

# 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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## PySDM contributors

Piotr Bartman (WMil), Michael Olesik (WFAiS),  
Grzegorz Łazarski (WCh/WMil), Anna Jaruga (Caltech);

+ students @ WMil:

Oleksii Bulenok, Kamil Górski, Bartosz Piasecki, Aleksandra Talar

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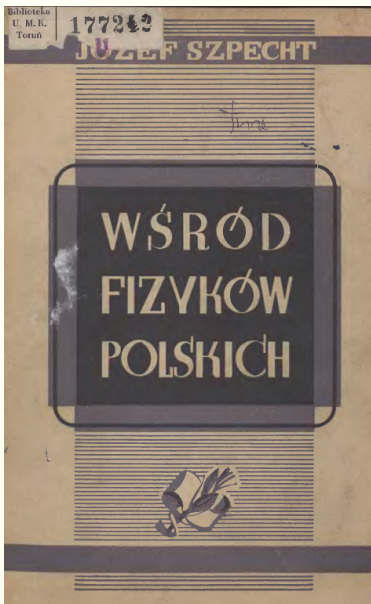
## funding

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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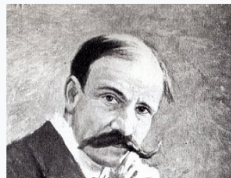
# Maurycy Pius Rudzki (1862–1916)

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From Wikipedia, the free encyclopedia

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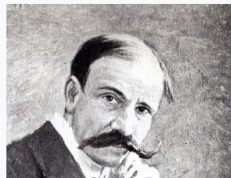
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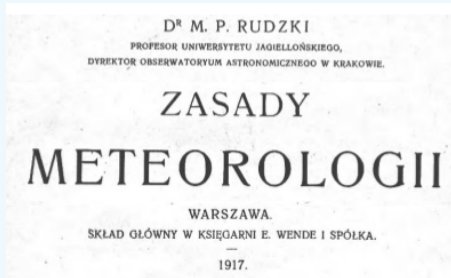
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Vol. XV, 1921, 8. 17-1  
1921

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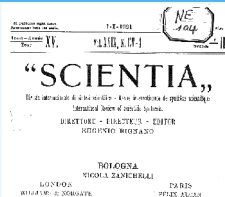
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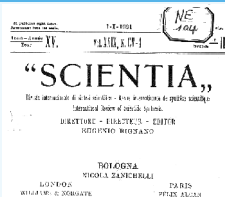
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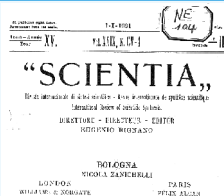
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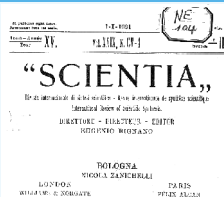
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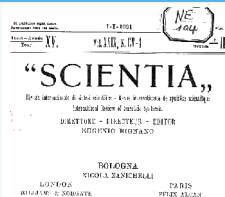
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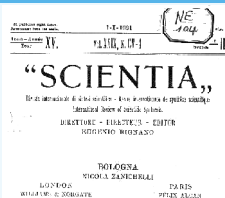
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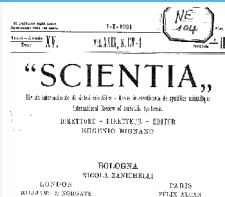
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Vol. 5                      SEPTEMBER 1921                      No. 3

**Rudzki, M. P.**  
**Zasady meteorologii.** 160 p. 1917. Wende, Warsaw.  
*Scientia*, v.29, 1921, no.5, p.389. 1 1/4 p.

REVUE SEMESTRIELLE

DES

## PUBLICATIONS MATHÉMATIQUES

RÉDIGÉE SOUS LES AUSPICES DE LA SOCIÉTÉ MATHÉMATIQUE D'AMSTERDAM.

AMSTERDAM

DELSMAN EN NOLTHENIUS

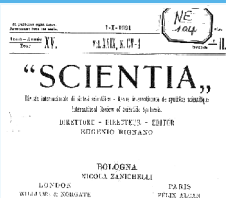
1922

**U 7. M. P. RUDZKI.** *Zasady meteorologii (Principes de météorologie).* Un vol. 8, p. 180. Varsovie, E. Wende, 1917. *Scientia*, XXIX, 1921 (p. 389-390).

<http://pbc.gda.pl/dlibra/docmetadata?id=18434> (+ Google Translate)

*... in the atmosphere, nuclei are needed for condensation ... the air contains a lot of smoke, molecules of acids e.t.c. ... all these are hygroscopic bodies that attract vapour even when the air is not saturated yet ... everything we have said so far only applies to to lonely drops, meanwhile, as rightly pointed out by Smoluchowski, usually it is not a single drop that falls but a whole plenty ... contrast between the sizes of drops, of which clouds are made up, and the size of raindrops, is so great that the latter, of course, can not come straight from the condensation, only from the merging of many small ones droplets ... the drops are all different, one smaller, the other bigger, but most often drops occur with weight ratios of 1,2,4,8 ... we thus conclude that droplets most often combine with those of equal size*

# Rudzki: "Principles of Meteorology" book (1917)



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# introduction: modelling coagulation

# cloud droplet collisional growth

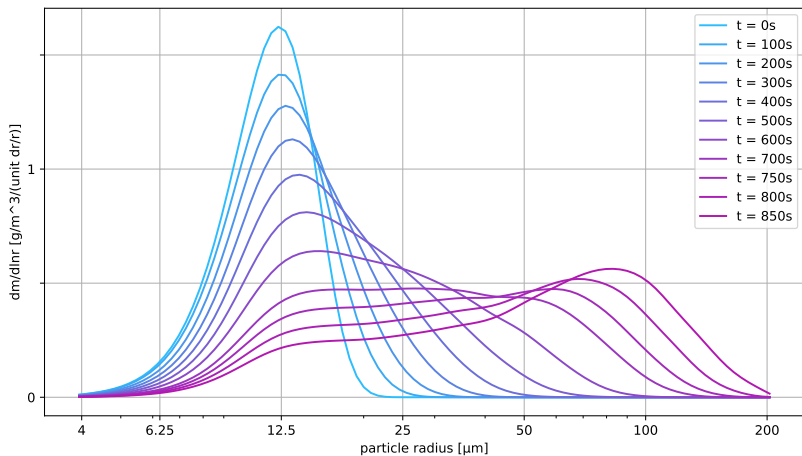


figure: Piotr Bartman

# 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:  $c_i = c(x_i)$

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

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

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

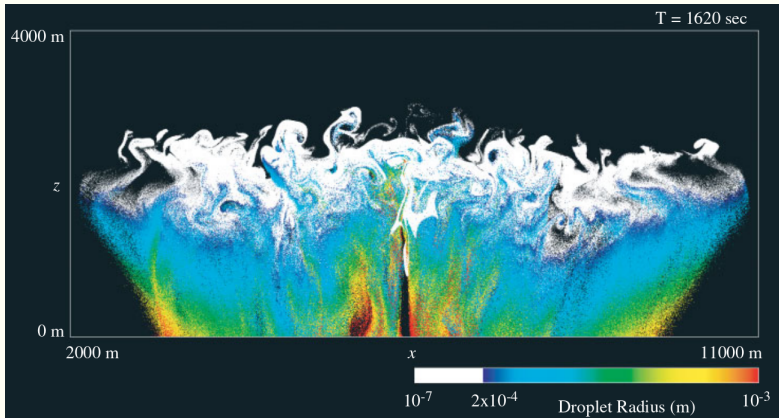


# context: aerosol-cloud-precipitation interactions (scales!)



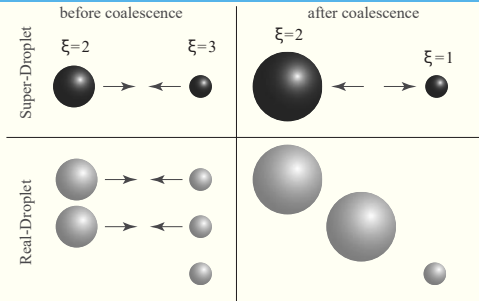
“Cloud and ship. Ukraine, Crimea, Black sea, view from Ai-Petri mountain”  
(photo: Yevgen Timashov / National Geographic)

# 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)

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

$$\phi_\gamma \sim \text{Uniform}[0, 1)$$

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

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

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

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

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

# 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.)

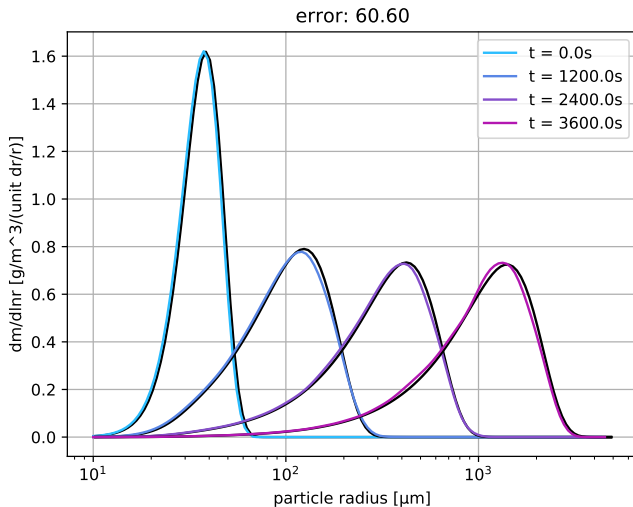


figure: Piotr Bartman

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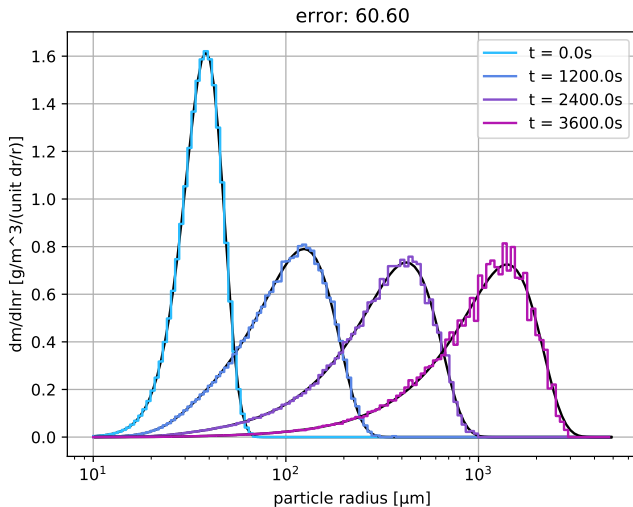
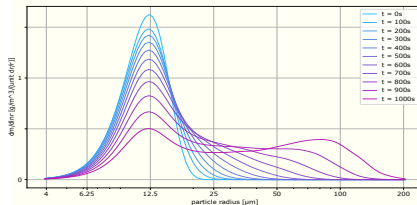
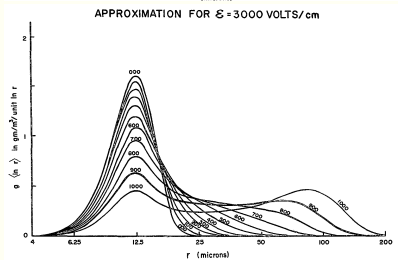
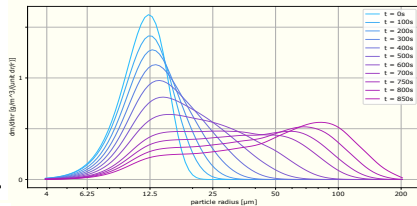
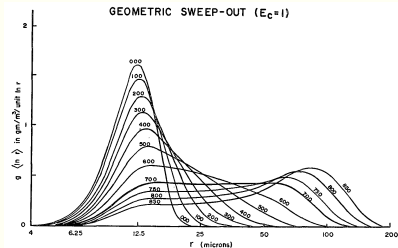


figure: Piotr Bartman



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



figures: E.X. Berry | P. Bartman

[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



## Atmospheric Cloud Simulation Group @ Jagiellonian University

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### Pinned repositories

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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 @njitable 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

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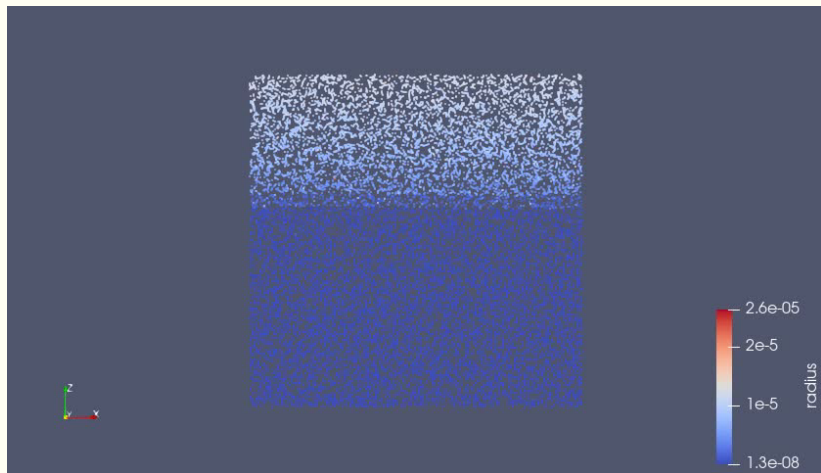


figure: Oleksii Bulenok

☰ 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  
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## 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.

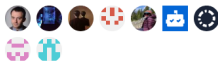
For an overview paper on PySDM v1 (and the preferred item to cite if using PySDM), see Bartman et al. 2021 arXiv e-print (submitted to JOSS). For a list of talks and other materials on PySDM, see the project wiki.

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

### Packages

No packages published  
[Publish your first package](#)

### Contributors 9



### Environments 1

[github-pages](#) Active

### Languages

● Python 100.0%

demo





- ▣ refactorable and maintainable code (Piotr Bartman)

# PySDM: highlights

- ❏ refactorable and maintainable code (Piotr Bartman)
- ❏ CPU and GPU backends (Piotr Bartman)

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- ❖ open and reproducible research ready

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

**PySDM: workflow**

**PySDM architecture**

PyMPDATA (eulerian advection)

PySDM (core)

Computational Backend (Numba, ThrustRTC) compilation, parallelization

microphysics logic

Jupyter

Control (blue arrow)  
Data (yellow arrow)  
Reductions (orange arrow)

Piotr Bartman

9:13 / 25:58

2021 ISS Conference Piotr Bartman

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Piotr Bartman (Jagiellonian University) gives a talk titled "Bridging Pythonicity with performance: Monte-Carlo on GPU case study using ThrustRTC and CURandRTC" at the 2021 SEA's Improving Scientific Software Conference.

(talk @ Improving Scientific Software Conference, NCAR, Boulder, Colorado) 26/45

*[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)

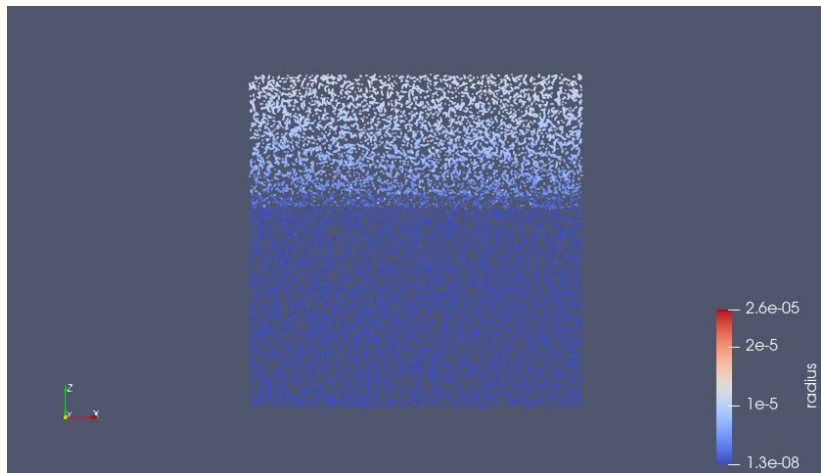


figure: Oleksii Bulenok

# MPDATA

a.k.a. the Smolarkiewicz method

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

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

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

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

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

$$\mathcal{C} = v\Delta t / \Delta x$$

← upwind

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

$$C = v\Delta t / \Delta x$$

← upwind

modified eq.: 
$$\frac{\partial \psi}{\partial t} + \frac{\partial}{\partial x} (v\psi) + \underbrace{K \frac{\partial^2 \psi}{\partial x^2}}_{\text{numerical diffusion}} + \dots = 0$$
 ← MEA



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$$\frac{\partial \psi}{\partial t} + \frac{\partial}{\partial x} (v\psi) + \frac{\partial}{\partial x} \left[ \underbrace{\left( -\frac{K \partial \psi}{\psi \partial x} \right) \psi}_{\text{antidiffusive flux}} \right] = 0 \quad \leftarrow$$

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

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

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

## **M**ultidimensional **P**ositive **D**efinite Advection Transport Algorithm

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- ❖ **Positive Definite:**  
sign-preserving + “infinite-gauge formulation for variable-sign fields
- ❖ **Conservative:**  
upstream for all iterations ( $\rightsquigarrow$  stability cond.)

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

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- ❖ **Positive Definite:**  
sign-preserving + “infinite-gauge formulation for variable-sign fields
- ❖ **Conservative:**  
upstream for all iterations ( $\rightsquigarrow$  stability cond.)
- ❖ **High-Order Accurate:**  
up to 3rd-order in time and space (dep. on options & flow)

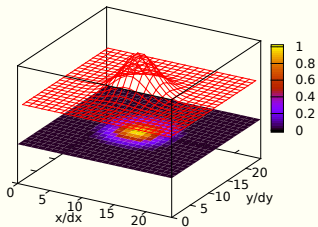
## Multidimensional **P**ositive **D**efinite Advection Transport Algorithm

- ❖ **Multidimensional:**  
antidiffusive fluxes include cross-dimensional terms, as opposed to dimensionally-split schemes
- ❖ **Positive Definite:**  
sign-preserving + “infinite-gauge formulation for variable-sign fields
- ❖ **Conservative:**  
upstream for all iterations ( $\rightsquigarrow$  stability cond.)
- ❖ **High-Order Accurate:**  
up to 3rd-order in time and space (dep. on options & flow)
- ❖ **Monotonic:**  
with Flux-Corrected Transport option

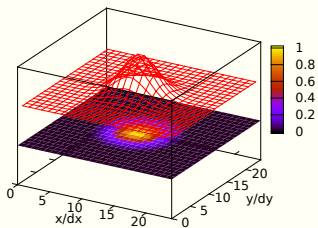


# MPDATA: 2D "hello-world" example

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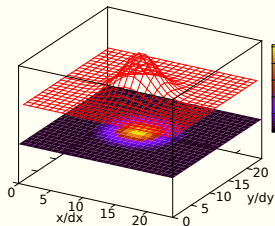


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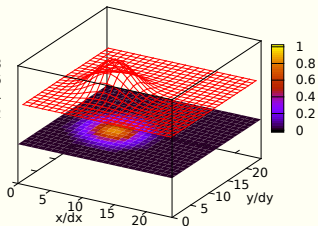


# MPDATA: 2D "hello-world" example

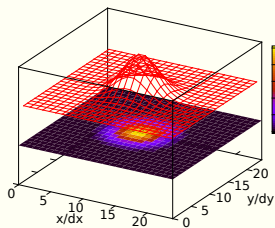
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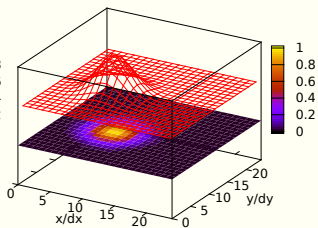
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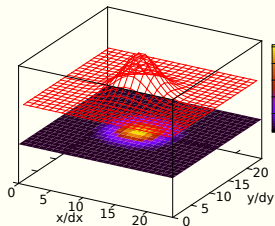


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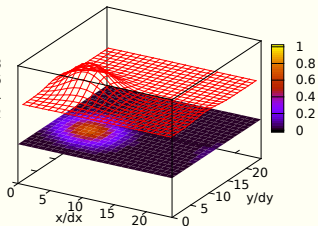


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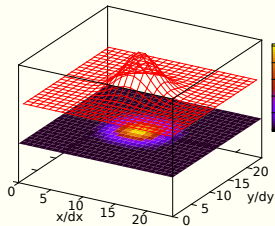
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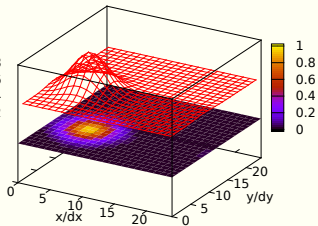
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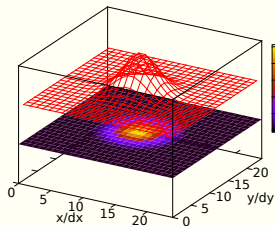


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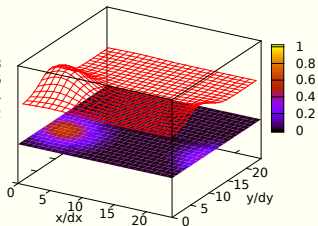


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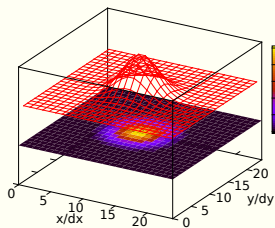
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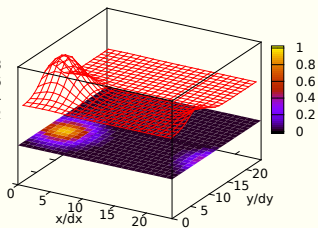
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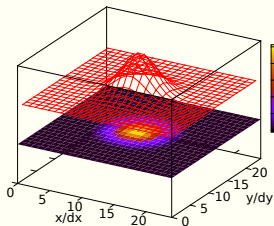


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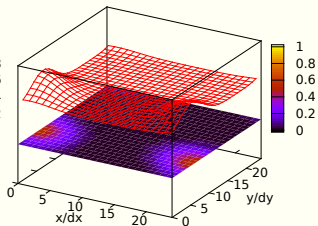


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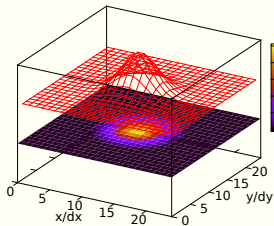
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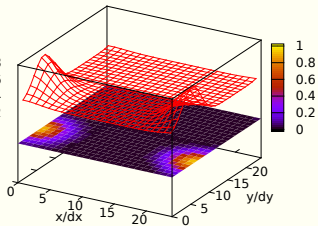
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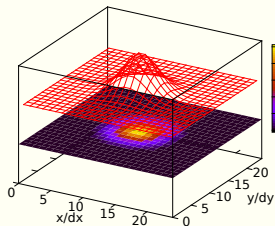


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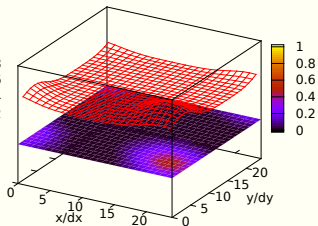


# MPDATA: 2D "hello-world" example

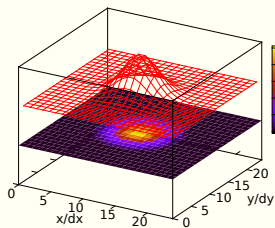
donorcell  $t/dt=0$



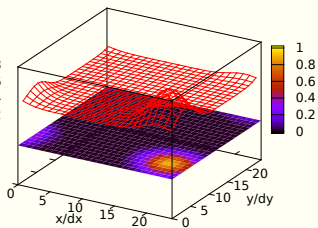
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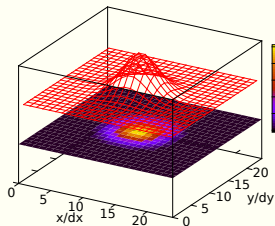


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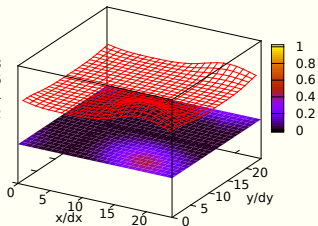


# MPDATA: 2D "hello-world" example

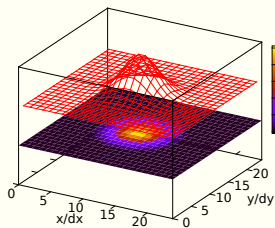
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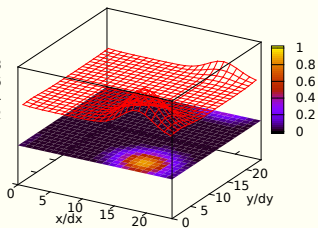
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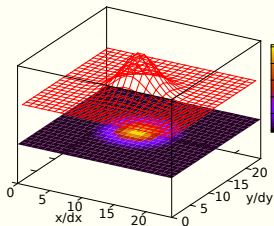


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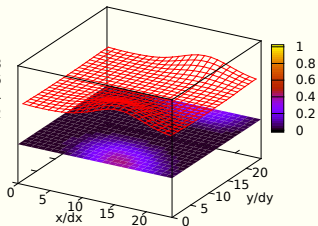


# MPDATA: 2D "hello-world" example

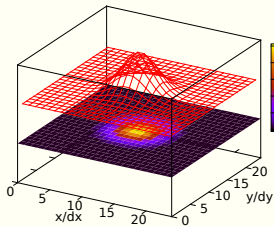
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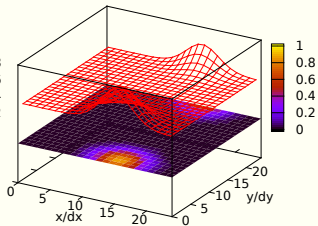
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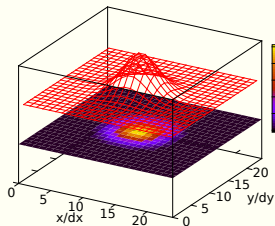
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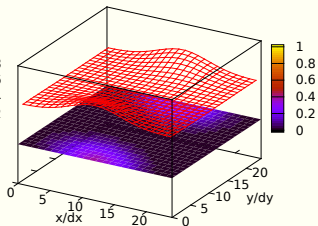


# MPDATA: 2D "hello-world" example

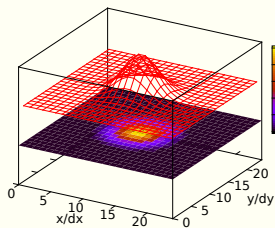
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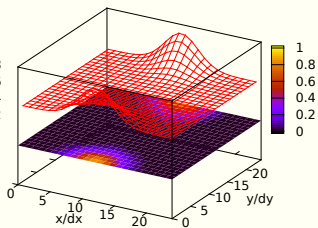
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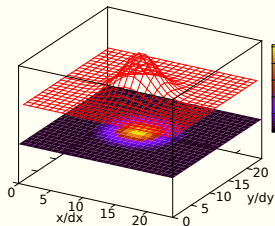


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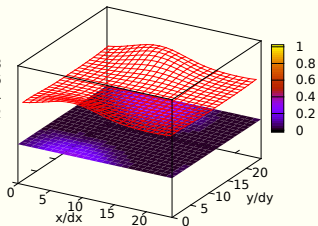


# MPDATA: 2D "hello-world" example

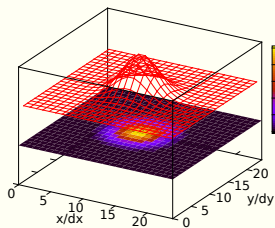
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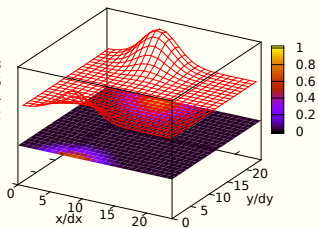
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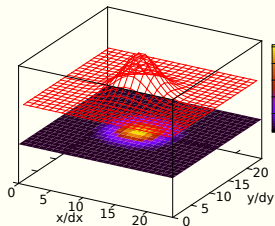


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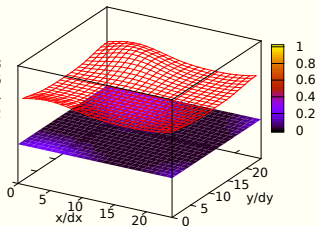


# MPDATA: 2D "hello-world" example

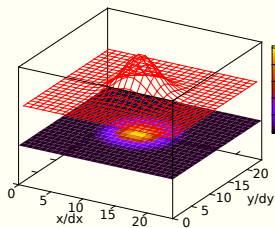
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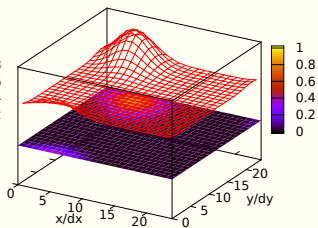
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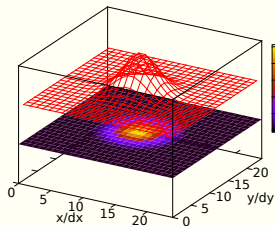


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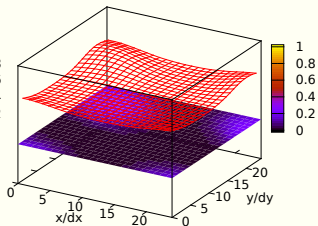


# MPDATA: 2D "hello-world" example

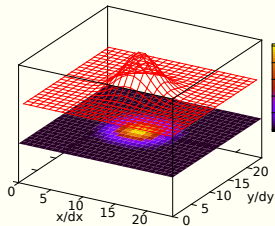
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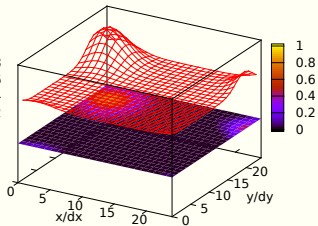
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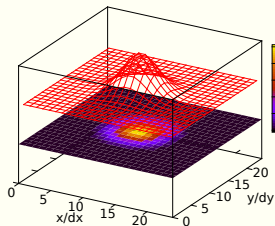


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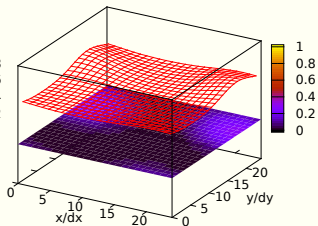


# MPDATA: 2D "hello-world" example

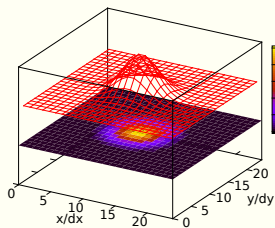
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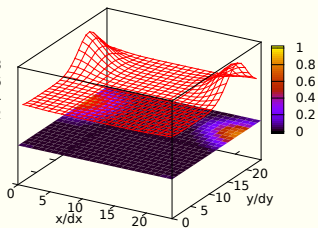
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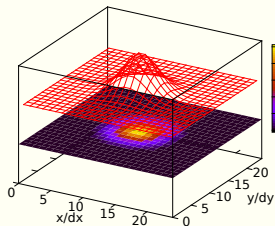


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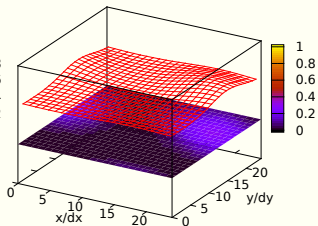


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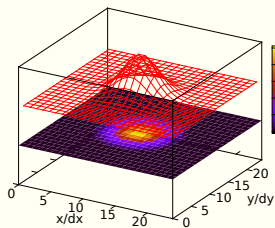
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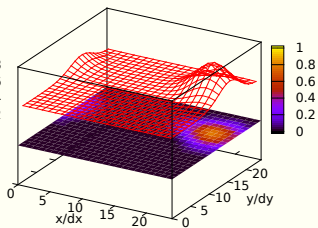
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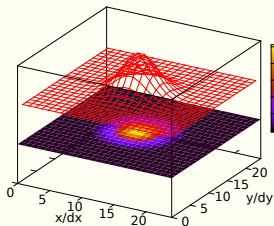


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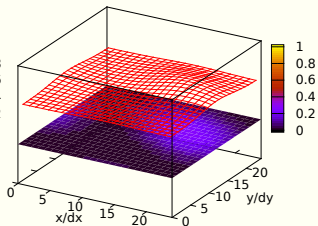


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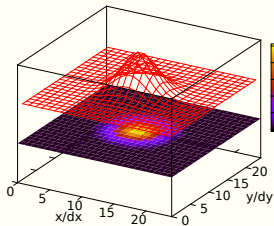
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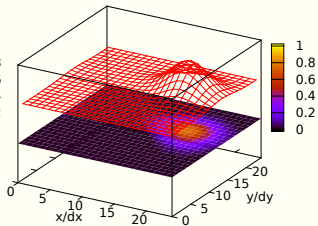
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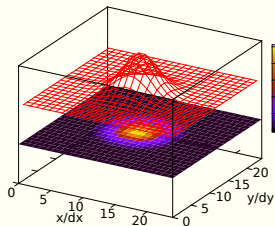


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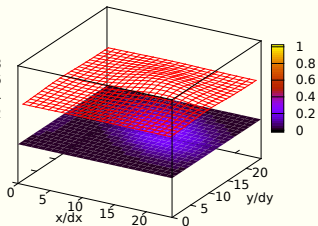


# MPDATA: 2D "hello-world" example

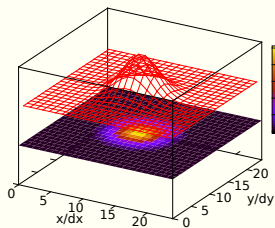
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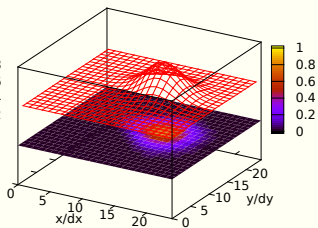
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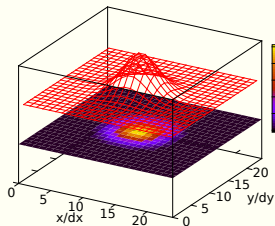
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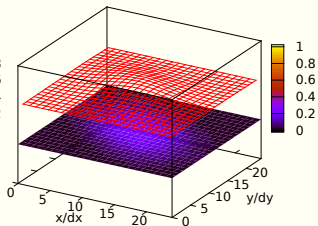


# MPDATA: 2D "hello-world" example

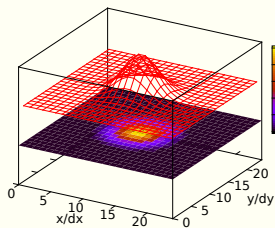
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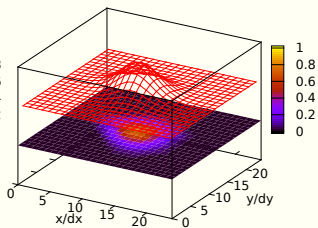
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# MPDATA: well established “classic” in geophysics



## Piotr Smolarkiewicz

Senior Scientist Emeritus  
Verified email at ucar.edu

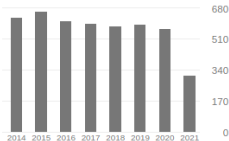
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TITLE	CITED BY	YEAR
<a href="#">A fully multidimensional positive definite advection transport algorithm with small implicit diffusion</a> PK Smolarkiewicz Journal of Computational Physics 54 (2), 325-362	790	1984
<a href="#">A simple positive definite advection scheme with small implicit diffusion</a> PK Smolarkiewicz Monthly weather review 111 (3), 479-486	642	1983
<a href="#">Low Froude number flow past three-dimensional obstacles. Part I: Baroclinically generated lee vortices</a> PK Smolarkiewicz, R Rotunno Journal of Atmospheric Sciences 46 (8), 1154-1164	511	1989
<a href="#">The multidimensional positive definite advection transport algorithm: Nonoscillatory option</a> PK Smolarkiewicz, WW Grabowski Journal of Computational Physics 86 (2), 355-375	440	1990
<a href="#">MPDATA: A finite-difference solver for geophysical flows</a> PK Smolarkiewicz, LG Margolin Journal of Computational Physics 140 (2), 459-480	429	1998

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# PyMPDATA



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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 @njitable 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

# 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.

*[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

- ❏ `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`



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



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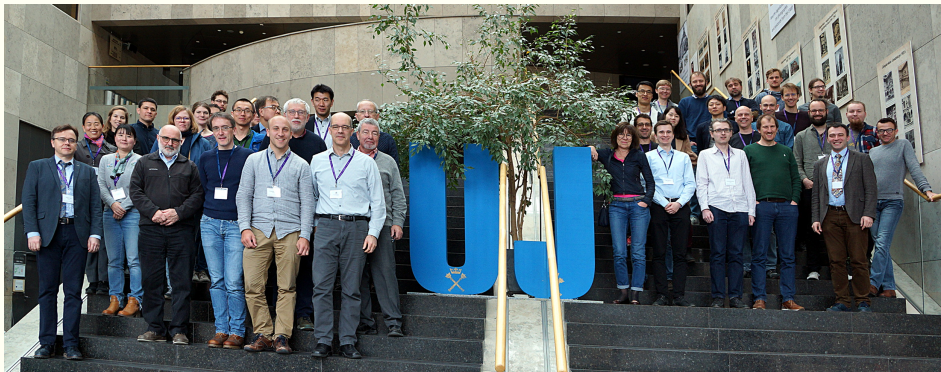
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# particle-based cloud modelling workshop at UJ (April '19)



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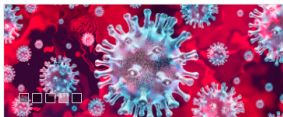
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Niezmiernie miło nam poinformować, iż w konkursach Narodowego Centrum Nauki oraz Narodowej Agencji Wymiany Akademickiej do finansowania zostało zakwalifikowanych aż 9 projektów pracowników naszego wydziału. Laureatami zostali:

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dr hab. Marcin Andrzej Kozik, [Puste przyzyczenia Thomasa Jerome Schaefera](#)

Szczegóły konkursu znaleźć można na stronie [Narodowego Centrum Nauki](#).

# acknowledgements

# acknowledgements: contributors & funding

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## PySDM contributors

Piotr Bartman (WMil), Michael Olesik (WFAiS),  
Grzegorz Łazarski (WCh/WMil), Anna Jaruga (Caltech);

+ students @ WMil:

Oleksii Bulenok, Kamil Górski, Bartosz Piasecki, Aleksandra Talar

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## funding

EU / Foundation for Polish Science (“POWROTY”)



Thank you for your attention!

