

Third-order accurate MPDATA for arbitrary flows

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Highlights of MPDATA

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

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

based on iterative application of the upwind algorithm

- The basic version with two iterations uses physical "velocity" \mathbf{V} in the first iteration and error-correcting antidiffusive velocity $\overline{\mathbf{V}}$ in the second
- The form of the antidiffusive velocity is derived by performing truncation analysis of the upwind scheme

Antidiffusive velocity on structured grids

$$\overline{\mathbf{V}} = \frac{1}{2} \delta \mathbf{x} \odot \uparrow \mathbf{V} \uparrow \odot \frac{\nabla \Psi}{\Psi} - \frac{1}{2} \delta t \frac{\mathbf{V} \cdot \nabla \cdot (\mathbf{V}\Psi)}{G\Psi}$$

where

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

denotes component-wise absolute value of a vector and

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

is the Hadamard product of two vectors,

Third-order accurate MPDATA for time and space dependant flows

The idea

- Find "third-order" antidiffusive velocity $\overline{\overline{\mathbf{V}}}$ that compensates MPDATA error for arbitrary flows
- Done for the constant velocity case in L. Margolin, P. K. Smolarkiewicz, SISC, 1998
- Here we consider homogeneous generalized transport equation with G independent of time and arbitrary \mathbf{V}

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

A glimpse at the result

$$\begin{aligned} \overline{\overline{\mathbf{V}}} = & - \frac{\delta \mathbf{x} \odot \delta \mathbf{x}}{24} \odot \left[4 \mathbf{V} \odot \frac{1}{\Psi} \nabla \odot \nabla \Psi + 2 \frac{\nabla \Psi}{\Psi} \odot \nabla \odot \mathbf{V} + \nabla \odot \nabla \odot \mathbf{V} \right] \\ & + \frac{\delta \mathbf{x}}{2} \odot \uparrow \overline{\mathbf{V}} \uparrow \odot \frac{\nabla \Psi}{\Psi} + \frac{\delta t}{2} \delta \mathbf{x} \odot \uparrow \mathbf{V} \uparrow \odot \frac{1}{\Psi} \nabla \left[\frac{1}{G} \nabla \cdot (\mathbf{V} \Psi) \right] \\ & + \frac{\delta t^2}{24} \left\{ - \frac{8 \mathbf{V}}{G \Psi} \nabla \cdot \left[\frac{\mathbf{V}}{G} \nabla \cdot (\mathbf{V} \Psi) \right] + \frac{\partial^2 \mathbf{V}}{\partial t^2} + \frac{2 \mathbf{V}}{G \Psi} \nabla \cdot \left(\frac{\partial \mathbf{V}}{\partial t} \Psi \right) - \frac{2}{G \Psi} \frac{\partial \mathbf{V}}{\partial t} \nabla \cdot (\mathbf{V} \Psi) \right\} \end{aligned}$$

Salient points of the derivation

- Starting point is modified equation analysis of the basic MPDATA scheme - different approach than for the constant velocity case
- Taylor expansion results in an equation of the form

$$\frac{\partial \Psi}{\partial t} + \frac{1}{G} \nabla \cdot (\mathbf{V} \Psi) = \frac{1}{G} \nabla \cdot (\mathbf{T}_0) - \frac{\delta t}{2} \frac{\partial^2 \Psi}{\partial t^2} - \frac{\delta t^2}{6} \frac{\partial^3 \Psi}{\partial t^3}$$

- Following Lax-Wendroff/Cauchy-Kovalevskaya procedure time derivatives are expressed in terms of spatial derivatives

$$\frac{\partial^2 \Psi}{\partial t^2} = \frac{1}{G} \nabla \cdot (\mathbf{T}_1) \quad \frac{\partial^3 \Psi}{\partial t^3} = \frac{1}{G} \nabla \cdot (\mathbf{T}_2)$$

- Combination of the above leads to

$$\frac{\partial \Psi}{\partial t} + \frac{1}{G} \nabla \cdot (\mathbf{V} \Psi) = \frac{1}{G} \nabla \cdot \left(\mathbf{T}_0 - \frac{\delta t}{2} \mathbf{T}_1 - \frac{\delta t^2}{6} \mathbf{T}_2 \right) := \frac{1}{G} \nabla \cdot (\overline{\overline{\mathbf{V}}} \Psi)$$

where the last equation defines third-order antidiffusive velocity $\overline{\overline{\mathbf{V}}}$

- Result depends on details of MPDATA implementation (velocity interpolation and extrapolation, antidiffusive velocities time level, ...)
- Finding \mathbf{T}_0 , \mathbf{T}_1 , and \mathbf{T}_2 is a tedious task suited for the use of computer algebra systems (CAS) e.g. SageMath

Interlude - hidden complexity and perils of CAS

First component of third-order antidiffusive velocity

$$\begin{aligned} & + \left[-\frac{dt dx U^2 G_x}{2G^2} + \frac{dt^2 U^3 G_x}{3G^3} + \frac{dt^2 U^2 V G_y}{3G^3} + \frac{dt^2 U^2 W G_z}{3G^3} - \frac{1}{12} dx^2 U_x + \frac{3 dt dx U U_x}{4G} - \frac{dt^2 U^2 U_x}{G^2} - \frac{dt^2 U V U_y}{3G^2} - \frac{dt^2 U W U_z}{3G^2} + \frac{dt dx U V_y}{4G} \right. \\ & - \frac{2 dt^2 U^2 V_y}{3G^2} + \frac{dt dx U W_z}{4G} - \frac{2 dt^2 U^2 W_z}{3G^2} \left. \right] \frac{\psi_x}{\psi} + \left[-\frac{1}{6} dx^2 U + \frac{dt dx U^2}{2G} - \frac{dt^2 U^3}{3G^2} \right] \frac{\psi_{xx}}{\psi} + \left[-\frac{dt dx U V G_x}{2G^2} + \frac{dt^2 U^2 V G_x}{3G^3} + \frac{dt^2 U V^2 G_y}{3G^3} + \frac{dt^2 U V W G_z}{3G^3} \right. \\ & - \frac{dt^2 V U_t}{12G} - \frac{2 dt^2 U V U_x}{3G^2} + \frac{dt^2 U V_t}{12G} + \frac{dt dx U V_x}{2G} - \frac{dt^2 U^2 V_x}{3G^2} - \frac{dt^2 U V V_y}{G^2} - \frac{dt^2 U W V_z}{3G^2} - \frac{2 dt^2 U V W_z}{3G^2} \left. \right] \frac{\psi_y}{\psi} + \left[\frac{dt dx U V}{2G} - \frac{2 dt^2 U^2 V}{3G^2} \right] \frac{\psi_{xy}}{\psi} \\ & + \left[-\frac{dt^2 U V^2}{3G^2} \right] \frac{\psi_{yy}}{\psi} + \left[-\frac{dt dx U W G_x}{2G^2} + \frac{dt^2 U^2 W G_x}{3G^3} + \frac{dt^2 U V W G_y}{3G^3} + \frac{dt^2 U W^2 G_z}{3G^3} - \frac{dt^2 W U_t}{12G} - \frac{2 dt^2 U W U_x}{3G^2} - \frac{2 dt^2 U W V_y}{3G^2} + \frac{dt^2 U W_t}{12G} + \frac{dt dx U W_x}{2G} \right. \\ & - \frac{dt^2 U^2 W_x}{3G^2} - \frac{dt^2 U V W_y}{3G^2} - \frac{dt^2 U W W_z}{G^2} \left. \right] \frac{\psi_z}{\psi} + \left[\frac{dt dx U W}{2G} - \frac{2 dt^2 U^2 W}{3G^2} \right] \frac{\psi_{xz}}{\psi} + \left[-\frac{2 dt^2 U V W}{3G^2} \right] \frac{\psi_{yz}}{\psi} + \left[-\frac{dt^2 U W^2}{3G^2} \right] \frac{\psi_{zz}}{\psi} + \frac{1}{24} dt^2 U_{tt} + \frac{dt^2 U U_{tx}}{12G} \\ & - \frac{dt dx U G_x U_x}{2G^2} + \frac{dt^2 U^2 G_x U_x}{3G^3} + \frac{dt^2 U V G_y U_x}{3G^3} + \frac{dt^2 U W G_z U_x}{3G^3} - \frac{dt^2 U_t U_x}{12G} - \frac{dt^2 U U_x^2}{3G^2} - \frac{1}{24} dx^2 U_{xx} + \frac{dt dx U U_{xx}}{2G} - \frac{dt^2 U^2 U_{xx}}{3G^2} - \frac{dt^2 U V U_{xy}}{3G^2} \\ & - \frac{dt^2 U W U_{xz}}{3G^2} + \frac{dt^2 U V_t V_y}{12G} + \frac{dt dx U V_{xy}}{2G} - \frac{dt^2 U^2 V_{xy}}{3G^2} - \frac{dt dx U G_x V_y}{2G^2} + \frac{dt^2 U^2 G_x V_y}{3G^3} + \frac{dt^2 U V G_y V_y}{3G^3} + \frac{dt^2 U W G_z V_y}{3G^3} - \frac{dt^2 U_t V_y}{12G} - \frac{2 dt^2 U U_x V_y}{3G^2} \\ & - \frac{dt^2 U V_y^2}{3G^2} - \frac{dt^2 U V V_{yy}}{3G^2} - \frac{dt^2 U W V_{yz}}{3G^2} + \frac{dt^2 U W_t z}{12G} + \frac{dt dx U W_{xz}}{2G} - \frac{dt^2 U^2 W_{xz}}{3G^2} - \frac{dt^2 U V W_{yz}}{3G^2} - \frac{dt dx U G_x W_z}{2G^2} + \frac{dt^2 U^2 G_x W_z}{3G^3} + \frac{dt^2 U V G_y W_z}{3G^3} \\ & + \frac{dt^2 U W G_z W_z}{3G^3} - \frac{dt^2 U_t W_z}{12G} - \frac{2 dt^2 U U_x W_z}{3G^2} - \frac{2 dt^2 U V_y W_z}{3G^2} - \frac{dt^2 U W^2}{3G^2} - \frac{dt^2 U W W_{zz}}{3G^2} + \frac{dx^2 U \psi_x^2}{4\psi^2} - \frac{dt dx U^2 \psi_x^2}{4G\psi^2} - \frac{dt dx U V \psi_x \psi_y}{4G\psi^2} - \frac{dt dx U W \psi_x \psi_z}{4G\psi^2} \end{aligned}$$

Implementation

- The differential expressions or interpolated variables that enter $\overline{\overline{\mathbf{V}}}$, for example $\frac{\partial^2 \mathbf{V}}{\partial t^2}$ or $\frac{\nabla \Psi}{\Psi}$, have to be known only to the first order
- The entire scheme can be done in two upwind passes, in the second pass
$$\tilde{\mathbf{V}} = \overline{\mathbf{V}}(\mathbf{V}) + \overline{\overline{\mathbf{V}}}(\overline{\mathbf{V}}, \mathbf{V})$$

Stability

- Upwind passes will be stable if the Courant numbers associated with physical and antidiffusive velocities are properly bounded
- Second-order antidiffusive velocity Courant number is bounded by the physical velocity Courant number given suitable timestep restriction, the same has not been proven for the third-order antidiffusive velocity
- Formally the third-order antidiffusive velocity is $O(\delta t, \delta \mathbf{x})$ correction to the second-order antidiffusive velocity and should be small for smooth problems in the high-resolution limit
- From stability point of view it may be beneficial to split second-order and third-order corrections into separate upwind passes
- Some form of antidiffusive velocity limiting may still be needed

A walk-through of the result

Considered term

$$\begin{aligned}\overline{\overline{\mathbf{V}}} = & -\frac{\delta \mathbf{x} \odot \delta \mathbf{x}}{24} \odot \left[4\mathbf{V} \odot \frac{1}{\Psi} \nabla \odot \nabla \Psi + 2\frac{\nabla \Psi}{\Psi} \odot \nabla \odot \mathbf{V} + \nabla \odot \nabla \odot \mathbf{V} \right] \\ & + \frac{\delta \mathbf{x}}{2} \odot \uparrow \overline{\mathbf{V}} \uparrow \odot \frac{\nabla \Psi}{\Psi} + \frac{\delta t}{2} \delta \mathbf{x} \odot \uparrow \mathbf{V} \uparrow \odot \frac{1}{\Psi} \nabla \left[\frac{1}{G} \nabla \cdot (\mathbf{V} \Psi) \right] \\ & + \frac{\delta t^2}{24} \left\{ -\frac{8\mathbf{V}}{G\Psi} \nabla \cdot \left[\frac{\mathbf{V}}{G} \nabla \cdot (\mathbf{V} \Psi) \right] + \frac{\partial^2 \mathbf{V}}{\partial t^2} + \frac{2\mathbf{V}}{G\Psi} \nabla \cdot \left(\frac{\partial \mathbf{V}}{\partial t} \Psi \right) - \frac{2}{G\Psi} \frac{\partial \mathbf{V}}{\partial t} \nabla \cdot (\mathbf{V} \Psi) \right\}\end{aligned}$$

Origin of the term: Upwind differencing with physical velocity

A walk-through of the result

Considered term

$$\begin{aligned}\overline{\overline{\mathbf{V}}} &= -\frac{\delta \mathbf{x} \odot \delta \mathbf{x}}{24} \odot \left[4\mathbf{V} \odot \frac{1}{\Psi} \nabla \odot \nabla \Psi + 2\frac{\nabla \Psi}{\Psi} \odot \nabla \odot \mathbf{V} + \nabla \odot \nabla \odot \mathbf{V} \right] \\ &+ \frac{\delta \mathbf{x}}{2} \odot \uparrow \overline{\mathbf{V}} \uparrow \odot \frac{\nabla \Psi}{\Psi} + \frac{\delta t}{2} \delta \mathbf{x} \odot \uparrow \mathbf{V} \uparrow \odot \frac{1}{\Psi} \nabla \left[\frac{1}{G} \nabla \cdot (\mathbf{V} \Psi) \right] \\ &+ \frac{\delta t^2}{24} \left\{ -\frac{8\mathbf{V}}{G\Psi} \nabla \cdot \left[\frac{\mathbf{V}}{G} \nabla \cdot (\mathbf{V} \Psi) \right] + \frac{\partial^2 \mathbf{V}}{\partial t^2} + \frac{2\mathbf{V}}{G\Psi} \nabla \cdot \left(\frac{\partial \mathbf{V}}{\partial t} \Psi \right) - \frac{2}{G\Psi} \frac{\partial \mathbf{V}}{\partial t} \nabla \cdot (\mathbf{V} \Psi) \right\}\end{aligned}$$

Origin of the term: Upwind differencing with antidiffusive velocity

A walk-through of the result

Considered term

$$\begin{aligned}\overline{\overline{\mathbf{V}}} &= -\frac{\delta \mathbf{x} \odot \delta \mathbf{x}}{24} \odot \left[4\mathbf{V} \odot \frac{1}{\Psi} \nabla \odot \nabla \Psi + 2\frac{\nabla \Psi}{\Psi} \odot \nabla \odot \mathbf{V} + \nabla \odot \nabla \odot \mathbf{V} \right] \\ &+ \frac{\delta \mathbf{x}}{2} \odot \uparrow \overline{\mathbf{V}} \uparrow \odot \frac{\nabla \Psi}{\Psi} + \frac{\delta t}{2} \delta \mathbf{x} \odot \uparrow \mathbf{V} \uparrow \odot \frac{1}{\Psi} \nabla \left[\frac{1}{G} \nabla \cdot (\mathbf{V} \Psi) \right] \\ &+ \frac{\delta t^2}{24} \left\{ -\frac{8\mathbf{V}}{G\Psi} \nabla \cdot \left[\frac{\mathbf{V}}{G} \nabla \cdot (\mathbf{V} \Psi) \right] + \frac{\partial^2 \mathbf{V}}{\partial t^2} + \frac{2\mathbf{V}}{G\Psi} \nabla \cdot \left(\frac{\partial \mathbf{V}}{\partial t} \Psi \right) - \frac{2}{G\Psi} \frac{\partial \mathbf{V}}{\partial t} \nabla \cdot (\mathbf{V} \Psi) \right\}\end{aligned}$$

Origin of the term: Iterative nature of MPDATA

A walk-through of the result

Considered term

$$\begin{aligned}\overline{\overline{\mathbf{V}}} &= -\frac{\delta \mathbf{x} \odot \delta \mathbf{x}}{24} \odot \left[4\mathbf{V} \odot \frac{1}{\Psi} \nabla \odot \nabla \Psi + 2\frac{\nabla \Psi}{\Psi} \odot \nabla \odot \mathbf{V} + \nabla \odot \nabla \odot \mathbf{V} \right] \\ &+ \frac{\delta \mathbf{x}}{2} \odot \uparrow \overline{\mathbf{V}} \uparrow \odot \frac{\nabla \Psi}{\Psi} + \frac{\delta t}{2} \delta \mathbf{x} \odot \uparrow \mathbf{V} \uparrow \odot \frac{1}{\Psi} \nabla \left[\frac{1}{G} \nabla \cdot (\mathbf{V} \Psi) \right] \\ &+ \frac{\delta t^2}{24} \left\{ -\frac{8\mathbf{V}}{G\Psi} \nabla \cdot \left[\frac{\mathbf{V}}{G} \nabla \cdot (\mathbf{V} \Psi) \right] + \frac{\partial^2 \mathbf{V}}{\partial t^2} + \frac{2\mathbf{V}}{G\Psi} \nabla \cdot \left(\frac{\partial \mathbf{V}}{\partial t} \Psi \right) - \frac{2}{G\Psi} \frac{\partial \mathbf{V}}{\partial t} \nabla \cdot (\mathbf{V} \Psi) \right\}\end{aligned}$$

Origin of the term: Forward-in-time differencing - transported field

A walk-through of the result

Considered term

$$\begin{aligned}\overline{\overline{\mathbf{V}}} &= -\frac{\delta \mathbf{x} \odot \delta \mathbf{x}}{24} \odot \left[4\mathbf{V} \odot \frac{1}{\Psi} \nabla \odot \nabla \Psi + 2\frac{\nabla \Psi}{\Psi} \odot \nabla \odot \mathbf{V} + \nabla \odot \nabla \odot \mathbf{V} \right] \\ &+ \frac{\delta \mathbf{x}}{2} \odot \uparrow \overline{\mathbf{V}} \uparrow \odot \frac{\nabla \Psi}{\Psi} + \frac{\delta t}{2} \delta \mathbf{x} \odot \uparrow \mathbf{V} \uparrow \odot \frac{1}{\Psi} \nabla \left[\frac{1}{G} \nabla \cdot (\mathbf{V} \Psi) \right] \\ &+ \frac{\delta t^2}{24} \left\{ -\frac{8\mathbf{V}}{G\Psi} \nabla \cdot \left[\frac{\mathbf{V}}{G} \nabla \cdot (\mathbf{V} \Psi) \right] + \frac{\partial^2 \mathbf{V}}{\partial t^2} + \frac{2\mathbf{V}}{G\Psi} \nabla \cdot \left(\frac{\partial \mathbf{V}}{\partial t} \Psi \right) - \frac{2}{G\Psi} \frac{\partial \mathbf{V}}{\partial t} \nabla \cdot (\mathbf{V} \Psi) \right\}\end{aligned}$$

Origin of the term: Forward-in-time differencing - physical velocity

Test description

- Method of manufactured solutions

$$\Psi(t, \mathbf{x}) = (2 + \sin t \sin x)(2 + \sin t \sin y)(2 + \sin t \sin z)$$

$$G(\mathbf{x}) = e^{\cos x + \cos y + \cos z}$$

$$V^I(t, \mathbf{x}) = \frac{G \cos t}{2 + \sin t \sin x^I}$$

where

$$\mathbf{x} = (x, y, z)$$

- Solved on $[0, 2\pi] \times [0, 2\pi] \times [0, 2\pi]$ domain with periodic boundary conditions using N^3 gridpoints

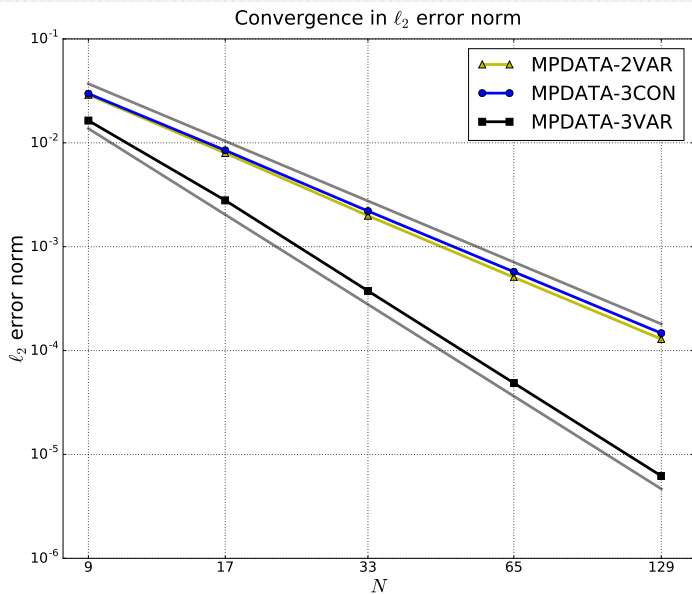
Error norms

$$l_2 = \left[\frac{I[(\Psi - \Psi_{\text{exact}})^2]}{I[(\Psi_{\text{exact}})^2]} \right]^{1/2}$$

$$l_\infty = \frac{\max |\Psi - \Psi_{\text{exact}}|}{\max |\Psi_{\text{exact}}|}$$

$$I(\Psi) = \int \Psi dV$$

Convergence test in 3D - results



Initial condition

$$\Psi(\lambda, \theta) = \frac{\Psi_0}{4} \left[1 + \cos \left(\frac{\pi R_g}{R_c} \right) \right]^2 \quad \text{if } R_g < R_c \text{ else } 0$$

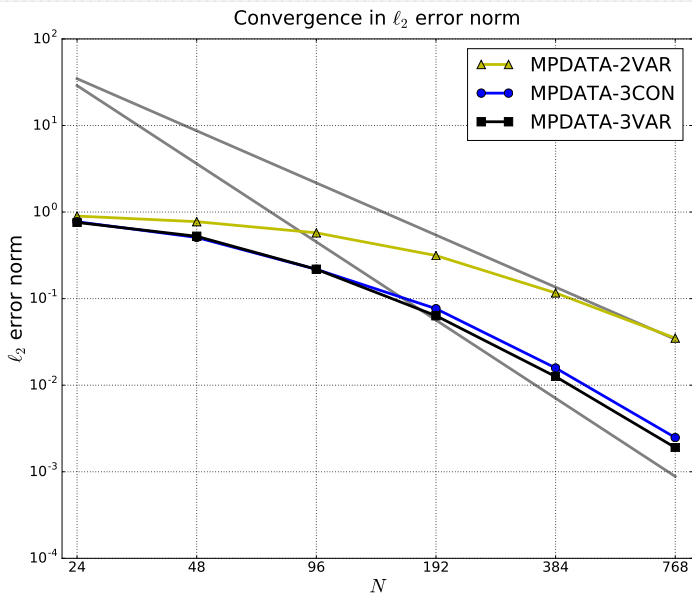
with $\Psi_0 = 1000$ and $R_c = \frac{1}{3}$

$$\Psi(\lambda, \theta) \in \mathcal{C}^3$$

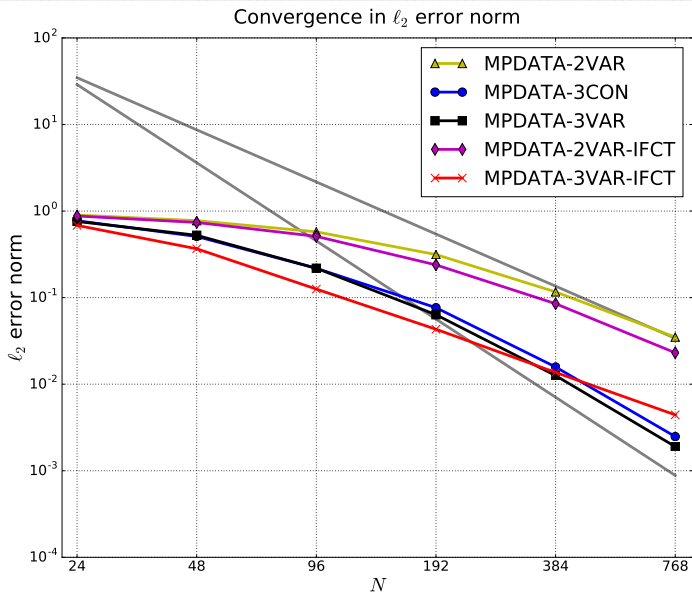
Grid

Regular latitude-longitude grid with $(2N + 1) \times N$ points (common to all tests in spherical geometry)

Solid-body advection of a cosine bell over the pole - results



Solid-body advection of a cosine bell over the pole - results with FCT



Wind field

- two vortices located on opposite sides of the sphere rotating with tangential velocity

$$V = v_0 \frac{3\sqrt{3}}{2} \frac{\tanh(\rho)}{\cosh^2(\rho)}$$

$$\rho = \rho_0 \cos(\theta')$$

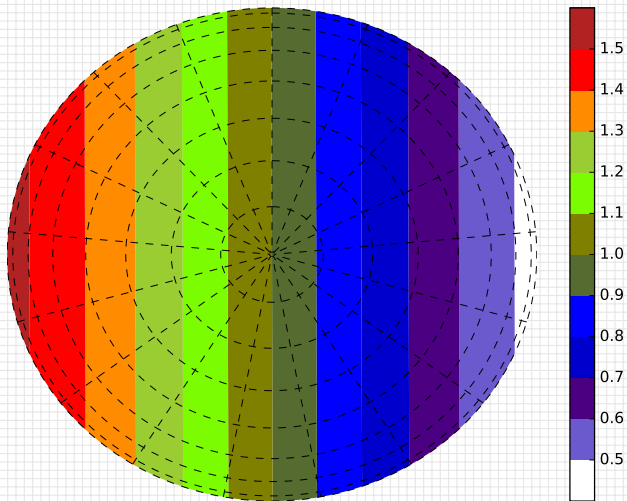
- location of one of the vortices is chosen to be $(\pi + 0.0025, \pi/2.2)$
- flow field is time-independent

Analytical solution known at any time

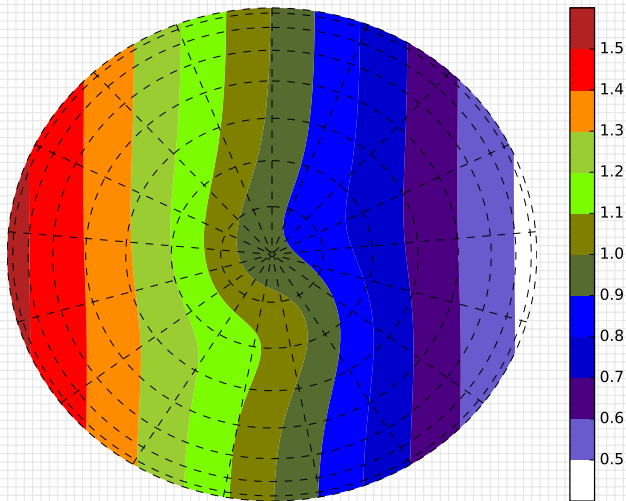
$$\Phi(t, \lambda', \theta') = 1 - \tanh \left[\frac{\rho}{\gamma} \sin(\lambda' - \omega_r t) \right]$$

where ω_r is the angular velocity

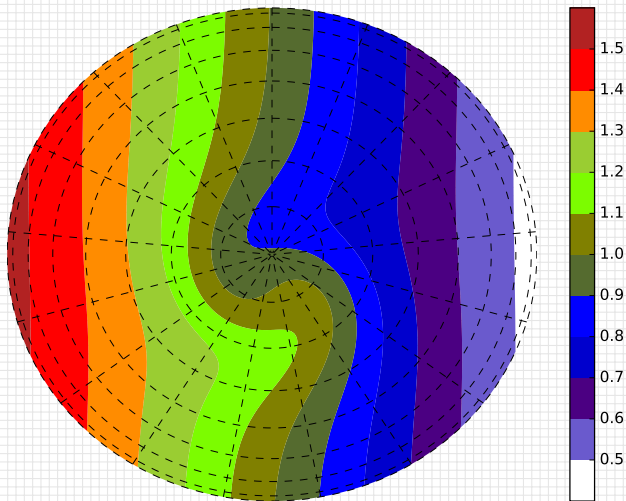
Stationary vortices on the sphere - Nair and Machenhauer 2002



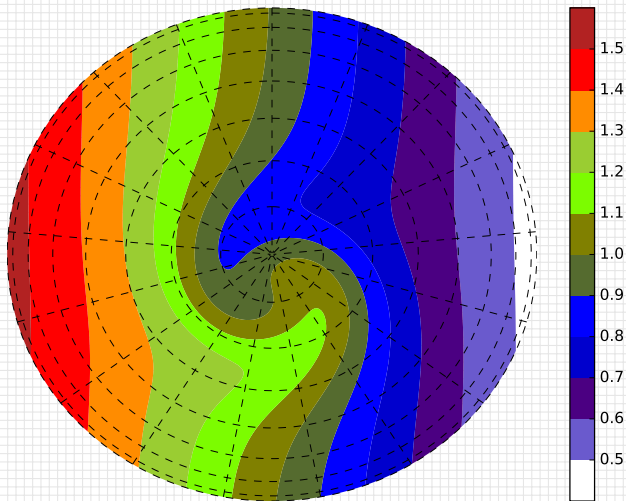
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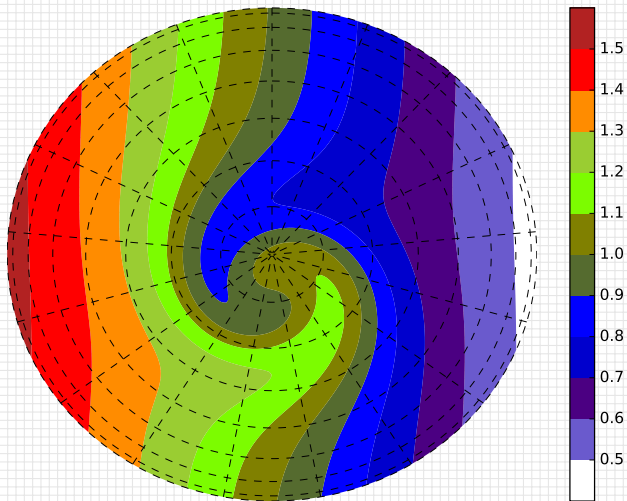
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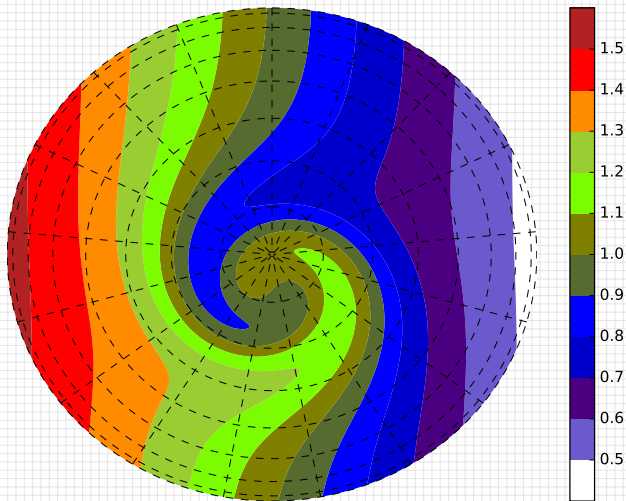
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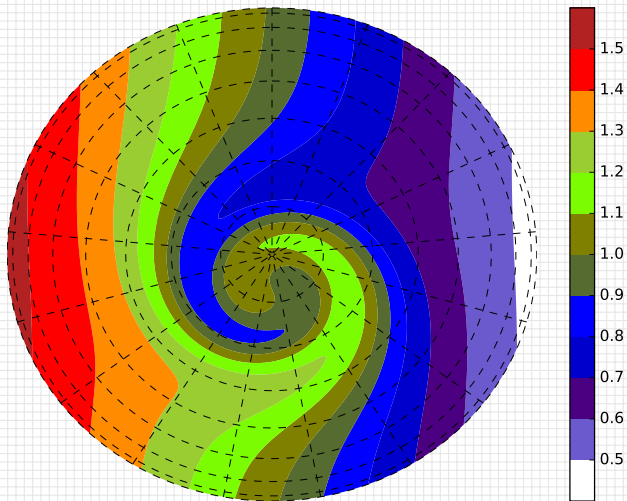
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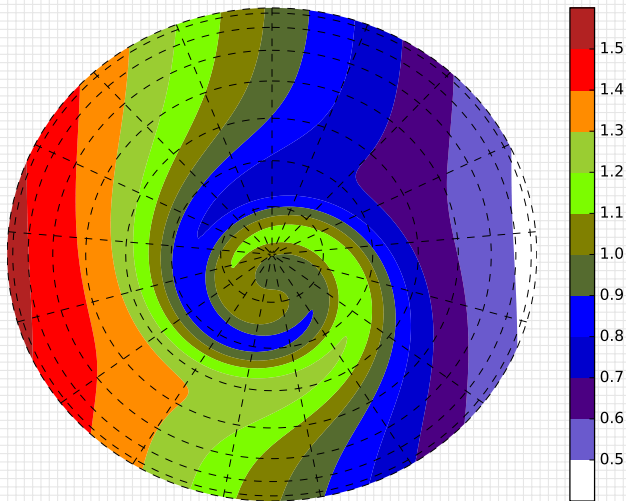
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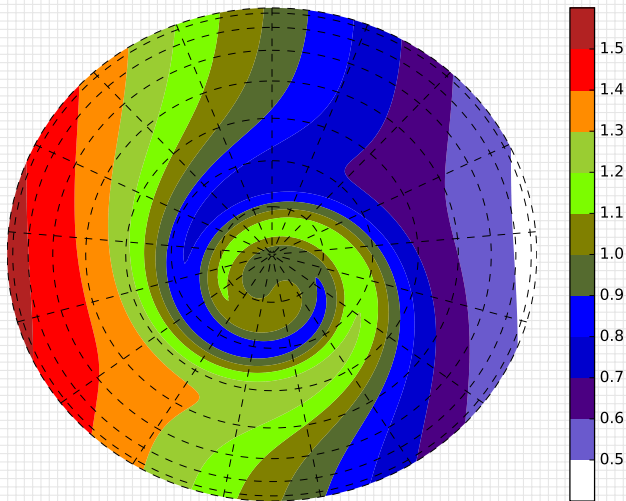
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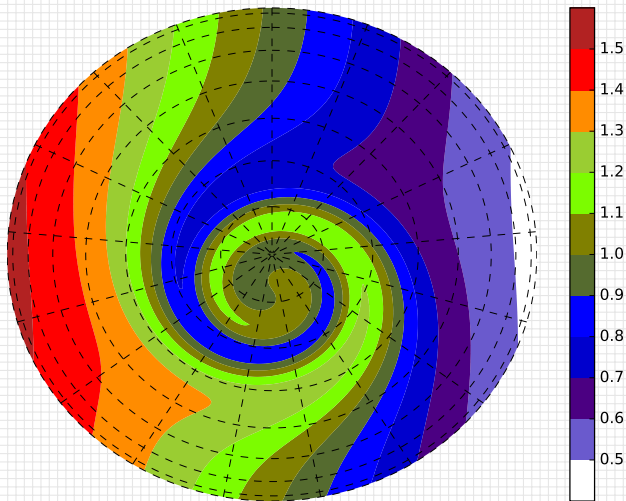
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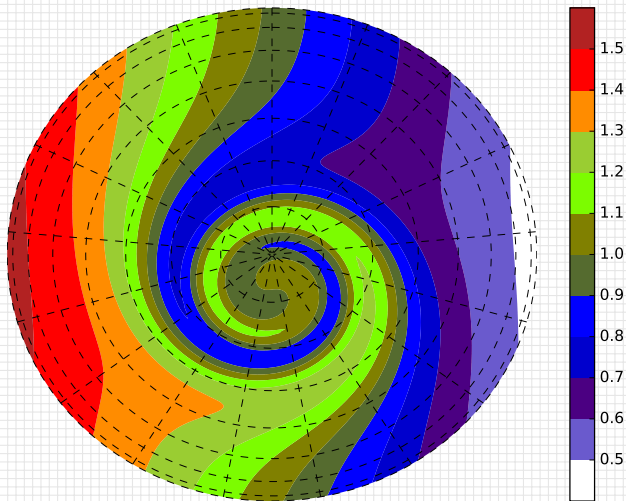
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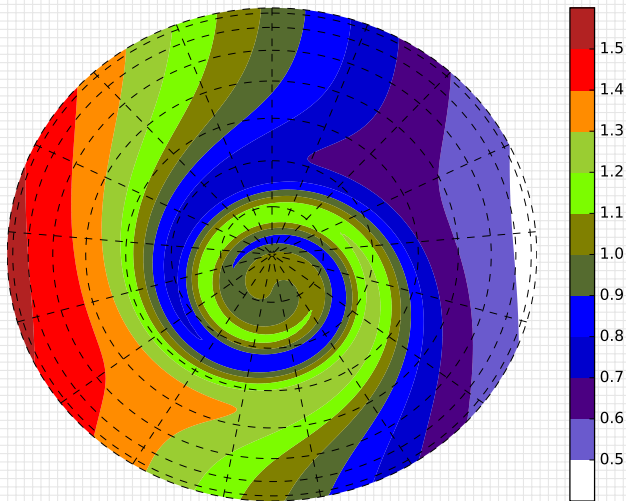
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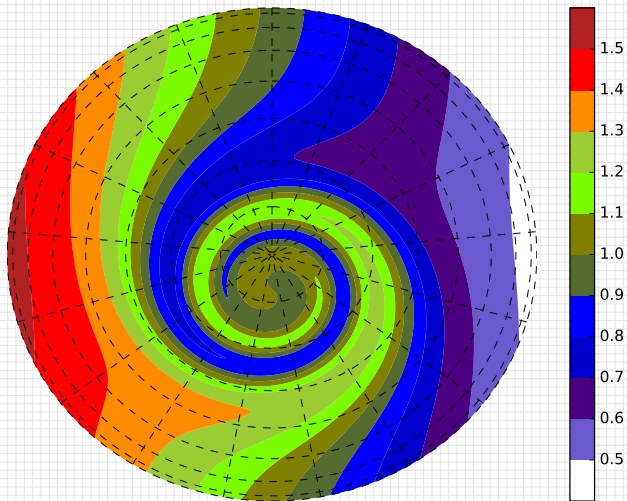
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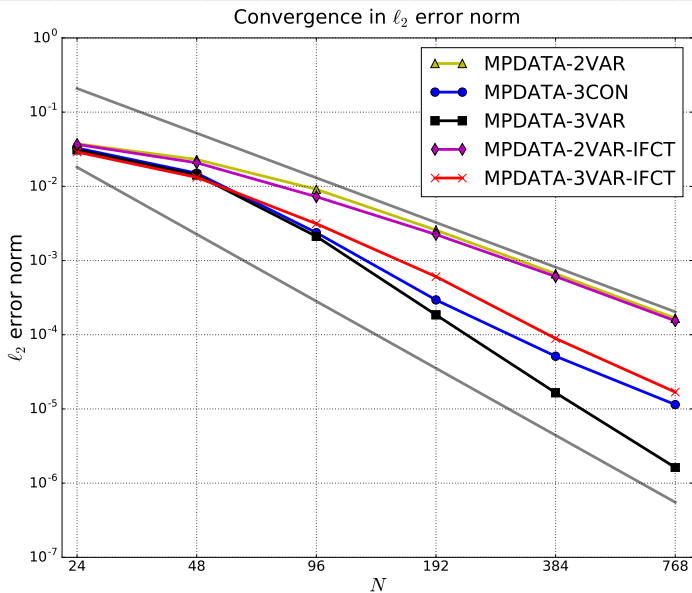
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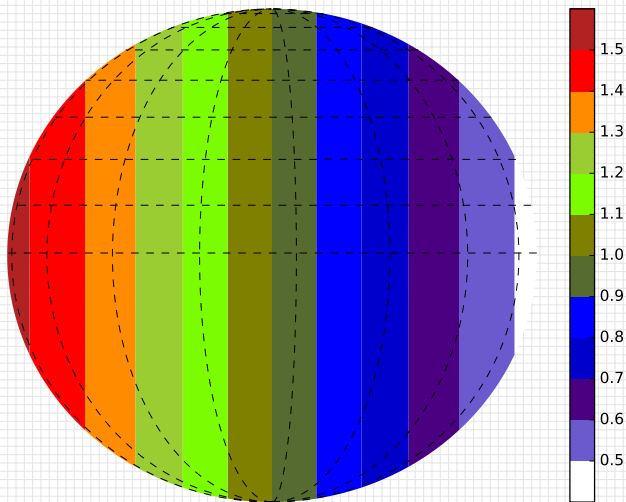
Stationary vortices on the sphere - Nair and Machenhauer 2002



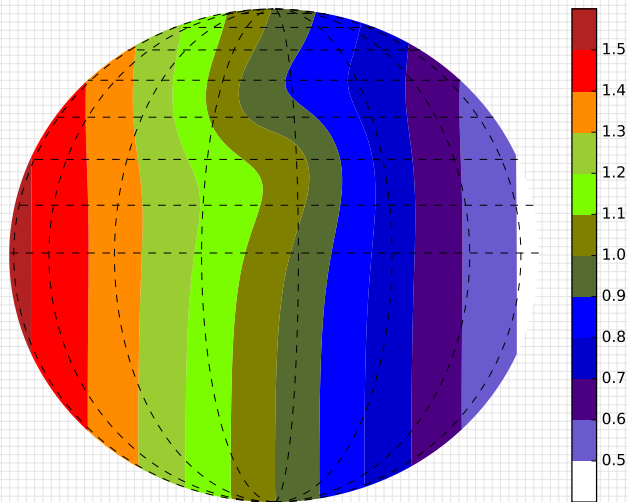
Stationary vortices on the sphere - results



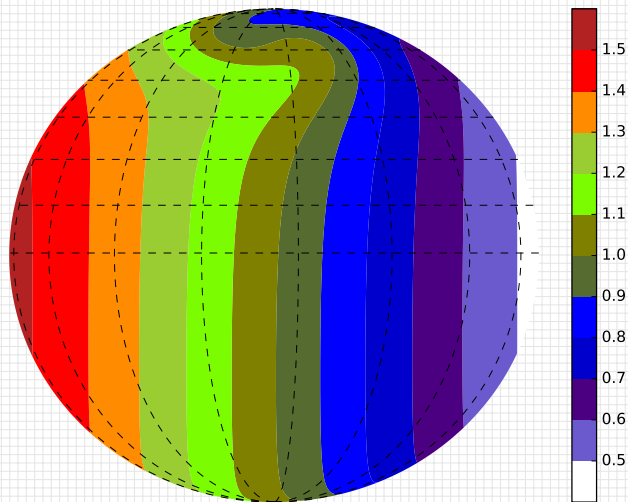
Moving vortices on the sphere - Nair and Jablonowski 2008



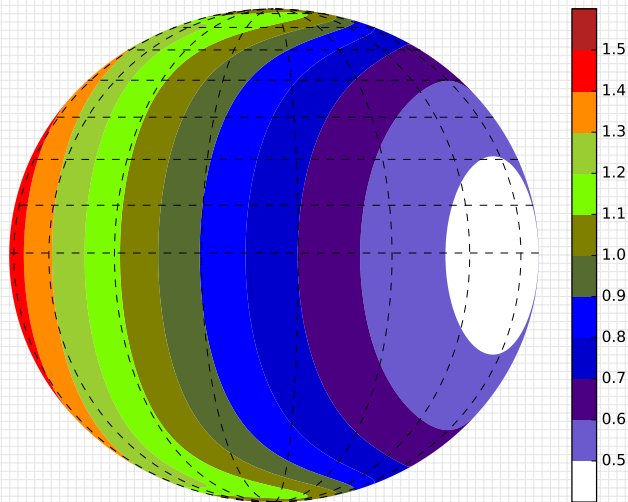
Moving vortices on the sphere - Nair and Jablonowski 2008



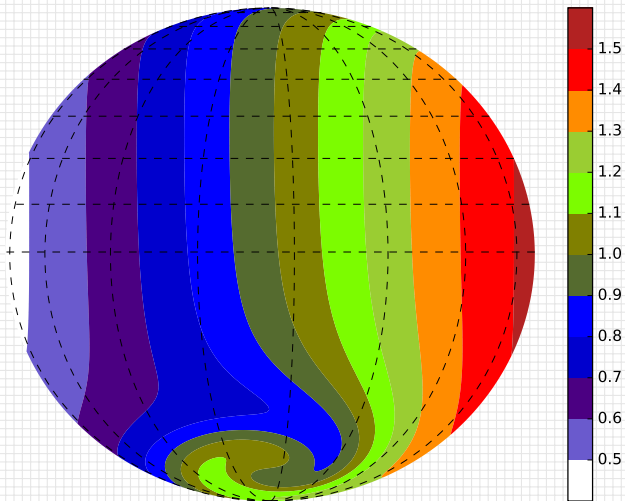
Moving vortices on the sphere - Nair and Jablonowski 2008



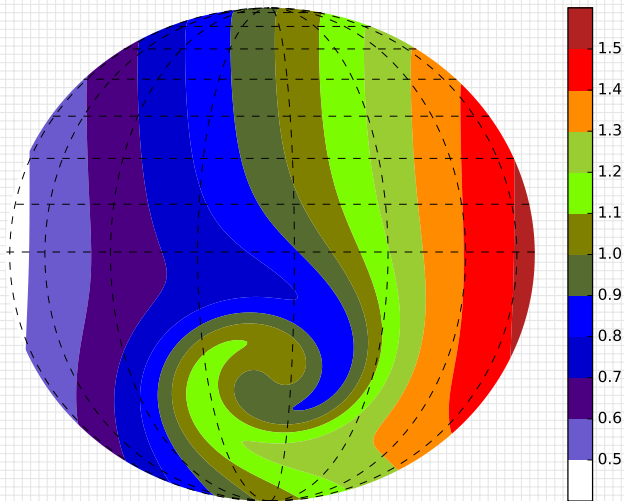
Moving vortices on the sphere - Nair and Jablonowski 2008



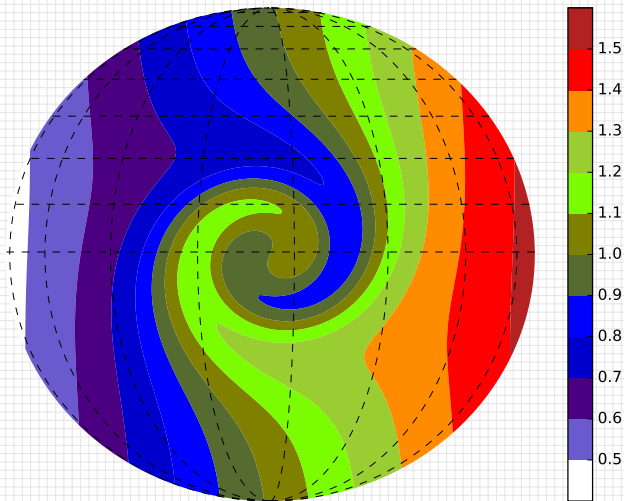
Moving vortices on the sphere - Nair and Jablonowski 2008



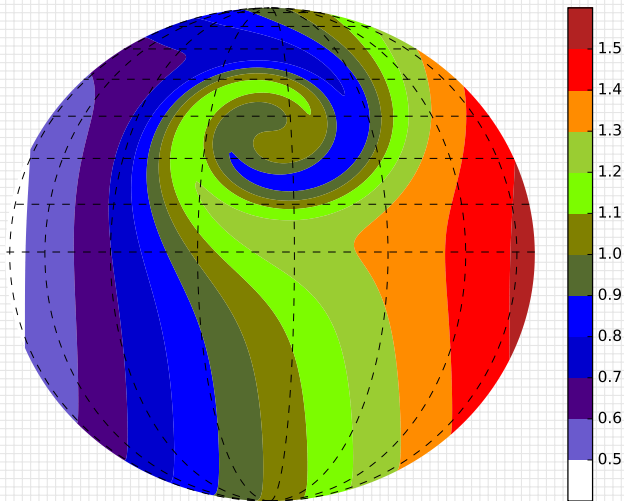
Moving vortices on the sphere - Nair and Jablonowski 2008



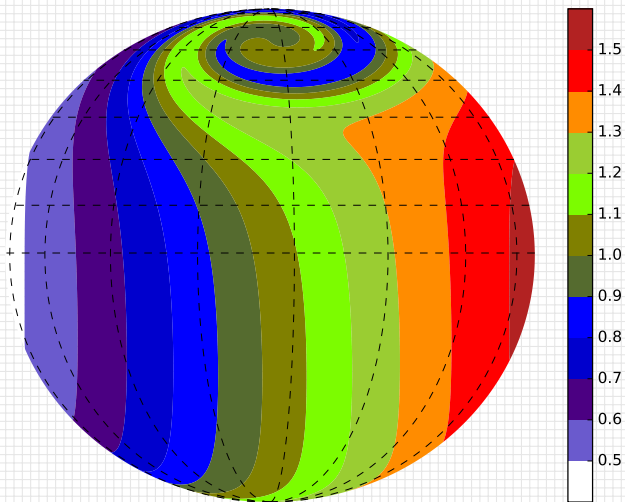
Moving vortices on the sphere - Nair and Jablonowski 2008



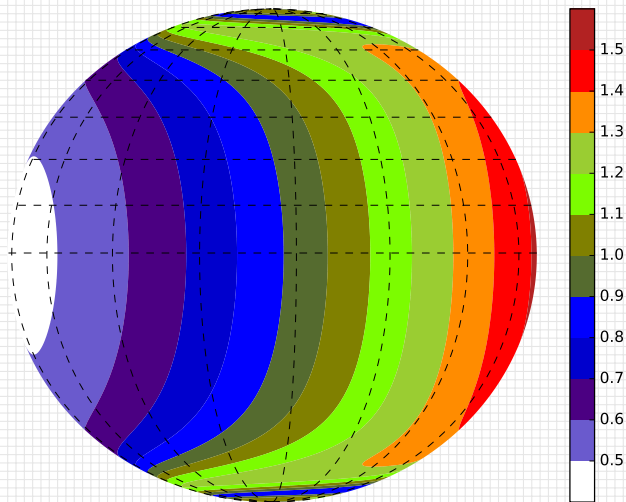
Moving vortices on the sphere - Nair and Jablonowski 2008



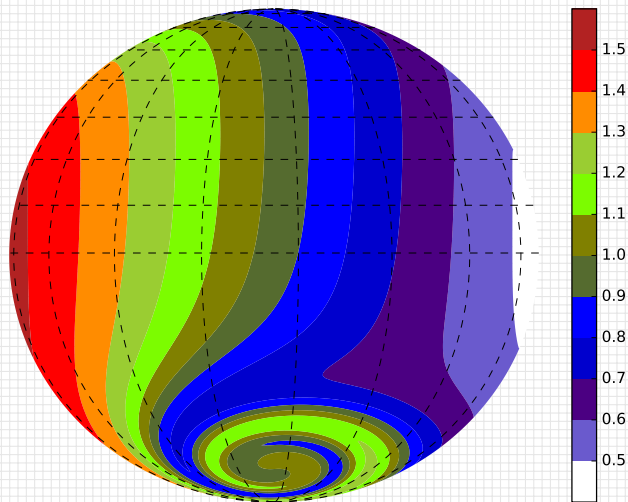
Moving vortices on the sphere - Nair and Jablonowski 2008



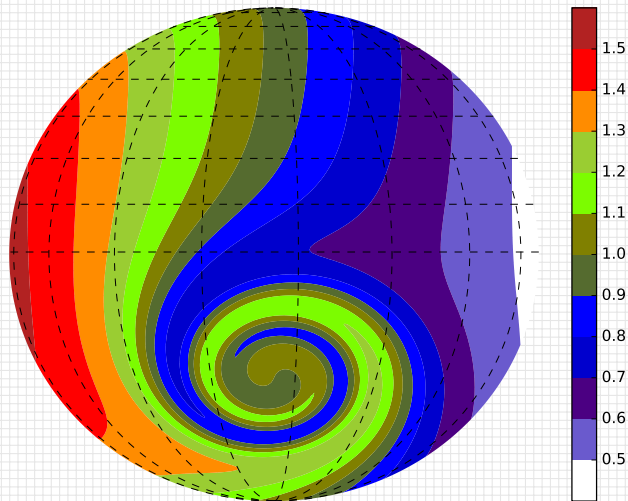
Moving vortices on the sphere - Nair and Jablonowski 2008



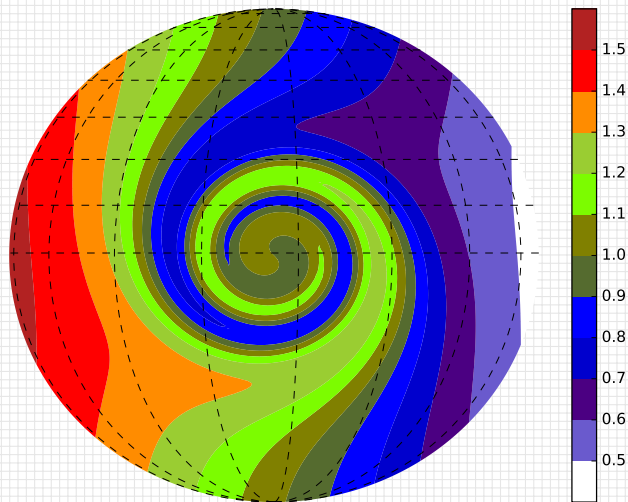
Moving vortices on the sphere - Nair and Jablonowski 2008



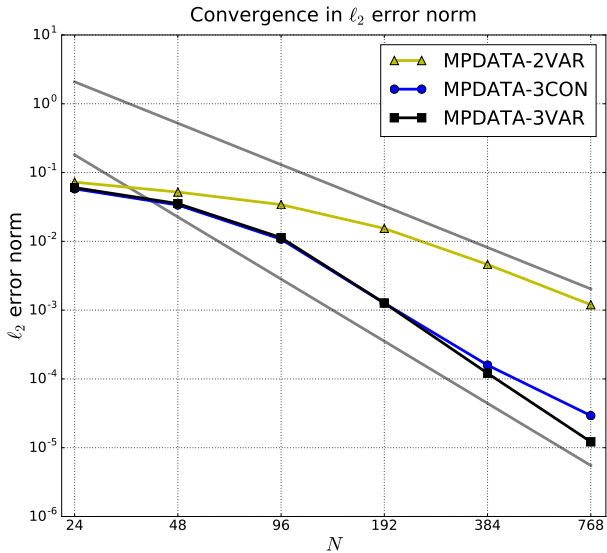
Moving vortices on the sphere - Nair and Jablonowski 2008



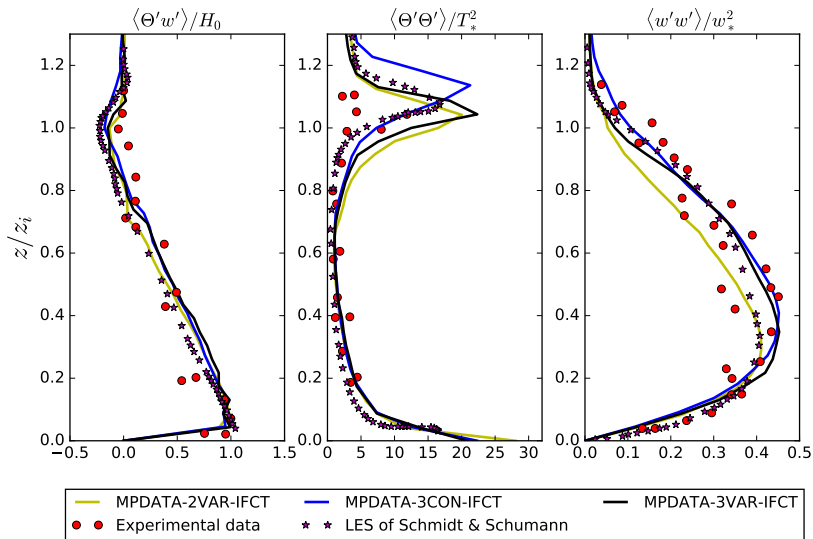
Moving vortices on the sphere - Nair and Jablonowski 2008



Moving vortices on the sphere - results



Beyond pure advection - simulation of convective boundary layer



Third-order accurate MPDATA coming soon to *libmpdata++*

libmpdata++

free & open source C++ library of MPDATA solvers

Repository

<https://github.com/igfuw/libmpdataxx>

Article

Jaruga et al. *libmpdata++ 0.1: a library of parallel MPDATA solvers for systems of generalised transport equations*

Geoscientific Model Development, 8, 1005-1032, 2015

Acknowledgments

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Thank you for your attention !