Third-order accurate MPDATA for variable flows

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Outline of the talk

1) Motivation

2) Main ideas of the scheme derivation

3) Benefits of the fully third-order MPDATA for global tracer transport

4) Benefits of the fully third-order MPDATA for fluid dynamics applications

5) Conclusions and outlook

Motivation

General motivation for high-order schemes

- Using a high-order scheme can be more cost-effective than increasing resolution with a lower order scheme.
- The functional form of a scheme leading-order truncation error determines its behavioural aspects such as respecting solution symmetries and minimising implicit diffusion or dispersion.
- High-order schemes with compact stencils make more efficient use of modern computers due to usually higher arithmetic intensity than lower order methods.

Motivation for third-order MPDATA for variable flows

- Third-order MPDATA for constant flows was derived in
  L. Margolin, P. K. Smolarkiewicz, SISC, 1998.
- This variant exhibits more uniform distribution of the truncation error as function of the Courant number leading to better preservation of the solution symmetries.
- It is especially beneficial for tracer transport.

Second-order accurate MPDATA

Background

- MPDATA is a sign-preserving second-order accurate scheme for numerical integration of the generalised transport equation

$$\frac{\partial G\Psi}{\partial t} + \nabla \cdot (\boldsymbol{V}\Psi) = 0$$

  based on iterative application of the first-order-accurate upwind algorithm.
- The basic version with two iterations uses physical velocity $\boldsymbol{V}$ in the first iteration and leading-error-compensating pseudo-velocity $\overline{\boldsymbol{V}}$ in the second.
- Pseudo-velocity is derived via truncation error analysis of the upwind scheme.

Pseudo-velocity on structured grids

$$\overline{\boldsymbol{V}} = \frac{1}{2}\boldsymbol{\delta x} \odot \uparrow\!\boldsymbol{V}\!\uparrow \odot \frac{\nabla\Psi}{\Psi} - \frac{1}{2}\delta t \frac{\boldsymbol{V}}{G}\left[\frac{\nabla \cdot (\boldsymbol{V}\Psi)}{\Psi}\right]$$

where

$$(\uparrow\!\boldsymbol{a}\!\uparrow)^I = |a^I|$$

denotes component-wise absolute value of a vector and

$$(\boldsymbol{a} \odot \boldsymbol{b})^I := a^I b^I$$

is the Hadamard product of two vectors

Third-order accurate MPDATA for time and space dependant flows

New idea

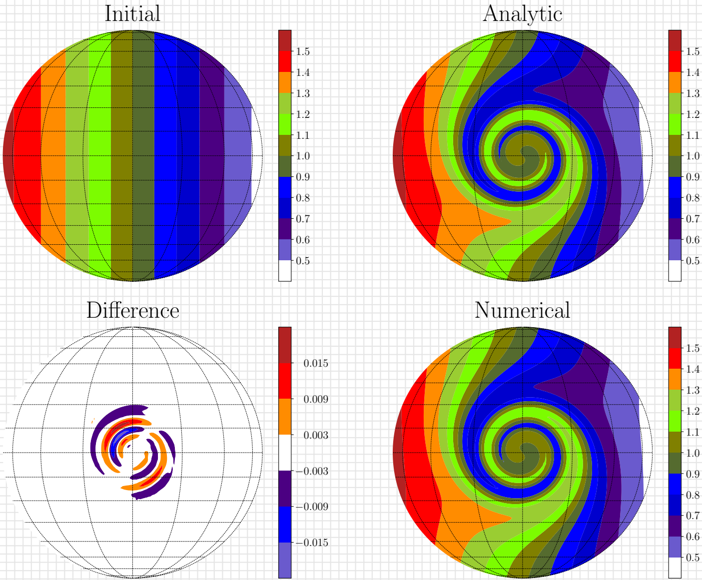
- Find a new pseudo-velocity $\overline{\overline{\boldsymbol{V}}}$ that compensates the leading-order MPDATA error for variable flows.
- The derivation of $\overline{\overline{\boldsymbol{V}}}$ uses MPDATA as a starting point in contrast to the derivation of the constant coefficients third-order scheme.
- Analytical calculation were verified and extended by using symbolic computer algebra.

Third-order error-compensating velocity

$$\overline{\overline{\boldsymbol{V}}} = -\frac{\boldsymbol{\delta x} \odot \boldsymbol{\delta x}}{24} \odot \left[4\boldsymbol{V} \odot \frac{1}{\Psi} \nabla \odot \nabla \Psi + 2 \frac{\nabla \Psi}{\Psi} \odot \nabla \odot \boldsymbol{V} + \alpha \nabla \odot \nabla \odot \boldsymbol{V} \right]$$
$$+ \beta_M \frac{\boldsymbol{\delta x}}{2} \odot \left\uparrow \overline{\boldsymbol{V}} \right\uparrow \odot \frac{\nabla \Psi}{\Psi} + \frac{\delta t}{2} \boldsymbol{\delta x} \odot \uparrow \boldsymbol{V} \uparrow \odot \frac{1}{\Psi} \nabla \left[\frac{1}{G} \nabla \cdot (\boldsymbol{V} \Psi) \right]$$
$$+ \frac{\delta t^2}{24} \left\{ -\frac{8\boldsymbol{V}}{G\Psi} \nabla \cdot \left[\frac{\boldsymbol{V}}{G} \nabla \cdot (\boldsymbol{V}\Psi) \right] + \gamma \frac{\partial^2 \boldsymbol{V}}{\partial t^2} + \frac{2\boldsymbol{V}}{G\Psi} \nabla \cdot \left(\frac{\partial \boldsymbol{V}}{\partial t} \Psi \right) - \frac{2}{G\Psi} \frac{\partial \boldsymbol{V}}{\partial t} \nabla \cdot (\boldsymbol{V}\Psi) \right\}$$

Benefits of the fully third-order MPDATA for global tracer transport

Moving vortices on the sphere – Nair & Jablonowski MWR 2008



Interlude – labels

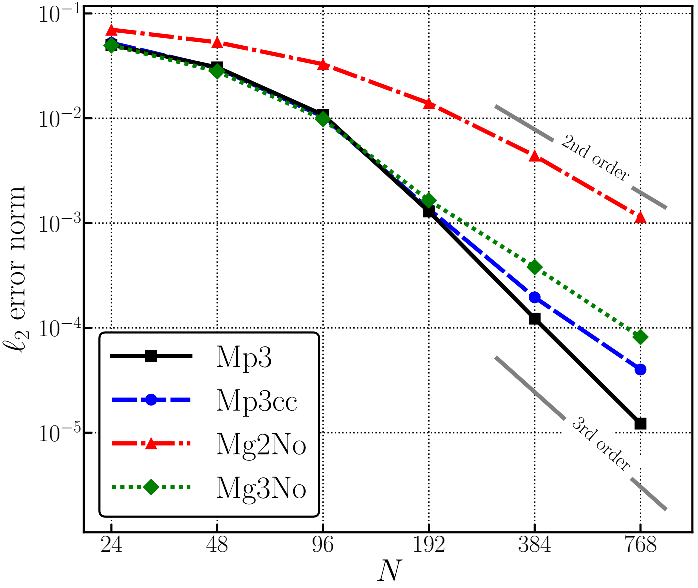
Sign-preserving MPDATA variants

- Mp2 – fully second-order-accurate MPDATA
- Mp3 – fully third-order-accurate MPDATA
- Mp3cc – third-order constant-coefficient MPDATA

Nonoscillatory infinite-gauge MPDATA variants

- Mg2No – nonoscillatory infinite-gauge variant of Mp2
- Mg3No – nonoscillatory infinite-gauge variant of Mp3
- Mg3ccNo – nonoscillatory infinite-gauge variant of Mp3cc

Moving vortices on the sphere – convergence results



Moving vortices – runtimes

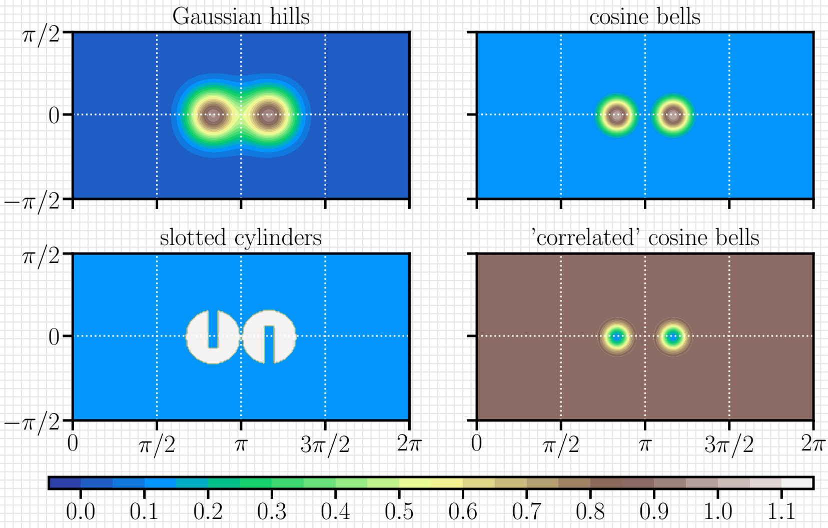
Selected runtimes relative to the upwind scheme

Upwind	Mp2	Mg2No	Mp3cc	Mp3	Mg3No
1.0	3.6	5.9	9.5	10.3	12.6

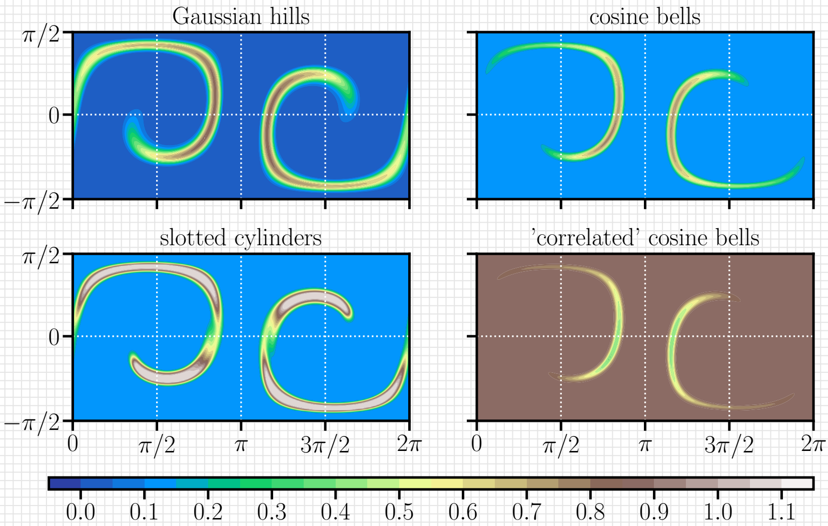
Remarks

- Negligible difference between the fully third-order scheme and the constant-coefficient third-order variant.
- Going from second to third-order is a factor of ~ 3 for the sign-preserving variant but only a factor of ~ 2 for the nonoscillatory infinite-gauge variant.

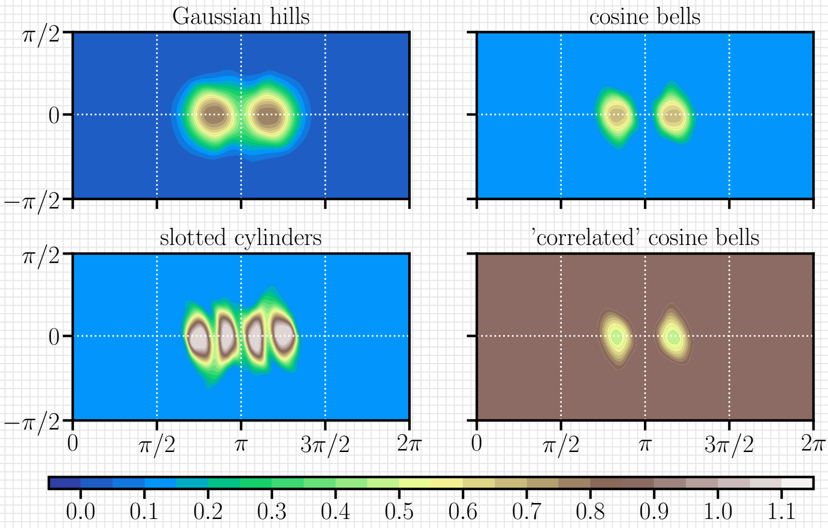
Reversing deformational flow – Lauritzen et al. GMD 2012



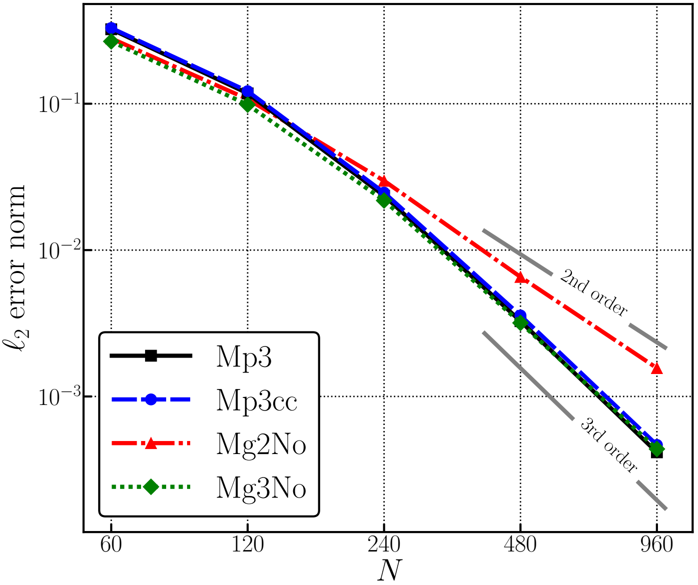
Reversing deformational flow – Lauritzen et al. GMD 2012



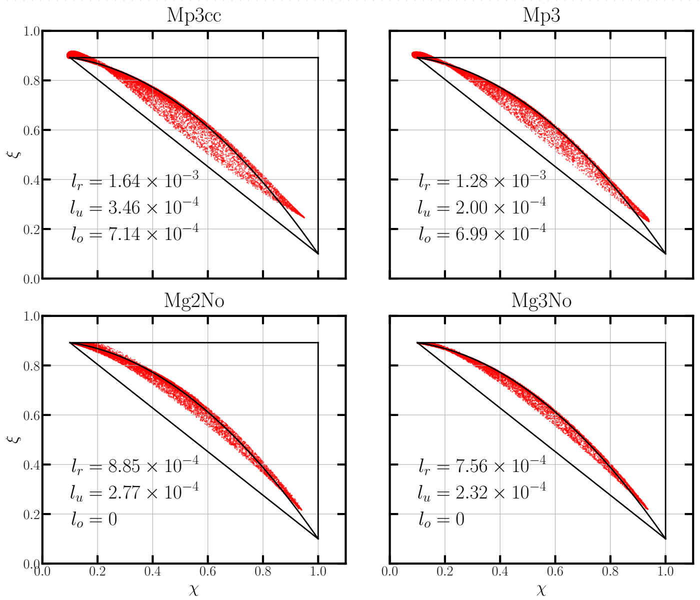
Reversing deformational flow – Lauritzen et al. GMD 2012



Reversing deformational flow – convergence results



Reversing deformational flow – numerical mixing results

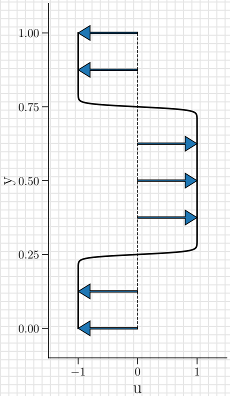


Benefits of the fully third-order MPDATA for fluid dynamics applications

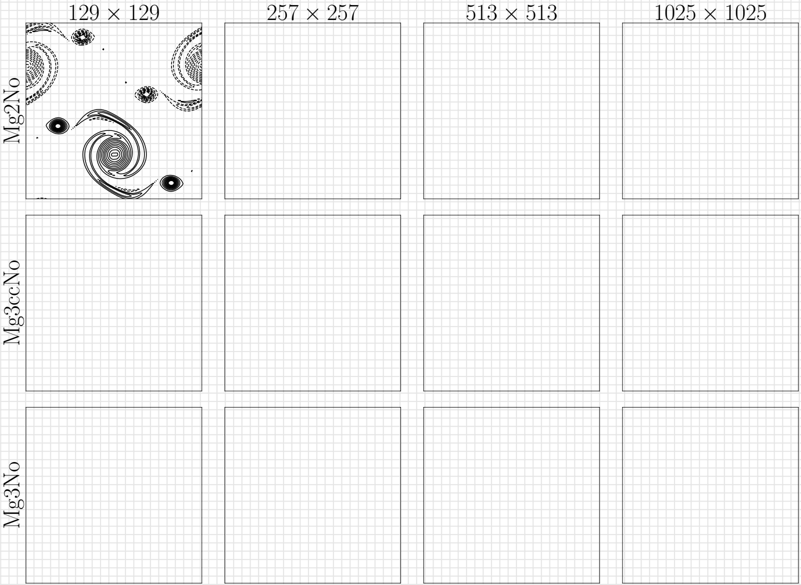
Double shear layer rollup – Brown & Minion 1995 JCP

Setup details

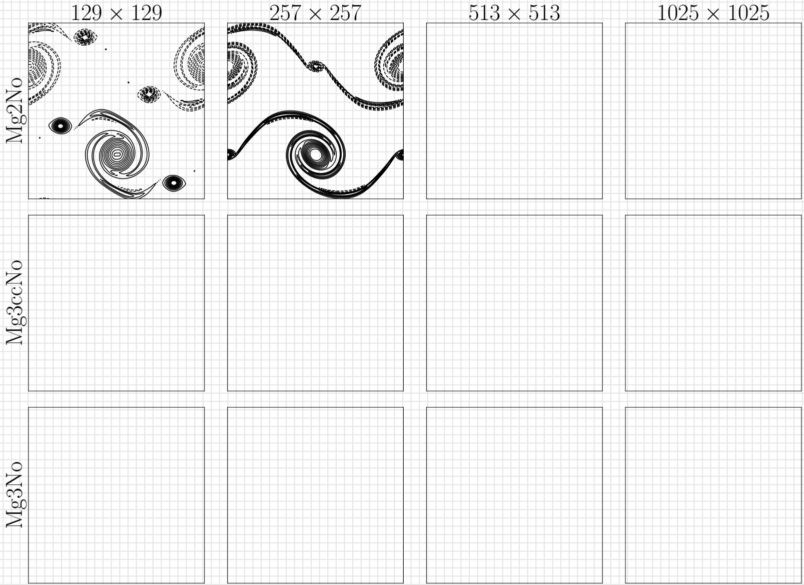
- Incompressible 2D Navier-Stokes in doubly periodic unit square.
- Only advection is integrated with third-order schemes.
- Explicit viscosity integrated to the first-order in time.
- Initial condition: shear profile $u(y)$ as seen on the right.
- Single harmonic perturbation of v to initiate the flow.
- Reynolds number Re = 10000.



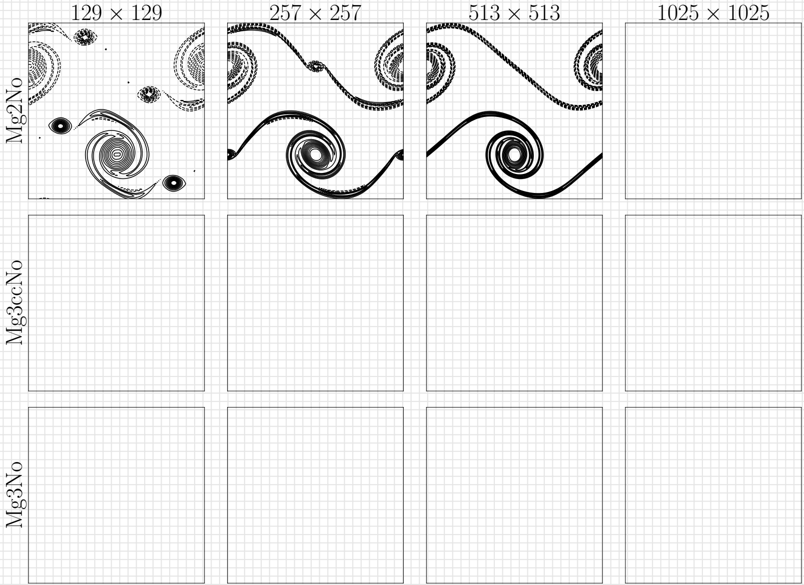
Double shear layer rollup – vorticity contours



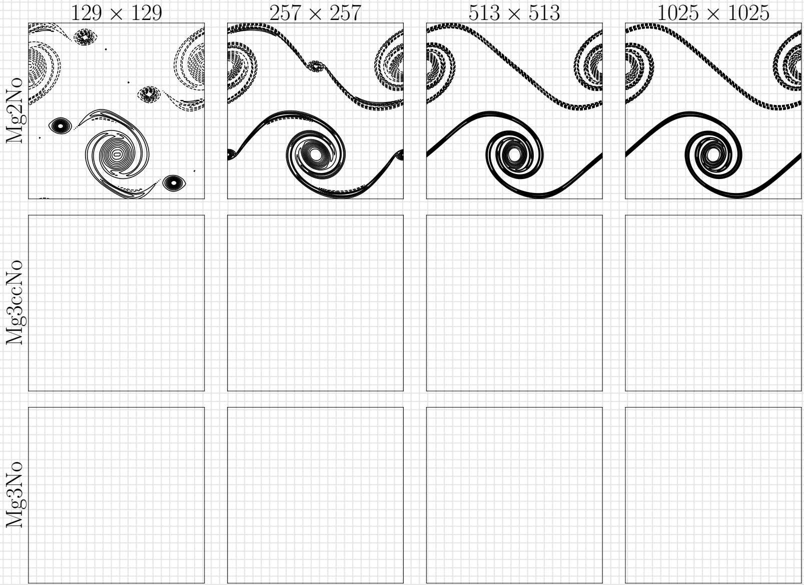
Double shear layer rollup – vorticity contours



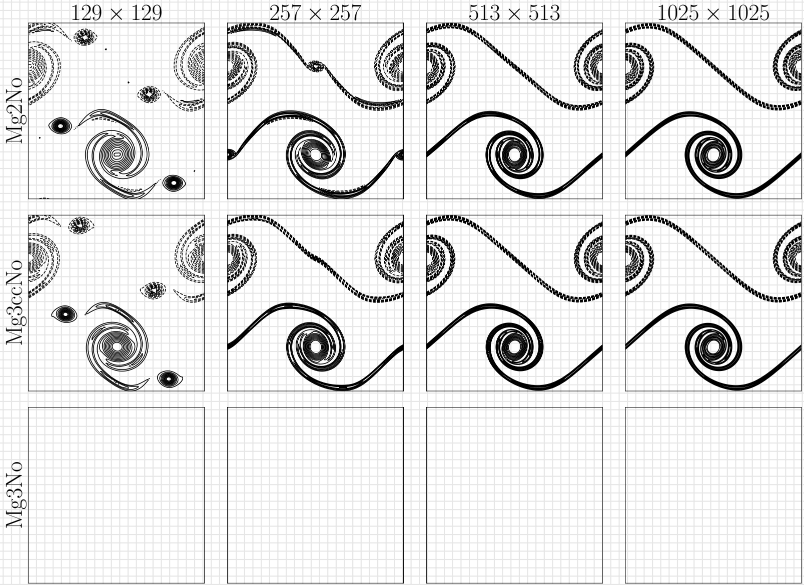
Double shear layer rollup – vorticity contours



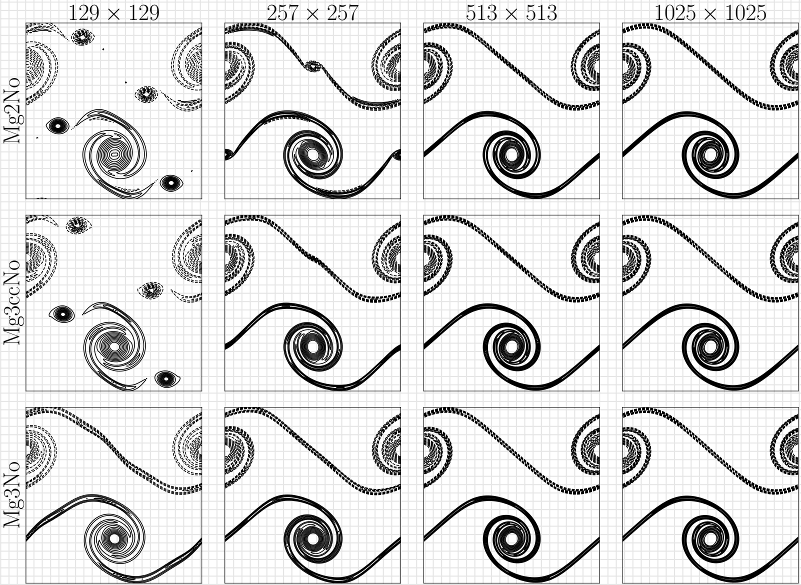
Double shear layer rollup – vorticity contours



Double shear layer rollup – vorticity contours



Double shear layer rollup – vorticity contours



Double shear layer rollup – errors

ℓ_2 error norms of u after $t = 1.5$ and convergence rates

Grid	Mg2No	Order	Mg3ccNo	Order	Mg3No	Order
129×129	3.35×10^{-1}	—	3.65×10^{-1}	—	5.96×10^{-2}	—
257×257	1.96×10^{-1}	0.77	1.09×10^{-1}	1.74	4.83×10^{-2}	0.30
513×513	7.21×10^{-2}	1.44	2.90×10^{-2}	1.91	1.57×10^{-2}	1.62
1025×1025	2.05×10^{-2}	1.82	7.06×10^{-3}	2.04	4.29×10^{-3}	1.87

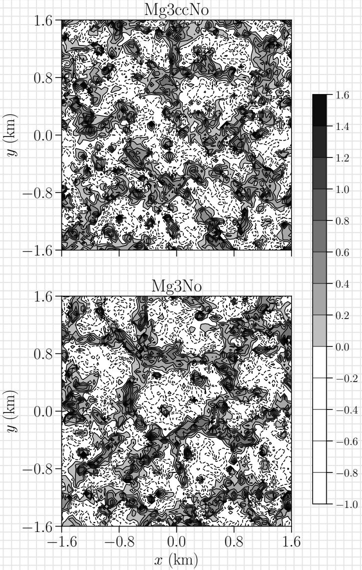
Remarks

- Errors calculated using the Mg3No result on 2049 $\times$ 2049 grid in lie of the true solution.
- Mg2No $>$ Mg3ccNo $>$ Mg3No error ordering even for the converged solutions.
- Overall convergence rates are around 2 (not formally assured).

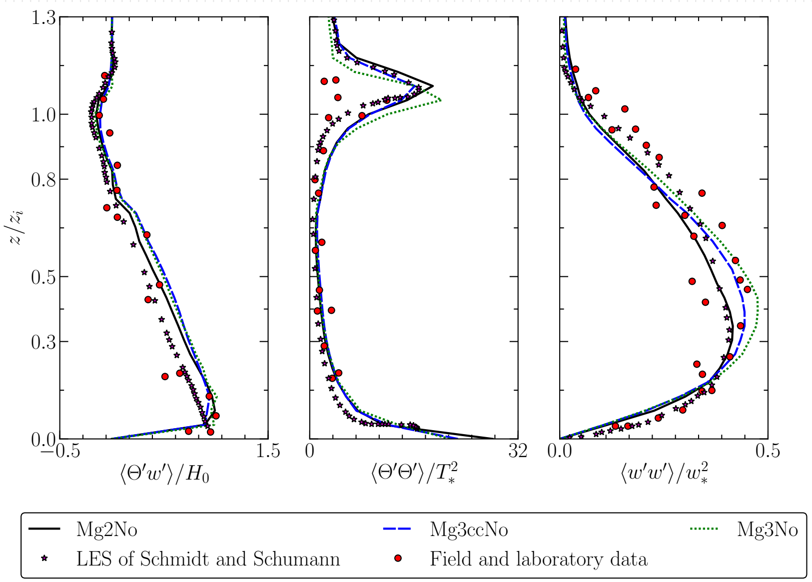
Dry convective boundary layer – Margolin & Smolarkiewicz 1999

Setup details

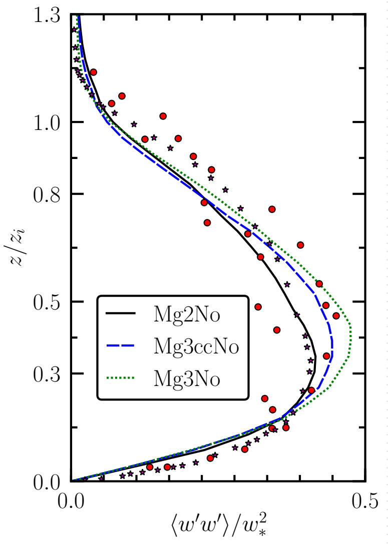
- Incompressible Boussinesq equations in 3D.
- No explicit subgrid model, ILES benchmark.
- Driven by a prescribed heat flux.
- Domain 3.2 km × 3.2 km × 1.5 km.
- Grid spacing 50 m × 50 m × 30 m (65 × 65 × 51 points).
- Time step 8 s, simulation time ∼ 4 h ∼ 13 eddy turnover times.

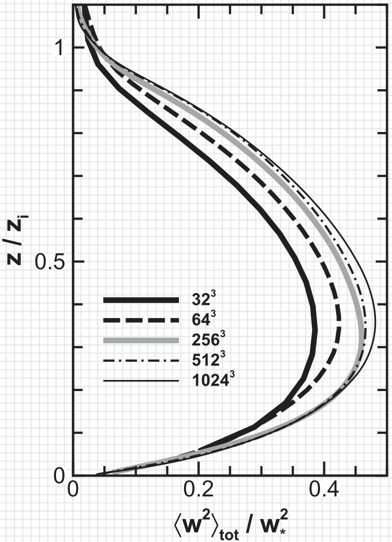


Convective boundary layer – profiles



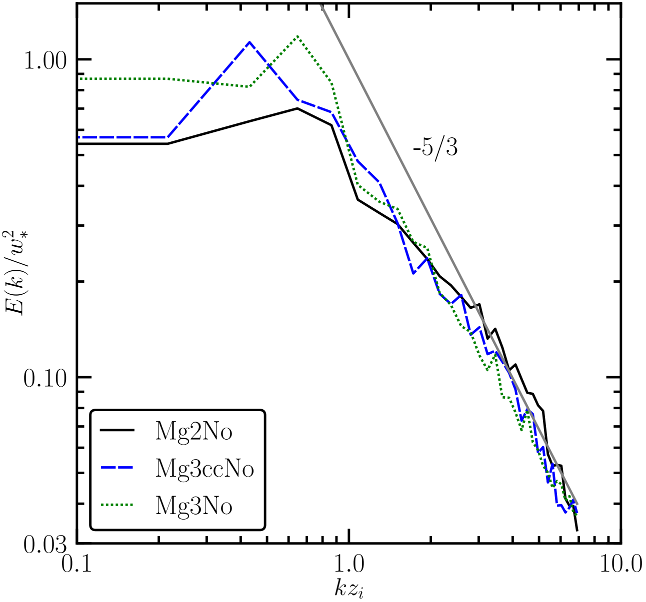
Convective boundary layer – vertical velocity variance





Taken from Sullivan, Patton, JAS, 2011

Convective boundary layer – spectra



For more information see the paper

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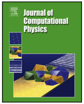

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MPDATA: Third-order accuracy for variable flows

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A B S T R A C T

This paper extends the multidimensional positive definite advection transport algorithm (MPDATA) to third-order accuracy for temporally and spatially varying flows. This is accomplished by identifying the leading truncation error of the standard second-order MPDATA, performing the Cauchy–Kowalevski procedure to express it in a spatial form and compensating its discrete representation—much in the same way as the standard MPDATA corrects the first-order accurate upwind scheme. The procedure of deriving the spatial form of the truncation error was automated using a computer algebra system. This enables various options in MPDATA to be included straightforwardly in the third-order scheme, thereby minimising the implementation effort in existing code bases. Following the spirit of MPDATA, the error is compensated using the upwind scheme resulting in a sign-preserving algorithm, and the entire scheme can be formulated using only two

Code availability

Fully third-order MPDATA is available in *libmpdata++*

free & open source C++ library of MPDATA solvers developed in our group

libmpdata++ repository

`https://github.com/igfuw/libmpdataxx`

Tracer transport examples from the paper

`https://github.com/igfuw/libmpdataxx/tests/mp3_paper_JCP_2018`

SageMath scripts used in the derivation

`https://github.com/igfuw/mpdata_mea`

Conclusions and outlook

Conclusions

- Third-order MPDATA is beneficial for tracer transport with the degree of improvement dependant on the flow and tracer field structure and measured statistics.
- Using third-order MPDATA results in improved resolution even when embedded in overall lower order accurate flow solver.
- Fully third-order MPDATA shows similar or better results than the constant-coefficient third-order variant at negligible computational expense.
- Fully third-order MPDATA can be used for ILES and the implicit subgrid model shows different scale-selectivity.

Outlook

- Closer investigation of the implicit turbulence model.
- Extension to unstructured meshes.