Overview of PySDM and PyMPDATA:
two new packages for numerically solving coagulation and transport problems in cloud physics and beyond

Sylwester Arabas
Jagiellonian University

acknowledgements: contributors & funding

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funding

EU / Foundation for Polish Science ("POWROTY")

introduction: cloud physics (@UJ)

Council of the Jagiellonian University Faculty of Philosophy in 1900
... August Witkowski - physicist, Rector in 1910-1911; Kazimierz Żorawski - mathematician, Rector in 1917-1918; **Maurycy Pius Rudzki - astronomer**

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TREŚĆ

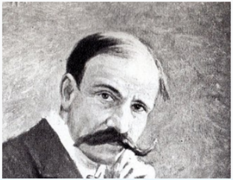
Maurycy Pius Rudzki (1862–1916)

Maurycy Pius Rudzki

From Wikipedia, the free encyclopedia

Maurycy Pius Rudzki (b. 1862, d. 1916) was the first person to call himself a professor of geophysics. He held the Chair of Geophysics at the Jagiellonian University in Kraków, and established the Institute of Geophysics there in 1895. His research specialty was elastic anisotropy, as applied to wave propagation in the earth, and he established many of the fundamental results in that arena. [1]

Maurycy Pius Rudzki



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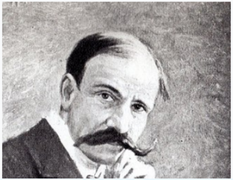
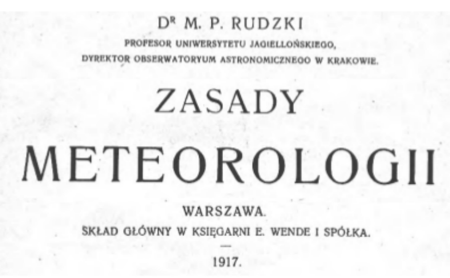


"Principles of Meteorology" book (1917)



DR M. P. RUDZKI

PROFESOR UNIWERSYTETU JAGIELLOŃSKIEGO,
DYREKTOR OBSERWATORYUM ASTRONOMICZNEGO W KRAKOWIE.

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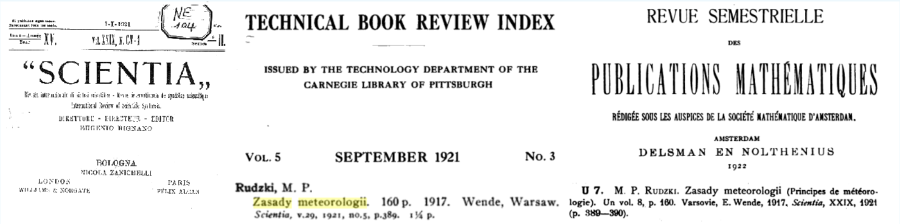

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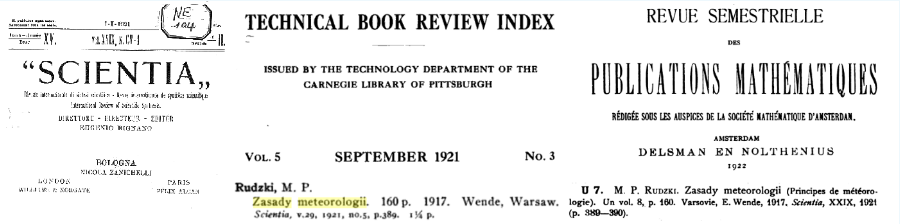
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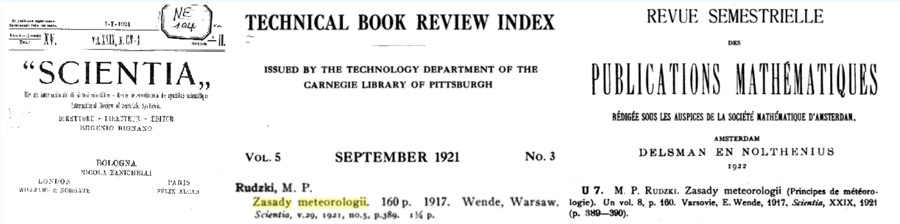

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introduction: modelling coagulation

cloud droplet collisional growth

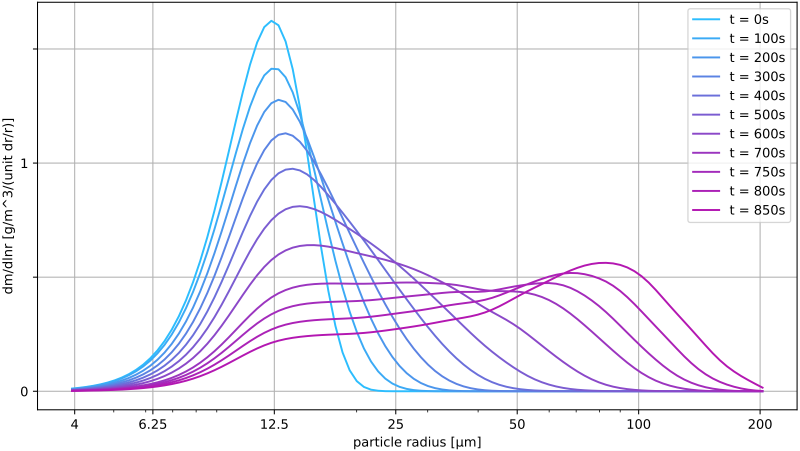

figure: Piotr Bartman

Smoluchowski's coagulation equation (SCE)

droplet concentration: $c(x,t) : \mathbb{R}^+ \times \mathbb{R}^+ \rightarrow \mathbb{R}^+$
collision kernel: $a(x_1, x_2) : \mathbb{R}^+ \times \mathbb{R}^+ \rightarrow \mathbb{R}^+$

$$\dot{c}(x) = \frac{1}{2}\int_0^x a(y, x-y)c(y)c(x-y)dy - \int_0^\infty a(y,x)c(y)c(x)dy \quad (1)$$

droplet concentration: $c_i = c(x_i)$

$$\dot{c}_i = \frac{1}{2}\sum_{k=1}^{i-1} a(x_k, x_{i-k})c_k c_{i-k} - \sum_{k=1}^{\infty} a(x_k, x_i)c_k c_i \quad (2)$$

SCE: challenges/problems

- analytic solutions to the equation are known only for simple kernels

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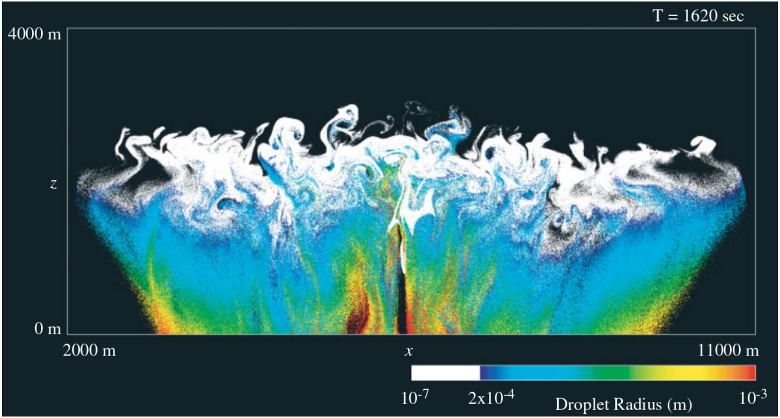
- the numerical methods for SCE suffer from the curse of dimensionality due to the need to distinguish particles of same size x but different properties
- in practice, the assumptions of the Smoluchowski equation may be difficult to meet:
  (i) the particle size changes at the same time
  (ii) it is assumed that the system is large enough and the droplets inside are uniformly distributed, which in turn is only true for a small volume in the atmosphere
- ...

context: aerosol-cloud-precipitation interactions (scales!)

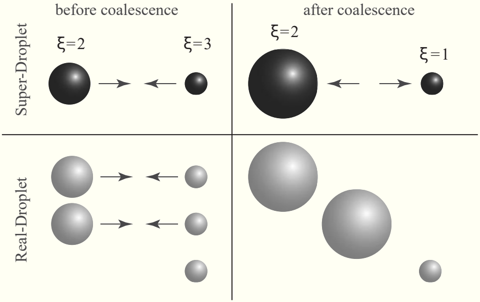
"Cloud and ship. Ukraine, Crimea, Black sea, view from Ai-Petri mountain"
(photo: Yevgen Timashov / National Geographic)

probabilistic particle-based simulations



Super-droplet simulation of a shallow convective cloud
(figure: Shima et al. 2009, QJRMS)

Super-Droplet Method (SDM)



Conceptual view of collision in SDM.
(figure: Shima et al. 2009, QJRMS)

$$\gamma = \left\lceil a(v_{[j]}, v_{[k]}) \frac{\Delta t}{V} \max\{\xi_{[j]}, \xi_{[k]}\} \frac{n_{sd}(n_{sd}-1)/2}{n_{sd}/2} - \phi_\gamma \right\rceil \quad (3)$$

$$\phi_\gamma \sim Uniform[0,1)$$

assume $\xi_{[j]} > \xi_{[k]}$ and $\tilde{\gamma} = \min\{\gamma, \lfloor \xi_{[j]}/\xi_{[k]} \rfloor\}$

1. $\xi_{[j]} - \tilde{\gamma}\xi_{[k]} > 0$

$$\begin{aligned} \hat{\xi}_{[j]} &= \xi_{[j]} - \tilde{\gamma}\xi_{[k]} & \hat{\xi}_{[k]} &= \xi_{[k]} \\ \hat{A}^{ex}_{[j]} &= A^{ex}_{[j]} & \hat{A}^{ex}_{[k]} &= A^{ex}_{[k]} + \tilde{\gamma}A^{ex}_{[j]} \end{aligned} \tag{4}$$

2. $\xi_{[j]} - \tilde{\gamma}\xi_{[k]} = 0$

$$\begin{aligned} \hat{\xi}_{[j]} &= \lfloor \xi_{[k]}/2 \rfloor & \hat{\xi}_{[k]} &= \xi_{[k]} - \lfloor \xi_{[k]}/2 \rfloor \\ \hat{A}^{ex}_{[j]} &= \hat{A}^{ex}_{[k]} & \hat{A}^{ex}_{[k]} &= A^{ex}_{[k]} + \tilde{\gamma}A^{ex}_{[j]} \end{aligned} \tag{5}$$

SCE vs SDM: differences

method type	
Mean-field, deterministic	Monte-Carlo, stochastic

considered pairs	
all (i,j) pairs	random set of $n_{sd}/2$ non-overlapping pairs, probability up-scaled by $(n_{sd}^2 - n_{sd})/2$ to $n_{sd}/2$ ratio

computation complexity	
$\mathcal{O}(n_{sd}^2)$	$\mathcal{O}(n_{sd})$

SCE vs SDM: differences

collisions	
colliding a fraction of $\xi_{[i]}, \xi_{[j]}$	collide all of $\min\{\xi_{[i]}, \xi_{[j]}\}$ (all or nothing)

collisions triggered	
every time step	by comparing probability with a random number

SCE vs SDM: solutions (Golovin kernel with analytic sol.)

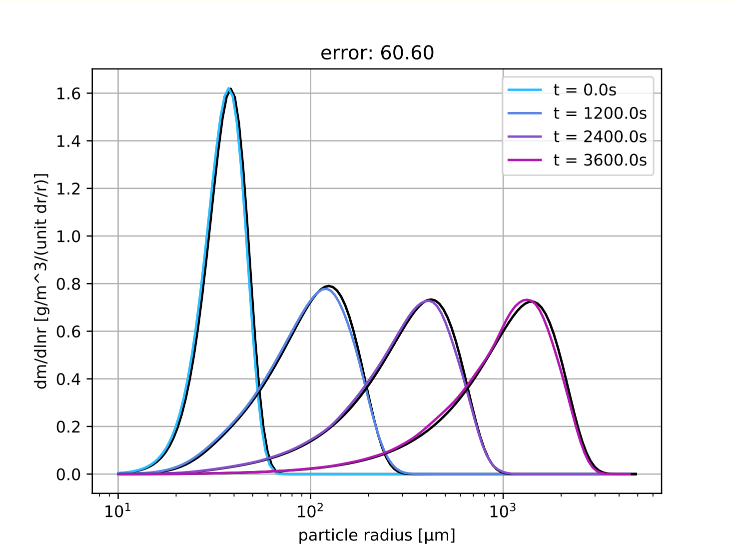


figure: Piotr Bartman

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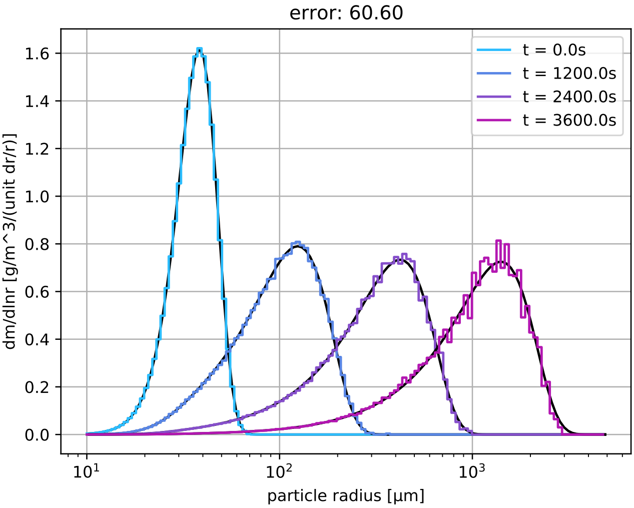
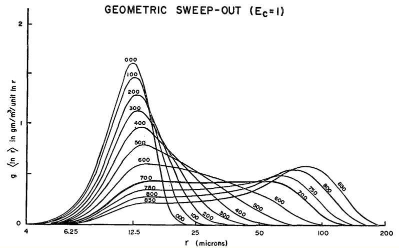
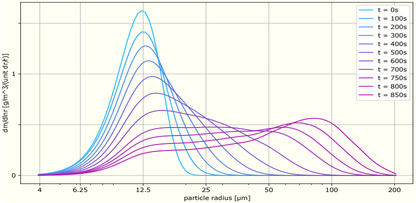
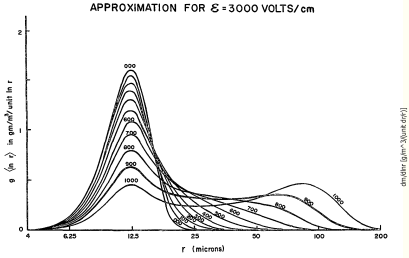


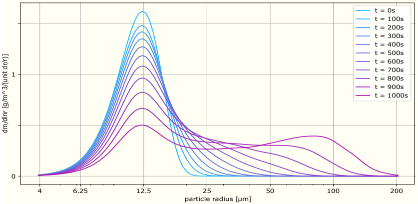
figure: Piotr Bartman

SDM: non-trivial kernels (vs. plots from Berry 1967)









figures: E.X. Berry | P. Bartman

more: https://arxiv.org/abs/2101.06318

arXiv.org > physics > arXiv:2101.06318

Physics > Computational Physics

[Submitted on 15 Jan 2021 (v1), last revised 3 Apr 2021 (this version, v2)]

On the design of Monte-Carlo particle coagulation solver interface: a CPU/GPU Super-Droplet Method case study with PySDM

Piotr Bartman, Sylwester Arabas

Super-Droplet Method (SDM) is a probabilistic Monte-Carlo-type model of particle coagulation process, an alternative to the mean-field formulation of Smoluchowski. SDM as an algorithm has linear computational complexity with respect to the state vector length, the state vector length is constant throughout simulation, and most of the algorithm steps are readily parallelizable. This paper discusses the design and implementation of two number-crunching backends for SDM implemented in PySDM, a new free and open-source Python package for simulating the dynamics of atmospheric aerosol, cloud and rain particles. The two backends share their application programming interface (API) but leverage distinct parallelism paradigms, target different hardware, and are built on top of different lower-level routine sets. First offers multi-threaded CPU computations and is based on Numba (using Numpy arrays). Second offers GPU computations and is built on top of ThrustRTC and CURandRTC (and does not use Numpy arrays). In the paper, the API is discussed focusing on: data dependencies across steps, parallelisation opportunities, CPU and GPU implementation nuances, and algorithm workflow. Example simulations suitable for validating implementations of the API are presented.

Comments: accepted to ICCS 2021
Subjects: **Computational Physics (physics.comp-ph)**
Cite as: arXiv:2101.06318 **[physics.comp-ph]**
(or arXiv:2101.06318v2 **[physics.comp-ph]** for this version)

Piotr's talk on Thu June 17 @ ICCS (paper accepted to LNCS): https://easychair.org/smart-program/ICCS2021/2021-06-17.html#talk:168705

PySDM

http://atmos.ii.uj.edu.pl

Atmospheric Cloud Simulation Group @ Jagiellonian University

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PySDM

Pythonic particle-based (super-droplet) warm-rain/aqueous-chemistry cloud microphysics package with box, parcel & 1D/2D prescribed-flow examples in Python, Julia and Matlab

Python 17 14

PyMPDATA

Forked from piotrbartman/PyMPDATA

Numba-accelerated Pythonic implementation of MPDATA with examples in Python, Julia and Matlab

Python 5 7

numba-mpi

Numba @njittable MPI wrappers tested on Linux, macOS and Windows

Python 2

PySDM-examples

PySDM usage examples (mostly reproducing results from literature) depicting how to use PySDM in Python, in particular from Jupyter notebooks

Jupyter Notebook 1 4

PyMPDATA-examples

PyMPDATA usage examples (mostly reproducing results from literature) depicting how to use PyMPDATA in Python, in particular from Jupyter notebooks

Jupyter Notebook 1 3

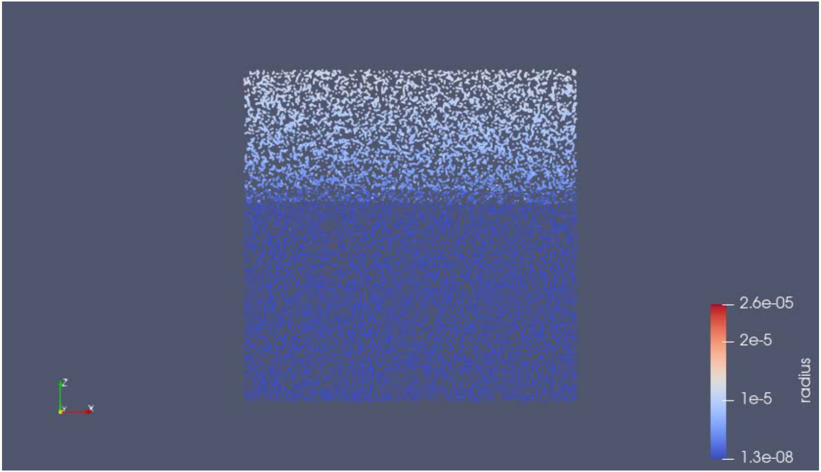

figure: Oleksii Bulenok

https://github.com/atmos-cloud-sim-uj/PySDM/

README.md

Python 3 | LLVM Numba | CUDA ThrustRTC | Linux ✓ | macOS ✓ | Windows ✓ | Jupyter ✓ | build passing
PySDM passing | PySDM-examples passing | build passing | Dependabot on | codecov 60% | Maintained? yes
issues 89 open | issues 225 closed | pull requests 2 open | pull requests 243 closed | Open Hub Metrics by Open Hub
EU Funding by FNP | Copyright Jagiellonian University | License GPL v3

PySDM

PySDM is a package for simulating the dynamics of population of particles. It is intended to serve as a building block for simulation systems modelling fluid flows involving a dispersed phase, with PySDM being responsible for representation of the dispersed phase. Currently, the development is focused on atmospheric cloud physics applications, in particular on modelling the dynamics of particles immersed in moist air using the particle-based (a.k.a. super-droplet) approach to represent aerosol/cloud/rain microphysics. The package core is a Pythonic high-performance implementation of the Super-Droplet Method (SDM) Monte-Carlo algorithm for representing collisional growth (Shima et al. 2009), hence the name.

PySDM has two alternative parallel number-crunching backends available: multi-threaded CPU backend based on Numba and GPU-resident backend built on top of ThrustRTC. The `Numba` backend (aliased `CPU`) features multi-threaded parallelism for multi-core CPUs, it uses the just-in-time compilation technique based on the LLVM infrastructure. The `ThrustRTC` backend (aliased `GPU`) offers GPU-resident operation of PySDM leveraging the SIMT parallelisation model. Using the `GPU` backend requires nVidia hardware and CUDA driver.

For an overview paper on PySDM v1 (and the preferred item to cite if using PySDM), see Bartman et al. 2021 arXiv e-print (submitted to JOSS). For a list of talks and other materials on PySDM, see the project wiki.

A pdoc-generated documentation of PySDM public API is maintained at: https://atmos-cloud-sim-uj.github.io/PySDM

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Contributors 9

Environments 1

github-pages Active

Languages

Python 100.0%

demo

PySDM: highlights

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- refactorable and maintainable code (Piotr Bartman)

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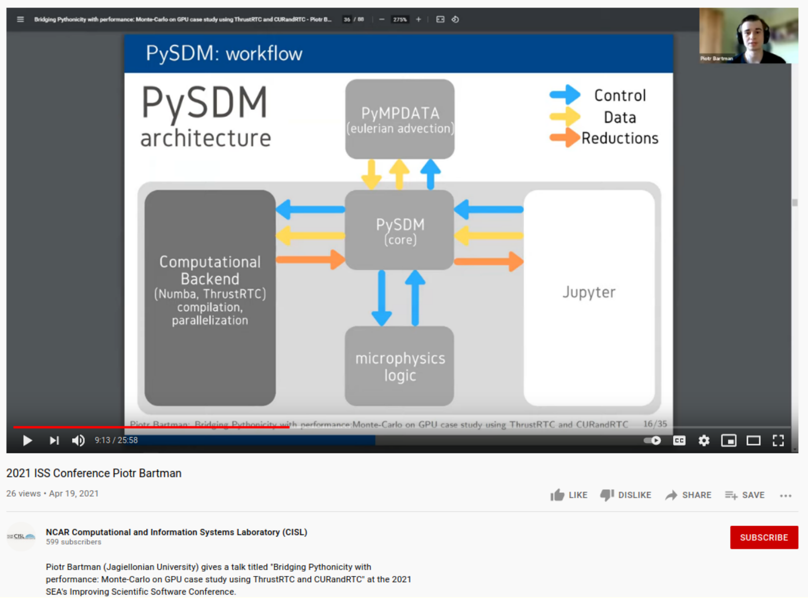
- open and reproducible research ready

more: https://www.youtube.com/watch?v=s7iM9RBtULU



(talk @ Improving Scientific Software Conference, NCAR, Boulder, Colorado)

more: https://arxiv.org/abs/2103.17238

arXiv.org > physics > arXiv:2103.17238

Physics > Atmospheric and Oceanic Physics

[Submitted on 31 Mar 2021]

PySDM v1: particle-based cloud modelling package for warm-rain microphysics and aqueous chemistry

Piotr Bartman, Sylwester Arabas, Kamil Górski, Anna Jaruga, Grzegorz Łazarski, Michael Olesik, Bartosz Piasecki, Aleksandra Talar

PySDM is an open-source Python package for simulating the dynamics of particles undergoing condensational and collisional growth, interacting with a fluid flow and subject to chemical composition changes. It is intended to serve as a building block for process-level as well as computational-fluid-dynamics simulation systems involving representation of a continuous phase (air) and a dispersed phase (aerosol), with PySDM being responsible for representation of the dispersed phase. The PySDM package core is a Pythonic high-performance implementation of the Super-Droplet Method (SDM) Monte-Carlo algorithm for representing collisional growth, hence the name. PySDM has two alternative parallel number-crunching backends available: multi-threaded CPU backend based on Numba and GPU-resident backend built on top of ThrustRTC. The usage examples are built on top of four simple atmospheric cloud modelling frameworks: box, adiabatic parcel, single-column and 2D prescribed flow kinematic models. In addition, the package ships with tutorial code depicting how PySDM can be used from Julia and Matlab.

(submitted to JOSS)

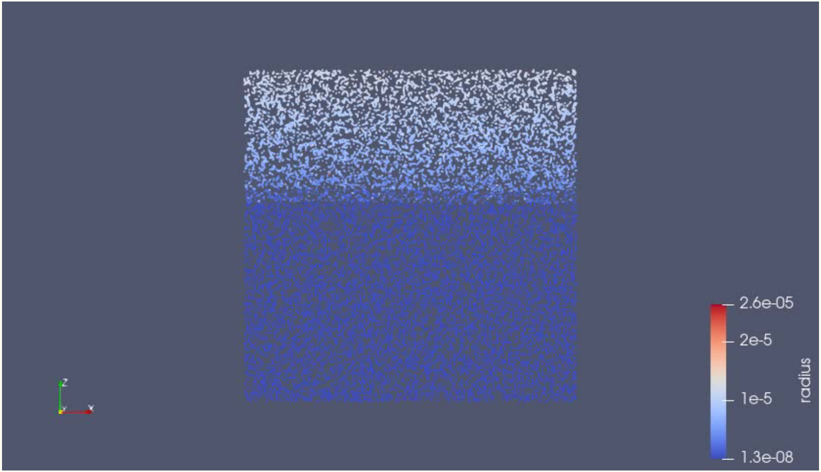


figure: Oleksii Bulenok

MPDATA

a.k.a. the Smolarkiewicz method

MPDATA in a nutshell (Smolarkiewicz 1983 MWR . . .)

transport PDE: $\frac{\partial \psi}{\partial t} + \frac{\partial}{\partial x}(v\psi) = 0$

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$$\psi_i^{n+1} = \psi_i^n - \left[F(\psi_i^n, \psi_{i+1}^n, \mathcal{C}_{i+1/2}) - F(\psi_{i-1}^n, \psi_i^n, \mathcal{C}_{i-1/2})\right]$$

$$F(\psi_L, \psi_R, \mathcal{C}) = \max(\mathcal{C}, 0) \cdot \psi_L + \min(\mathcal{C}, 0) \cdot \psi_R$$

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upwind

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$$\mathcal{C}'_{i+1/2} = (|\mathcal{C}_{i+1/2}| - \mathcal{C}^2_{i+1/2})A_{i+1/2}$$

$$A_{i+1/2} = \frac{\psi_{i+1} - \psi_i}{\psi_{i+1} + \psi_i}$$

MPDATA: reverse numerical diffusion by integrating the antidiffusive flux using upwind (in a corrective iteration)

MPDATA: key features (review: e.g. Smolarkiewicz 2006)

Multidimensional **P**ositive **D**efinite Advection Transport Algorithm

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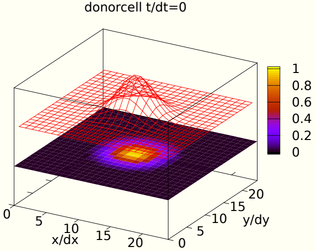
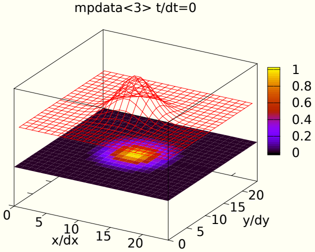
- Monotonic:
  with Flux-Corrected Transport option

MPDATA: 2D “hello-world” example





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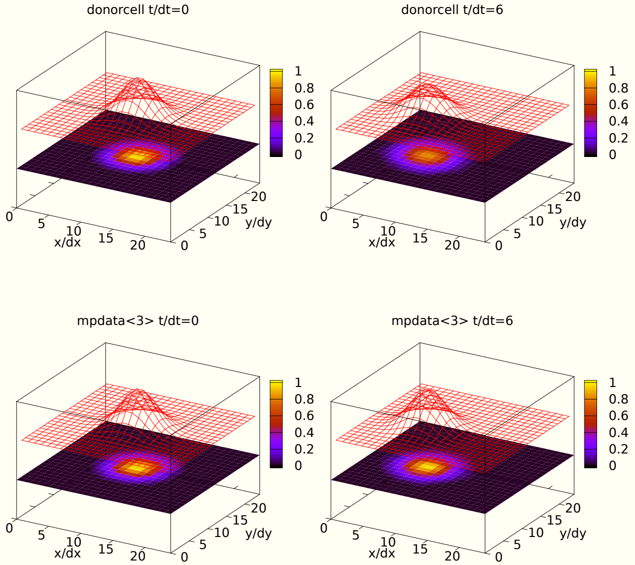

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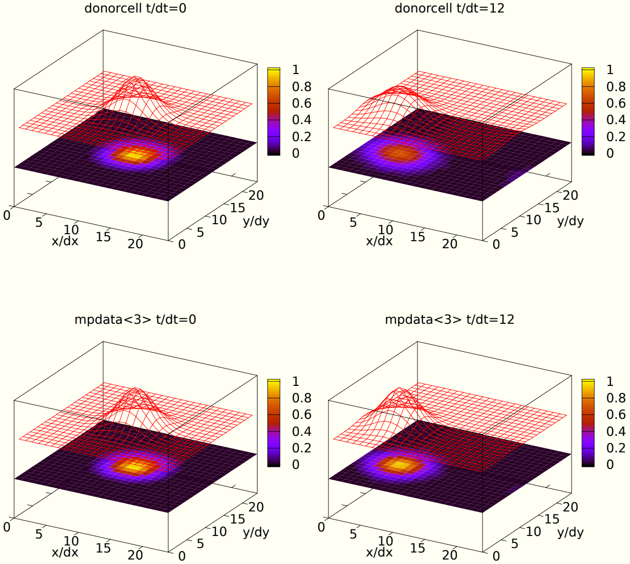

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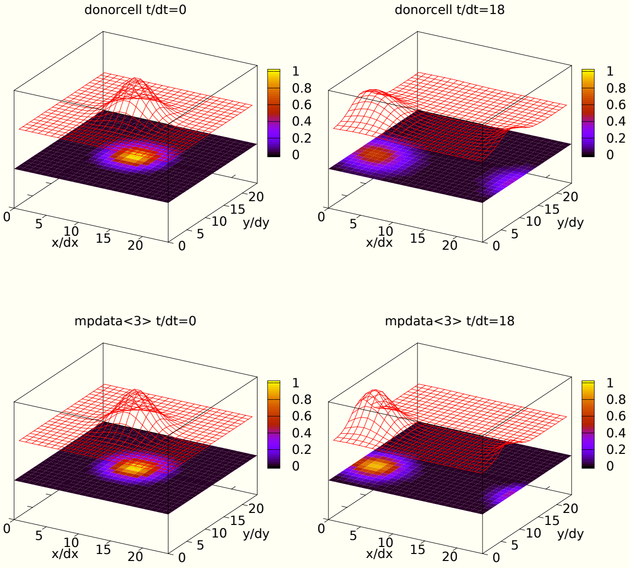

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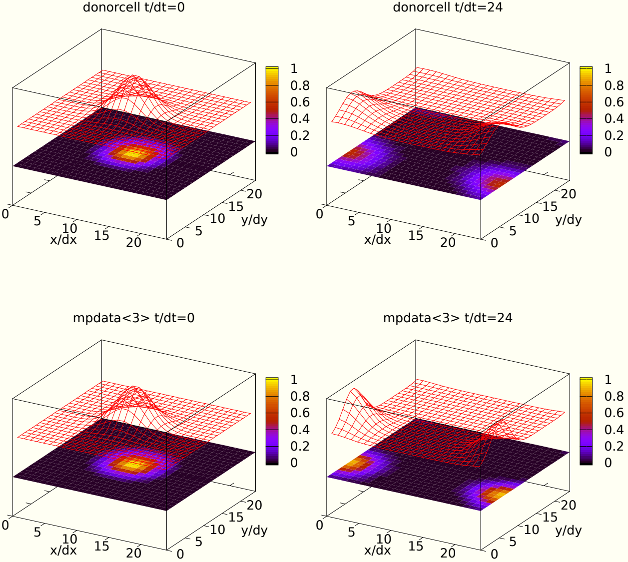

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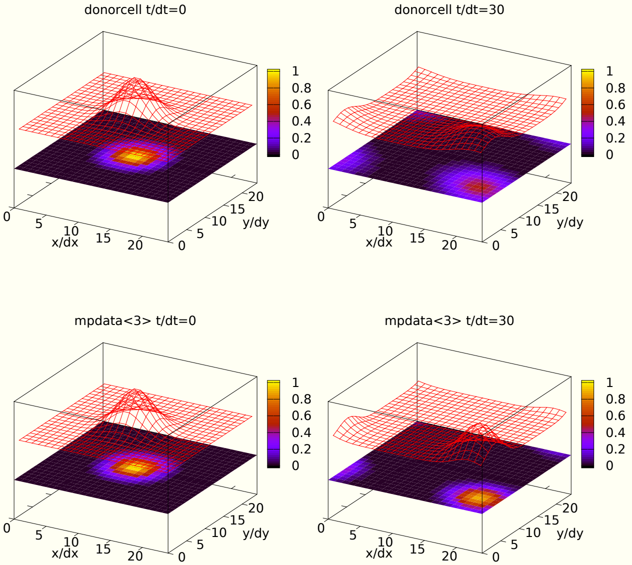

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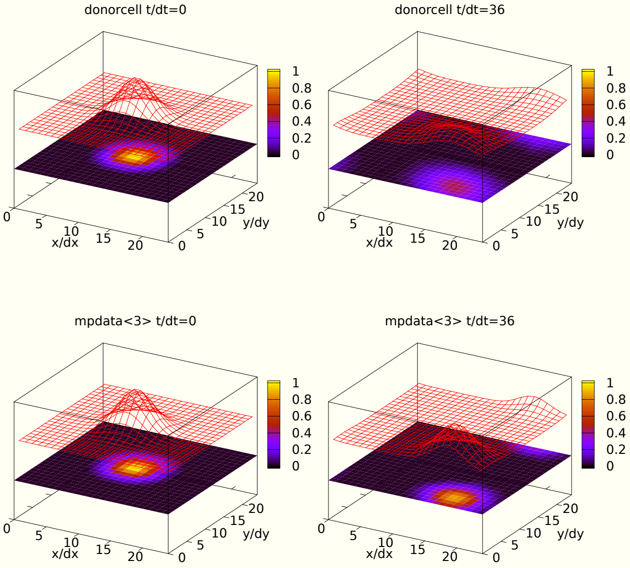

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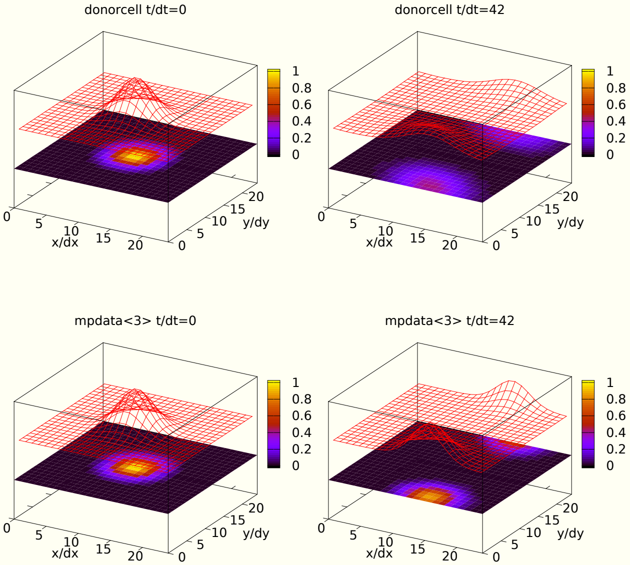

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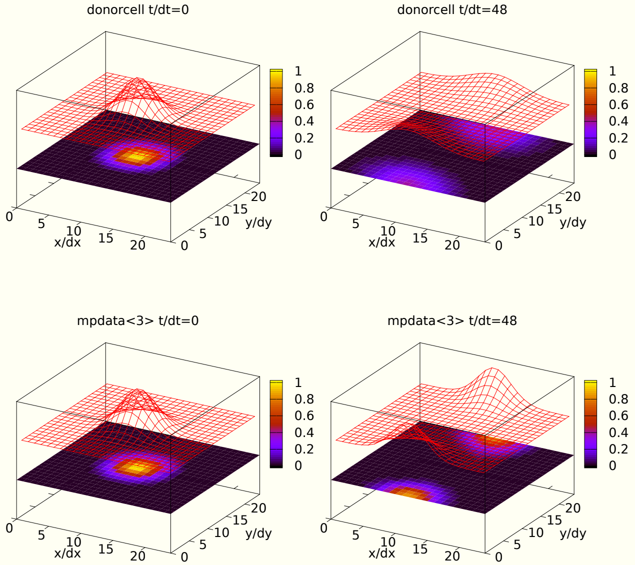

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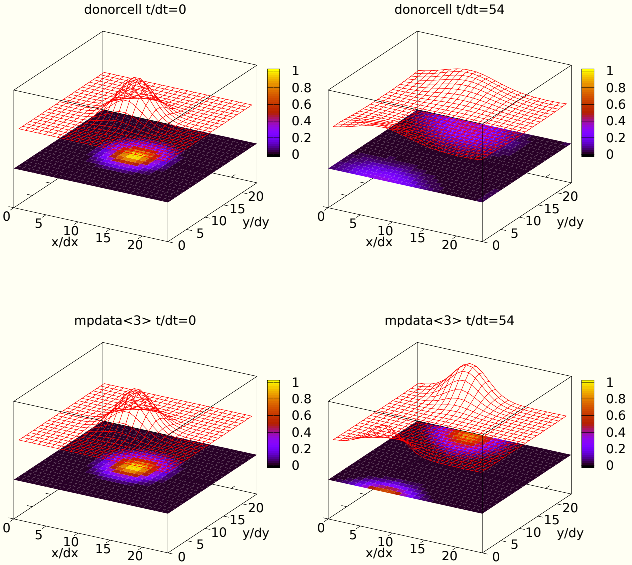

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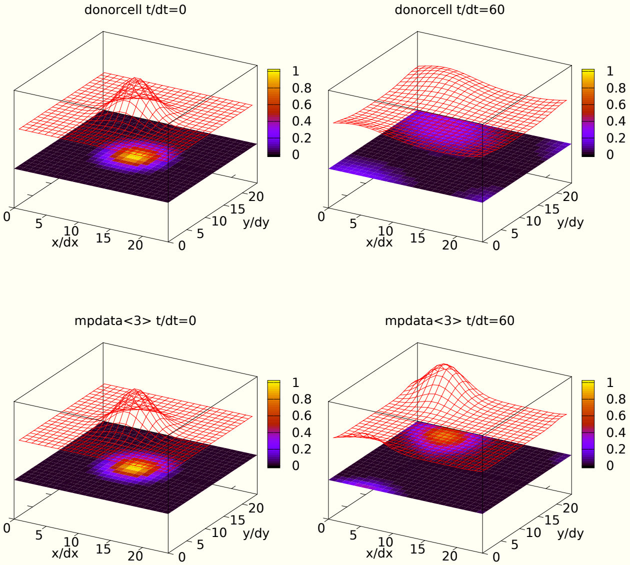

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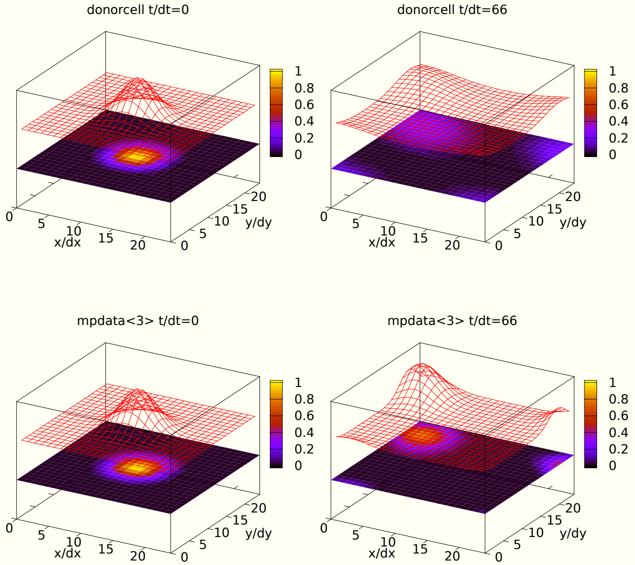

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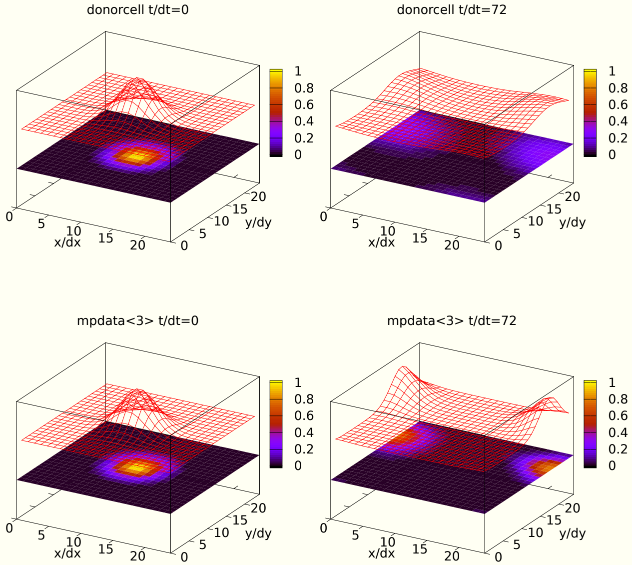

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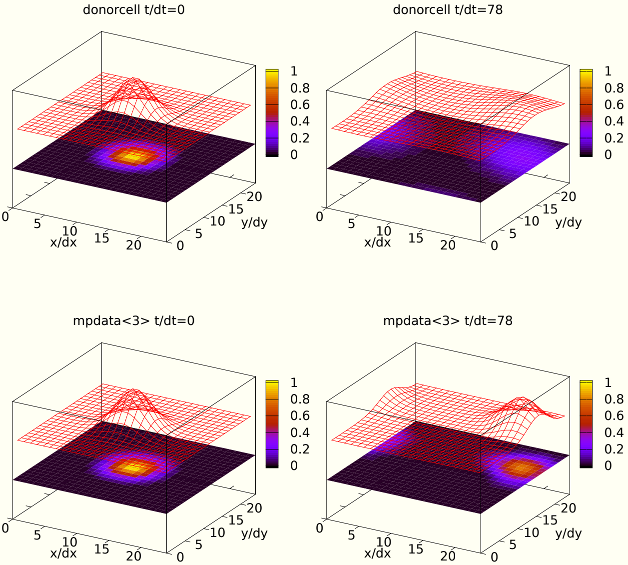

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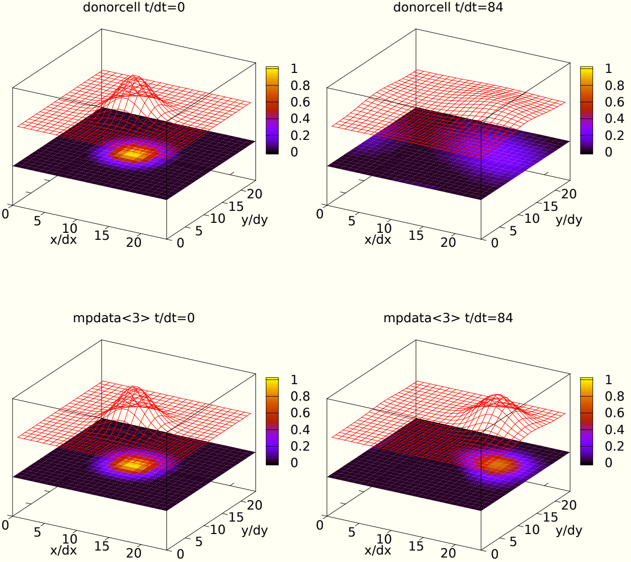

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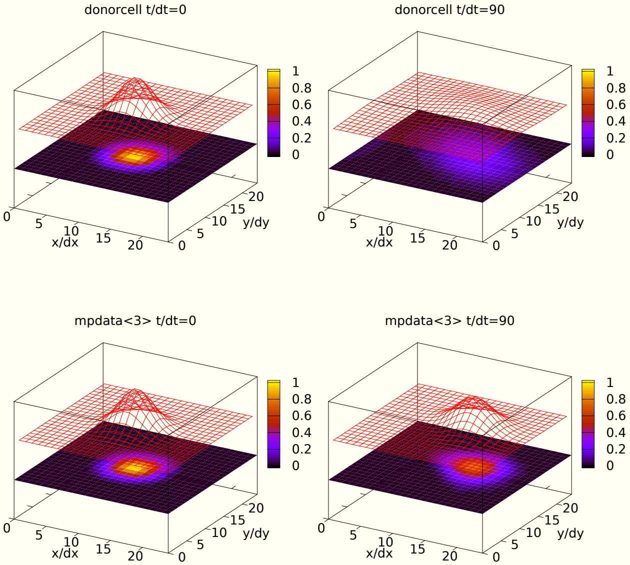

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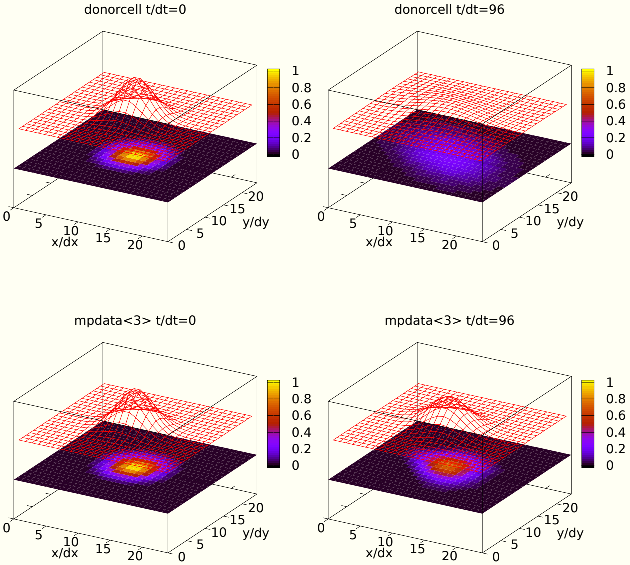

MPDATA: well established “classic” in geophysics

Piotr Smolarkiewicz

Senior Scientist Emeritus
Verified email at ucar.edu

atmospheric physics   geophysical fluid dynamics   MHD   numerical methods

TITLE	CITED BY	YEAR
A fully multidimensional positive definite advection transport algorithm with small implicit diffusion PK Smolarkiewicz Journal of Computational Physics 54 (2), 325-362	790	1984
A simple positive definite advection scheme with small implicit diffusion PK Smolarkiewicz Monthly weather review 111 (3), 479-486	642	1983
Low Froude number flow past three-dimensional obstacles. Part I: Baroclinically generated lee vortices PK Smolarkiewicz, R Rotunno Journal of Atmospheric Sciences 46 (8), 1154-1164	511	1989
The multidimensional positive definite advection transport algorithm: Nonoscillatory option PK Smolarkiewicz, WW Grabowski Journal of Computational Physics 86 (2), 355-375	440	1990
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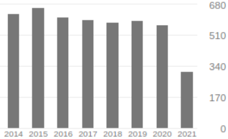

PyMPDATA

http://atmos.ii.uj.edu.pl

Atmospheric Cloud Simulation Group @ Jagiellonian University

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PySDM

Pythonic particle-based (super-droplet) warm-rain/aqueous-chemistry cloud microphysics package with box, parcel & 1D/2D prescribed-flow examples in Python, Julia and Matlab

Python ☆ 17 Forks 14

PyMPDATA

Forked from piotrbartman/PyMPDATA

Numba-accelerated Pythonic implementation of MPDATA with examples in Python, Julia and Matlab

Python ☆ 5 Forks 7

numba-mpi

Numba @njittable MPI wrappers tested on Linux, macOS and Windows

Python Forks 2

PySDM-examples

PySDM usage examples (mostly reproducing results from literature) depicting how to use PySDM in Python, in particular from Jupyter notebooks

Jupyter Notebook ☆ 1 Forks 4

PyMPDATA-examples

PyMPDATA usage examples (mostly reproducing results from literature) depicting how to use PyMPDATA in Python, in particular from Jupyter notebooks

Jupyter Notebook ☆ 1 Forks 3

PyMPDATA: new open-source Python/Numba package

README.md

Python 3 | LLVM Numba | Linux ✓ | macOS ✓ | Windows ✓ | Jupyter ✓ | build passing | PyMPDATA passing
PyMPDATA-examples passing | build passing | Dependabot on | codecov 67% | Maintained? yes | issues 35 open
issues 66 closed | pull requests 1 open | pull requests 129 closed | Open Hub 7 Developers | EU Funding by FNP
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PyMPDATA

PyMPDATA is a high-performance **Numba-accelerated Pythonic implementation of the MPDATA algorithm of Smolarkiewicz et al.** for numerically solving generalised transport equations - partial differential equations used to model conservation/balance laws, scalar-transport problems, convection-diffusion phenomena (in geophysical fluid dynamics and beyond). As of the current version, PyMPDATA supports homogeneous transport in 1D, 2D and 3D (work in progress) using structured meshes, optionally generalised by employment of a Jacobian of coordinate transformation. PyMPDATA includes implementation of a set of MPDATA **variants including the non-oscillatory option, infinite-gauge, divergent-flow, double-pass donor cell (DPDC) and third-order-terms options**. It also features support for integration of Fickian-terms in advection-diffusion problems using the pseudo-transport velocity approach. In 2D and 3D simulations, domain-decomposition is used for multi-threaded parallelism.

PyMPDATA is engineered purely in Python targeting both performance and usability, the latter encompassing research users', developers' and maintainers' perspectives. From researcher's perspective, PyMPDATA offers **hassle-free installation on multitude of platforms including Linux, OSX and Windows**, and eliminates compilation stage from the perspective of the user. From developers' and maintainers' perspective, PyMPDATA offers a suite of unit tests, multi-platform continuous integration setup, seamless integration with Python development aids including debuggers and profilers.

more: https://arxiv.org/abs/2011.14726

arXiv.org > physics > arXiv:2011.14726

Physics > Computational Physics

[Submitted on 30 Nov 2020]

On numerical broadening of particle size spectra: a condensational growth study using PyMPDATA

Michael Olesik, Sylwester Arabas, Jakub Banaśkiewicz, Piotr Bartman, Manuel Baumgartner, Simon Unterstrasser

The work discusses the diffusional growth in particulate systems such as atmospheric clouds. It focuses on the Eulerian modeling approach in which the evolution of the probability density function describing the particle size spectrum is carried out using a fixed-bin discretization. The numerical diffusion problem inherent to the employment of the fixed-bin discretization is scrutinized. The work focuses on the applications of MPDATA family of numerical schemes. Several MPDATA variants are explored including: infinite-gauge, non-oscillatory, third-order-terms and recursive antidiffusive correction (double pass donor cell, DPDC) options. Methodology for handling coordinate transformations associated with both particle size distribution variable choice and numerical grid layout are expounded. The study uses PyMPDATA - a new open-source Python implementation of MPDATA. Analysis of the performance of the scheme for different discretization parameters and different settings of the algorithm is performed using an analytically solvable test case pertinent to condensational growth of cloud droplets. The analysis covers spatial and temporal convergence, computational cost, conservativeness and quantification of the numerical broadening of the particle size spectrum. Presented results demonstrate that, for the problem considered, even a tenfold decrease of the spurious numerical spectral broadening can be obtained by a proper choice of the MPDATA variant (maintaining the same spatial and temporal resolution).

(submitted to GMD)

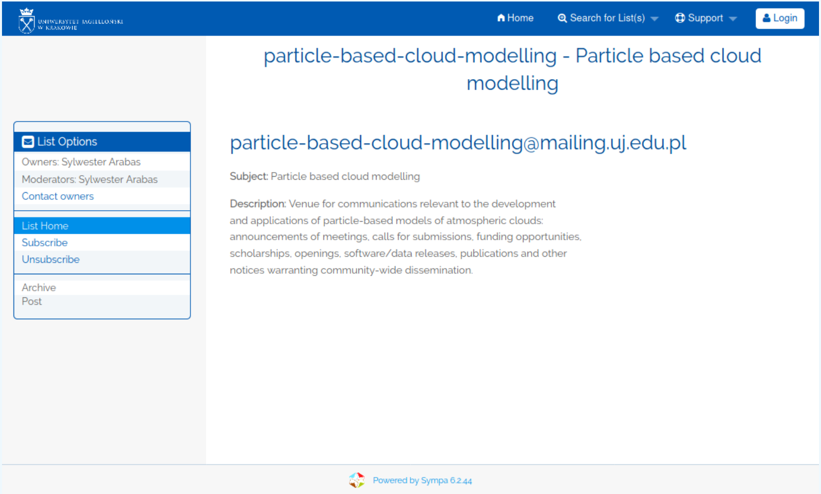
future

ideas...

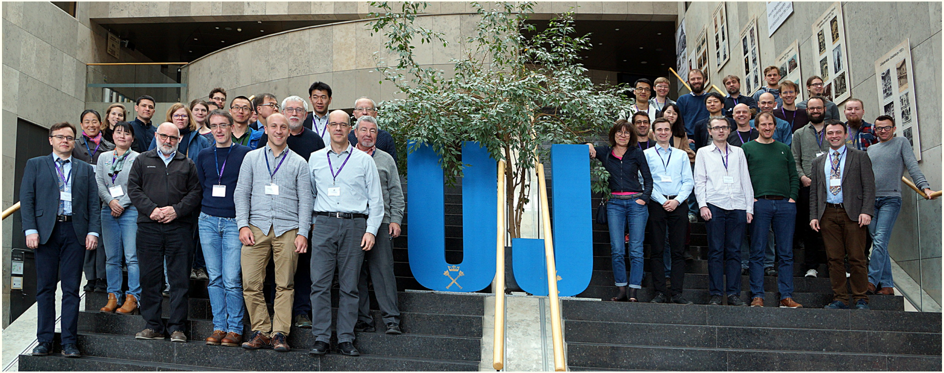
- https://github.com/atmos-cloud-sim-uj/PySDM/wiki/Ideas-for-new-features-and-examples
- https://github.com/atmos-cloud-sim-uj/PyMPDATA/wiki/Ideas-for-new-features-and-examples

users & developers

https://mailing.uj.edu.pl/sympa/info/particle-based-cloud-modelling



particle-based cloud modelling workshop at UJ (April '19)



44 researchers from 28 institutions from 11 countries

`http://www.ii.uj.edu.pl/~arabas/workshop_2019/`

NCN SONATA: "Modelling isotopic signatures in precipitation ..."

acknowledgements

acknowledgements: contributors & funding

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PySDM contributors

Piotr Bartman (WMiI), Michael Olesik (WFAiIS),
Grzegorz Łazarski (WCh/WMiI), Anna Jaruga (Caltech);

+ students @ WMiI:
Oleksii Bulenok, Kamil Górski, Bartosz Piasecki, Aleksandra Talar

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