Seamless integration of hydrostatic, soundproof, and fully compressible equations

(with application to balanced data assimilation)

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CRC 1114
Scaling Cascades in Complex Systems

Unified numerics

Some results

Balanced data assimilation

Outlook

Compressible flow equations

$$
\begin{aligned}
\rho_t + \nabla_\parallel \cdot (\rho \boldsymbol{u}) + (\rho w)_z &= 0 \\
(\rho \boldsymbol{u})_t + \nabla_\parallel \cdot (\rho \boldsymbol{u} \circ \boldsymbol{u}) + (\rho w \boldsymbol{u})_z + c_p P \nabla_\parallel \pi &= -f \boldsymbol{k} \times \rho \boldsymbol{u} \\
(\rho w)_t + \nabla_\parallel \cdot (\rho \boldsymbol{u} \circ w) + (\rho w w)_z + c_p P \pi_z &= -\rho g \\
\underline{P_t + \nabla_\parallel \cdot (P \boldsymbol{u}) + (P w)_z} &= 0 \\
\pi &= P^{\gamma-1} \\
(\underline{P} &= \underline{\rho\theta})
\end{aligned}
$$

Asymptotic flow regimes of the atmosphere

$$
\begin{aligned}
\rho_t + \nabla_\| \cdot (\rho \boldsymbol{u}) + (\rho w)_z &= 0 \\
(\rho \boldsymbol{u})_t + \nabla_\| \cdot (\rho \boldsymbol{u} \circ \boldsymbol{u}) + (\rho w \boldsymbol{u})_z + c_p P \nabla_\| \pi &= -f \boldsymbol{k} \times \rho \boldsymbol{u} \\
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P_t + \nabla_\| \cdot (P \boldsymbol{u}) + (P w)_z &= 0 \\
\pi &= P^{\gamma - 1} \\
(P &= \rho \theta)
\end{aligned}
$$

drop terms (roughly speaking) for:

- geostrophic
- hydrostatic
- pseudo-incompressible (soundproof)

Asymptotic flow regimes of the atmosphere

$$
\begin{aligned}
\rho_t + \nabla_\| \cdot (\rho \boldsymbol{u}) + (\rho w)_z &= 0 \\
(\rho \boldsymbol{u})_t + \nabla_\| \cdot (\rho \boldsymbol{u} \circ \boldsymbol{u}) + (\rho w \boldsymbol{u})_z + c_p P \nabla_\| \pi &= -f \boldsymbol{k} \times \rho \boldsymbol{u} \\
(\rho w)_t + \nabla_\| \cdot (\rho \boldsymbol{u} \circ w) + (\rho w w)_z + c_p P \pi_z &= -\rho g \\
P_t + \nabla_\| \cdot (P \boldsymbol{u}) + (P w)_z &= 0 \\
\pi &= P^{\gamma - 1} \\
(P &= \rho \theta)
\end{aligned}
$$

Unified numerics – what for?

- “fair” math model comparison*
- asymptotic consistency†
- **balanced data assimilation**

* Smolarkiewicz & Dörnbrack, IJ Num. Meth. Fluids, **56** (2007)

† M.J.P. Cullen, Acta Numer., **16** (2007)

Slight change of perspective on advection

$$
\begin{aligned}
(P\chi)_t + \nabla_\parallel \cdot (P\boldsymbol{u}\chi) + (Pw\chi) &= 0 \\
(P\chi\boldsymbol{u})_t + \nabla_\parallel \cdot (P\boldsymbol{u} \circ \chi\boldsymbol{u}) + (Pw\chi\boldsymbol{u})_z + c_p P \nabla_\parallel \pi &= -f\boldsymbol{k} \times P\chi\boldsymbol{u} \\
(P\chi w)_t + \nabla_\parallel \cdot (P\boldsymbol{u} \circ \chi w) + (Pw\chi w)_z + c_p P \pi_z &= -P\chi g
\end{aligned}
$$

$$
\begin{aligned}
P_t + \nabla_\parallel \cdot (P\boldsymbol{u}) + (Pw)_z &= 0 \\
\pi &= P^{\gamma-1} \\
(\rho &= P\chi) \qquad (\chi = 1/\theta)
\end{aligned}
$$

Change of variables:

P is the central variable for Low-Mach divergence control

System rewritten with $P\boldsymbol{u}$, Pw as the "advecting fluxes"

Fast-slow separation

Perturbation entropy

$$\chi(t, \boldsymbol{x}, z) = \overline{\chi}(z) + \chi'(t, \boldsymbol{x}, z)$$

Slow-fast sorting of terms

$$\begin{aligned}
\rho_t \quad + \quad \nabla_\parallel \cdot (P\boldsymbol{u}\,\chi') + (Pw\,\chi')_z \quad &= -Pw\,\frac{d\overline{\chi}}{dz} \\
(\rho\boldsymbol{u})_t + \nabla_\parallel \cdot (P\boldsymbol{u} \circ \chi\boldsymbol{u}) + (Pw\,\chi\boldsymbol{u})_z &= -P\left(c_p \nabla_\parallel \pi + f\boldsymbol{k} \times \chi\boldsymbol{u}\right) \\
(\rho w)_t + \ \nabla_\parallel \cdot (P\boldsymbol{u}\,\chi w) + (Pw\,\chi w)_z \ &= -P\left(c_p \pi_z + \chi g\right) \\
P_t \qquad\qquad\qquad\qquad\qquad\qquad &= -\nabla_\parallel \cdot (P\boldsymbol{u}) + (Pw)_z\,.
\end{aligned}$$

Advection (slow) — Sound & IGWs (fast)

IGW: internal gravity waves

Primary (full) and auxiliary variables

Primary variables and equations with evolution of $\boldsymbol{Pv}$

$$
\begin{aligned}
\rho_t \quad + \quad \nabla_\parallel \cdot (P\boldsymbol{u}\,\chi) + (Pw\,\chi)_z &= 0 \\
(P\chi\boldsymbol{u})_t + \nabla_\parallel \cdot (P\boldsymbol{u} \circ \chi\boldsymbol{u}) + (Pw\,\chi\boldsymbol{u})_z &= -\Big(c_p P \nabla_\parallel \pi + f\boldsymbol{k} \times \chi P\boldsymbol{u} \Big) \\
(P\chi w)_t + \nabla_\parallel \cdot (P\boldsymbol{u}\,\chi w) + (Pw\,\chi w)_z &= -\left(c_p P \pi_z + P(\overline{\chi} + \chi')g \right) \\
P_t \quad + \quad \nabla_\parallel \cdot (P\boldsymbol{u}) + (Pw)_z &= 0
\end{aligned}
$$

Auxiliary variables and equations for balanced flux/source calculations

$$
\begin{aligned}
(P\chi')_t + \nabla_\parallel \cdot (P\boldsymbol{u}\,\chi') + (Pw\,\chi')_z &= -Pw\,\frac{d\overline{\chi}}{dz} \\
\frac{\partial P}{\partial \pi}\,\pi_t &= -\nabla_\parallel \cdot (P\boldsymbol{u}) + (Pw)_z \,.
\end{aligned}
$$

Decomposition into linear substeps I

Given $P\boldsymbol{u}, Pw \quad \Rightarrow$

compressible*† linear advection of $(\chi, \chi\boldsymbol{u}, \chi w, \chi')$ **& full evolution of** (ρ, P)

$$
\begin{aligned}
(P\chi)_t + \nabla_\parallel \cdot (P\boldsymbol{u}\,\chi) + (Pw\,\chi)_z &= 0 \\
(P\chi\boldsymbol{u})_t + \nabla_\parallel \cdot (P\boldsymbol{u} \circ \chi\boldsymbol{u}) + (Pw\,\chi\boldsymbol{u})_z &= -\left((c_p P/\chi)\nabla_\parallel \pi + f\boldsymbol{k} \times P\boldsymbol{u}\right) \\
(P\chi w)_t + \nabla_\parallel \cdot (P\boldsymbol{u}\,\chi w) + (Pw\,\chi w)_z &= -\left((c_p P/\chi)\pi_z + Pg\right) \\
P_t + \nabla_\parallel \cdot (P\boldsymbol{u}) + (Pw)_z &= 0
\end{aligned}
$$

$$
\begin{aligned}
(P\chi')_t + \nabla_\parallel \cdot (P\boldsymbol{u}\,\chi') + (Pw\,\chi')_z &= -Pw\,\frac{d\overline{\chi}}{dz} \\
\frac{\partial P}{\partial \pi}\pi_t &= -\nabla_\parallel \cdot (P\boldsymbol{u}) + (Pw)_z\,.
\end{aligned}
$$

* Blossey, Durran, J. Comput. Phys., **227** (2008)

† K., TCFD, **23** (2009)

Decomposition into linear substeps II

Given $\rho, P, \chi = \rho/P \quad \Rightarrow$

"linear" acoustic/inertia-gravity wave system for $(P\boldsymbol{u}, Pw, \chi', \pi)$

$$
\begin{aligned}
\rho_t \quad &+ \quad \nabla_\parallel \cdot (P\boldsymbol{u}\,\chi) + (P\boldsymbol{w}\,\chi)_z &&= 0 \\
\chi(P\boldsymbol{u})_t &+ \nabla_\parallel \cdot (P\boldsymbol{u} \circ \chi\boldsymbol{u}) + (Pw\,\chi\boldsymbol{u})_z &&= -P\,c_p \nabla_\parallel \pi + f\boldsymbol{k} \times \chi P\boldsymbol{u} \\
\chi(Pw)_t &+ \nabla_\parallel \cdot (P\boldsymbol{u}\,\chi w) + (Pw\,\chi w)_z &&= -P\left(c_p \pi_z + g(\overline{\chi} + \chi')\right) \\
P_t \quad &+ \quad \nabla_\parallel \cdot (P\boldsymbol{u}) + (Pw)_z &&= 0
\end{aligned}
$$

$$
\begin{aligned}
(P\chi')_t \; &+ \; \nabla_\parallel \cdot (P\boldsymbol{u}\,\chi') + (Pw\,\chi')_z &&= -Pw\,\frac{d\overline{\chi}}{dz} \\
\frac{\partial P}{\partial \pi}\,\pi_t & &&= -\nabla_\parallel \cdot (P\boldsymbol{u}) + (Pw)_z\,.
\end{aligned}
$$

Decomposition into linear substeps II

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\begin{aligned}
\rho_t \quad &+ \quad \nabla_{\|} \cdot (P\boldsymbol{u}\,\chi) + (P\boldsymbol{w}\,\chi)_z &&= 0 \\
\chi(P\boldsymbol{u})_t &+ \nabla_{\|} \cdot (P\boldsymbol{u} \circ \chi\boldsymbol{u}) + (Pw\,\chi\boldsymbol{u})_z &&= -P\,c_p \nabla_{\|} \pi + f\boldsymbol{k} \times \chi P\boldsymbol{u} \\
\chi(Pw)_t &+ \nabla_{\|} \cdot (P\boldsymbol{u}\,\chi w) + (Pw\,\chi w)_z &&= -P\,(c_p \pi_z + g(\overline{\chi} + \chi')) \\
P_t \quad &+ \quad \nabla_{\|} \cdot (P\boldsymbol{u}) + (Pw)_z &&= 0
\end{aligned}
$$

$$
\begin{aligned}
(P\chi')_t \quad &+ \quad \nabla_{\|} \cdot (P\boldsymbol{u}\,\chi') + (Pw\,\chi')_z &&= -Pw\,\frac{d\overline{\chi}}{dz} \\
\frac{\partial P}{\partial \pi}\,\pi_t & &&= -\nabla_{\|} \cdot (P\boldsymbol{u}) + (Pw)_z\,.
\end{aligned}
$$

The only (VERY WEAK) linearization in the entire scheme

Borrowing from Piotr's compact notation*

Define

$$\Psi = (\chi, \chi \boldsymbol{u}, \chi w, \chi')$$

and subsume the Euler system ***(incl. auxiliary variables)*** **as**

$$(P\Psi)_t + \mathcal{A}(\Psi; P\boldsymbol{v}) = Q(\Psi, P; \pi)$$

$$P_t + \nabla \cdot (P\boldsymbol{v}) = 0 \,.$$

(2 incarnations for P, π)

* **see, e.g., P.K. Smolarkiewicz and L.G. Margolin, Atmosphere-Ocean Special, 127–157 (1997)**

Borrowing from Piotr's time stepping ideas*

Given $(P\boldsymbol{v})^{n+1/2}$, ...

$$
\begin{aligned}
(P\Psi)^{*} &= (P\Psi)^{n} + \frac{\Delta t}{2} Q\left(\Psi^{n}, P^{n}; \pi^{n}\right) \\
(P\Psi)^{**} &= \mathcal{A}_{2_{\text{nd}}}^{\Delta t}\left(\Psi^{*}; (P\boldsymbol{v})^{n+1/2}\right) \\
(P\Psi)^{n+1} &= (P\Psi)^{**} + \frac{\Delta t}{2} Q\left(\Psi^{n+1}, P^{n+1}; \pi^{n+1}\right) .
\end{aligned}
$$

(slow) robust Advection by Δt bracketed by

$(\Delta t/2)$-steps of the implicit trapezoidal rule for the (fast) Ac/IGW-terms

* **see, e.g., Kühnlein, et al., *A nonhydrostatic finite-volume formulation of IFS*, Geosci. Mod. Dev. Disc., 12 (2019)**

Borrowing from Piotr's time stepping ideas

Given $(P\boldsymbol{v})^{n+1/2}$, ...

$$(P\Psi)^{*} = (P\Psi)^{n} + \frac{\Delta t}{2} Q\left(\Psi^{n}, P^{n}; \pi^{n}\right)$$

$$(P\Psi)^{**} = \mathcal{A}_{2_{\text{nd}}}^{\Delta t}\left(\Psi^{*}; (P\boldsymbol{v})^{n+1/2}\right)$$

$$(P\Psi)^{n+1} = (P\Psi)^{**} + \frac{\Delta t}{2} Q\left(\Psi^{n+1}, P^{n+1}; \pi^{n+1}\right) .$$

Remarks

- **This is a second-order split* scheme, but ...**
- **... it is *NOT* standard Strang-splitting**
  (1st and last step are first-order only)
- $(P\boldsymbol{v})^{n+1/2}$ **remains to be determined**

* Please excuse my language here, Piotr ☺

Intermediate time advective fluxes

Desired: second order full time step for P

$$P^{n+1} = P^n - \Delta t \nabla \cdot (P\boldsymbol{v})^{n+\frac{1}{2}}$$

implicit midpoint rule!

(Semi-)Implicit midpoint update for P

$(\Delta t/2)$ Advection step

$$
\begin{aligned}
(P\Psi)^{\#} &= \mathcal{A}_{\text{1st}}^{\frac{\Delta t}{2}}\left(\Psi^n; (P\boldsymbol{v})^n\right) \\
P^{\#} &= P^n - \frac{\Delta t}{2}\widetilde{\nabla}\cdot(P\boldsymbol{v})^n \,.
\end{aligned}
$$

$(\Delta t/2)$ **backward Euler** step for the fast system

$$
\begin{aligned}
(P\Psi)^{n+\frac{1}{2}} &= (P\Psi)^{\#} + \frac{\Delta t}{2} Q\left(\Psi^{n+1/2}, P^{\#}; \pi^{n+1/2}\right) \,, \\
P^{n+\frac{1}{2}} &= P^n - \frac{\Delta t}{2}\nabla\cdot(P\boldsymbol{v})^{n+\frac{1}{2}}
\end{aligned}
$$

linearized or iterated closure via eqn. of state

$$
P^{n+\frac{1}{2}} = P^n + \left(\frac{\partial P}{\partial \pi}\right)^{\#}\left(\pi^{n+\frac{1}{2}} - \pi^n\right)
$$

- Semi-implicit Euler step for $P^{n+\frac{1}{2}}$
- Generates advecting fluxes $(P\boldsymbol{v})^{n+\frac{1}{2}}$
- Generates P^{n+1} via implicit midpoint rule

Summary

$\boldsymbol{P}^{\boldsymbol{n+1}} = P^n - \Delta t \nabla \cdot (\boldsymbol{P v})^{\boldsymbol{n+1/2}}$	**implicit midpoint**	(slow/fast)
$(P\boldsymbol{\Psi})^* = (P\Psi)^n + \frac{\Delta t}{2} Q\left(\Psi^n, P^n; \pi^n\right)$	**forward Euler**	(fast)
$(P\boldsymbol{\Psi})^{**} = \mathcal{A}_{\text{2nd}}^{\Delta t}\left(\Psi^*; (P\boldsymbol{v})^{n+1/2}\right)$	**2nd order upwind**	(slow)
$(P\boldsymbol{\Psi})^{n+1} = (P\Psi)^{**} + \frac{\Delta t}{2} Q\left(\boldsymbol{\Psi}^{\boldsymbol{n+1}}, P^{n+1}; \boldsymbol{\pi}^{\boldsymbol{n+1}}\right)$	**backward Euler**	(fast)

Sole linearization (compressible case only):

$$P^{n+*} = P^n + \left(\frac{\partial P}{\partial \pi}\right)^{\#} \left(\pi^{n+*} - \pi^n\right)$$

Seamless access to reduced models

Backward Euler for Ac/IGW subsystem

$$
\begin{aligned}
\boldsymbol{U}^{n+1} &= \boldsymbol{U}^{n} - \Delta t \left(c_p P\theta \;\; \nabla_{\|} \pi'^{\,n+1} - f \boldsymbol{k} \times \boldsymbol{U}^{n+1} \right) \\
\alpha_{\text{hy}} W^{n+1} &= \alpha_{\text{hy}} W^{n} - \Delta t \left(c_p P\theta \;\; \partial_z \pi'^{\,n+1} + (g/\chi) \; \widetilde{\chi}^{n+1} \right) \\
\widetilde{\chi}^{n+1} &= \widetilde{\chi}^{n} - \Delta t \left(\frac{d\overline{\chi}}{dz} \, W^{n+1} \right) \\
\alpha_{\text{pi}} \frac{\partial P}{\partial \pi} \pi'^{\,n+1} &= \alpha_{\text{pi}} \frac{\partial P}{\partial \pi} \pi'^{\,n} - \Delta t \; \left(\nabla_{\|} \cdot \boldsymbol{U}^{n+1} + \partial_z W^{n+1} \right) .
\end{aligned}
$$

$$
\begin{aligned}
(\boldsymbol{U}, W) &= (P\boldsymbol{u}, Pw) \\
\widetilde{\chi} &= P\chi'
\end{aligned}
$$

Switches

α_{hy} : hydrostatic / non-hydrostatic $\qquad$ α_{pi} : compressible / pseudo-inc.

Unified numerics

Some results

Balanced data assimilation

Outlook

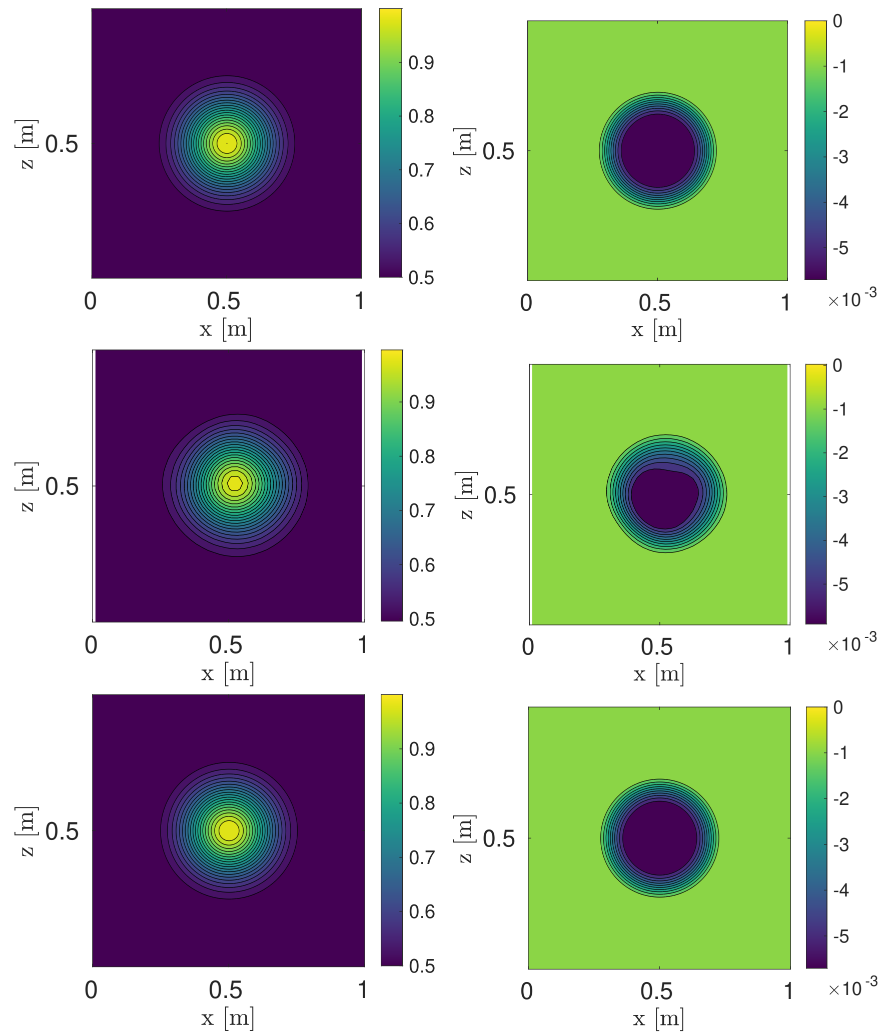
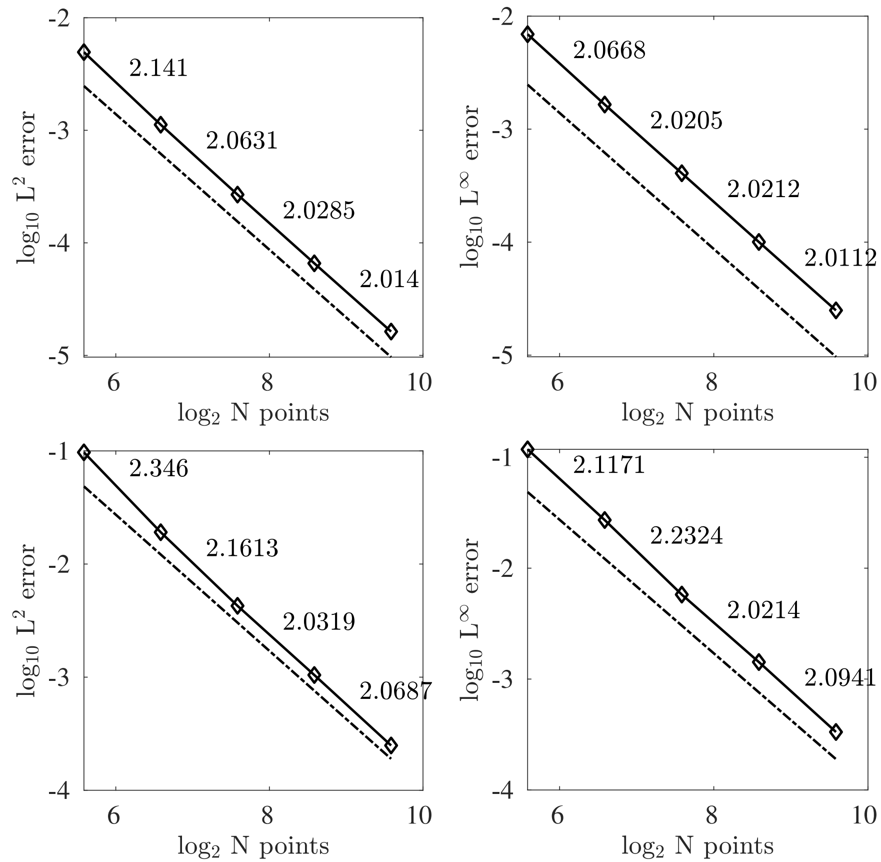


Figure 1: Density (left) and nodal pressure perturbation (right) in the travelling vortex case, initial data (top), computed solution at $T = 1\,\mathrm{s}$ on a grid with 48×48 points (middle) and 768×768 points (bottom).

Travelling vortex test case*

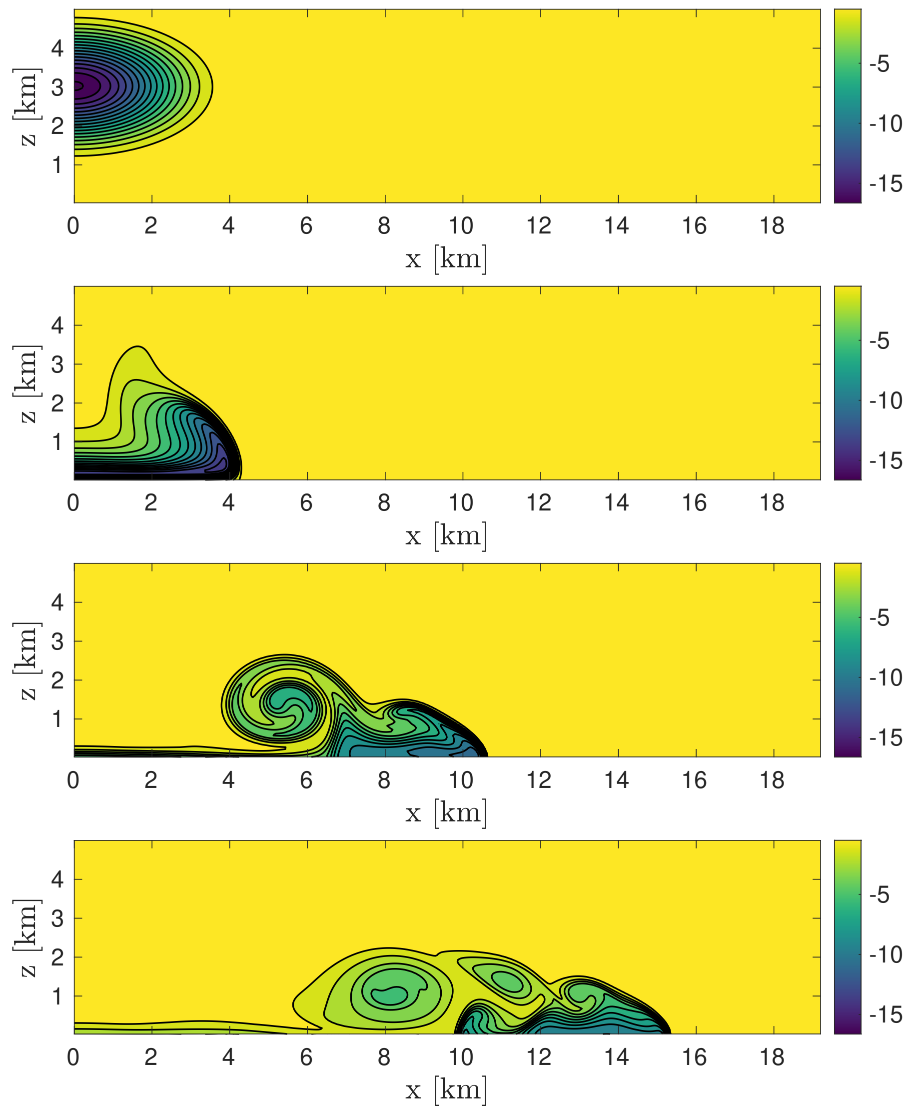


Empirical convergence

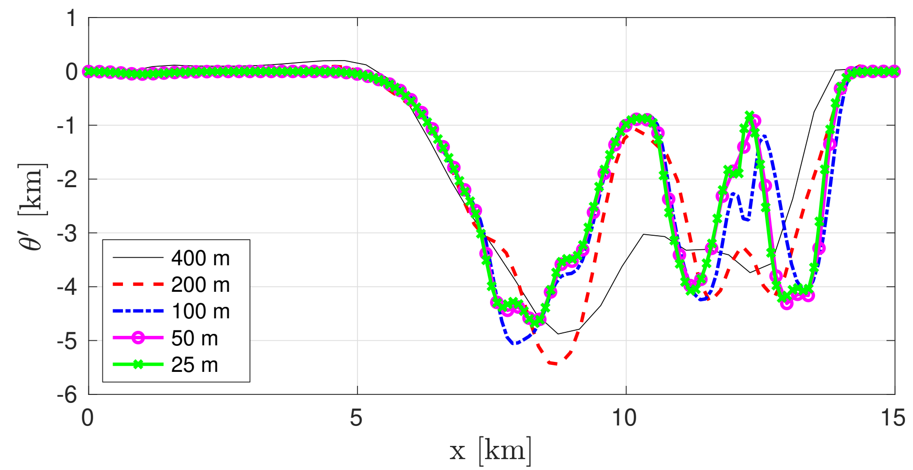
Top: Density; Bottom: Pressure

Benacchio, R. K., Mon. Wea. Rev., **147** (2019)

* Kadioglu et al., J. Comput. Phys., **227** (2008)



Straka's gravity current test*

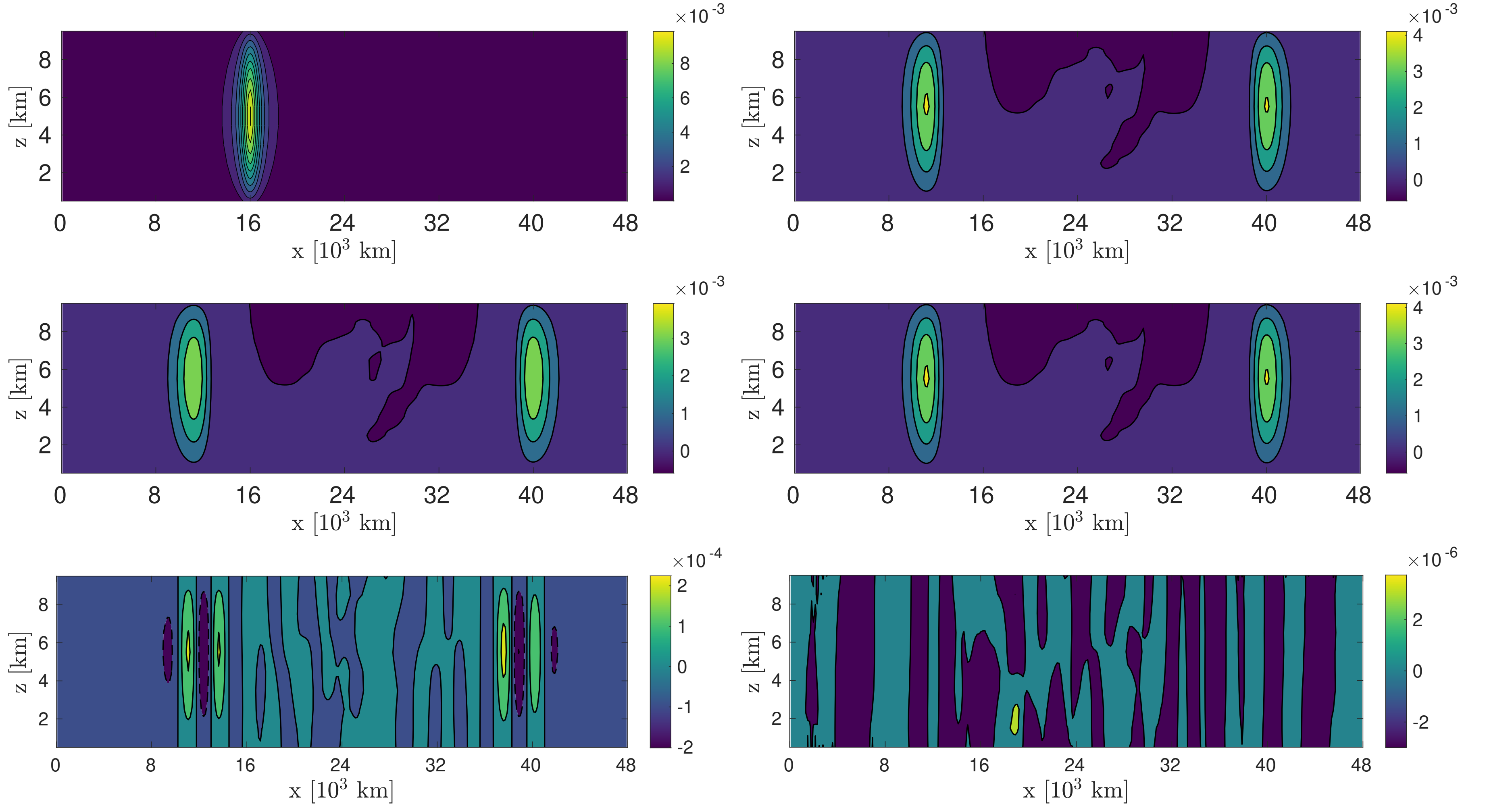


Qualitative empirical convergence
Potential temperature

Benacchio, K., Mon. Wea. Rev., **147** (2019)

* J.M. Straka et al., Int. J. Numer. Meth. Fluids, **17**, 1–22 (1993)

Planetary scale internal gravity wave test* ($\Delta t = 7\,100\,\mathrm{s}$; $N\Delta t = 71$)



top left: potential temperature perturbation initial data; **top right:** compressible solution $t = 480\,000\,\mathrm{s}$

middle left: pseudo-incompressible solution; **middle right:** hydrostatic solution

bottom row: differences to compressible solution

Benacchio, K., Mon. Wea. Rev., **147** (2019)

* Skamarock, Klemp, Mon. Wea. Rev., **122** (1994)

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Some results

Balanced data assimilation

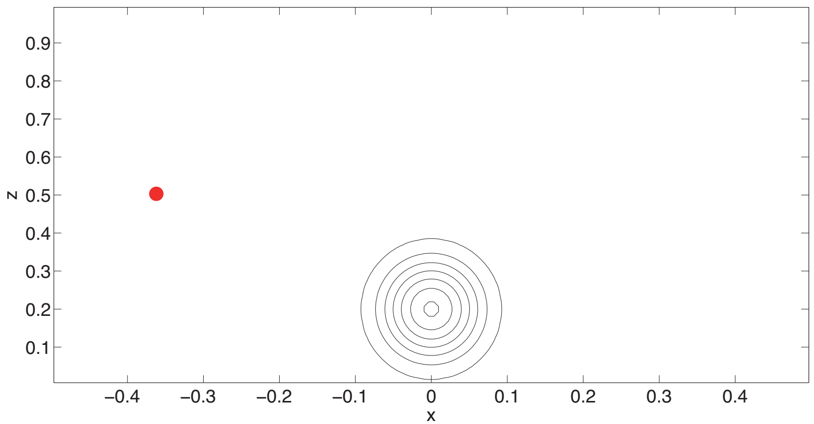
Outlook

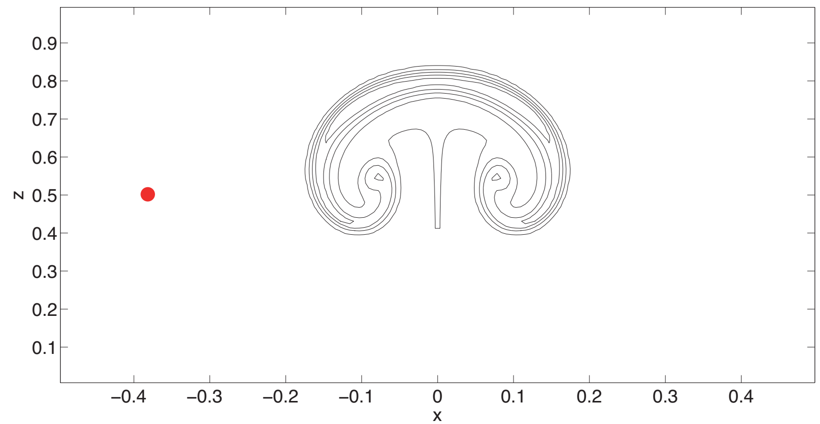
Imbalanced data / semi-implicit time integration

Rising Bubble test case

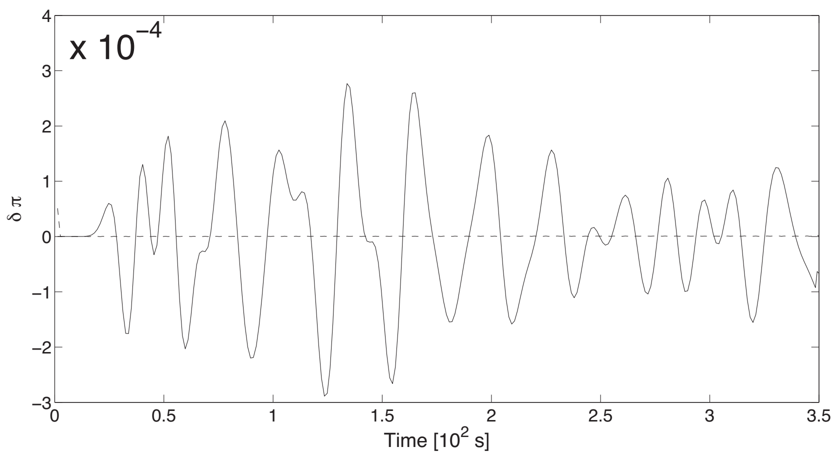
($\delta\theta = 2$ K; $[-10, 10] \times [0, 10]$ km; $t \in \{0, 1050\}$ s)

$\boldsymbol{\theta}$





$\boldsymbol{\delta\pi}$ at ●



compressible simulation, $\delta\pi = \pi^{n+1} - \pi^{n}$

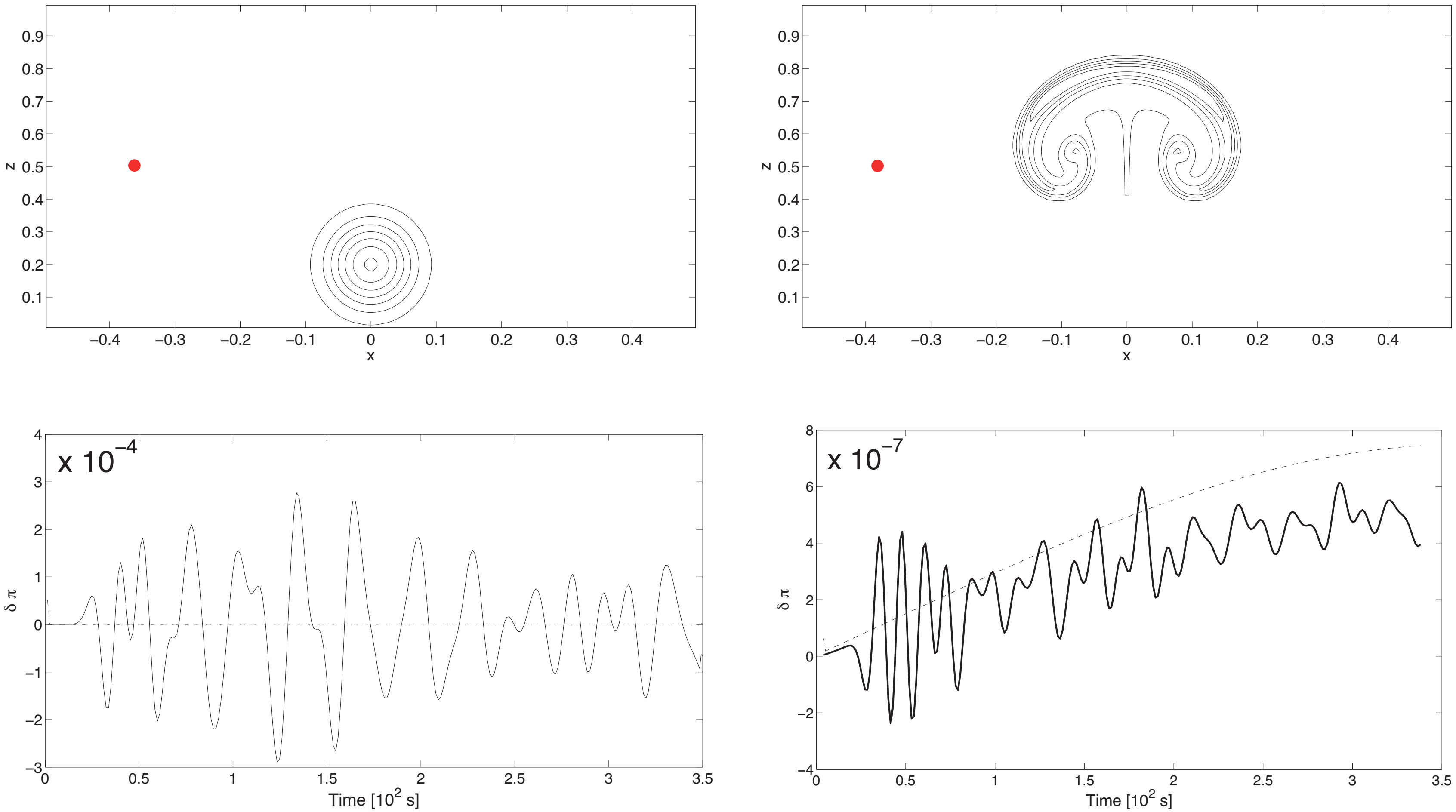
Balanced initialization for data assimilation

Rising Bubble test case

($\delta\theta = 2$ K; $[-10, 10] \times [0, 10]$ km; $t \in \{0, 1050\}$ s)

θ

$\delta\pi$ at ●



compressible $\delta\pi \sim 10^{-4}$

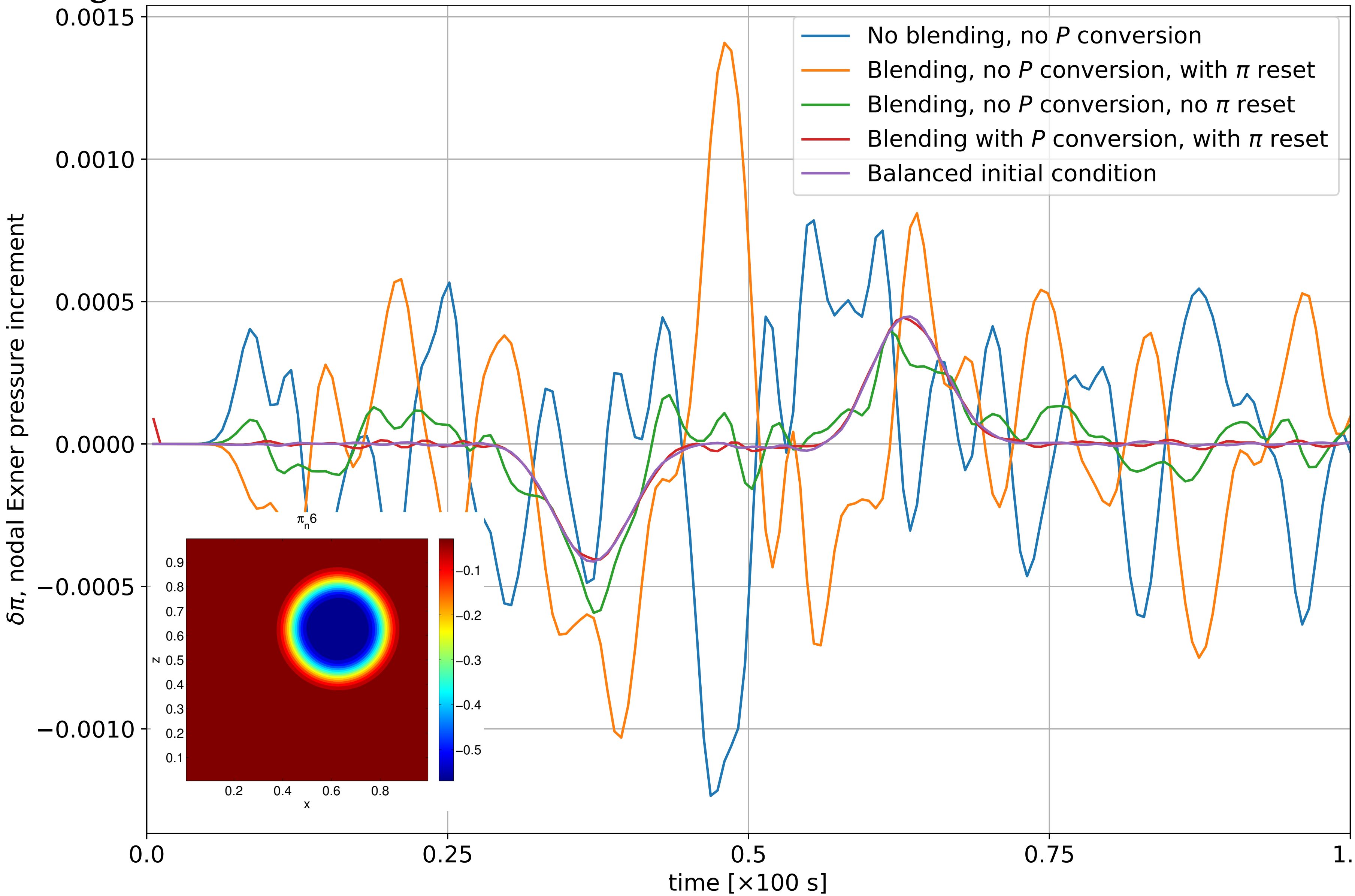
$\alpha_{pi} \equiv \mathbf{1.0}$

blended $\delta\pi \sim 10^{-7}$

$\alpha_{pi} = [\mathbf{0.0, 0.733, 1.0, 1.0, \ldots}]$

Balanced initialization for data assimilation

Travelling vortex test



Improved balance I

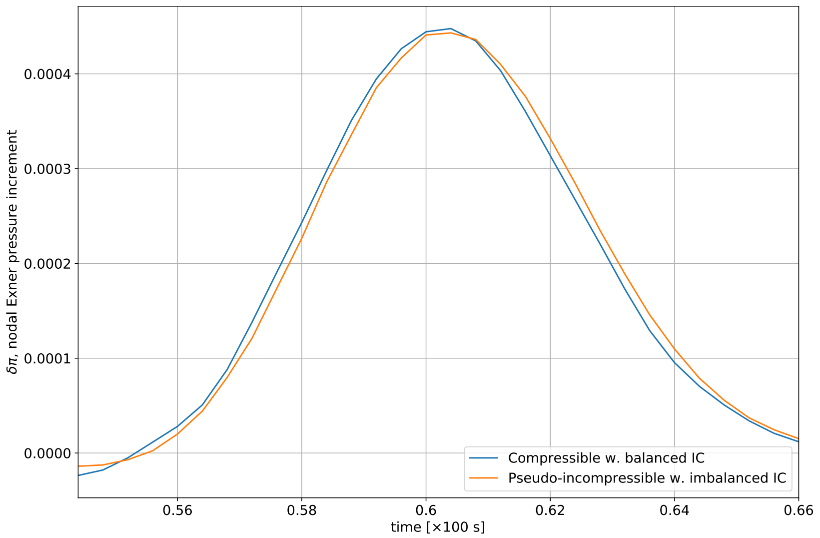
Use analytical insights to reset P, π:

1) Low Mach number ($\mathrm{M} \ll 1$) asymptotic adjustment of $P = \rho\theta$

$$P_{\text{comp}} = \overline{P}_{\text{pi}} + \mathrm{M}^2 \frac{\partial P}{\partial \pi} \left(\pi^{(2)}_{\text{pi}} - \overline{\pi^{(2)}_{\text{pi}}}\right) + \text{h.o.t}$$

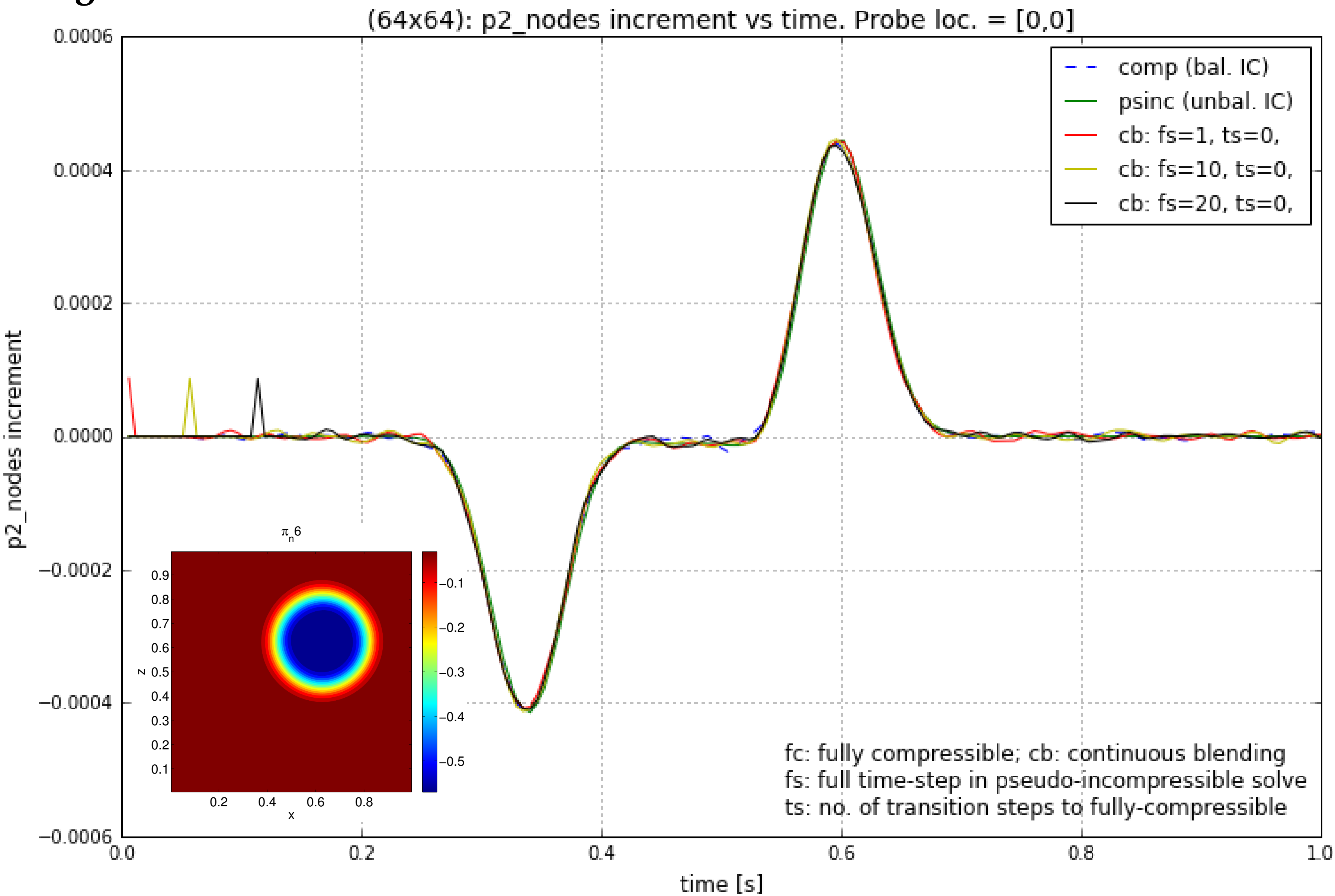
2) Optimized match of pressure time levels

$$\pi^{(2),n+1}_{\text{pi}} = \frac{1}{2}\left(\pi^{(2),n+1}_{\text{comp}} + \pi^{(2),n}_{\text{comp}}\right)$$



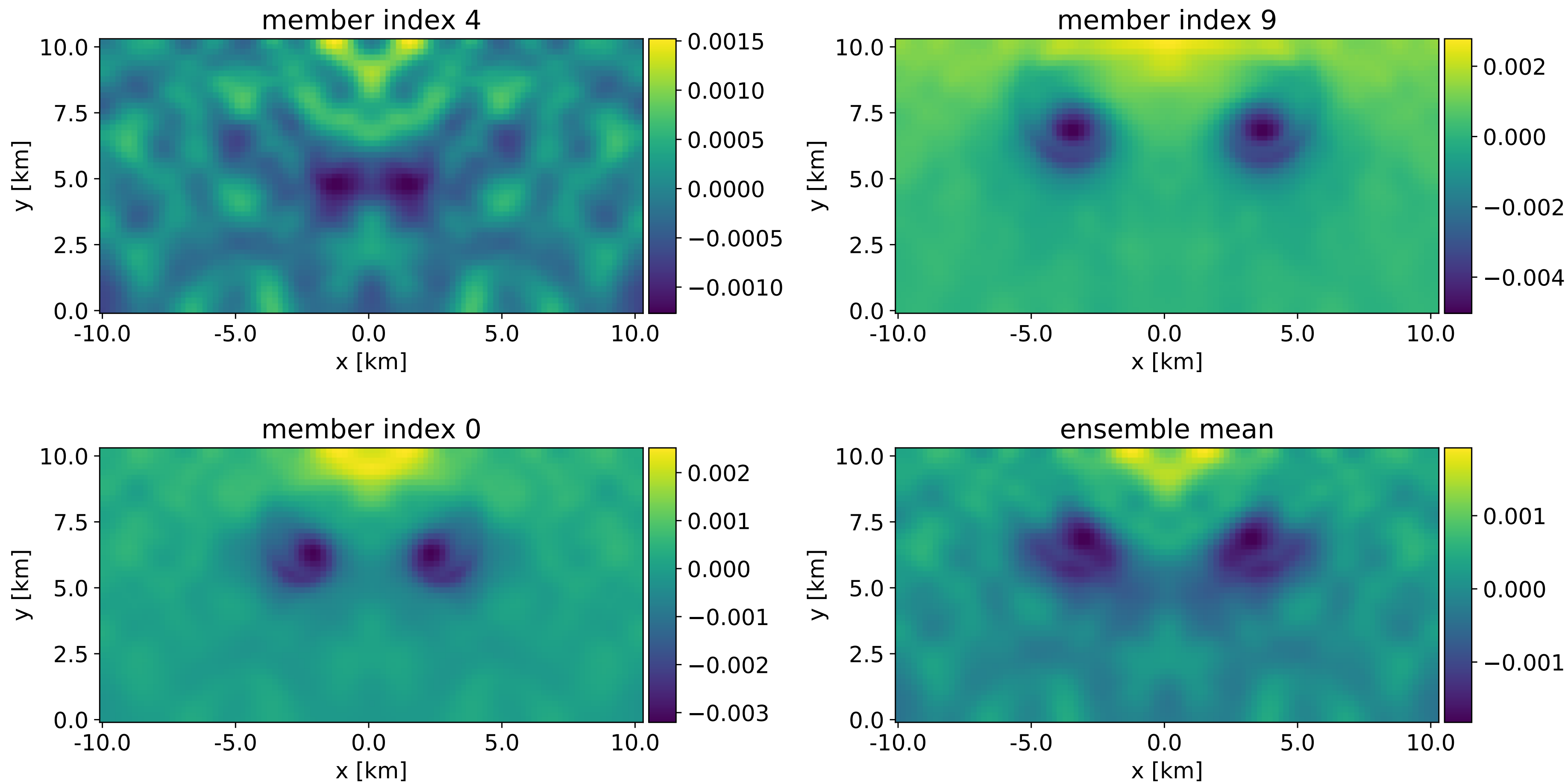
Optimized balance I

Travelling vortex test



Rising bubble, LETKF-based data assimilation

Ensemble with data assimilation without blending. Quantity is π, nodal Exner pressure at output time $t = 1000.0$s.

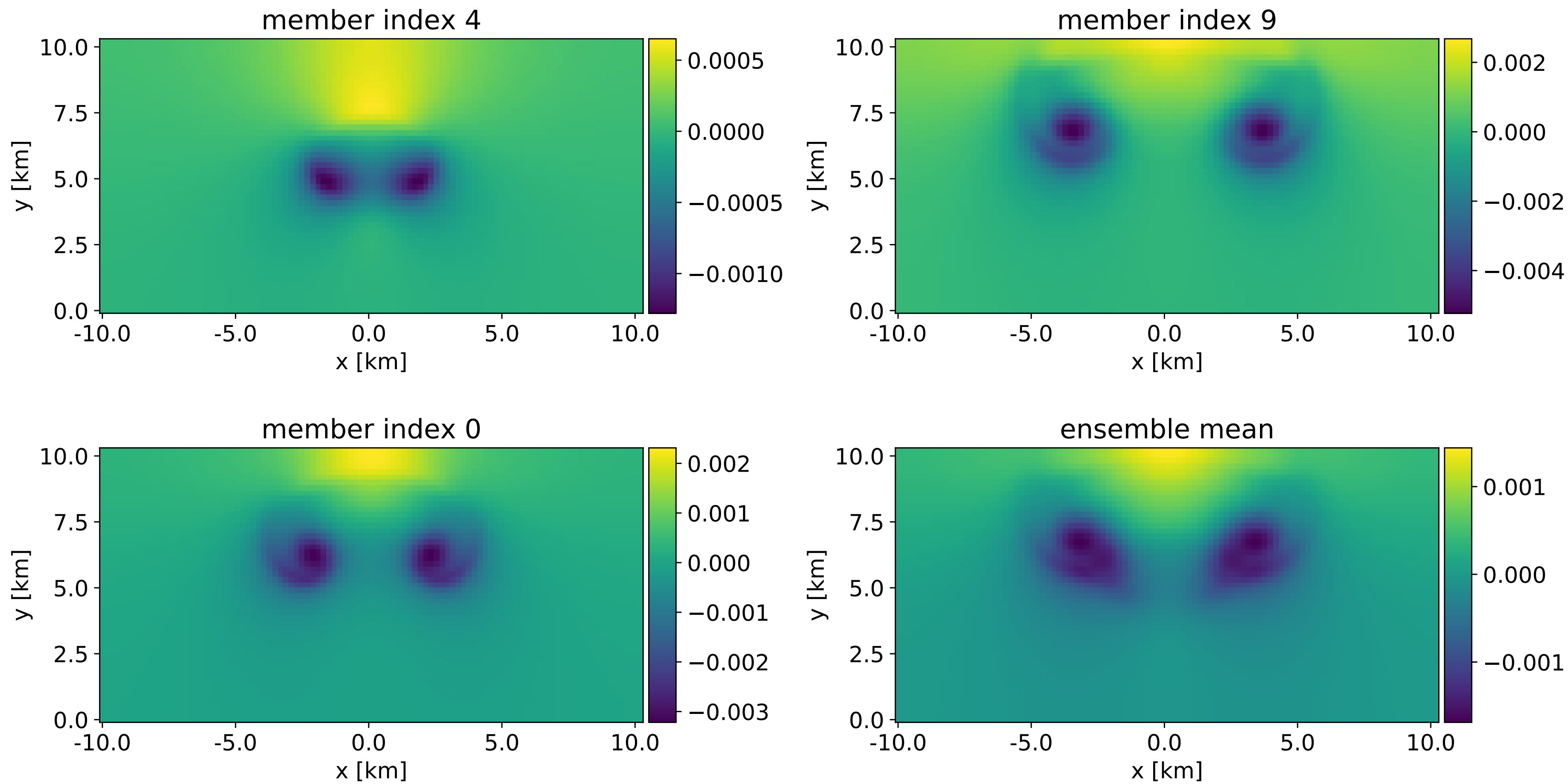


w/o blending

Optimized balance I

Rising bubble, LETKF-based data assimilation

Ensemble with data assimilation with blending. Quantity is π, nodal Exner pressure at output time $t = 1000.0$s.



w blending

Optimized balance II

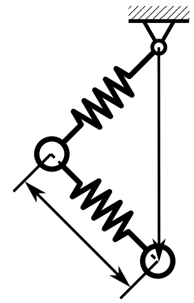
Approach to balance accelerated by selective damping for $\alpha \in (0, 1)$
(akin to divergence damping)

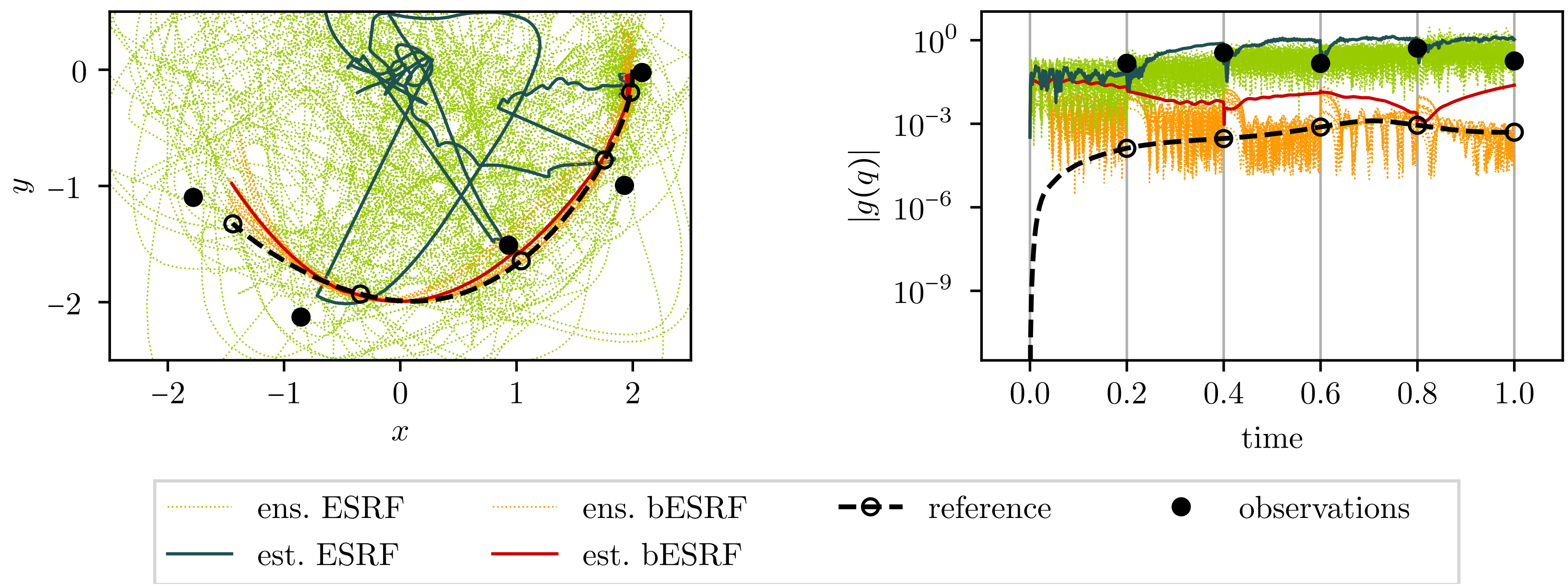
Symplectic integration for $\alpha \in \{0, 1\}$

Optimized balance II

Stiff-spring double pendulum test

$$H^{\varepsilon}(q,p) = \frac{1}{2}p^{\top}p + \frac{1}{2\varepsilon^2}g(q)^{\top}Kg(q) + V(q),$$





Unified numerics

Some results

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Outlook

Summary & Outlook

- "Splitting" of the Euler equations in (almost) linear substeps
- Combination of implicit trapezoidal & implicit midpoint for fast system
- Seamless access to compressible, pseudo-incompressible & hydrostatic models

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- Access to QG dynamics ?
- Access to Arakawa & Konor's unified model ?*
- Rigorous analysis of the scheme ? ⇒ **Gottfried Hastermann**
- Multiscale data assimilation ? ⇒ **Ray Chew**

* Arakawa, Konor, Mon. Wea. Rev., **137** (2009)