particle-based modelling of water-isotope fractionation in aerosol-cloud-precipitation systems using PySDM

Sylwester Arabas, Sanket Bhiogade & Kazimierz Różański
AGH University in Krakow

ENVIRONMENTAL
PHYSICS
GROUP

plan of the presentation

- **particle-based cloud μ-physics modelling**
  - aerosol-cloud-precip interactions: a conceptual picture
  - cloud μ-physics: Eulerian vs. Lagrangian models
  - particle-based μ-physics: key concepts
  - particle-based μ-physics: coupling with the host model
  - super-particles as an alternative to bulk or bin μ-physics
- **PySDM: design goals and features overview**
  - PySDM: open-source particle-based μ-physics modelling package
  - PySDM users & use cases
- **water-isotope-related developments in PySDM**
  - Pierchała et al. '22 – triple isotope analysis, kinetic fractionation
  - Różański & Sonntag '82 – multibox cloud/precip column model
  - water isotopes in PySDM: summary, next steps

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aerosol-cloud-precip interactions: a conceptual picture

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graphic: vitsly / Hokusai

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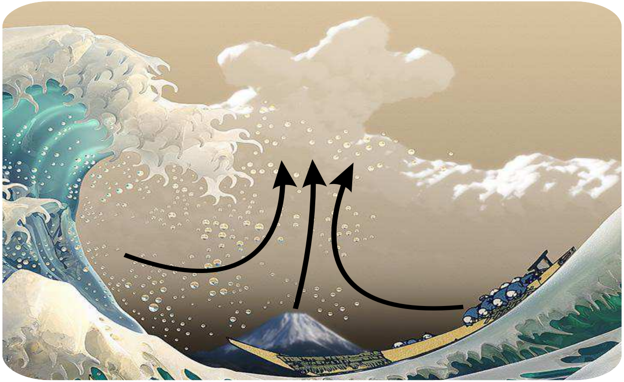
aerosol-cloud-precip interactions: a conceptual picture

- aerosol particles of natural and anthropogenic origin act as condensation/crystallisation nuclei



graphic: vitsly / Hokusai

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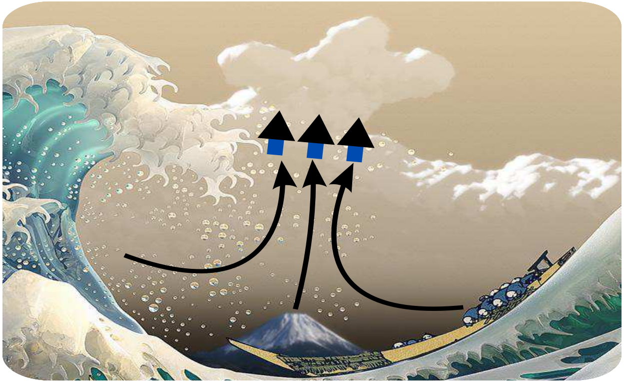

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- particles evaporating before reaching surface (with potentially altered size/composition) contribute to ambient aerosol

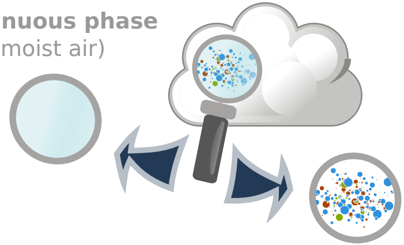
two-way interactions:
- aerosol characteristics influence cloud microstructure
- cloud processes influence aerosol size and composition

graphic: vitsly / Hokusai

cloud μ-physics: Eulerian vs. Lagrangian models

cloud μ-physics: Eulerian vs. Lagrangian models

continuous phase
(moist air)



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(aerosol particles, cloud droplets, drizzle, rain, snow, ...)

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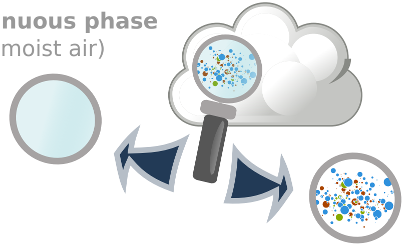

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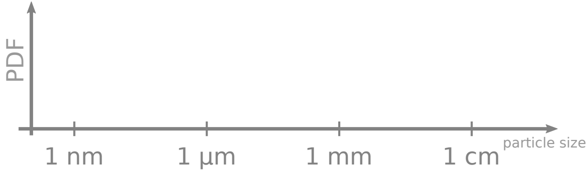

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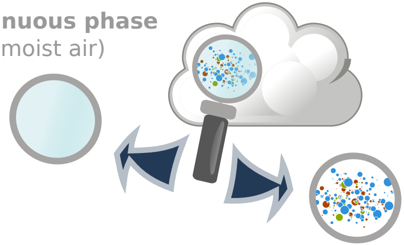

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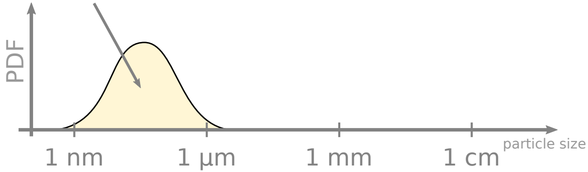

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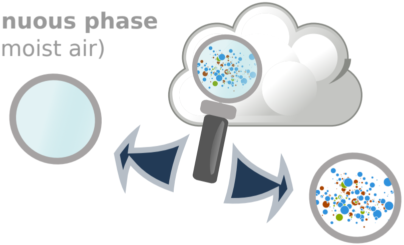

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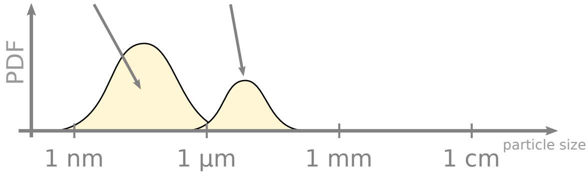

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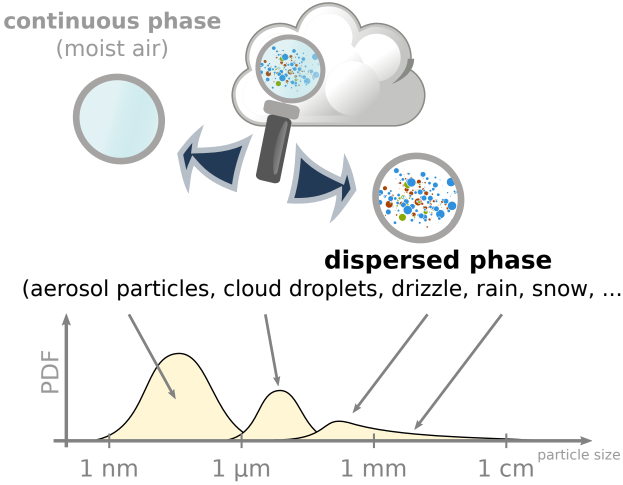

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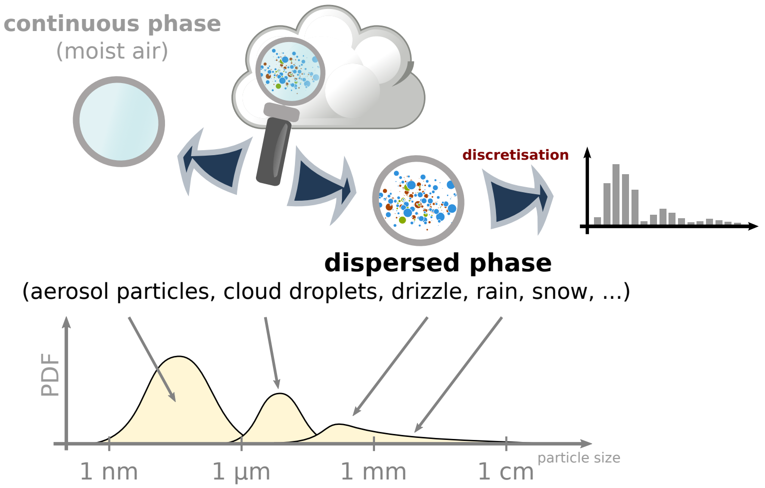

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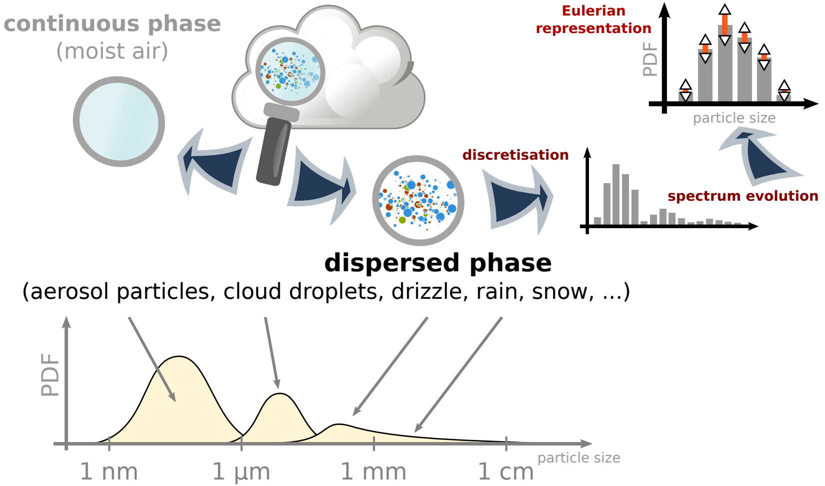

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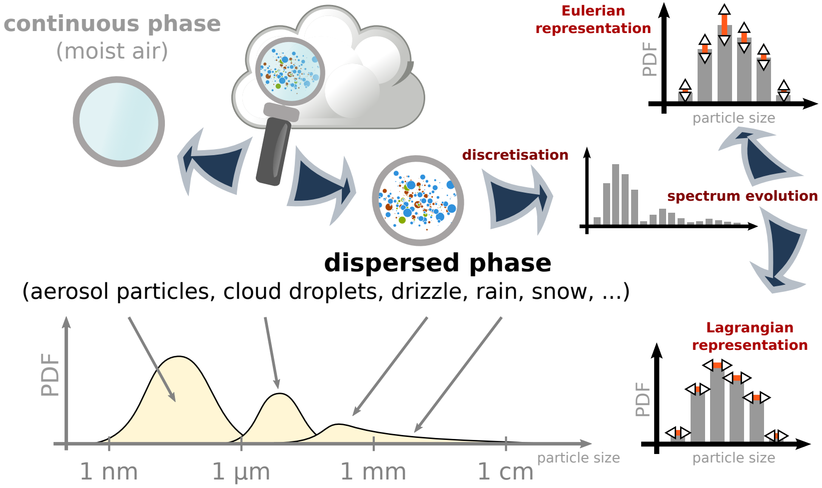

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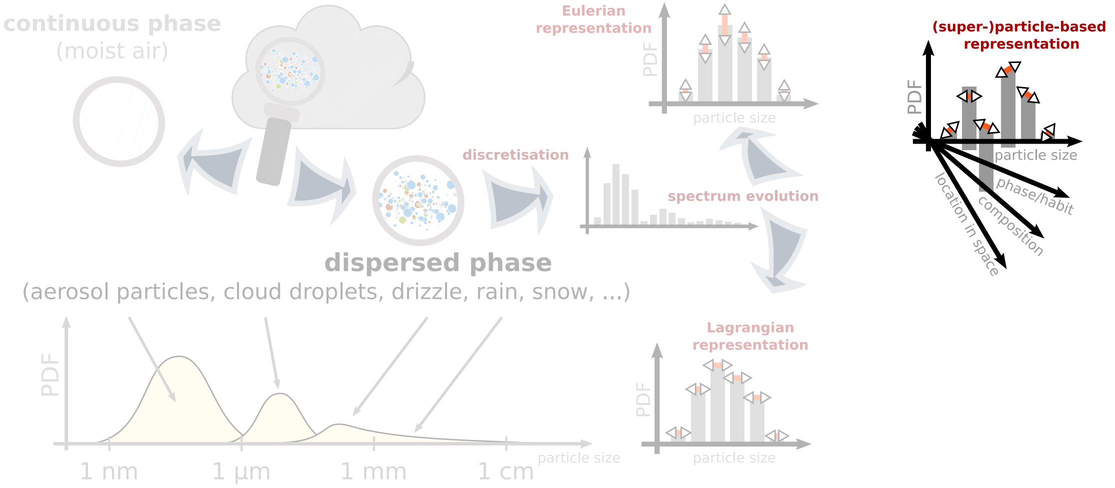

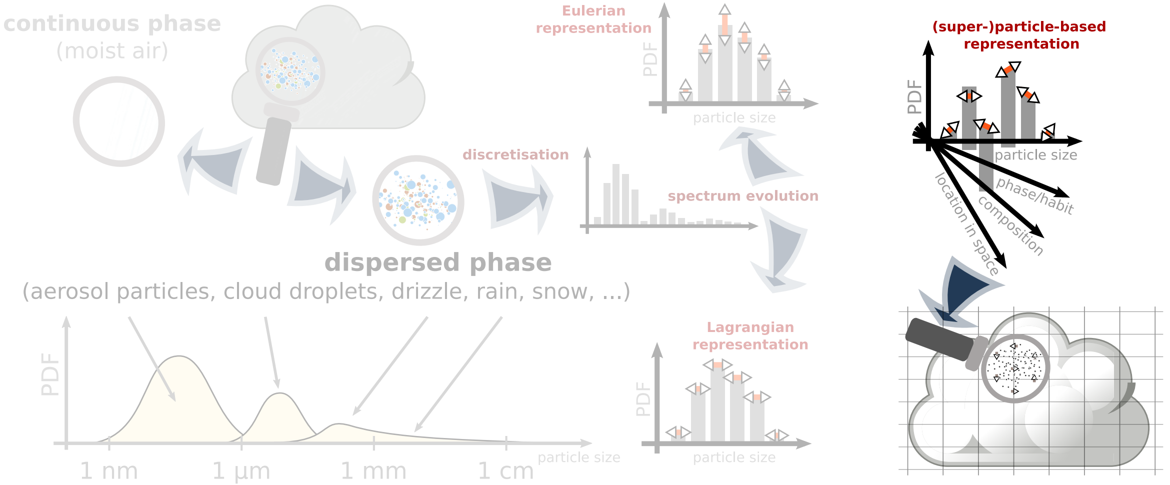
continuous phase
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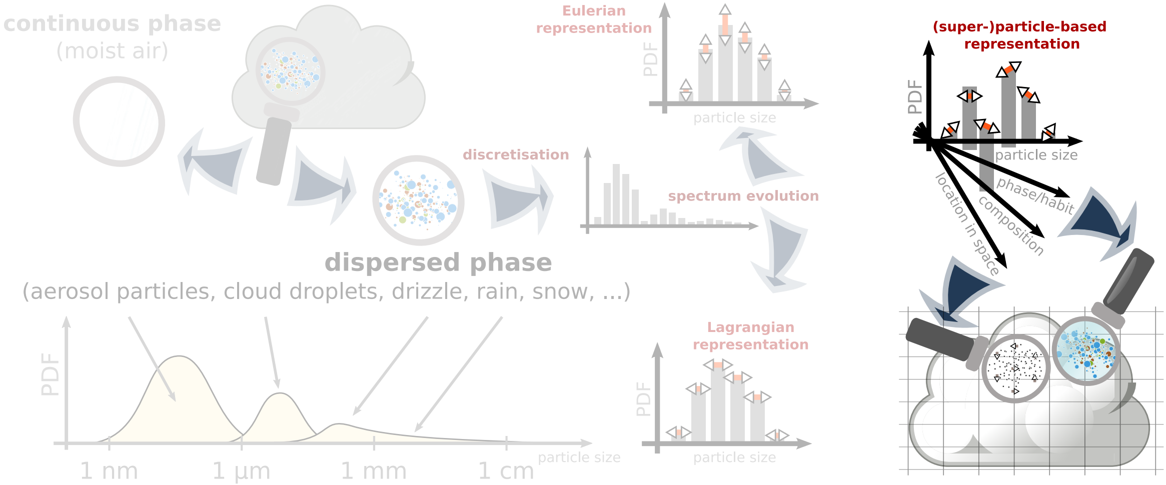
PDF
1 nm
1 µm
1 mm
1 cm
particle size
discretisation
Eulerian representation
spectrum evolution
Lagrangian representation
(super-)particle-based representation
phase/habit
composition
location in space

cloud μ-physics: Eulerian vs. Lagrangian models



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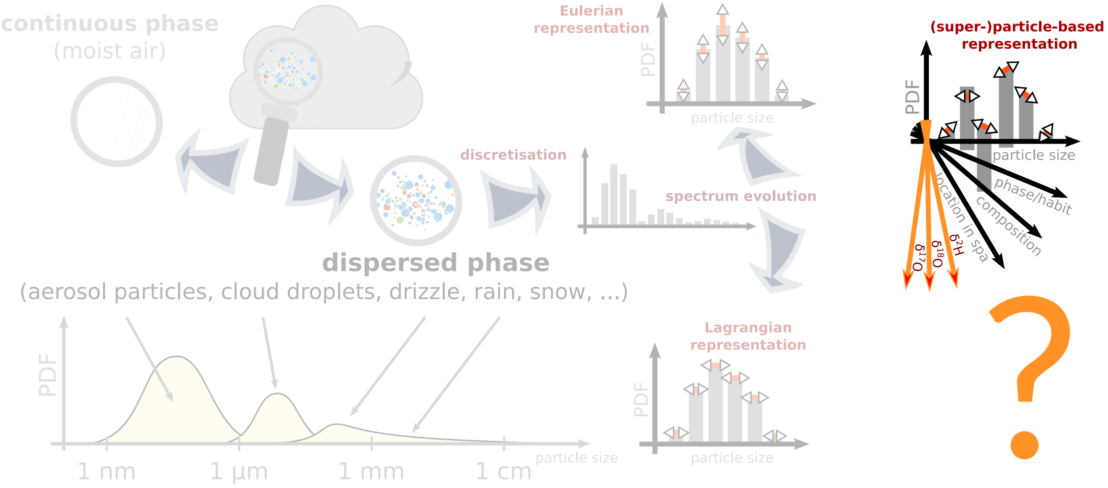
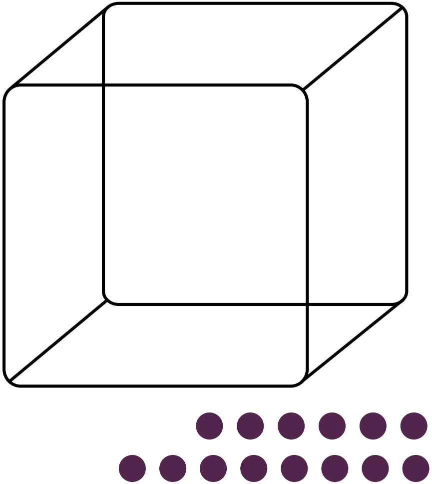
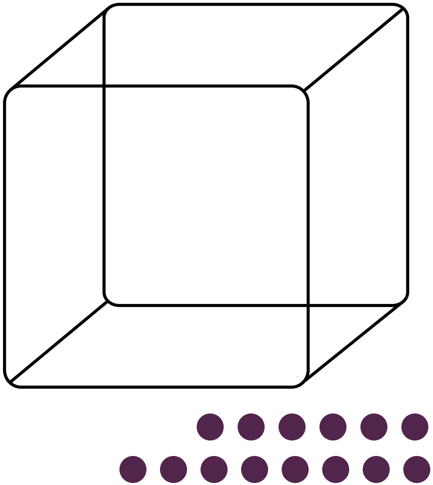




Domain randomly populated with "μ-physics information carriers"

(super particles / super droplets)

particle-based μ-physics: key concepts



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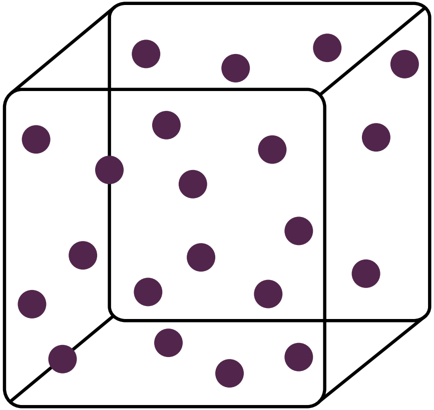

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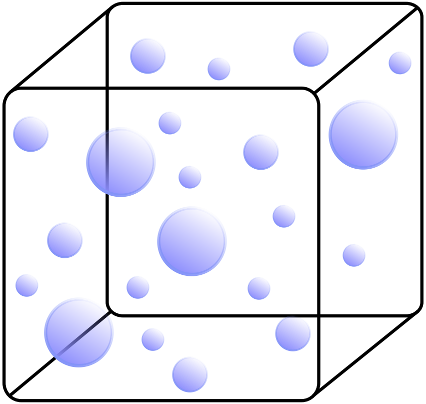

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- wet radius

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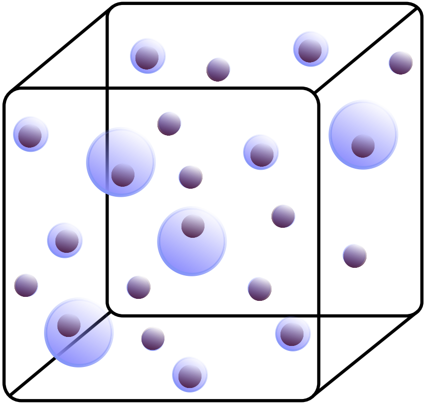

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carrier attributes:

- location
- wet radius
- dry radius

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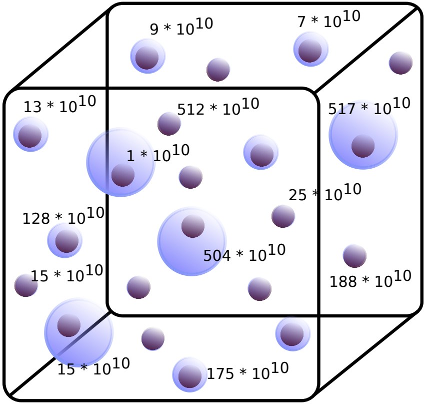

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- dry radius
- multiplicity

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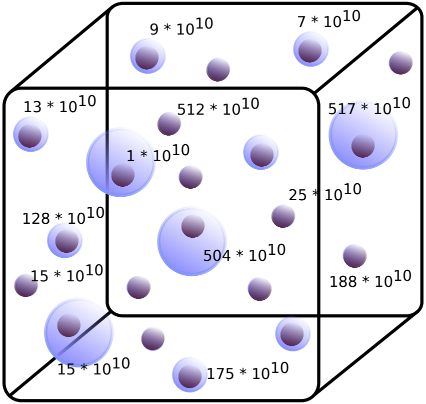

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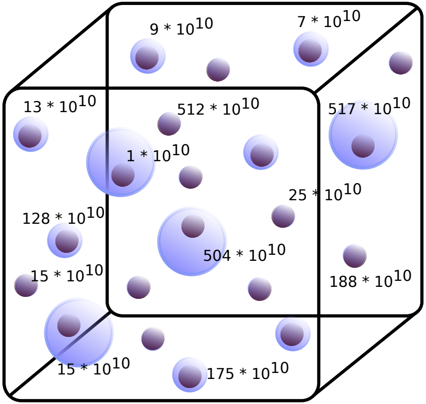

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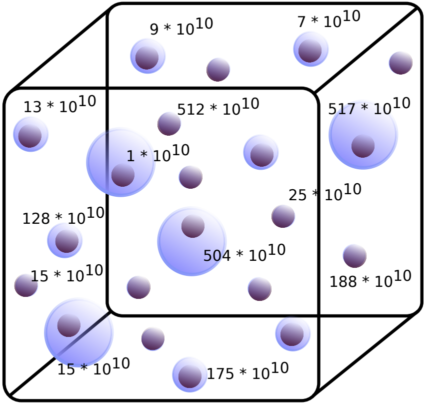

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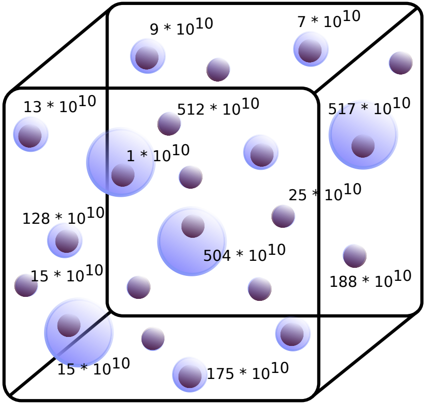

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advantages over Eulerian approach: no "categorisation"; adding attributes does not increase dimensionality
(e.g., isotopic composition)

particle-based μ-physics: coupling with the host model

Eulerian / PDE	Lagrangian / ODE

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Eulerian / PDE	Lagrangian / ODE
advection of heat	particle transport by the flow
advection of moisture	

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advection of moisture	condensational growth/evap
	collisional growth/breakage
	sedimentation

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$\partial_t(\rho_d \theta) + \nabla \cdot (\vec{v}\rho_d \theta) = \rho_d \dot{\theta}$	$\dot{\theta} = \sum\limits_{\text{particles} \in \Delta V} \ldots$

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advection of trace gases ambient vapour isotopic budget	in-particle aqueous chemistry hydrometeor isotopic composition

super-particles as an alternative to bulk or bin μ-physics

Arabas & Shima 2013 (JAS)

AMS | Journals

Large-Eddy Simulations of Trade Wind Cumuli Using Particle-Based Microphysics with Monte Carlo Coalescence

Sylwester Arabas and Shin-ichiro Shima

Print Publication: 01 Sep 2013

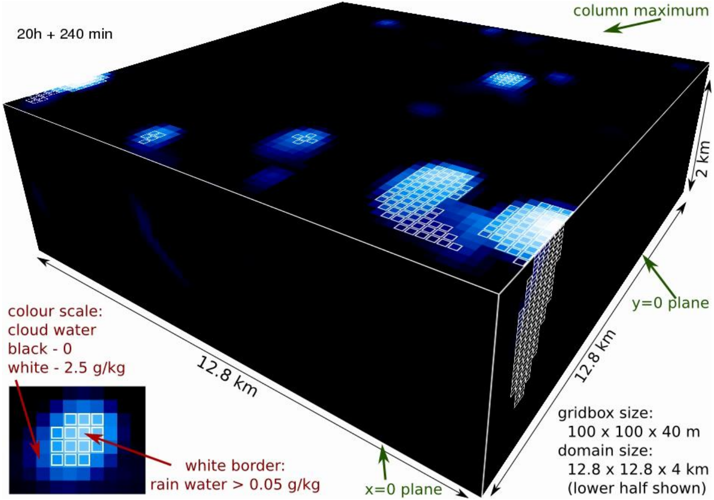
DOI: https://doi.org/10.1175/JAS-D-12-0295.1

Page(s): 2768–2777

Abstract

A series of simulations employing the superdroplet method (SDM) for representing aerosol, cloud, and rain microphysics in large-eddy simulations (LES) is discussed. The particle-based formulation treats all particles in the same way, subjecting them to condensational growth and evaporation, transport of the particles by the flow, gravitational settling, and collisional growth. SDM features a Monte Carlo–type numerical scheme for representing the collision and coalescence process. All processes combined cover representation of cloud condensation nuclei (CCN) activation, drizzle formation by autoconversion, accretion of cloud droplets, self-collection of raindrops, and precipitation, including aerosol wet deposition. The model setup used in the study is based on observations from the Rain in Cumulus over the Ocean (RICO) field project. Cloud and rain droplet size spectra obtained in the simulations are discussed in context of previously published analyses of aircraft observations carried out during RICO. The analysis covers height-resolved statistics of simulated cloud microphysical parameters such as droplet number concentration, effective radius, and parameters describing the width of the cloud droplet size spectrum. A reasonable agreement with measurements is found for several of the discussed parameters. The sensitivity of the results to the grid resolution of the LES, as well as to the sampling density of the probabilistic Monte Carlo–type model, is explored.

Corresponding author address: Sylwester Arabas, Institute of Geophysics, Faculty of Physics, University of Warsaw, Pasteura 7, 02-093 Warsaw, Poland. E-mail: sarabas@igf.fuw.edu.pl



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Morrison et al. 2020 (JAMES)

JAMES | Journal of Advances in Modeling Earth Systems

COMMISSIONED MANUSCRIPT

10.1029/2019MS001689

Confronting the Challenge of Modeling Cloud and Precipitation Microphysics

Hugh Morrison[1], Marcus van Lier-Walqui[2], Ann M. Fridlind[3], Wojciech W. Grabowski[1], Jerry Y. Harrington[4], Corinna Hoose[5], Alexei Korolev[6], Matthew R. Kumjian[4], Jason A. Milbrandt[7], Hanna Pawlowska[8], Derek J. Posselt[9], Olivier P. Prat[10], Karly J. Reimel[4], Shin-Ichiro Shima[11], Bastiaan van Diedenhoven[2], and Lulin Xue[1]

Key Points:

- Microphysics is an important component of weather and climate models, but its representation in current models is highly uncertain

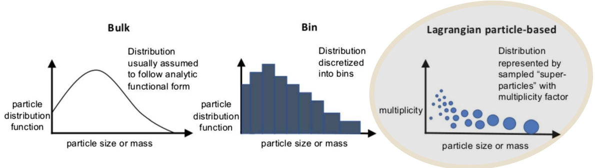

Figure 3. Representation of cloud and precipitation particle distributions in the three main types of microphysics

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PySDM: open-source particle-based μ-physics modelling package

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PySDM 2.20

`pip install PySDM`

Latest version

Released: Apr 21, 2023

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

Navigation

- Project description
- Release history
- Download files

Project links

- Homepage
- Documentation
- Source
- Tracker

Statistics

GitHub statistics:

- **Stars:** 40
- **Forks:** 21
- **Open issues:** 101
- **Open PRs:** 13

Project description

PySDM

Python 3 | LLVM Numba | CUDA ThrustRTC | Linux ✓ | macOS ✓ | Windows ✓ | Jupyter ✓ | Maintained? yes | Open Hub PySDM | JOSS 10.21105/joss.03219 | DOI 10.5281/zenodo.7851352 | EU Funding by FNP | PL Funding by NCN | US DOE Funding by ASR

License GPL v3

tests+artifacts+pypi passing | build passing | codecov 78% | pypi package 2.20 | API docs pdoc3

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 features 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

PySDM: open-source particle-based μ-physics modelling package

- particle diffusional growth/evaporation (incl. CCN activation)

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- multi-core CPU (LLVM) & GPU (NVRTC) backends
- 100% Python code!

PySDM users & use cases

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

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An Efficient Bayesian Approach to Learning Droplet Collision Kernels: Proof of Concept Using "Cloudy," a New *n*-Moment Bulk Microphysics Scheme

M Bieli, ORA Dunbar, EK De Jong… - Journal of Advances …, 2022 - Wiley Online Library

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E de Jong, JB Mackay, A Jaruga, S Arabas - EGUsphere, 2022 - egusphere.copernicus.org

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plan of the presentation

- **particle-based cloud μ-physics modelling**
  - aerosol-cloud-precip interactions: a conceptual picture
  - cloud μ-physics: Eulerian vs. Lagrangian models
  - particle-based μ-physics: key concepts
  - particle-based μ-physics: coupling with the host model
  - super-particles as an alternative to bulk or bin μ-physics
- **PySDM: design goals and features overview**
  - PySDM: open-source particle-based μ-physics modelling package
  - PySDM users & use cases
- **water-isotope-related developments in PySDM**
  - Pierchała et al. '22 – triple isotope analysis, kinetic fractionation
  - Różański & Sonntag '82 – multibox cloud/precip column model
  - water isotopes in PySDM: summary, next steps

Pierchała et al. '22 – triple isotope analysis, kinetic fractionation[a]

[a] launch-in-the-cloud URL: `https://mybinder.org/v2/gh/open-atmos/PySDM.git/main?urlpath=lab/tree/examples/PySDM_examples/Pierchala_et_al_2022`

new PySDM "example" (incl. numerous automated tests) based on:

doi:10.1016/j.gca.2022.01.020

Geochimica et Cosmochimica Acta 322 (2022) 244–259

www.elsevier.com/locate/gca

Quantification the diffusion-induced fractionation of $^{1}H_2^{17}O$ isotopologue in air accompanying the process of water evaporation

Anna Pierchala *, Kazimierz Rozanski, Marek Dulinski, Zbigniew Gorczyca

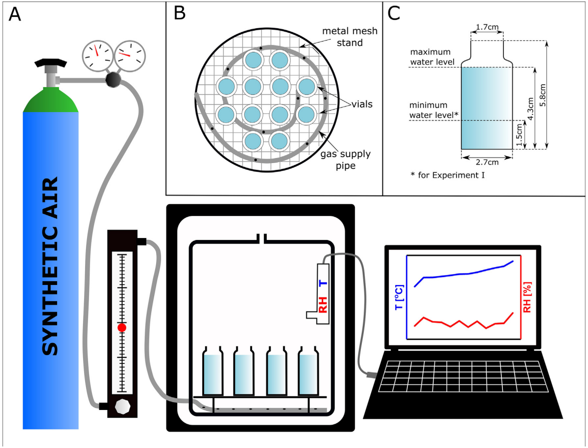
AGH University of Science and Technology, Faculty of Physics and Applied Computer Science, al. Mickiewicza 30, 30-059 Krakow, Poland

Received 25 February 2021; accepted in revised form 15 January 2022; Available online 24 January 2022

Pierchała et al. '22 – triple isotope analysis, kinetic fractionation[a]

[a] launch-in-the-cloud URL: https://mybinder.org/v2/gh/open-atmos/PySDM.git/main?urlpath=lab/tree/examples/PySDM_examples/Pierchala_et_al_2022

Fig. 1 (paper): lab experiment setup



Pierchała et al. '22 – triple isotope analysis, kinetic fractionation[a]

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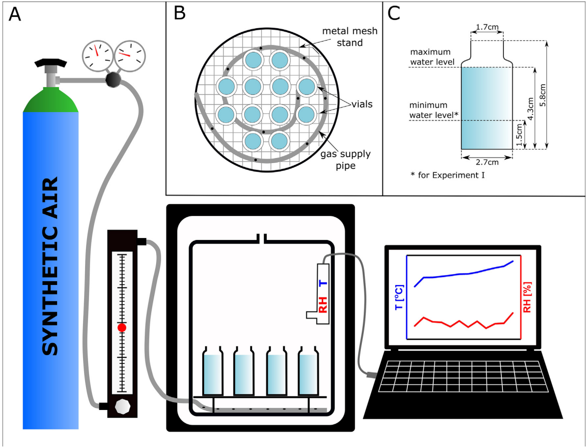
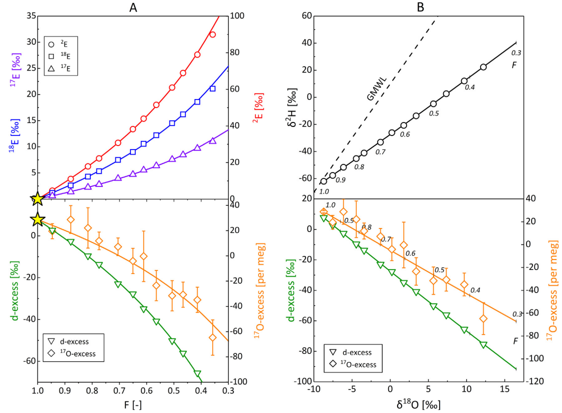


- diffusion-induced fractionation upon evaporation
- multi-day experiments (up to two weeks)
- Picarro L2140-i cavity ring-down laser spectrometer (probing liquid water vaporised for analysis)
- constant T/RH, variable T or variable RH setups

Pierchała et al. ’22 – triple isotope analysis, kinetic fractionation[a]

[a] launch-in-the-cloud URL: `https://mybinder.org/v2/gh/open-atmos/PySDM.git/main?urlpath=lab/tree/examples/PySDM_examples/Pierchala_et_al_2022`

Fig. 3 (paper): $E = \delta_{R/R_0}$, measurements + model



Pierchała et al. '22 – triple isotope analysis, kinetic fractionation[a]

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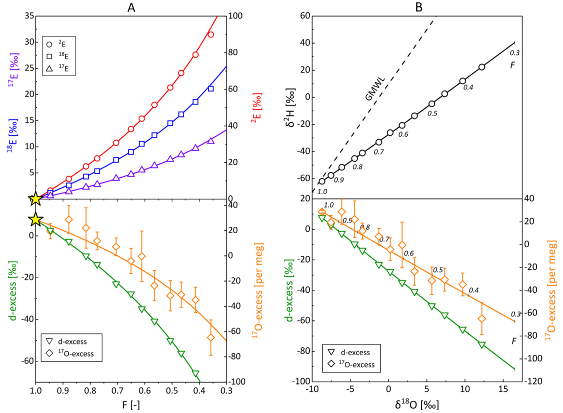

PySDM: theoretical curves (Craig-Gordon model)

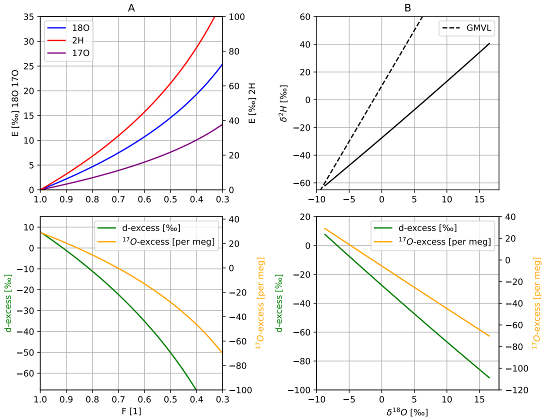

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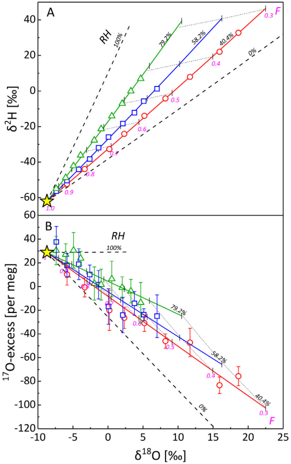
Fig. 4 (paper): RH varied



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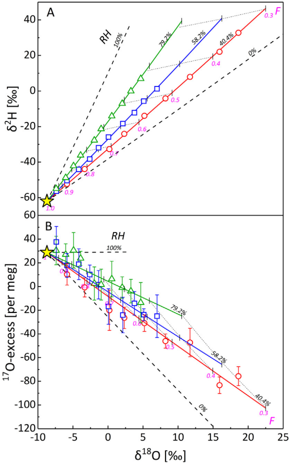
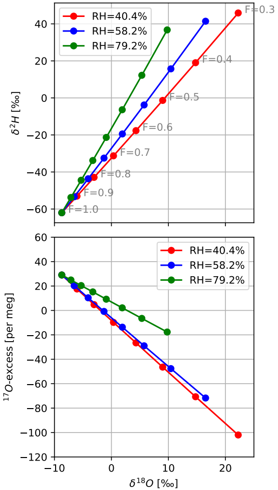


PySDM: model curves



Różański & Sonntag '82 – multibox cloud/precip column model[a]

[a] launch-in-the-cloud URL: https://mybinder.org/v2/gh/slayoo/PySDM.git/isotopes_rozanski_and_sonntag_example?urlpath=lab/tree/examples/PySDM_examples

new PySDM "example" (work in progress):

doi:10.3402/tellusa.v34i2.10795

Tellus (1982), *34*, 135–141

Vertical distribution of deuterium in atmospheric water vapour

By K. ROZANSKI[1] and C. SONNTAG, *Institute of Environmental Physics, University of Heidelberg, Im Neuenheimer Feld 366, D-6900 Heidelberg, F. R. Germany*

(Manuscript received September 26, 1980; in final form May 12, 1981)

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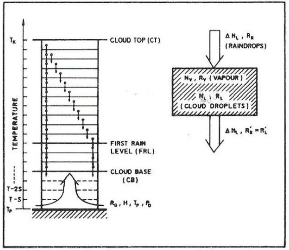

Fig. 3. Schematic diagram of the multibox cloud model. Input data: initial temperature, T_p; final temperature, T_k; initial pressure, P_0; relative humidity, H; initial isotopic composition of water vapour, R_0; cloud water mixing ratio, N_L; temperature step, S; isotope exchange factor, K.

Tellus 34 (1982), 2

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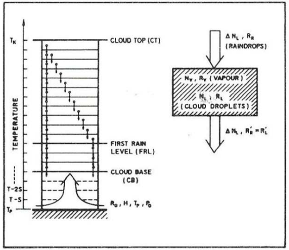

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Tellus 34 (1982), 2

- hydrostatic/adiabatic rainshaft with precip removal

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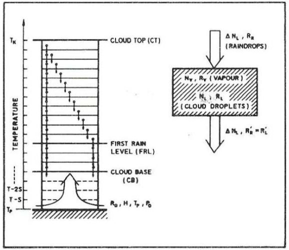

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Tellus 34 (1982), 2

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- condensation: saturation adjustment

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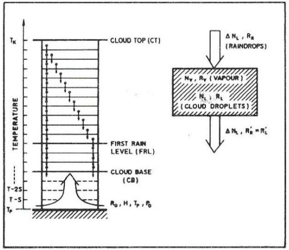

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Tellus 34 (1982), 2

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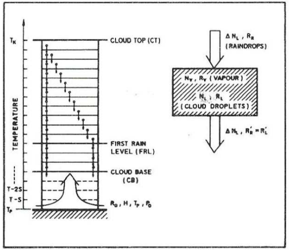

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Tellus 34 (1982), 2

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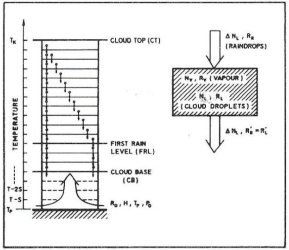

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Tellus 34 (1982), 2

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- condensation: saturation adjustment
- rain formation: liquid water content threshold
- iterations towards quasi-stationary state (no explicit role of time)
- parameter controlling efficiency of rain isotopic equilibration with ambient vapour

[a] launch-in-the-cloud URL: https://mybinder.org/v2/gh/slayoo/PySDM.git/isotopes_rozanski_and_sonntag_example?urlpath=lab/tree/examples/PySDM_examples

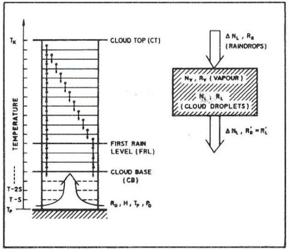

Fig. 3. Schematic diagram of the multibox cloud model. Input data: initial temperature, T_p; final temperature, T_k; initial pressure, P_0; relative humidity, H; initial isotopic composition of water vapour, R_0; cloud water mixing ratio, N_L; temperature step, S; isotope exchange factor, K.

Tellus 34 (1982), 2

- hydrostatic/adiabatic rainshaft with precip removal
- condensation: saturation adjustment
- rain formation: liquid water content threshold
- iterations towards quasi-stationary state (no explicit role of time)
- parameter controlling efficiency of rain isotopic equilibration with ambient vapour
- minimal model for capturing isotope exchange between precip, ambient vapour and cloud water

Różański & Sonntag '82 – multibox cloud/precip column model[a]

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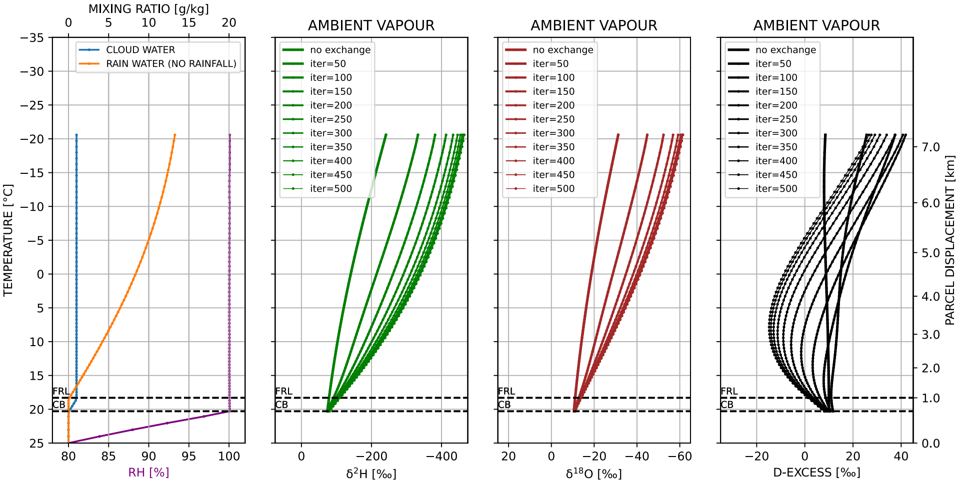

extended wrt paper with oxygen-18, aerosol-coupled supersaturation dynamics, ...

README.md

PySDM-examples

no-model examples depicting isotope-related formulae:

- Merlivat & Nief 1967:
  - Fig. 2: render on GitHub | launch binder | Open in Colab
- Van Hook 1968:
  - Fig. 1: render on GitHub | launch binder | Open in Colab
- Bolot et al. 2013:
  - Fig. 1: render on GitHub | launch binder | Open in Colab
- Graf et al. 2019:
  - Table. 1: render on GitHub | launch binder | Open in Colab
- Pierchala et al. 2022:
  - Fig. 3: render on GitHub | launch binder | Open in Colab
  - Fig. 4: render on GitHub | launch binder | Open in Colab

0D box-model coalescence and breakup examples:

- Shima et al. 2009 (Box model, coalescence only, test case employing Golovin analytical solution):
  - Fig. 2: render on GitHub | launch binder | Open in Colab

plan for upcoming months:

- below-cloud kinetic fractionation

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water isotopes in PySDM: summary, next steps

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- exploring dependence on droplet and precip size spectra (and hence aerosol)
- ice-phase processes
- ...

Thank you for your attention!

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