarkiewicz scheme

Continuity equation for advection of non-diffusive quantity in flow field

$$\frac{\partial \psi}{\partial t} + div(V\psi) = 0$$

Upstream advection scheme

$$\psi_i^{N+1} = \psi_i^N - [F(\psi_i^N, \psi_{i+1}^N, u_{i+\frac{1}{2}}^N) - F(\psi_{i-1}^N, \psi_i^N, u_{i-\frac{1}{2}}^N)]$$

where

$$F(\psi_i, \psi_{i+1}, u) = [(u + |u|)\psi_i + (u - |u|)\psi_{i+1}]\frac{\Delta t}{2\Delta x}$$

Eventually the scheme has the following look:

$$\psi_i^* = \psi_i^N - [F(\psi_i^N, \psi_{i+1}^N, u_{i+\frac{1}{2}}^N) - F(\psi_{i-1}^N, \psi_i^N, u_{i-\frac{1}{2}}^N)]$$

$$\psi_i^{N+1} = \psi_i^* - [F(\psi_i^*, \psi_{i+1}^*, \bar{u}_{i+\frac{1}{2}}) - F(\psi_{i-1}^*, \psi_i^*, \bar{u}_{i-\frac{1}{2}})]$$

$$\bar{u}_{i+\frac{1}{2}} = \frac{(|u_{i+\frac{1}{2}}|\Delta x - \Delta t u_{i+\frac{1}{2}}^2)(\psi_{i+1}^* - \psi_i^*)}{(\psi_i^* + \psi_{i+1}^* + \epsilon)\Delta x}$$

Theoretical study of numerical schemes

Von Neumann stability analysis of Bott's scheme

For error of schemes we have : $E_j^n = e^{\gamma nh} e^{i\beta jk} = \xi^n e^{i\beta jk}$

Write numerical approximation for the error of finite difference schemes.

$$\xi^{n+1} e^{i\beta jk} = \xi^n e^{i\beta jk} - \alpha(\xi^n e^{i\beta jk} - \xi^n e^{i\beta(j-1)k})$$

Cancellation of common terms yields: $\xi = 1 - \alpha(1 - e^{-i\beta k})$

Condition for stability is that the amplification $\xi = \left|\frac{E_j^{n+1}}{E_j^n}\right| = |e^{\gamma h}| \leq 1$

We have developed an expression for the amplification factor ξ for Bott's approximation. we now merely need to see what requirements are involved such that $|\ \xi\ | < 1$ hold for all βk.

we get if $1 - \alpha \leq 0$ then $|\xi| \leq 1$. This means that $\alpha = u\frac{\Delta t}{\Delta x} \leq 1$ is the stability condition. This is CFL condition.

Artificial source term method for adjoint schemes

- Adjoint advection equation $$\rho\frac{\partial q^*}{\partial t} + \nabla\cdot(\rho q^*\vec{v}) = q^*\nabla\cdot(\rho\vec{v})$$

- Adjoint advection scheme

Numerical flux using forward scheme

$$\bar{\rho}_j^n\frac{q_j^{*,n+1}-q_j^{*,n}}{\Delta t} + \frac{1}{|\Omega_j|}\sum_{i\in I_j} F_{ji}(\{\bar{\rho}_j^n, \bar{v}_k^n, q_k^{*,n}\}_{k\in K_{ji}}, \vec{n}_{ji}, l_{ji}) = \frac{1}{|\Omega_j|}\sum_{i\in I_j} F_{ji}(\{\bar{\rho}_j^n, \bar{v}_k^n, q_j^{*,n}\}_{k\in K_{ji}}, \vec{n}_{ji}, l_{ji})$$

New fast and efficient method for adjoint development. The method can be used when the numerical flux function is limited with or without flux limiters

Numerical experiments

- Advection experiments for forward schemes
  - Rotational flow field test
  - Smolarkiewicz deformational flow field test
  - Divergent flow field test

- Advection experiments for adjoint schemes
  - Rotational flow field test
- divergence flow field test

- Data assimilation experiments
  - Convergence of iterative process
  - Manipulating with weights of background and observation terms
  - Impact of number of observations

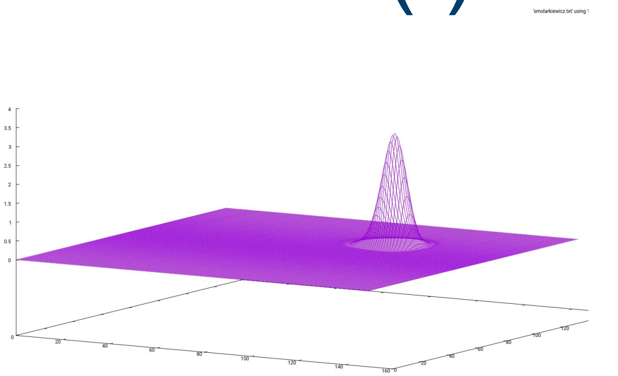
Experiment 1: Rotational flow field test

Goals :

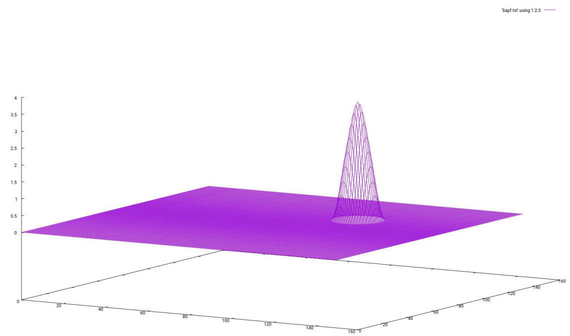
- Studying advection schemes of EURAD-IM model for different initial data.
- Comparison of schemes.

- Velocity vector components : $u(x,y)=-0.1(y-70)$; $v(x,y)=0.1(x-70)$
- Domain 150x150 nodes; Spatial steps $\Delta x=\Delta y=1$; Time step $\Delta t=0.04$;
- One full rotation -1570 time steps.
- initial conditions :
  - cone with maximum height 4, with base radius 10 unit .
  - cylinder with radius 10 and height 4 center at (100, 100).
  - the slotted cylinder.

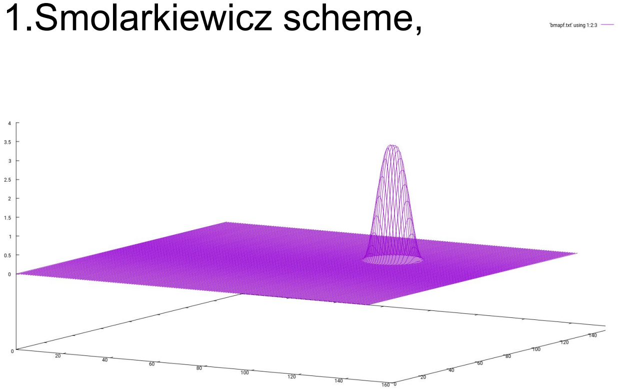
Results (I)



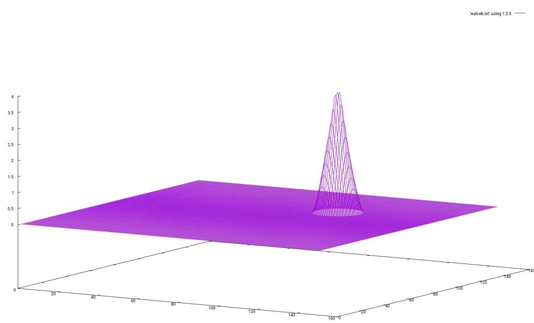
1.Smolarkiewicz scheme,



2. Bott scheme

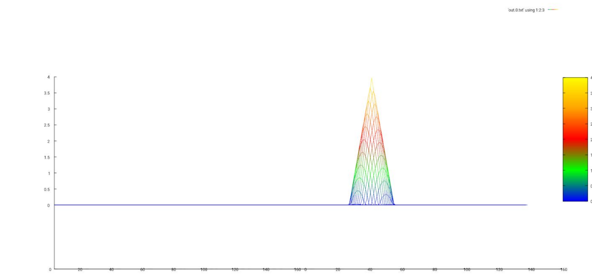


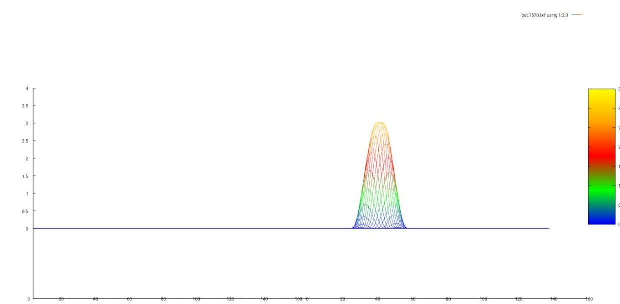
3.Bott monotone scheme



4. Walcek scheme

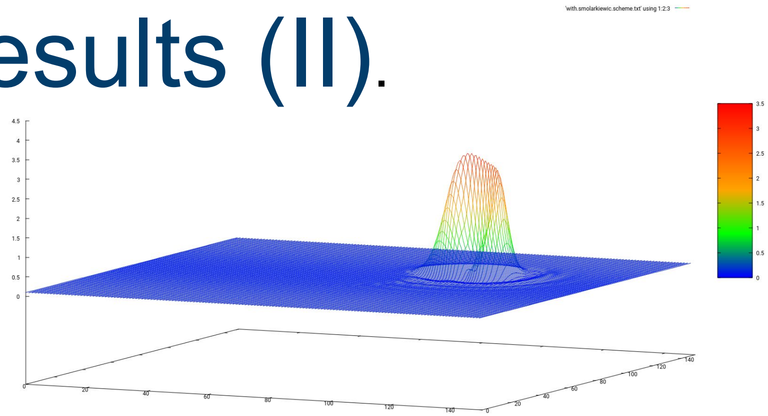
Result for Rotational Cone after one full rotation,
1570 time steps,



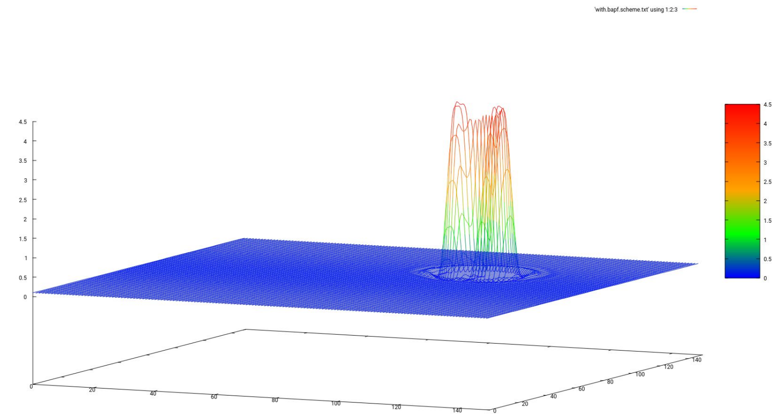


Bott scheme
initial condition and result after one rotation, 1570 time steps,

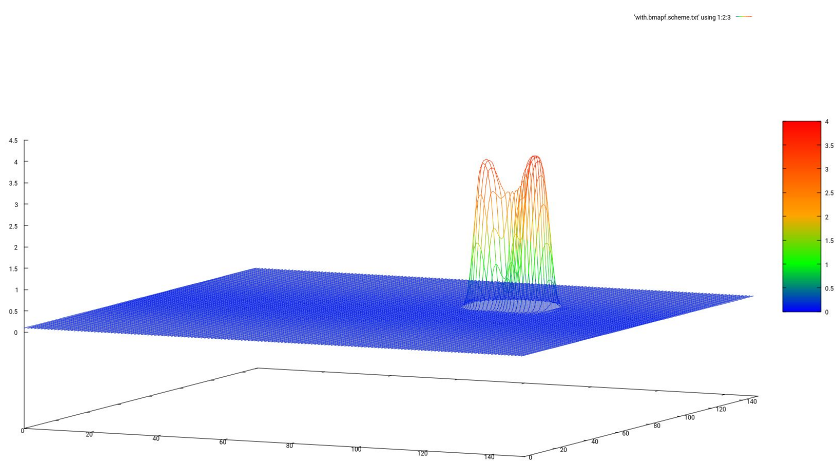
Results (II).



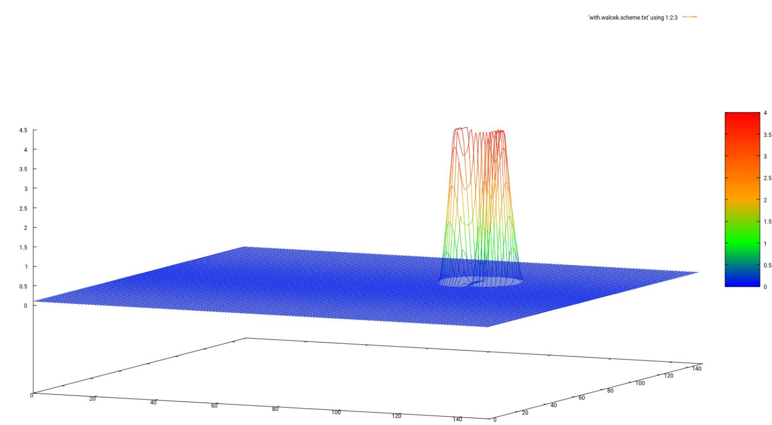
1. Smolarkiewicz scheme,



2. Bott scheme



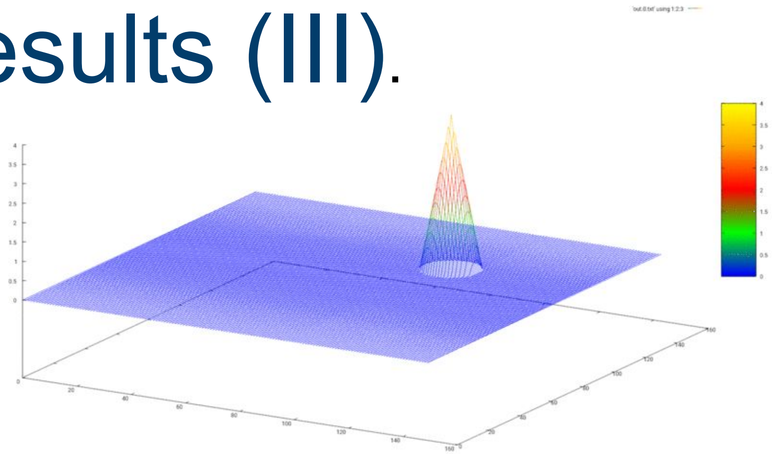
3. Bott monotone scheme



4. Walcek scheme

Slotted cylinder after one full rotation, 1570 time steps

Results (III).



$$l_{1,rel} = \frac{\sum_{i=1}^{N} |\Omega_i||q_i - q_i^{true}|}{\sum_{i=1}^{N} |\Omega_i||q_i^{true}|}, \quad l_{1,abs} = \sum_{i=1}^{N} |q_i - q_i^{true}|$$

$$l_{2,rel} = \frac{\sqrt{\sum_{i=1}^{N} |\Omega_i|(q_i - q_i^{true})^2}}{\sqrt{\sum_{i=1}^{N} |\Omega_i(q_i^{true})^2}}, \quad l_{1,abs} = \sqrt{\sum_{i=1}^{N} (q_i - q_i^{true})^2}$$

$$l_{\infty,rel} = \frac{\max_{i=1,N} |q_i - q_i^{true}|}{\max_{i=1,N} |q_i^{true}|}, \quad l_{\infty,abs} = \max_{i=1,N} |q_i - q_i^{true}|$$

initisl Data	norms	Smolarkiewicz scheme	Bott scheme	Bott non-monotone scheme	Walcek scheme
Cone	Absolute firs norm	164.67596	23.5887794	33.9459610	29.2817116
	Absolute second norm	8.94577026	1.52778172	2.69549799	1.81237614
	Absolute infinite norm	1.39720035	0.499090195	0.984883547	0.245351791
	Relative firs norm	0.393162668	5.63551225E -02	8.10991004E -02	6.99559078E-02
	Relative second norm	0.308932424	5.27602769E -02	9.30860862E-02	6.5884384E -02
	Relative infinite norm	0.349300086	0.124772549	0.246220887	6.13379478E -02
Cylinder	Absolute firs norm	676.746826	289.457520	274.378540	275.241180
	Absolute second norm	30.3927231	18.3770294	8.4850121	18.9958382
	Absolute infinite norm	2.80773306	2.42684531	2.23414564	2.25216651
	Relative firs norm	0.554710507	0.237260267	0.224900439	0.225607529
	Relative second norm	0.435070574	0.263066411	0.264612198	0.271924645
	Relative infinite norm	0.701933265	0.606711328	0.558536410	0.563041627
Slotted cylinder	Absolute firs norm	915.308960	352.183105	522.810181	369.109100
	Absolute second norm	40.9977875	20.2291603	27.7285976	22.0090618
	Absolute infinite norm	3.77520108	2.90145874	3.32671690	2.80783129
	Relative firs norm	0.299341649	0.115177572	0.170979261	0.120713033
	Relative second norm	0.689548671	0.340237647	0.466371924	0.370174110
	Relative infinite norm	0.943800271	0.725364685	0.831679225	0.701957822

Experiment 2:

Goal:

- Check stability of numerical schemes

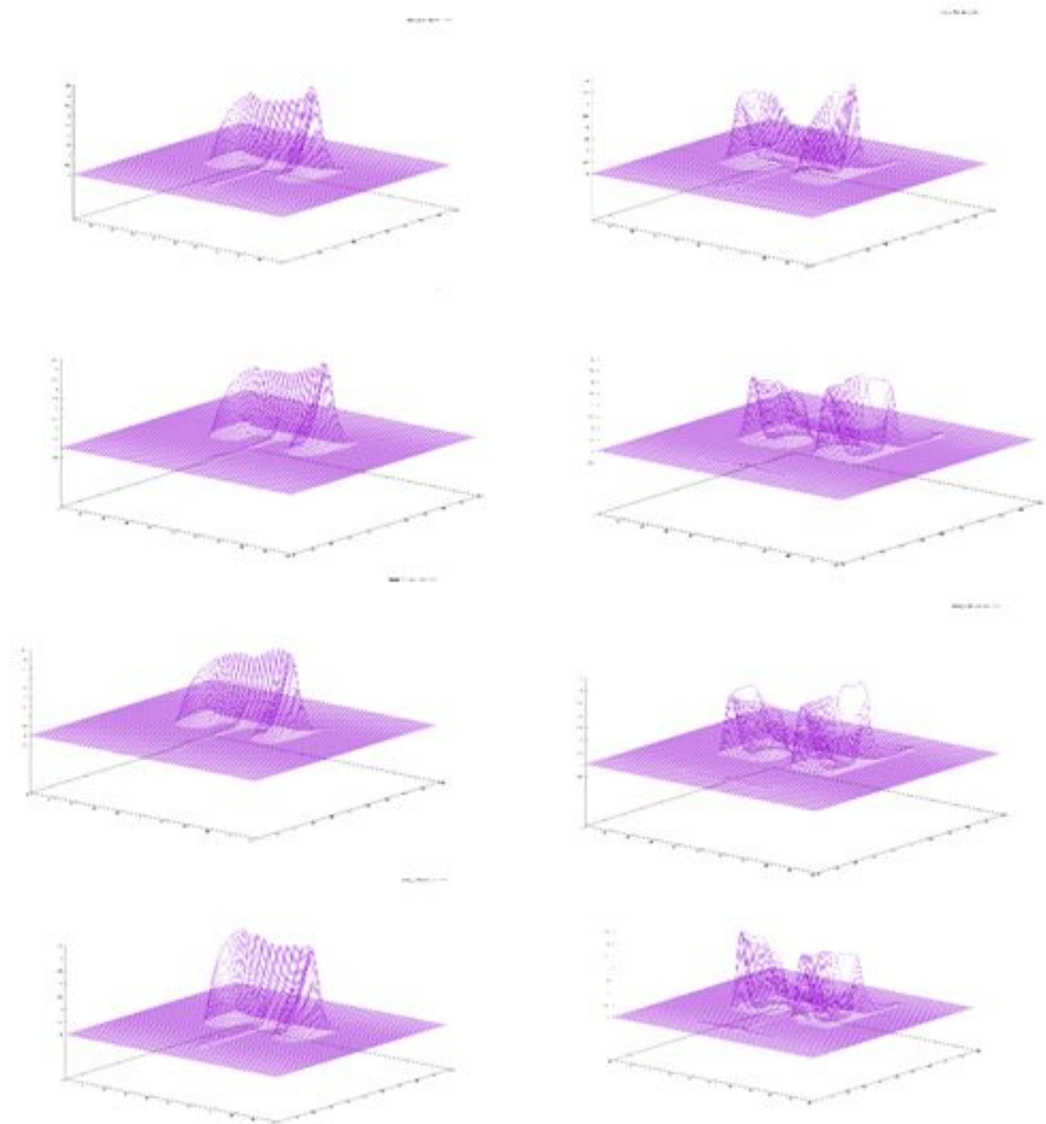
Smolarkiewicz deformational flow field test.

- ❑ Domain is [0,100]X [0,100], with spatial step 1.
- ❑ Initial condition is cone with center at (50 ,50), height 4, radius 15 unit.

The velocity field is :

$$u(x,y) = \frac{8\pi}{25} sin(\frac{\pi x}{25}) sin(\frac{\pi y}{25})$$

$$v(x,y) = \frac{8\pi}{25} cos(\frac{\pi x}{25}) cos(\frac{\pi y}{25})$$

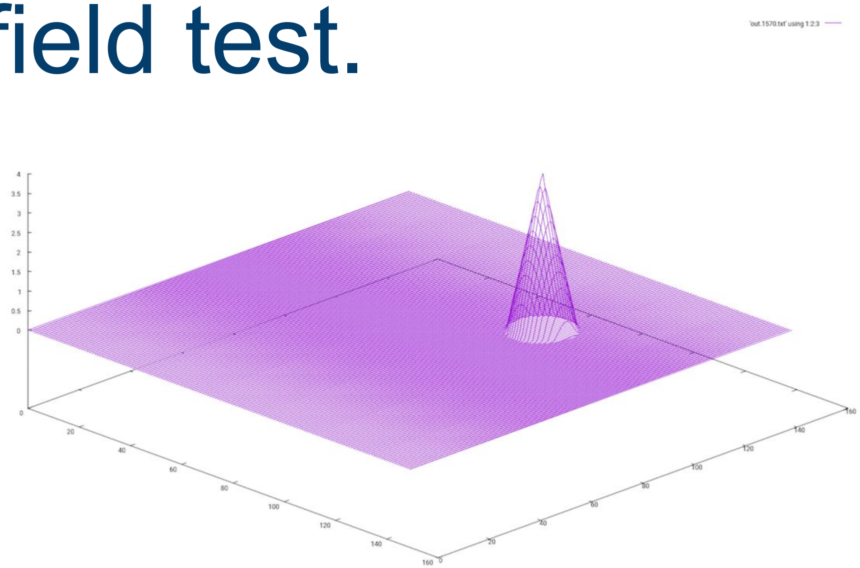


results after 38 and 75 iteration:

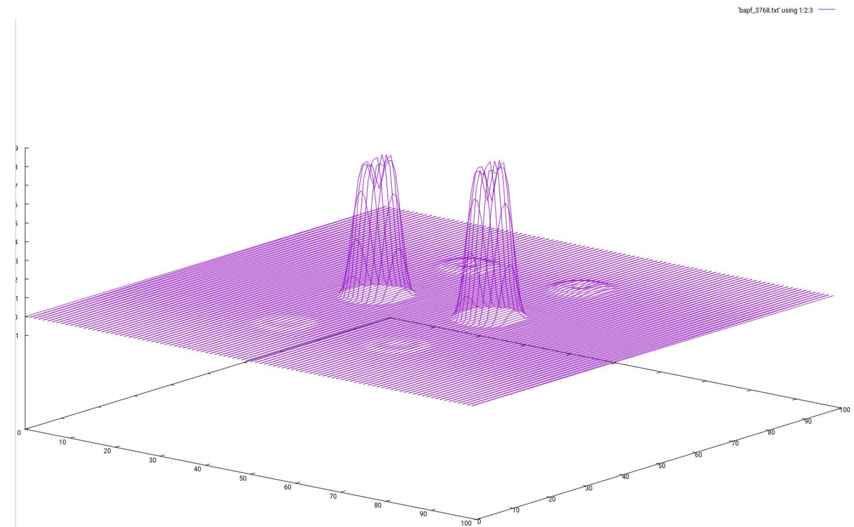
1.Smolarkiewicz scheme, 2. Bott scheme;

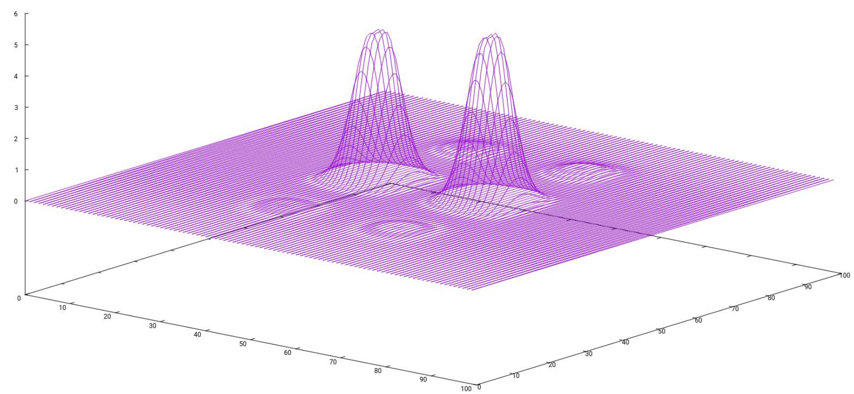
3. Bott monotone scheme 4. Walcek scheme

Results: Smolarkiewicz deformational flow field test.



First 100 time step with Bott scheme





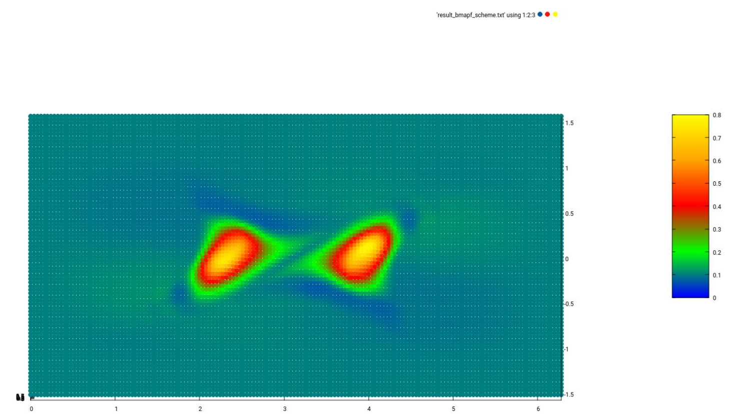
Results after 3768 time steps:
1.Smolarkiewicz scheme, 2. Bott scheme

Experiment 3: Divergent flow field test

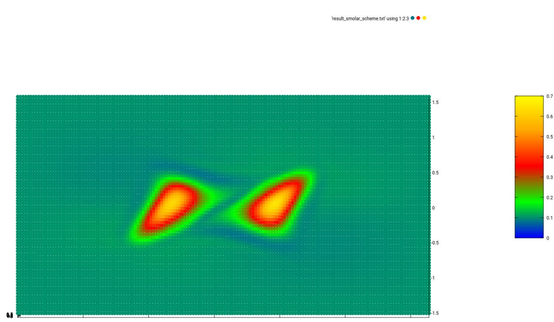
- Domain is [0 ; 2π]× [- π/2; π/2].
- Initial condition is two cone with center at (3/4 π ;0) and in (5/4 π ; 0) points, with radius π/8 and height 1 unit.
- Velocity vector fields:

$$u(x,y,t) = -sin^2(x/2)sin(2y)cos^2(y)cos(\pi t/T),$$

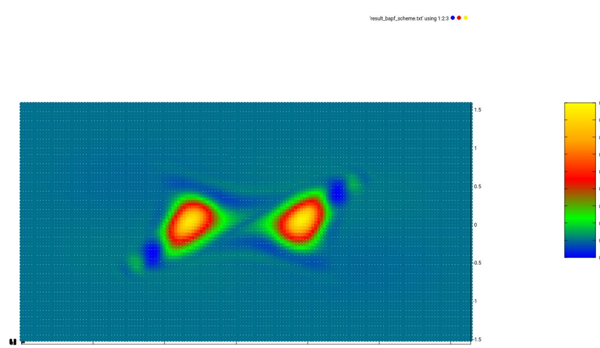
$$v(x,y,t) = \frac{1}{2}sin(x)cos^3(y)cos(\pi t/T),$$



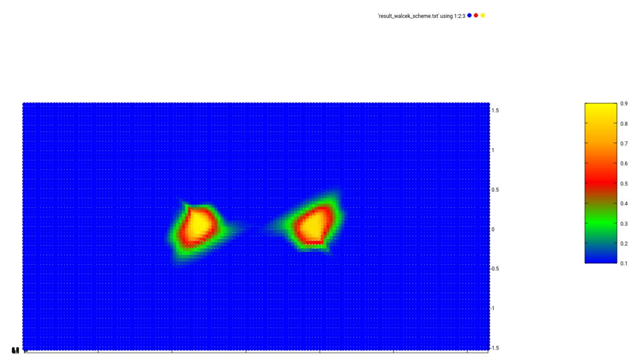
3. Bott monotone scheme



1. Smolarkiewicz scheme,



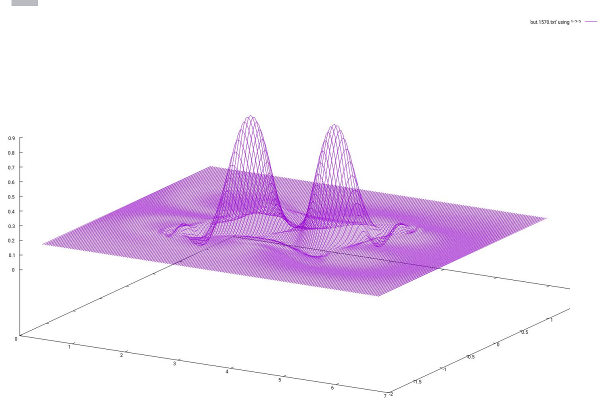
2. Bott scheme



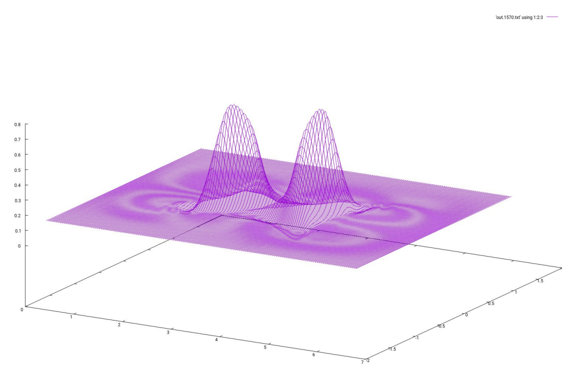
4. Walcek scheme

Results: Divergent flow field test

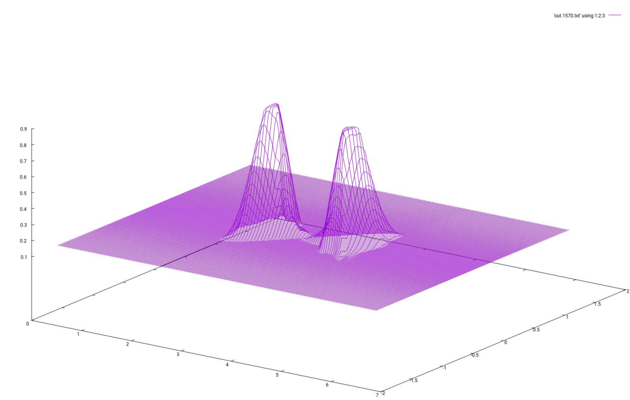
$schemes$	$Smolarkiewicz$ $scheme$	$BAPF$ $scheme$	$BMAPF$ $scheme$	$Walcek$ $scheme$
$l_{1,abs}$	0.234864667	0.159404129	0.206967369	$8.89417753E-02$
$l_{1,rel}$	$9.90675688E-02$	$6.72377795E-02$	$8.73002931E-02$	$3.75162661E-02$
$l_{2,abs}$	0.183403566	0.109545931	0.148490980	$9.58164409E-02$
$l_{2,rel}$	0.279403597	0.166886210	0.226216495	0.145970210
$l_{\infty,abs}$	0.446476221	0.221779764	0.336575985	0.232931197
$l_{\infty,rel}$	0.416936547	0.207106426	0.314307511	0.217520058



1. Bott monotone scheme



2. Bott scheme



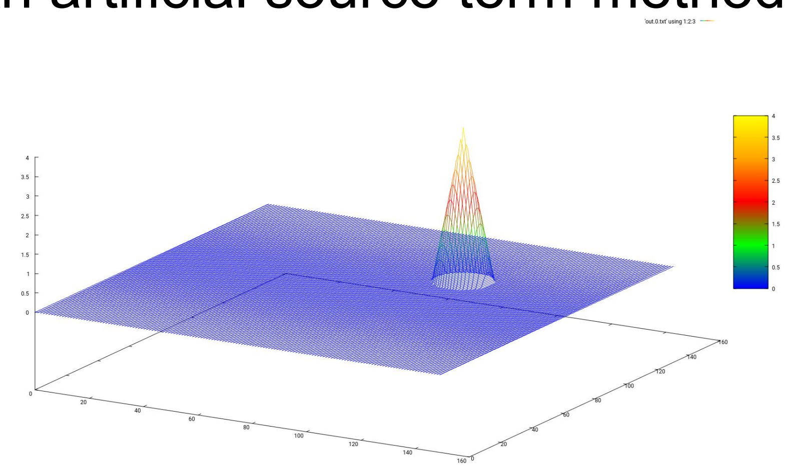
3. Walcek scheme

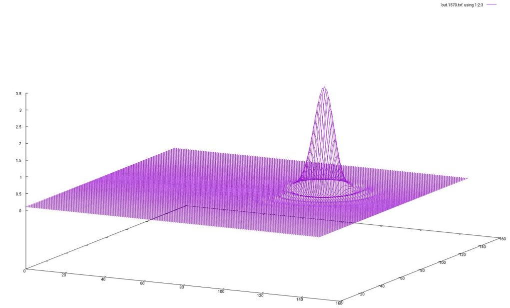
Experiment 4: Advection tests for adjoint advection schemes

Goal:

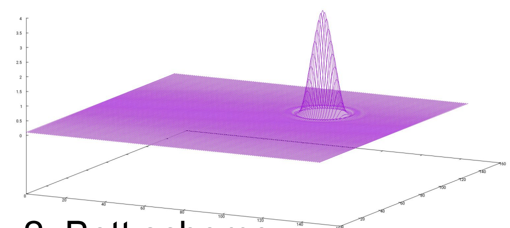
- comparison of adjoints of advection schemes;
- chek new artificial source term method

- ❑ This numerical experiment is same as numerical experiment 1;
- ❑ Adjoint of schemes is built with artificial source term method.
- ❑ Initial condition are :
- ❑ cone
- ❑ slotted cylinder

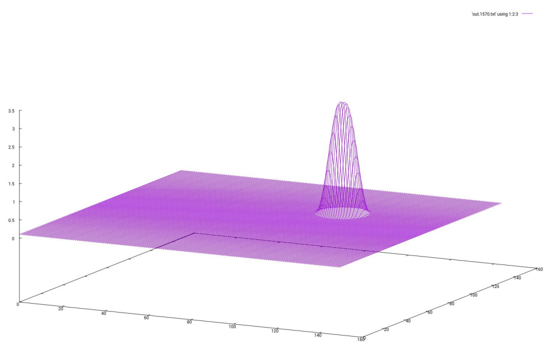




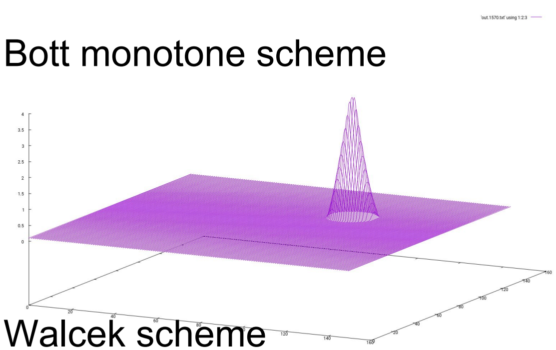
1. Smolarkiewicz scheme,



2. Bott scheme



3. Bott monotone scheme

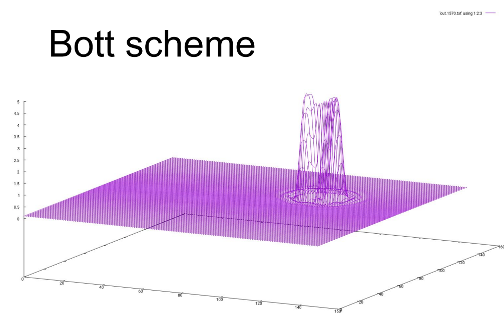


4. Walcek scheme

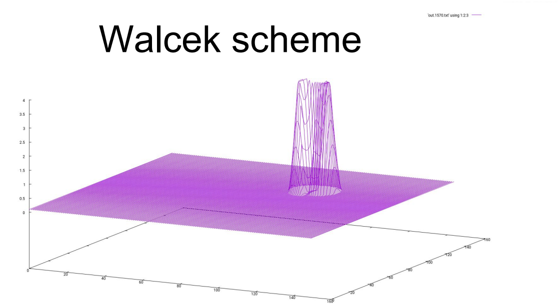
schemes	*Smolarkiewicz scheme*	*BAPF scheme*	*BMAPF scheme*	*Walcek scheme*
$l_{1,abs}$	188.782913	31.9276543	35.0605850	25.4268589
$l_{1,rel}$	$7.07334131E-02$	$1.19626932E-02$	$1.31365433E-02$	$9.52696707E-03$
$l_{2,abs}$	9.08317280	1.59539938	2.71032405	1.63549256
$l_{2,rel}$	0.268162996	$4.71010618E-02$	$8.00170451E-02$	$4.82847355E-02$
$l_{\infty,abs}$	1.35477161	0.494075775	0.985207558	0.265397787
$l_{\infty,rel}$	0.330432117	0.120506287	0.240294531	$6.47311658E-02$

error norms for moving cone after 1570 time iteration

Bott scheme



Walcek scheme



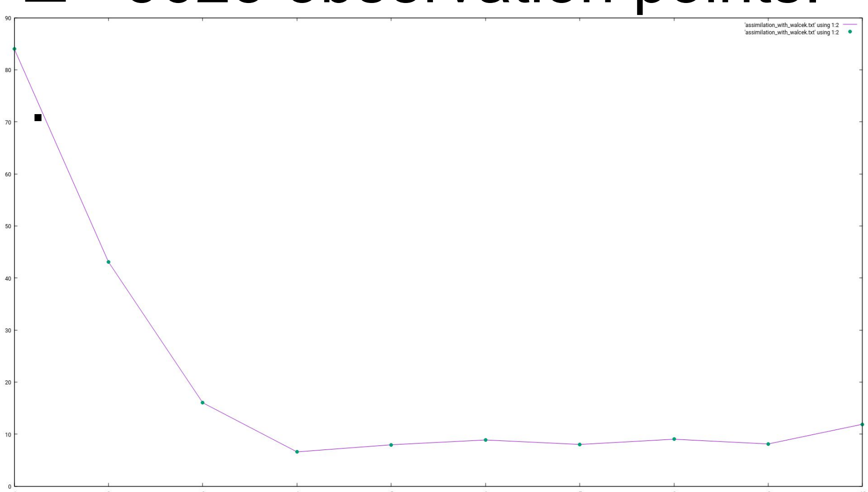
schemes	*Smolarkiewicz*	*BAPF*	*BMAPF*	*Walcek*
$l_{1,abs}$	931.690430	353.013550	502.949432	351.707336
$l_{1,rel}$	0.304699004	0.115449160	0.164484024	0.115021981
$l_{2,abs}$	41.0834274	20.2251072	27.4740562	21.4147530
$l_{2,rel}$	0.690989077	0.340169460	0.462090760	0.360178322
$l_{\infty,abs}$	3.46076822	3.00966358	3.42613435	2.73499990
$l_{\infty,rel}$	0.865192056	0.752415895	0.856533587	0.683749974

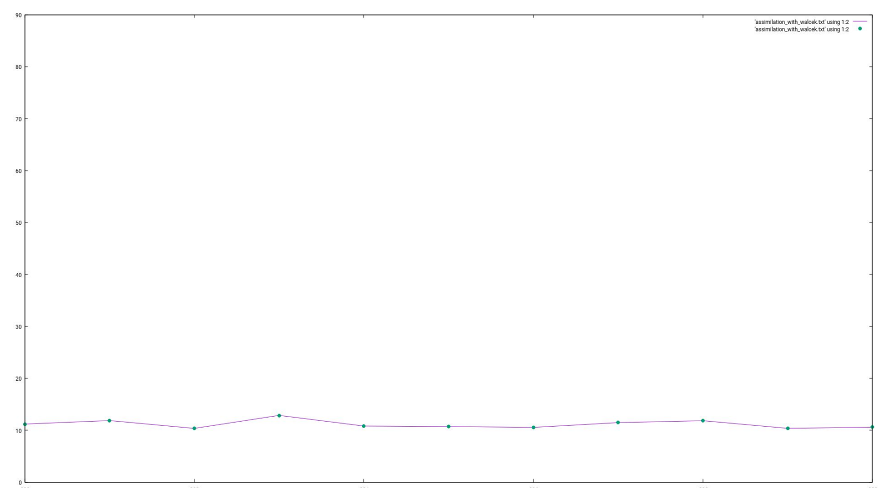
error norms for moving slotted cylinder after 1570 time iteration

Experiment 5: test for data assimilation

Convergence of iteration process

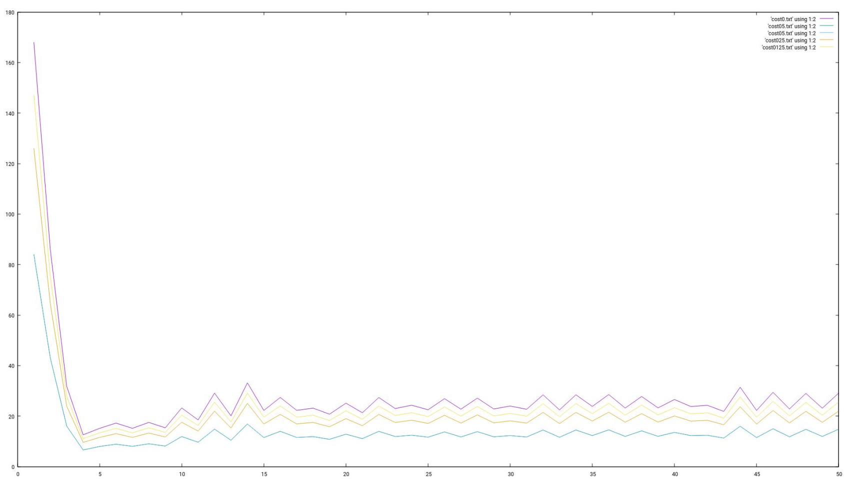
- Data assimilation experiment for rotational cone test;
- Walcek scheme.
- 300 LBFGS iterations.
- 5625 observation points.

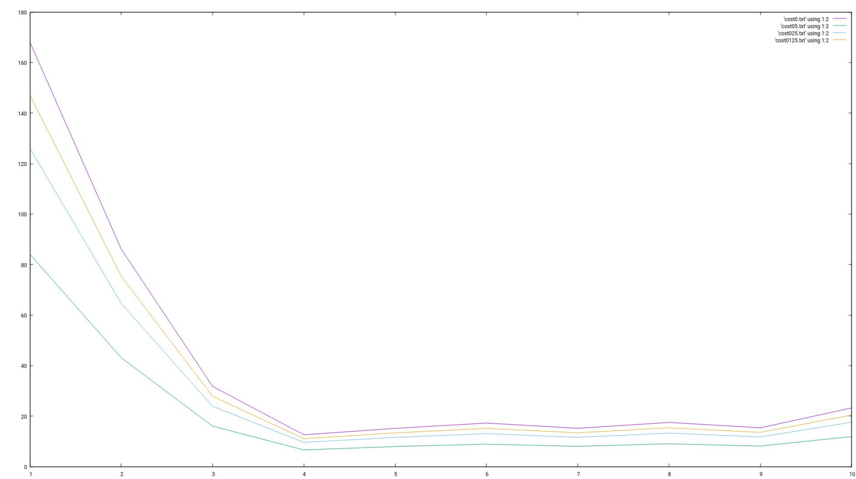


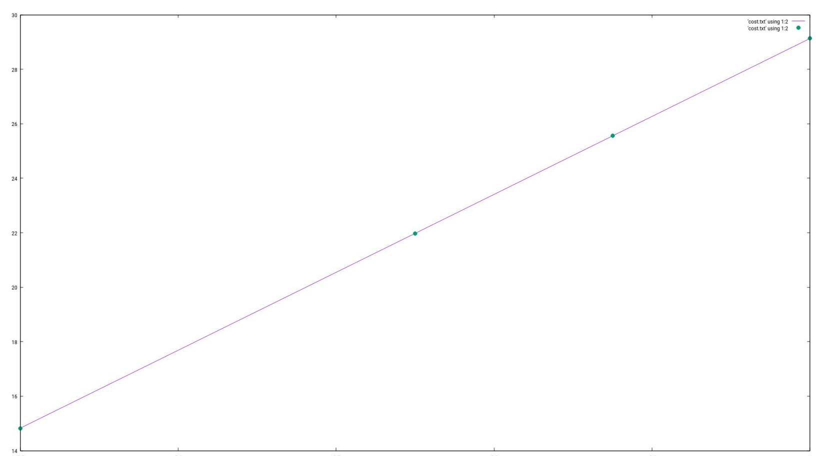


Cost function for first 10 LBFGS iterations and the second picture shows cost functions for 290-300 LBFGS iterations.

Experiment 6: Manipulating with weights of background and observation terms

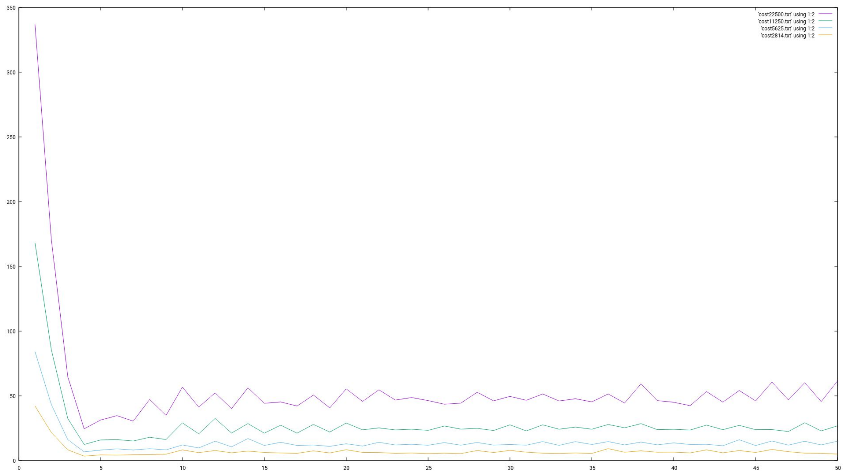


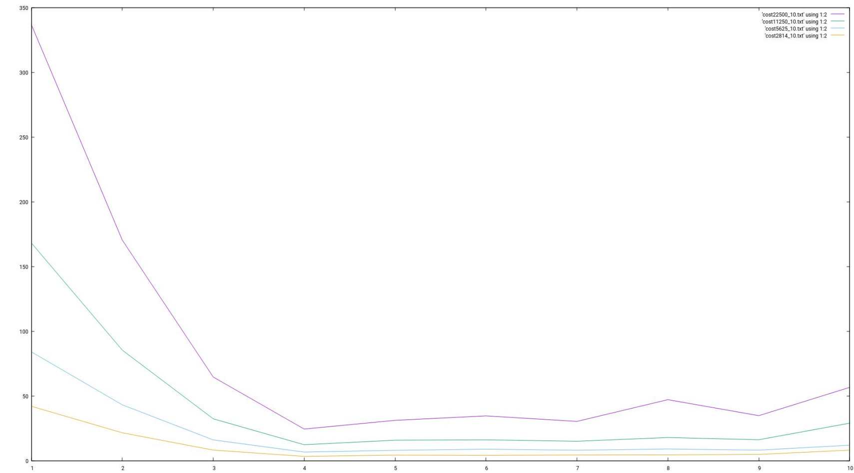




- Cost functions for different weights for first 10 LBFGS iteration and for 50 LBFGS iteration.
- increase weight of observation term up to 1 and at the same time we decrease weight of background term down to 0.
- Coefficient of observation term and Cost function after 50 LBFGS interation

Experiment 7: Impact of number of observations





- 22500 grid points
- Observation points: 2814, 5625,11250 and 22500
- 50 LBFGS iterations.

Idealized case when observations are given in all nodal points of the grid.

schemes	11250 *observation points*	22500 *observation points*
$l_{1,abs}$	36.5611954	35.6330681
$l_{1,rel}$	$8.73470679E-02$	$8.51297081E-02$
$l_{2,abs}$	2.14778638	2.08128095
$l_{2,rel}$	$7.41714612E-02$	$7.18747675E-02$
$l_{\infty,abs}$	0.344787598	0.261573553
$l_{\infty,rel}$	$8.61968994E-02$	$6.53933883E-02$

Thank you for your attention!

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