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Novel adjoint advection schemes for Atmospheric Chemistry

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Tbilisi

Outline

- ***Motivation***
  - ***atmospheric chemistry & 4D-var data assimilation***

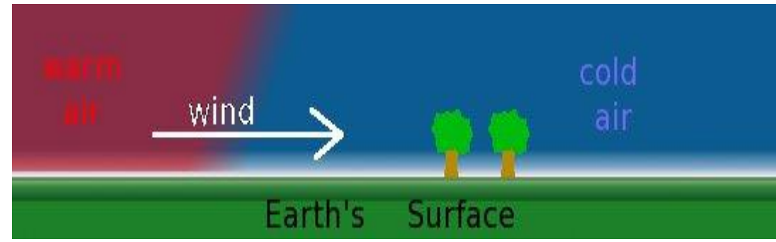
- ***Adjoint developments***

- ***Numerical results***

Atmospheric chemistry transport modeling

General atmospheric processes

- emission
- **transport**
- chemistry
- deposition



Numerical models are used to simulate atmospheric motion and provide better understanding of the processes determining the dynamical and chemical state

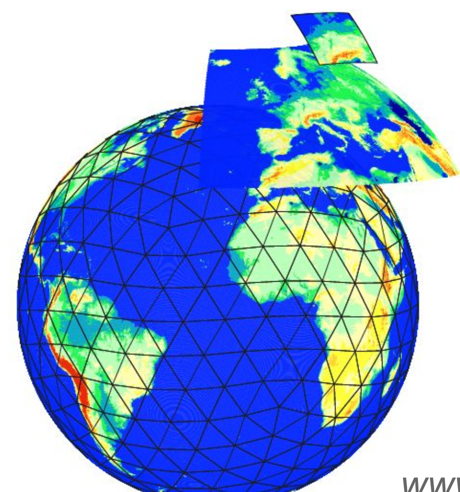
Transport continuity equation

$$\frac{\partial(\rho q)}{\partial t} + \nabla \cdot (\rho q v) = 0$$

ρ $- density$

q $- mass \quad concnetration$

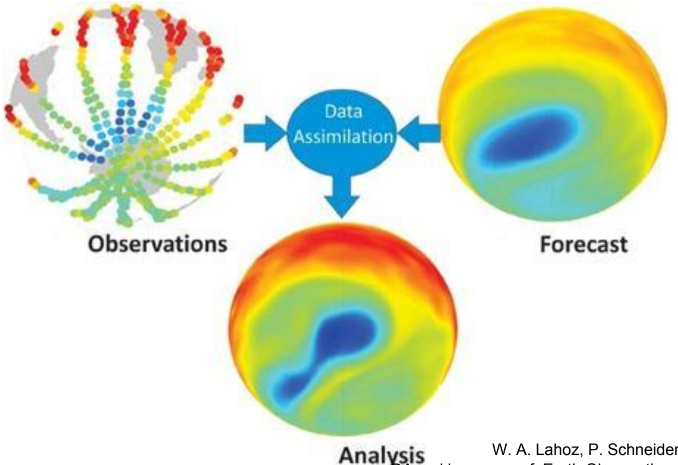
v $- wind \quad velocity \quad vector$



www.dwd.de

4D-var data assimilation (I)
(= space-time DA)

Benefit from satellite observation data for improved atmospheric chemistry and Climate Model performance



W. A. Lahoz, P. Schneider
DA:making sence of Earth Observations

Combining models with observations: a complex mathematical optimisation task

Result: the accuracy of the forecast is greatly improved

ICON Model

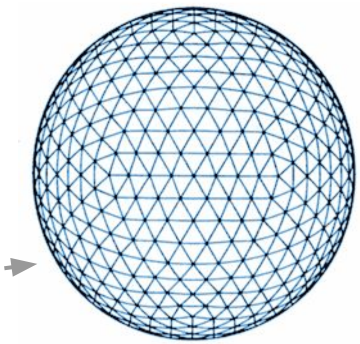
Joint project of German Weather Service (DWD) and Max-Plank Institute of Meteorology (MPI-M)

ICON model icosahedral grid, Zängl et. al, 2014

4D-var data assimilation (II)

Cost function

$$J(q_0) = f^b(q_0, q^b) + \int_0^T \int_\Omega f^o(q, q^o, t, \lambda, \theta) d\lambda d\theta dt$$



Source: ICON Database- Reference Manual

Ω - surface of the sphere

(λ, θ) - longitude-latitude coordinates

$\vec{q}_0$ - initial concentation (eg. greenhouse gases)

$\vec{q}^o$ - observational data (satellite or ground-based measurements)

$\vec{q}^b$ - background information

Data assimilation problem: find the initial state q_0 that minimizes the cost function subject to the constraints:

$$\frac{\partial(\rho q)}{\partial t} + \nabla \cdot (\rho q \vec{v}) = 0 \quad q(0, \lambda, \theta) = q_0(\lambda, \theta)$$

Solution approach

Gradient

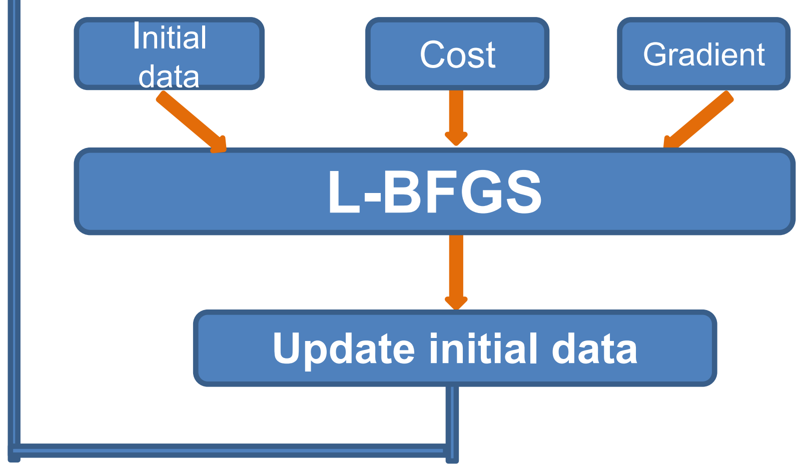
$$\nabla_{q_0} J(q_0) = \nabla_{q_0} f^b(q_0, q^b) - \rho(0, \lambda, \theta) q^*(0, \lambda, \theta)$$

$q^*(0, \lambda, \theta)$ -solution at $t = 0$ of the adjoint equation

Adjoint equation

$$\rho\left(\frac{\partial q^*}{\partial t} + v \cdot \nabla q^*\right) = \nabla_q f^o(q, q^o, t, \lambda, \theta), \quad q^*(T, \lambda, \theta) = 0$$

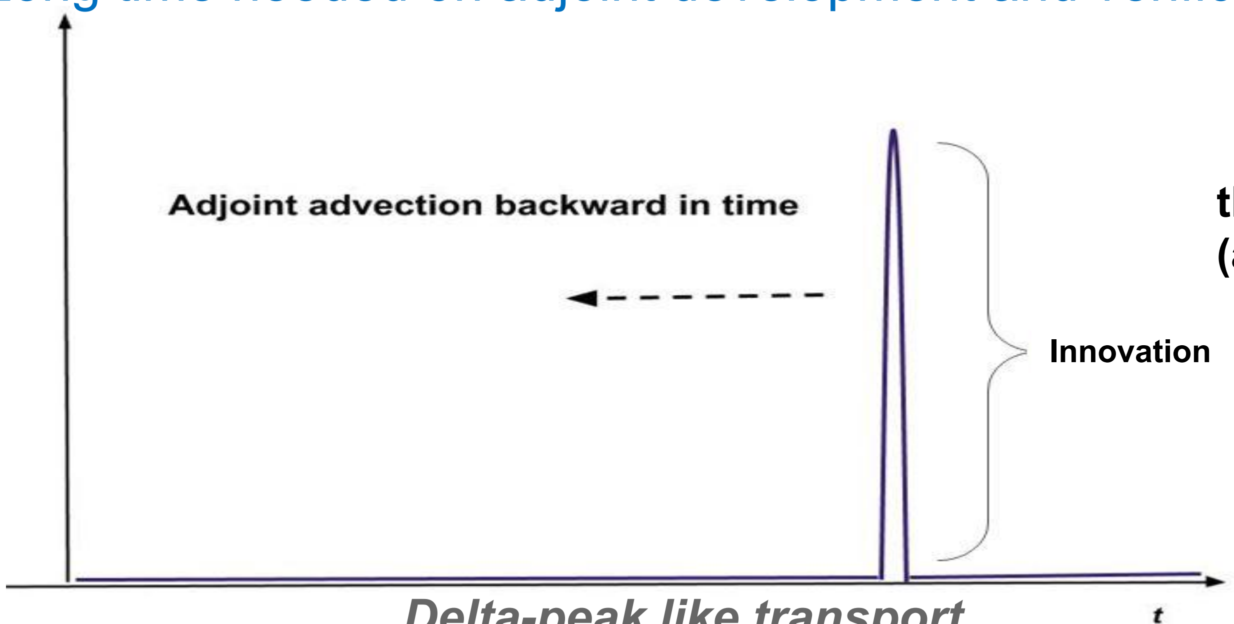
- **Forward run – Cost function**
- **Backward run – Gradient**



L-BFGS -Limited-memory Broyden-Fletcher-Goldfarb-Shanno, minimisation algorithm

Numerical challenge for adjoint development

- Delta-peak like transport during backward transport of $\nabla_q f^o(q, q^o, t, \lambda, \theta)$ requires **non-linear schemes**
- MPI based parallel computations
- Long time needed on adjoint development and verification

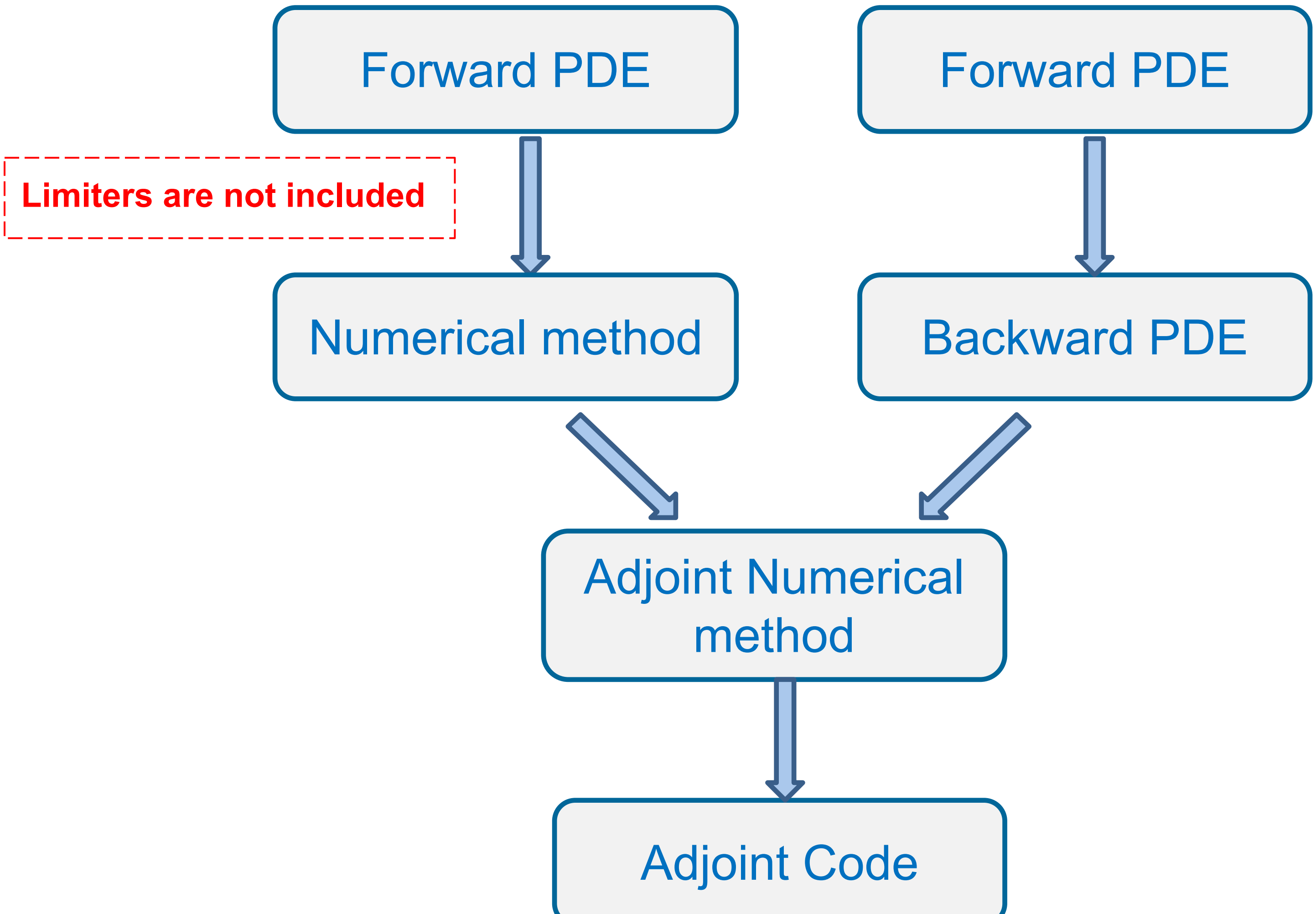


the worst case for (adjoint) advection

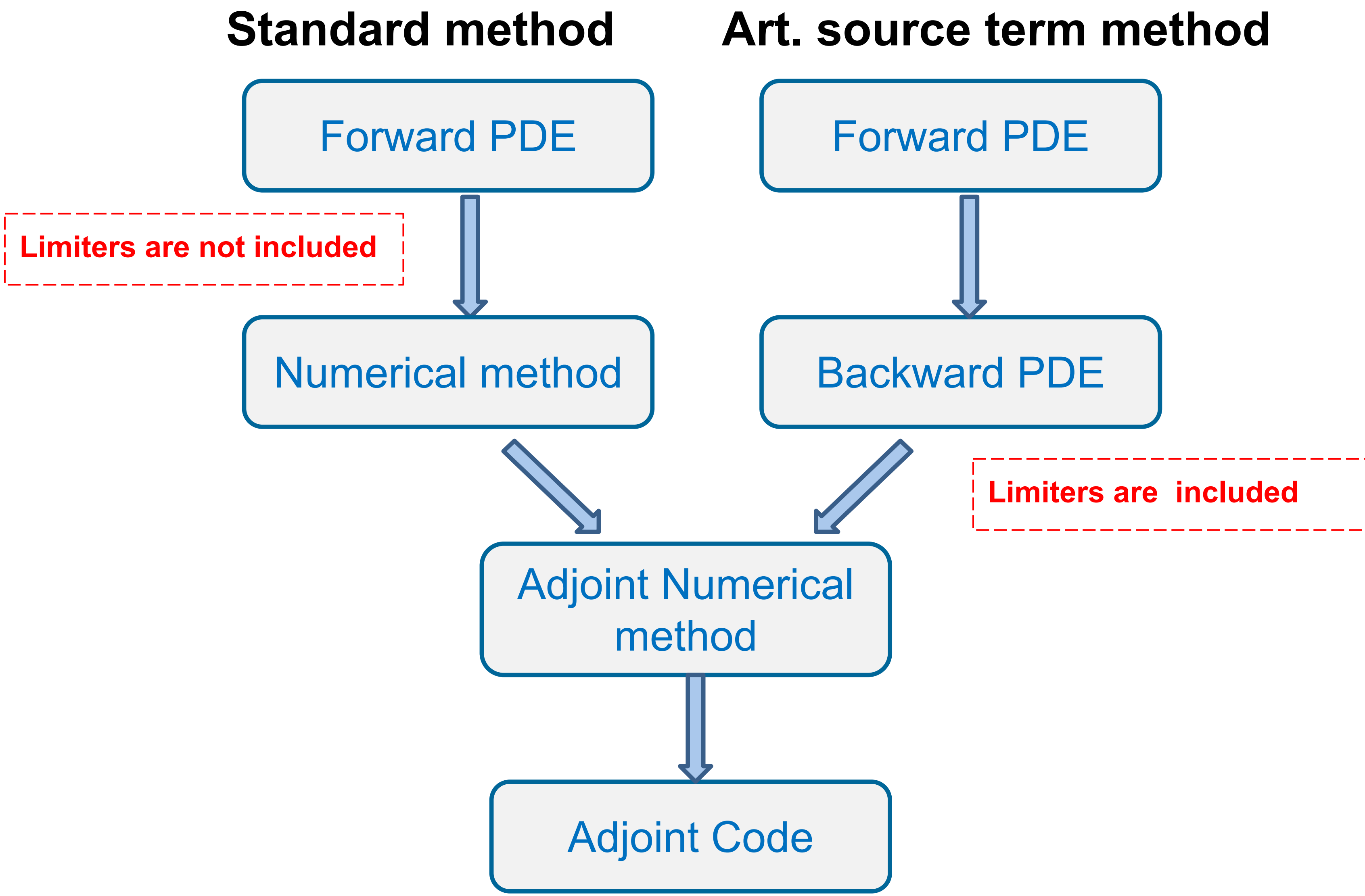
Delta-peak like transport

Paths to build the adjoint code

Standard method



Paths to build the adjoint code



Adjoint operators for ICON advection schemes

Splitted 3D continuity equation

Horizontal   Vertical

$$\frac{\partial(\rho q)}{\partial t} = \mathcal{H}(\rho q) + \mathcal{V}(\rho q)$$

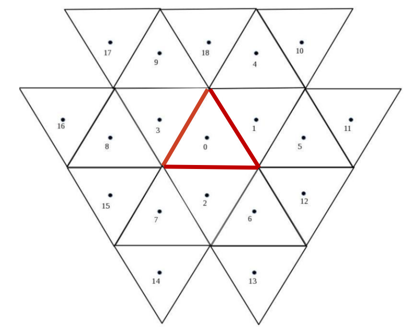
ICON Schemes

- Miura's scheme with third order least square reconstruction → Adjoint for **horizontal** scheme
- Third order Piecewise Parabolic Method (PPM) → Adjoint for **vertical** scheme

FCT Zalesak limiter (1979)

ICON-FFSL and its adjoint: standard method

Numerical scheme → Adjoint numerical scheme



Scheme stencil

- **Forward scheme**

$$\frac{\rho_j^{n+1} q_j^{n+1} - \rho_j^n q_j^n}{\Delta t} + \frac{1}{|\Omega_j|} \sum_{i \in S_j} \alpha_{ji}(\{\bar{\rho}_k^n, \bar{v}_k^n\}_{k \in K_{ji}}) q_i^n = 0, \quad S_j = \cup_{i \in I_j} K_{ji}$$

- **Adjoint scheme**

$$\bar{\rho}_j^n \frac{q_j^{*,n+1} - q_j^{*,n}}{\Delta t} + \frac{1}{|\Omega_j|} \sum_{i \in S_j^*} \alpha_{ij}(\{\bar{\rho}_k^n, \bar{v}_k^n\}_{k \in K_{ij}}) q_i^{*,n} = 0$$

K_{ji} -reference number of cells for flux F_{ji}
S_j -reference number of cells on the stencil
$I_j = \{1, 2, 3\}$

New method: artificial source term adjoint (I)

- Suitable form for **forward** problem

equivalent

$$\frac{\partial(\rho q)}{\partial t} + \nabla \cdot (\rho q \vec{v}) = 0$$

$$\frac{\partial(\rho q)}{\partial t} + (\rho q)\nabla \cdot (\vec{v}) + \vec{v}\nabla(\rho q) = 0$$

- Suitable form for **adjoint** problem

equivalent

$$\frac{\partial(\rho q)}{\partial t} + \vec{v}\nabla(\rho q) = 0$$

$$\frac{\partial(\rho q)}{\partial t} + \nabla \cdot (\rho q \vec{v}) = (\rho q)\nabla \cdot \vec{v}$$

$$\frac{\partial(\rho q)}{\partial t} + \nabla \cdot (\rho q \vec{v}) = (\rho q)\nabla \cdot \vec{v}$$

- Reuse existing forward code
- No need for extra parallelisation, use existing
- For discretisation of source term use existing solver with *q=const*
- No need for special adjoint limiting procedure

New method: artificial source term adjoint (II)

Theory:

- **If forward scheme is stable adjoint scheme is also stable**
- **If accuracy of forward scheme is $O(h^k)$ then accuracy of adjoint scheme is $O(h^k)$**
- **If forward scheme is convergent then adjoint scheme is also convergent for smooth solution**

ICON-FFSL and its adjoint: art. source term method

Backward PDE → Adjoint numerical scheme

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

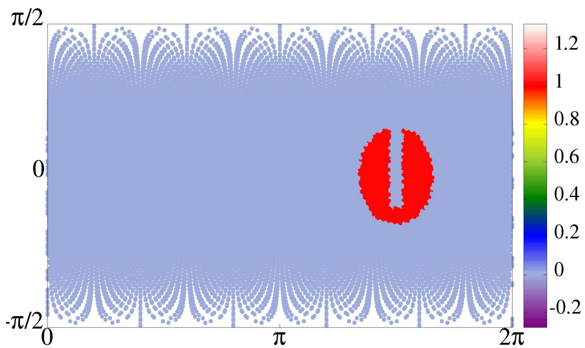
$$\bar{\rho}_j^n \frac{q_j^{*,n+1} - q_j^{*,n}}{\Delta t} + \frac{1}{|\Omega_j|} \sum_{i \in I_j} F_{ji}(\{\bar{\rho}_j^n, \bar{v}_k^n, q_k^{*,n}\}_{k \in K_{ji}}, \vec{n}_{ji}, l_{ji}) = \frac{1}{|\Omega_j|} \sum_{i \in I_j} F_{ji}(\{\bar{\rho}_j^n, \bar{v}_k^n, q_j^{*,n}\}_{k \in K_{ji}}, \vec{n}_{ji},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

Using new method, limiters are directly inherited in adjoint equation, while for standard adjoint numerical scheme development extra procedure is necessary to include limiters.

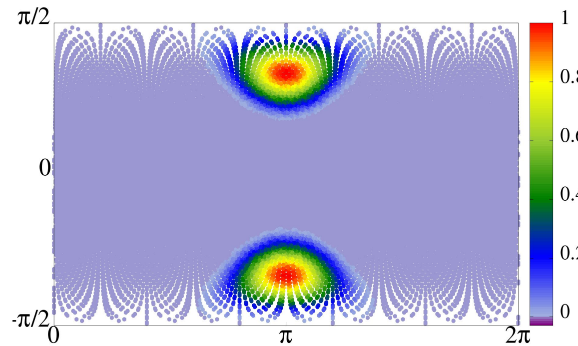
Numerical experiments - do the methods work ?

- **Linear horizontal advection**

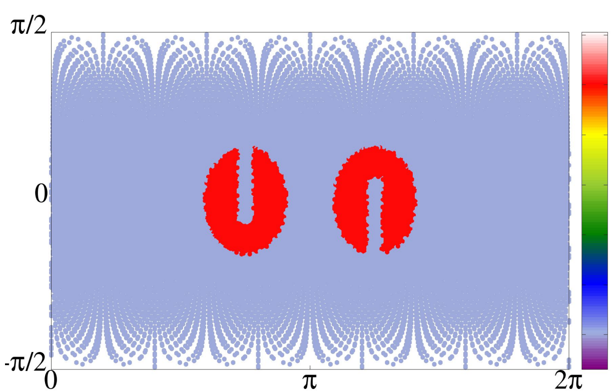
Solid body rotation



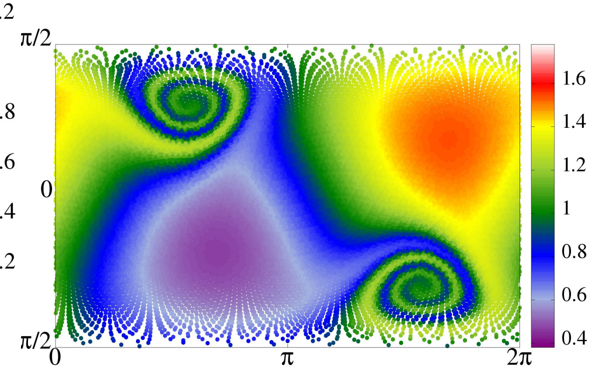
Deformational flow



Deformational flow



Moving vortex



- Divergent velocity
- Non-divergent velocity
- FCT Zalesak Flux limiter (1979)
- One full rotation-12 days

Error norms

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

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

$$l_{\infty,rel} = \frac{\max_{i=\overline{1,n_c}} |q_i - q_i^{true}|}{\max_{i=\overline{1,n_c}} |q_i^{true}|}$$

$$l_{1,abs} = \sum_{i=1}^{n_c} |q_i - q_i^{true}|$$

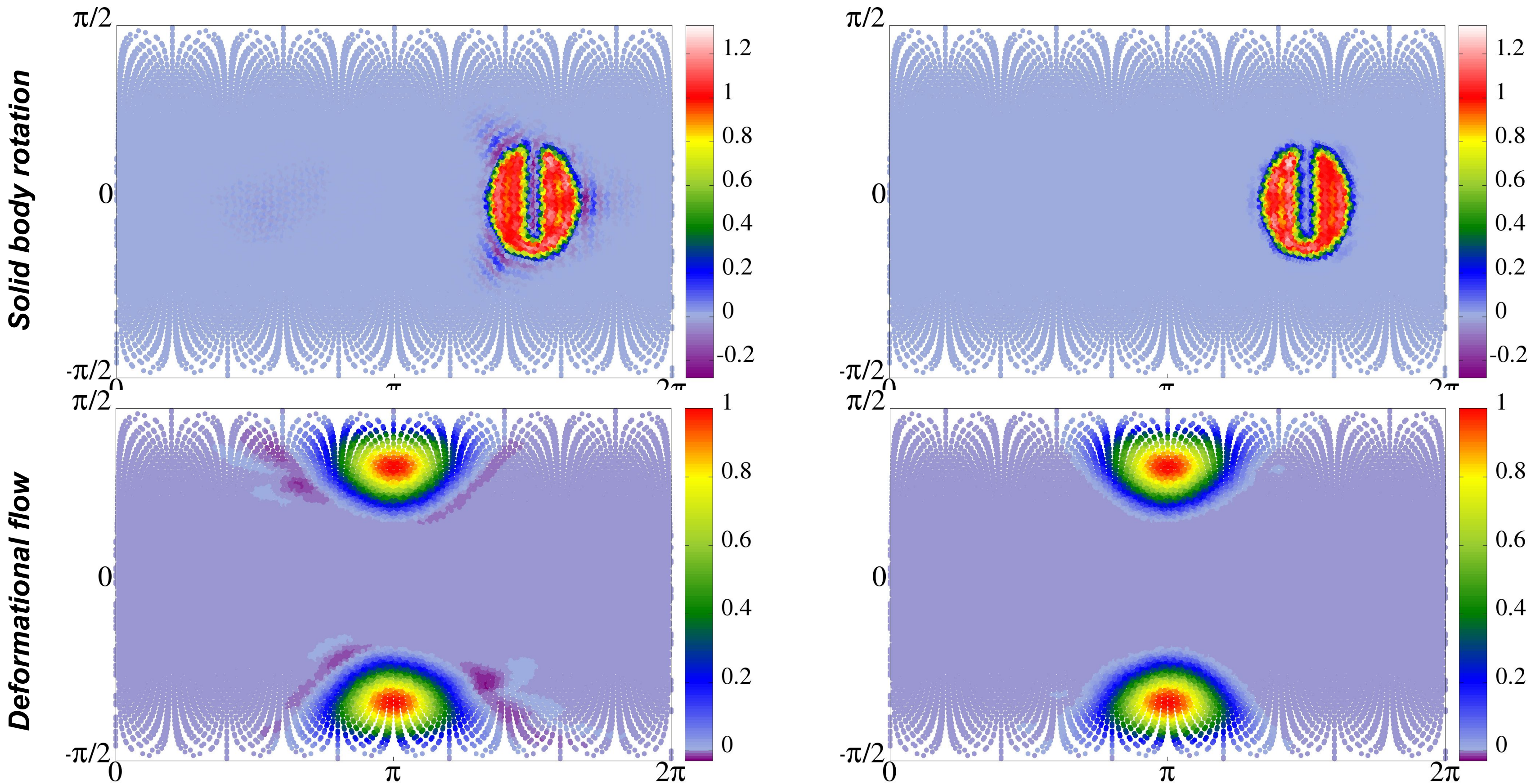
$$l_{2,abs} = \sqrt{\sum_{i=1}^{n_c} (q_i - q_i^{true})^2}$$

$$l_{\infty,abs} = \max_{i=\overline{1,n_c}} |q_i - q_i^{true}|$$

Results: linear advection (I)

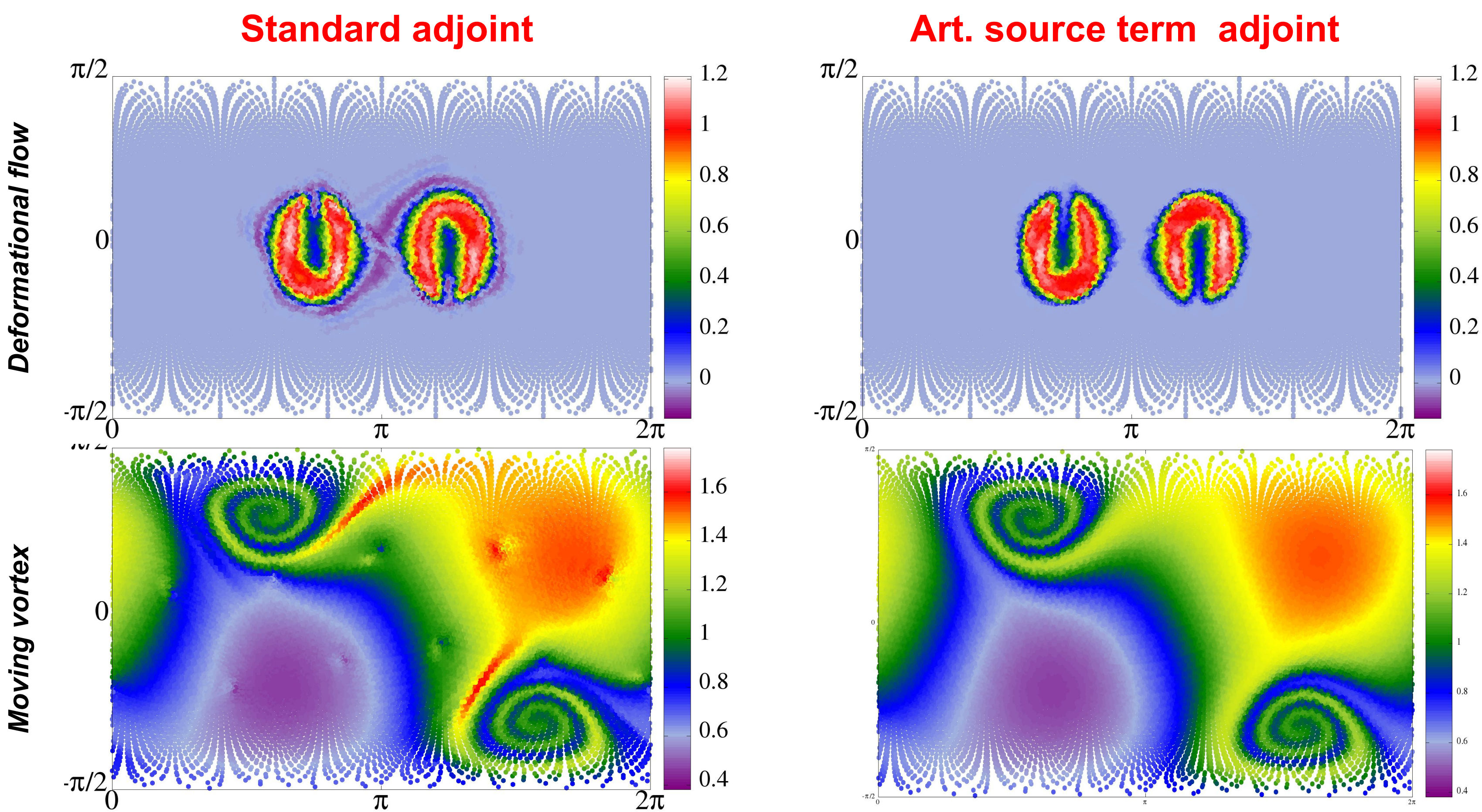
- **Standard adjoint method introduces oscillations and might leads to negative concentration**

Standard adjoint | **Art. source term adjoint**



Results: linear advection (II)

- Artificial source term method has better shape precervance, smaller error norms



Numerical experiments

- **Data assimilation**
  - Convergence
  - Impact of observation points
  - Mesh refinement
  - Manipulating with weights

- Deformational flow with non-divergent velocity vector
- Moving vortex

- *Identical twin experiment*
- *12 hr assimilation window*
- *Grids: R2B4, R2B5, R2B6, R2B7*
- *Observations: 12.5%, 25%, 50%, 100%*
- *Initial error: 10%, or 1% if concentration=0*
- *Observation at each time-step*

Results: data assimilation (I)

- **Convergence**

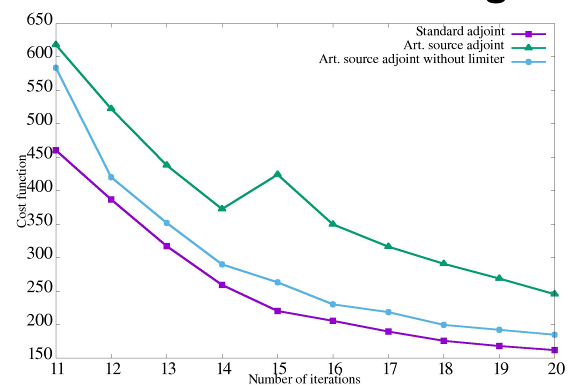
Both methods ensure convergence with increasing number of iterations

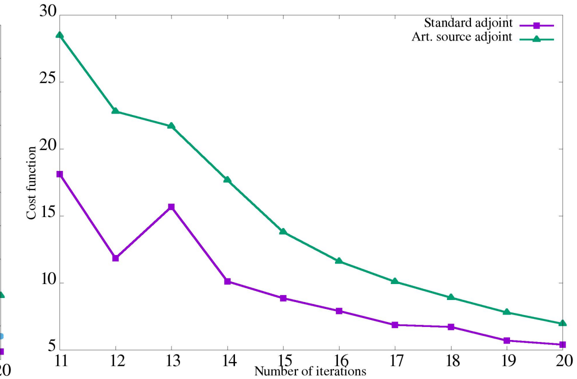
- **Number of observations**

The choice of adjoint solver influences the minimisation process

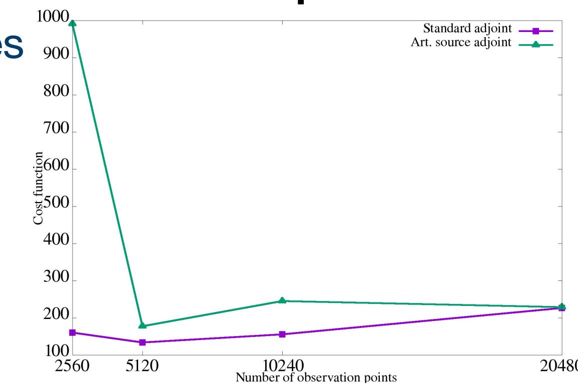
Moving vortex | Deforational flow

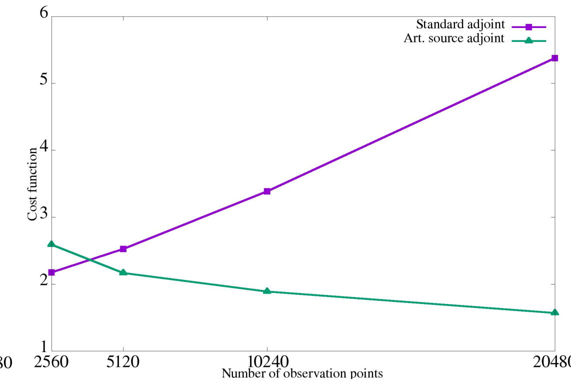
Convergence test





Impact of number of observations





Artificial source term method offers more reliable behavior in most cases

Results: data assimilation (II)

- **Mesh refinement**

Art. source term method yelds smaller final cost function

Mesh refinement

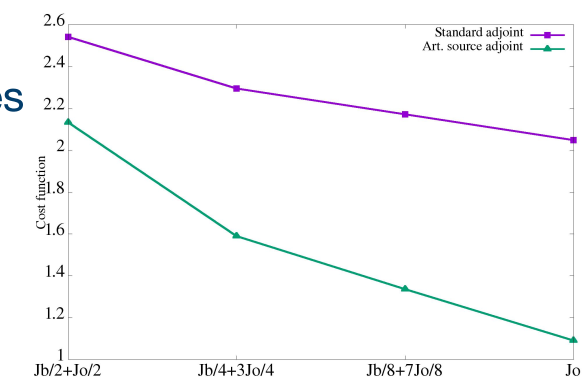
Deformational flow

Grid	Cost	Art. source adjoint without limiter	Art. source adjoint with limiter
R2B4	Final	5.43400710	1.568333807
R2B5	Final	7.25133893	7.422831065
R2B6	Final	6.07498723E+04	6.838604955E+01
R2B7	Final	1.38570810E+05	2.653808533E+02
R2B4	Final	7.42488109E+04	1.24677839E+02
R2B5	Final	2.89551111E+04	2.49163938E+02
R2B6	Final	4.64099399E+05	6.98240016E+02
R2B7	Final	1.12492223E+06	1.38281501E+03

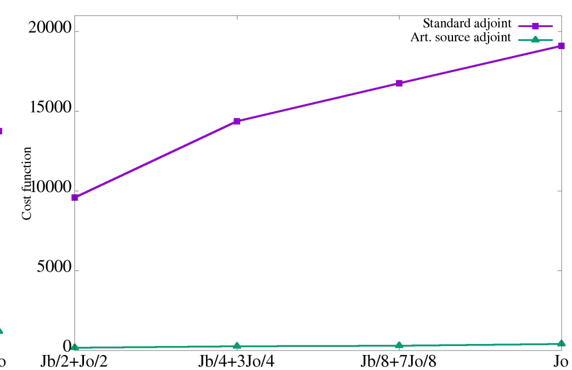
- **Manipulating with weights**

The choice of adjoint solver influences the minimisation process

Manipulating with weights



Moving vortex



Deformational flow

Artificial source term method gives good results when standard approach fails

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3D pure tracer advection test (Jablonowski, 2008)

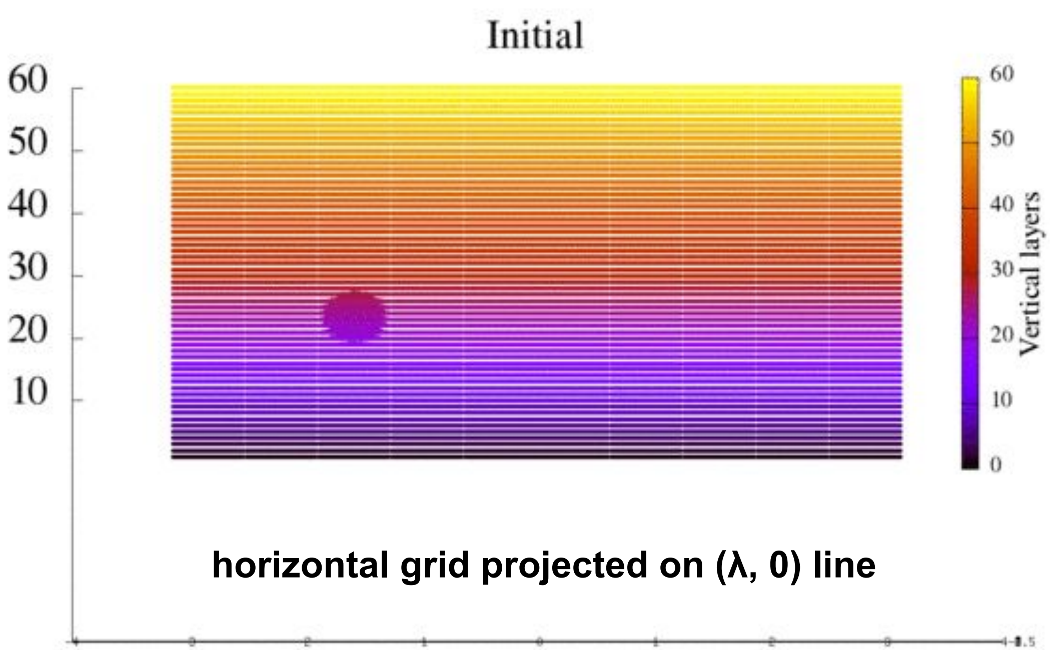
- **Horizontal velocity vector**

$$u(\lambda, \theta, \eta) = u_0 \cos(\theta \cos\alpha + \sin\theta \cos\lambda \sin\alpha),$$
$$v(\lambda, \theta, \eta) = -u_0 \sin\lambda \sin\alpha$$

- **Vertical velocity vector**

$$\dot{\eta}(\lambda, \theta, \eta) = \frac{\omega_0}{p_0} \cos(\frac{2\pi}{\tau} t) \sin(s(\eta)\frac{\pi}{2})$$

➢ Solid body rotation in horizontal direction with a period of 12 days
➢ Wave-like trajectory in the vertical direction with a period of 4 days
➢ 60 vertical layers up to ≈12 km.

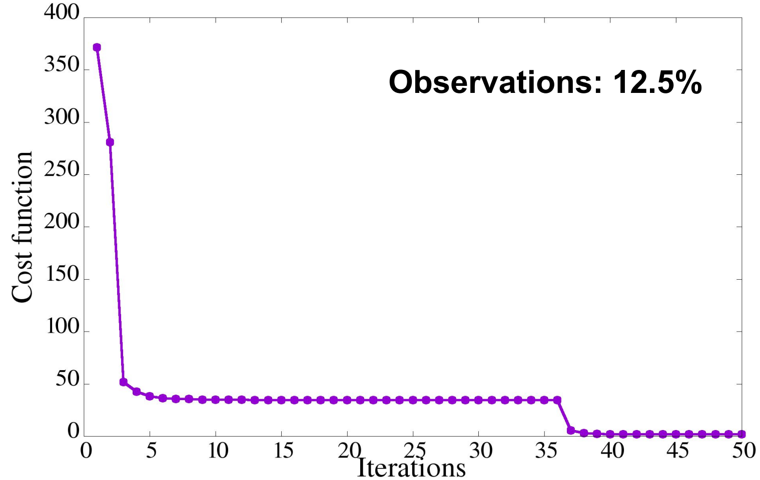


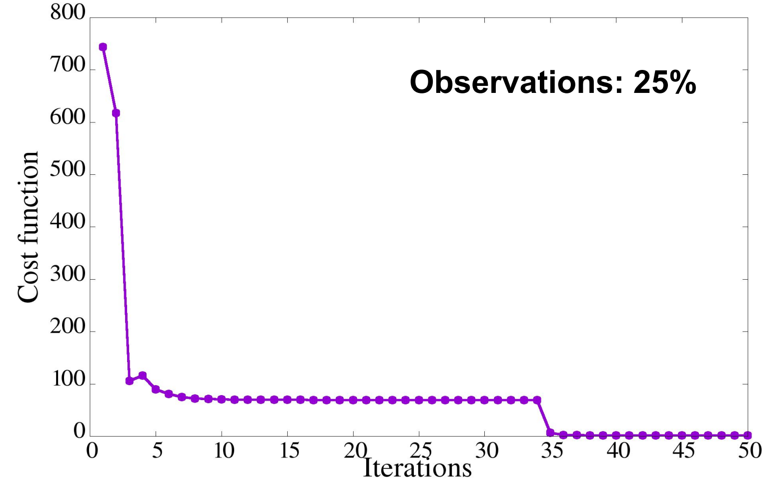
Art. source term adjoint scheme gives the same result as forward scheme

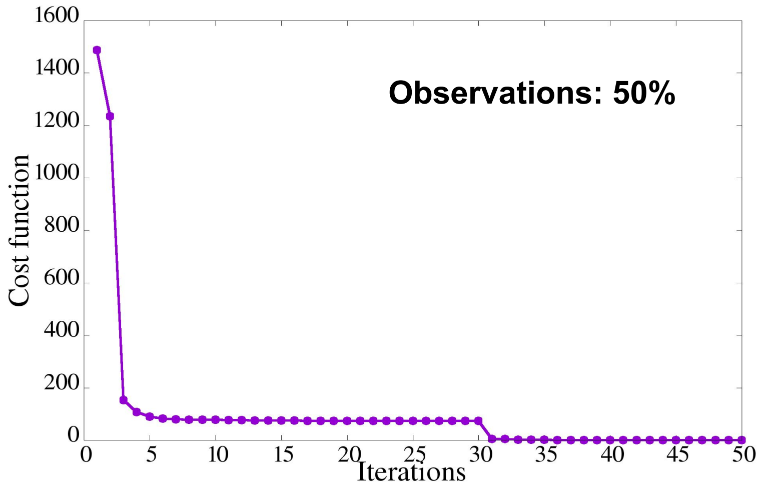
Data assimilation results

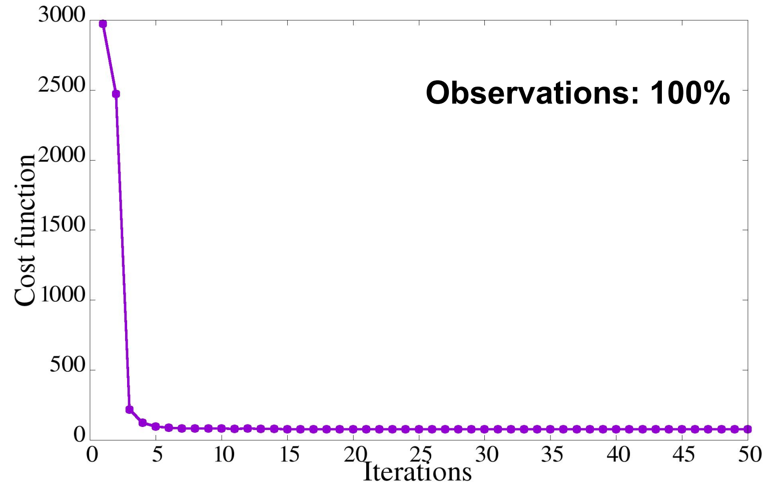
- *6 hr assimilation window*
- *Grids: R2B4*
- *Observations: 12.5%, 25%, 50%, 100%*

- *Initial error: 10%, or 1% if concentration=0, on the layers 34-42*
- *Observation at each time-step*









Thank you !