Elements of modern cloud modelling

PhD thesis defense

candidate:

Sylwester Arabas

supervisor:

Hanna Pawłowska

UNIVERSITAS VARSOVIENSIS

Thesis structure

- **Introductory chapters (or a guide through the papers):**

- **Appendix (the papers):**
  - Arabas & Pawlowska 2011, GMD
    Adaptive method of lines for multi-component aerosol condensational growth and CCN activation
  - Arabas & Shima 2013, JAS
    Large-Eddy Simulations of Trade Wind Cumuli Using Particle-Based Microphysics with Monte Carlo Coalescence
  - Arabas, Jaruga, Pawlowska & Grabowski 2013, arXiv
    libcloudph++ 0.1: single-moment bulk, double-moment bulk, and particle-based warm-rain microphysics library in C++

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  - Model formulation
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Aerosol-cloud interactions: conceptual picture

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background image: vitsly.ru / Hokusai

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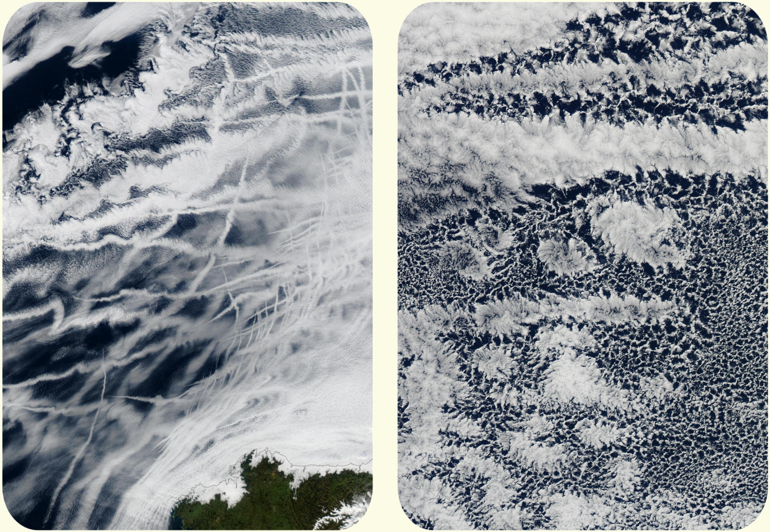
Aerosol-cloud interactions: conceptual picture

- aerosol particles of natural and anthropogenic origin act as condensation nuclei
- cloud droplets grow by water vapour condensation
- rain drops form through collisions of cloud droplets
- aqueous chemical reactions irreversibly modify the drop composition
- rain drops precipitate washing out aerosol
- rain drops evaporate into aerosol particles of potentially altered size and/or composition (collisions, chemistry)

background image: vitsly.ru / Hokusai

Aerosol-cloud interactions: as seen from space



NASA/MODIS (27 Jan 2003 – Bay of Biscay; 17 Apr 2010 – off the coast of Peru)
http://visibleearth.nasa.gov/view.php?id=64992
http://earthobservatory.nasa.gov/IOTD/view.php?id=43795

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Lagrangian μ-physics

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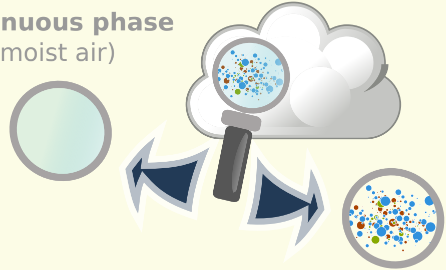
continuous phase
(moist air)



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

Lagrangian μ-physics

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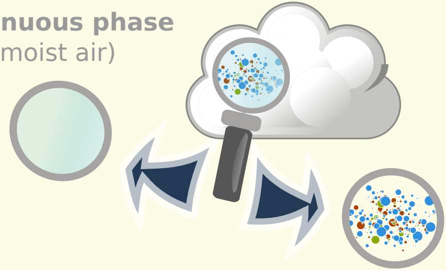

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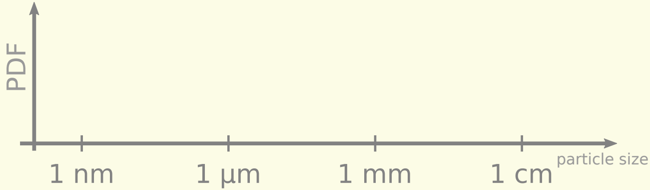
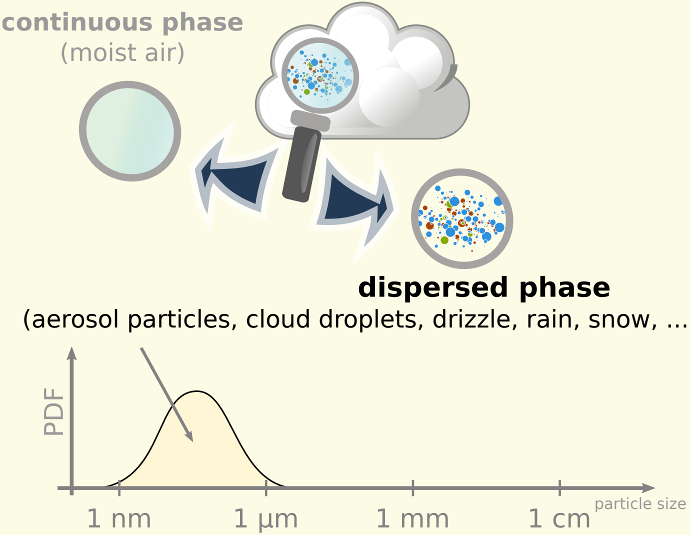


Lagrangian μ-physics



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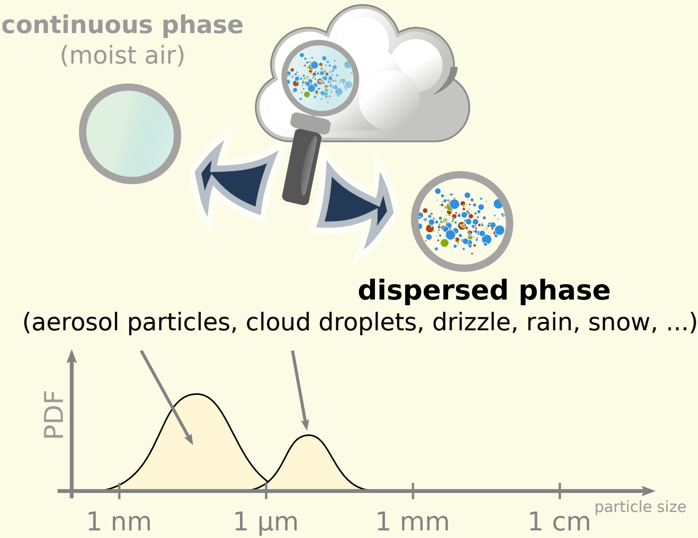

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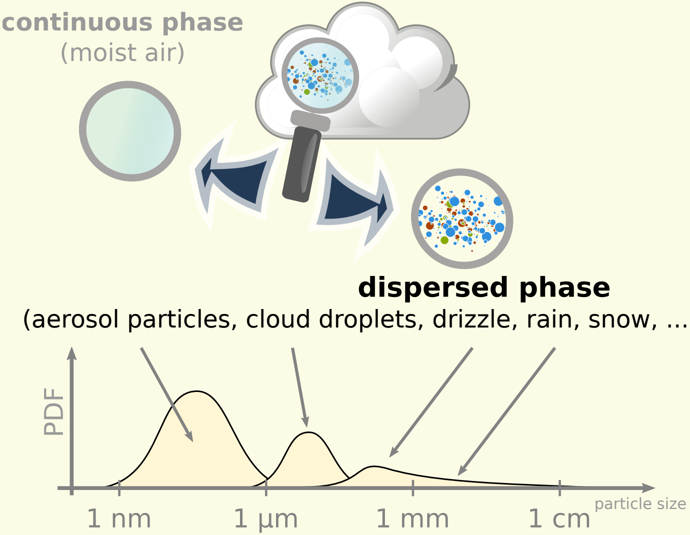

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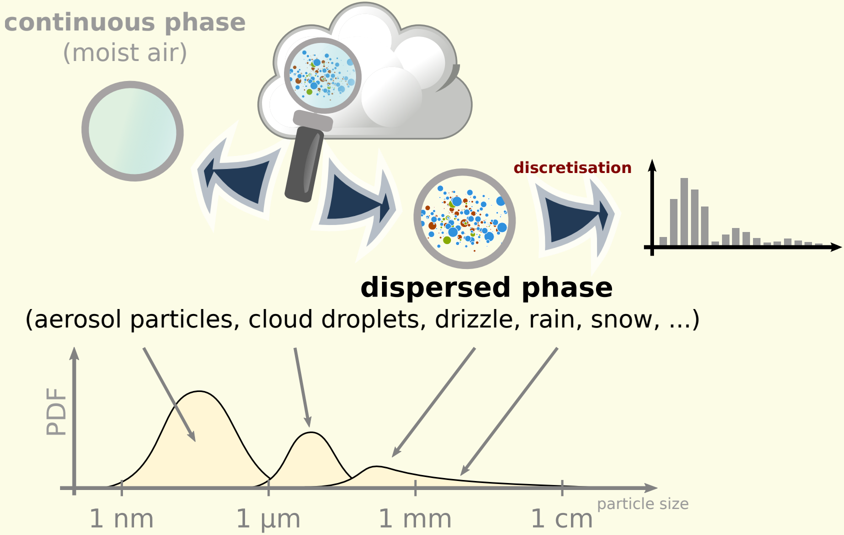

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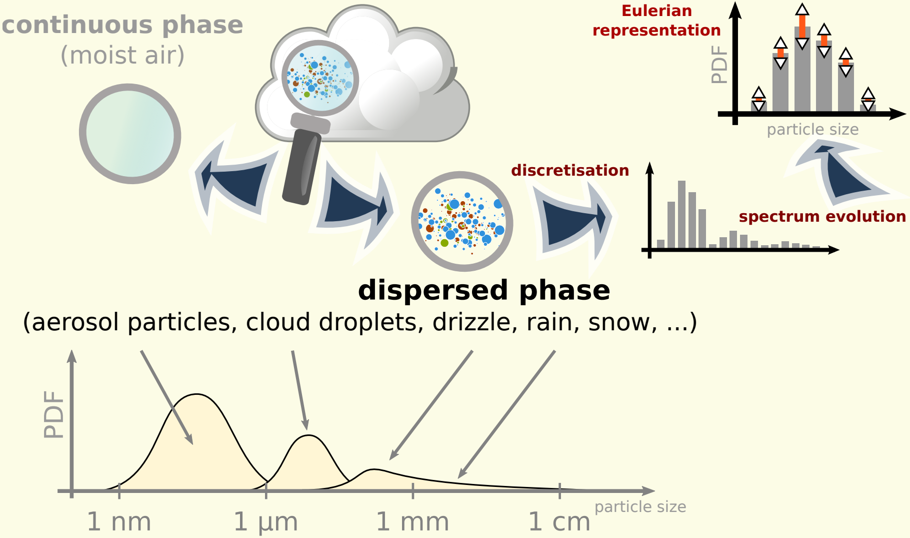

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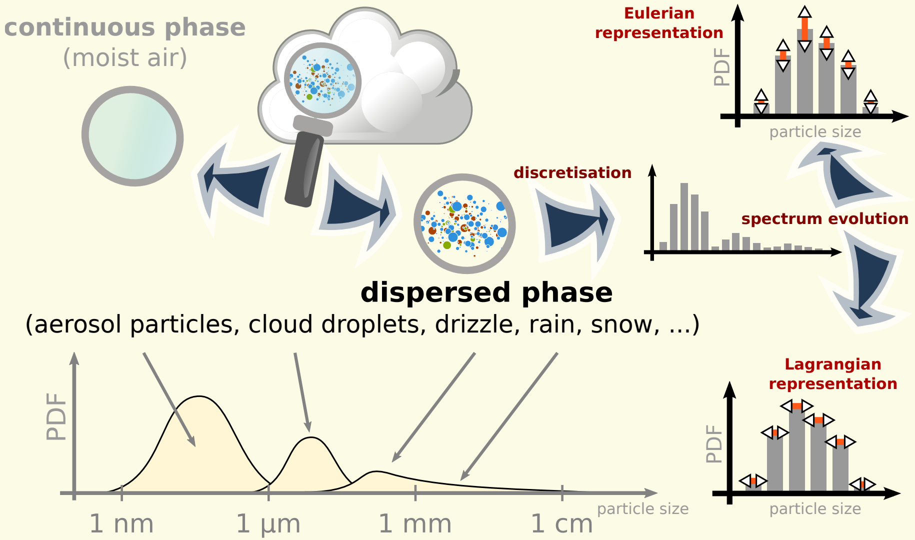
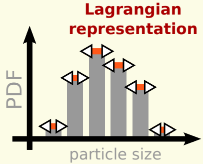


Lagrangian μ-physics in 0D, 2D and 3D



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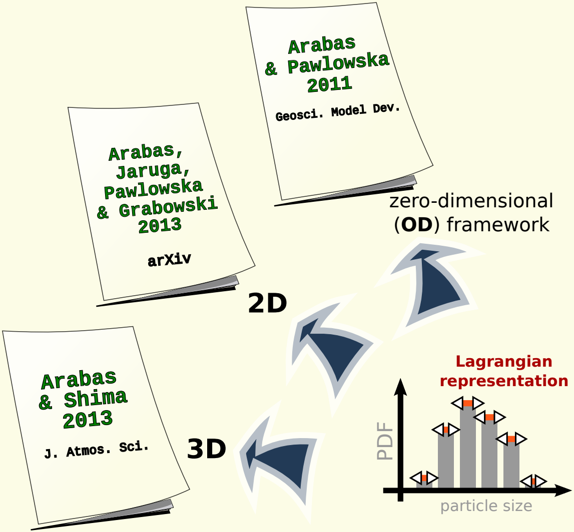

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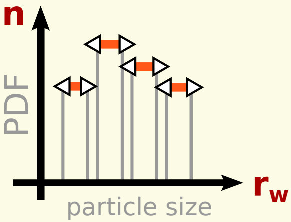

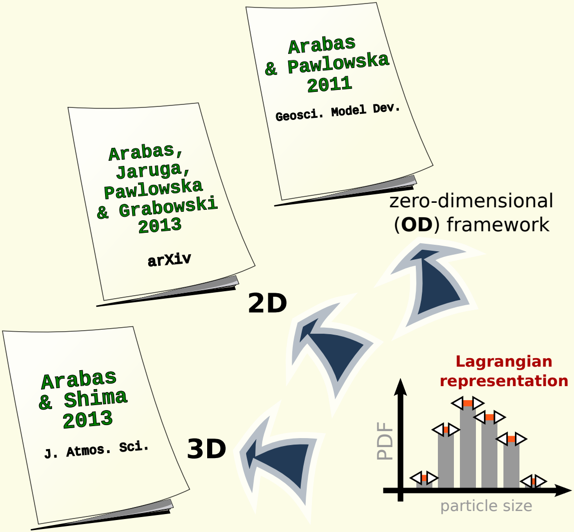

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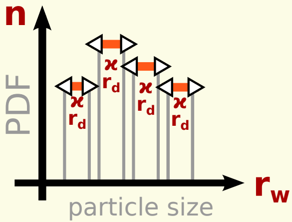

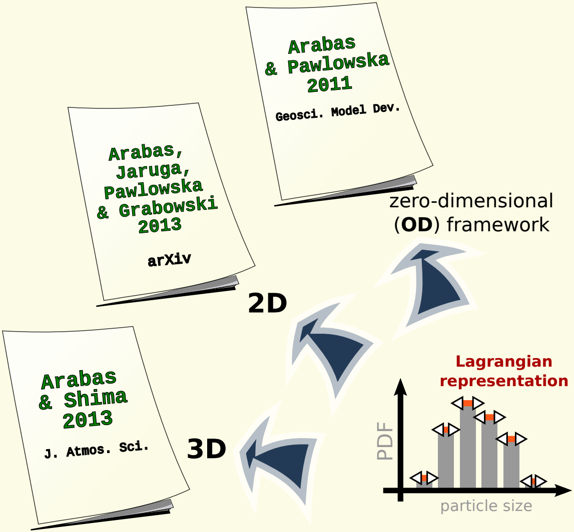

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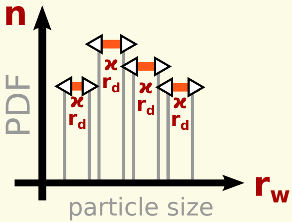

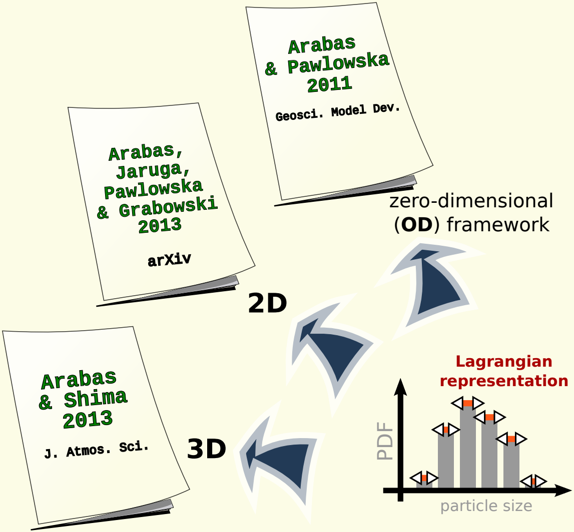

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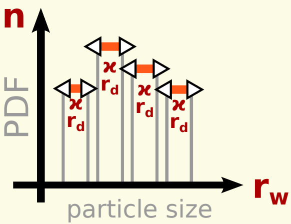
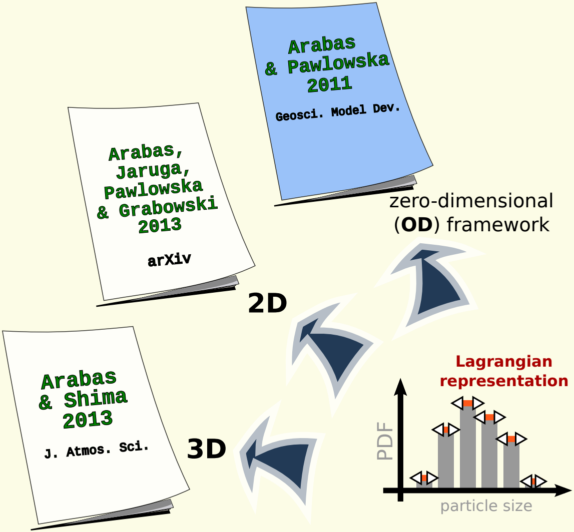
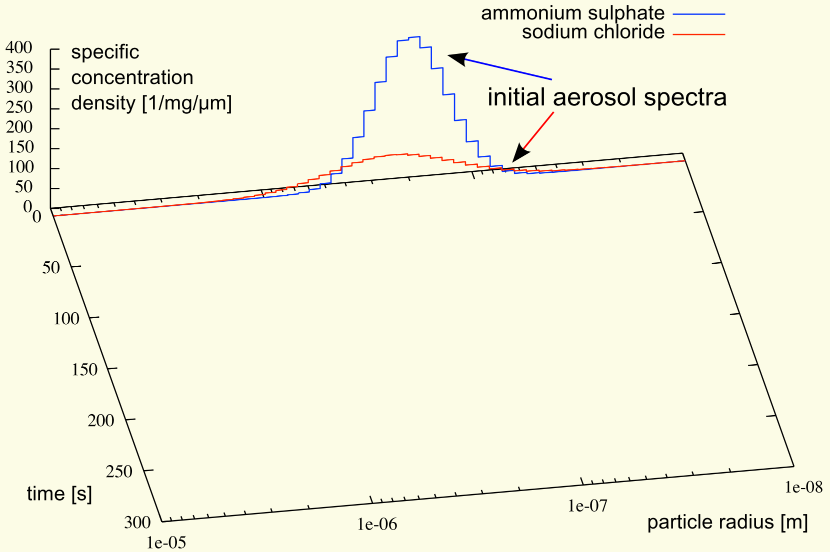




Lagrangian μ-physics in 0D (parcel model)



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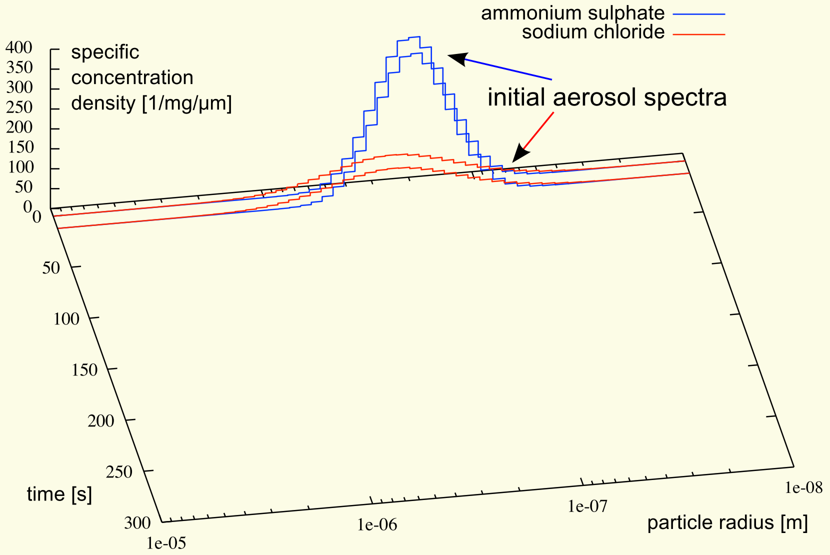

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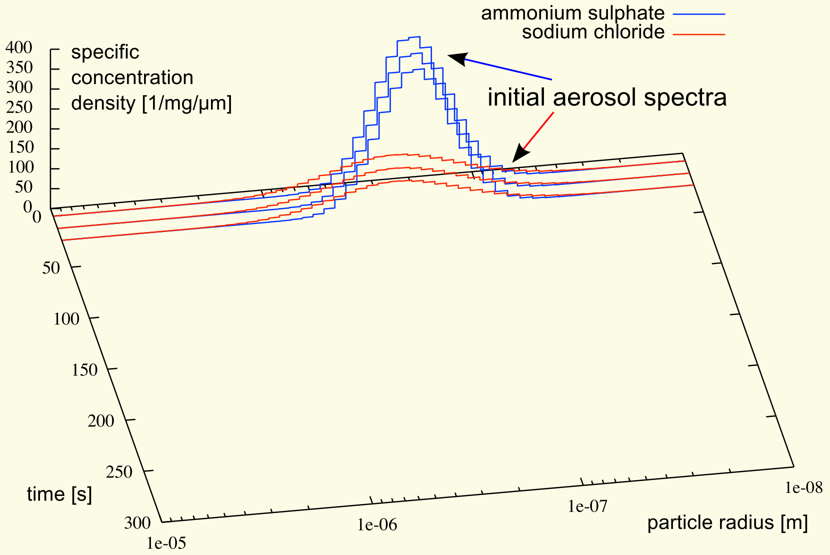

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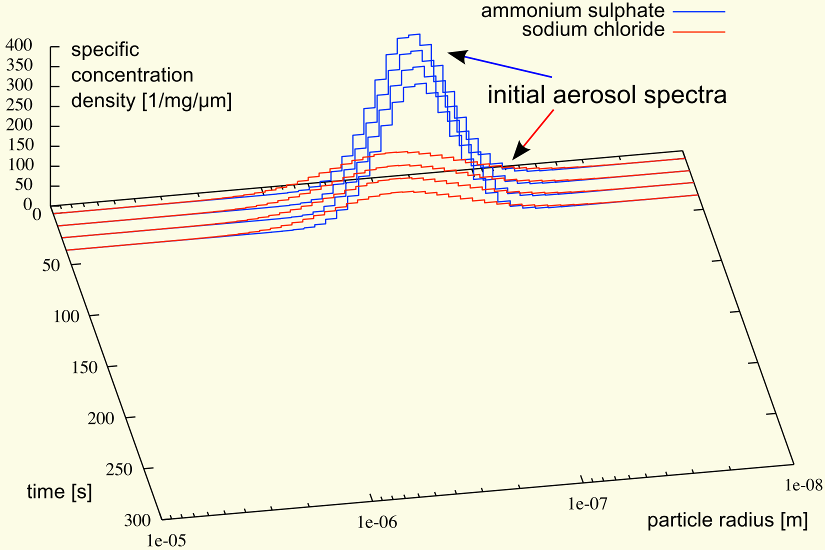

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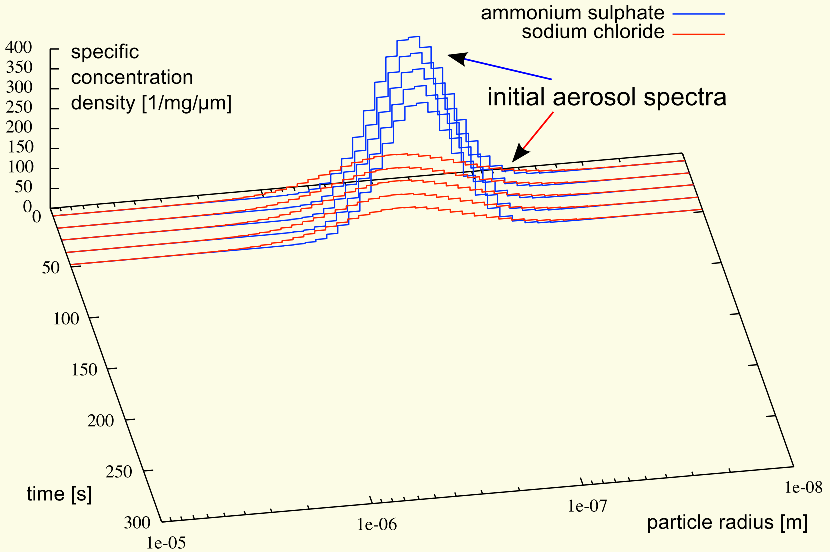

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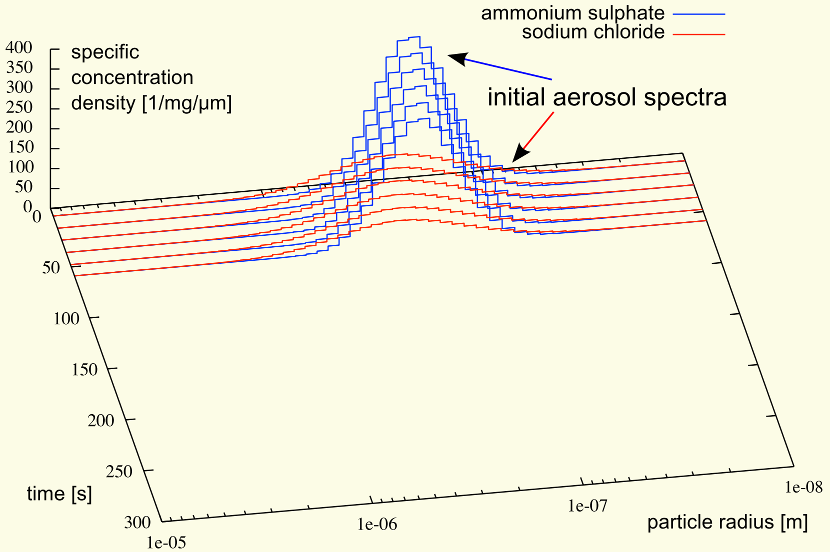

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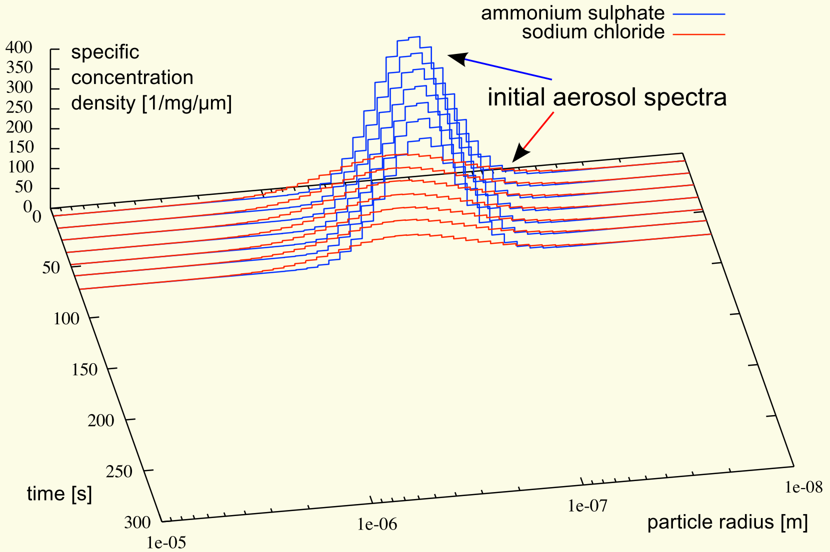

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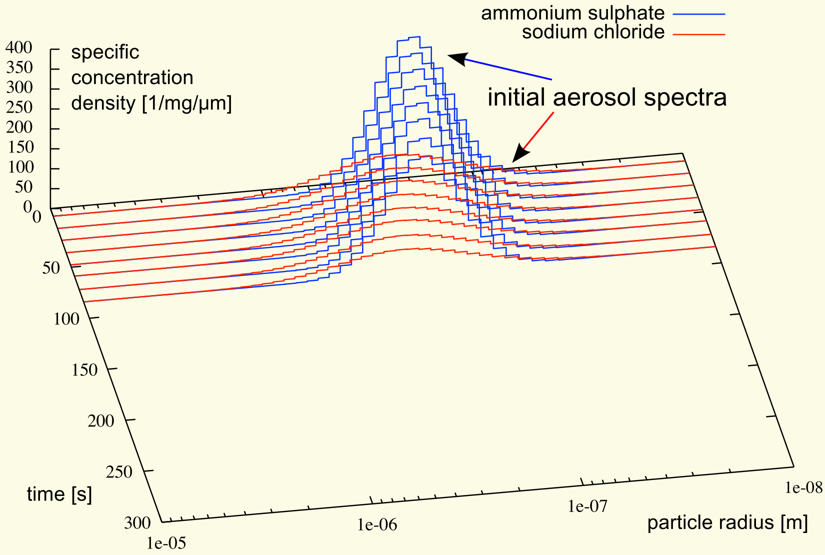

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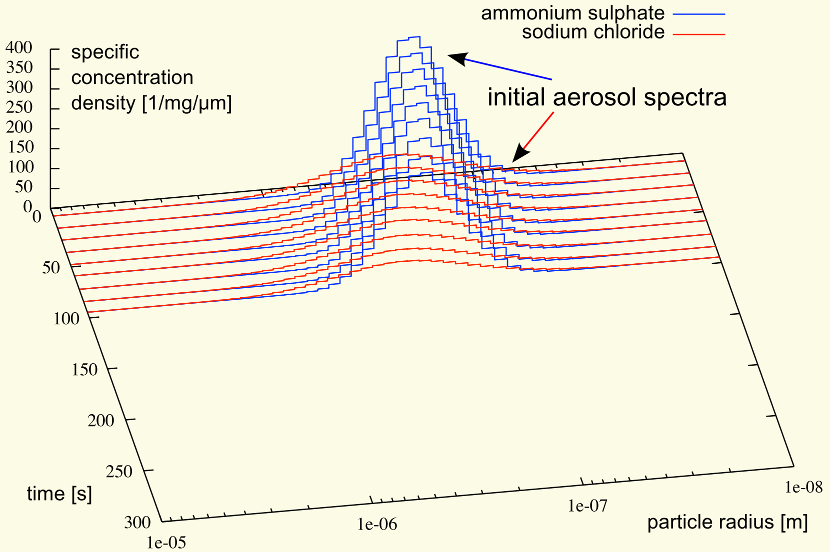

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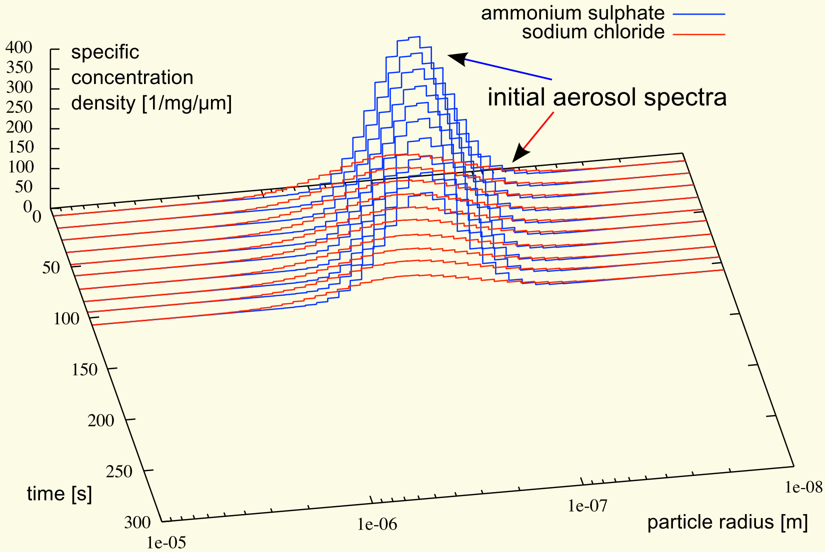

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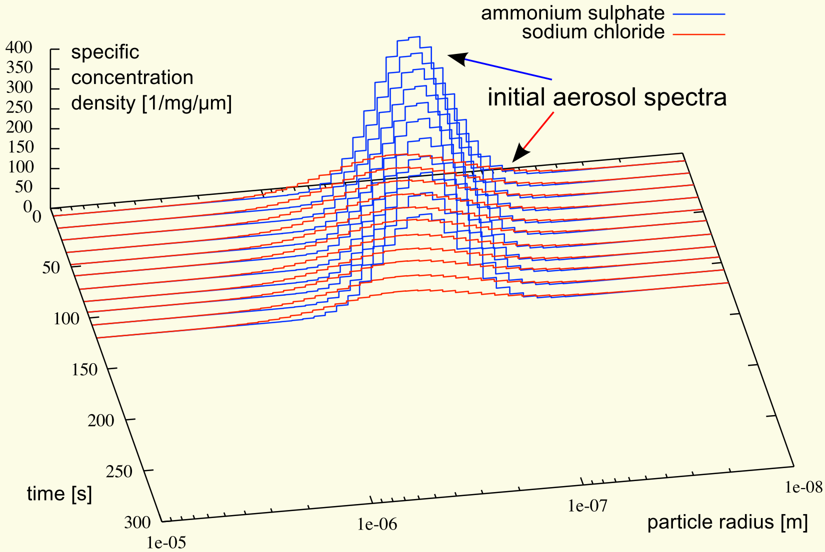

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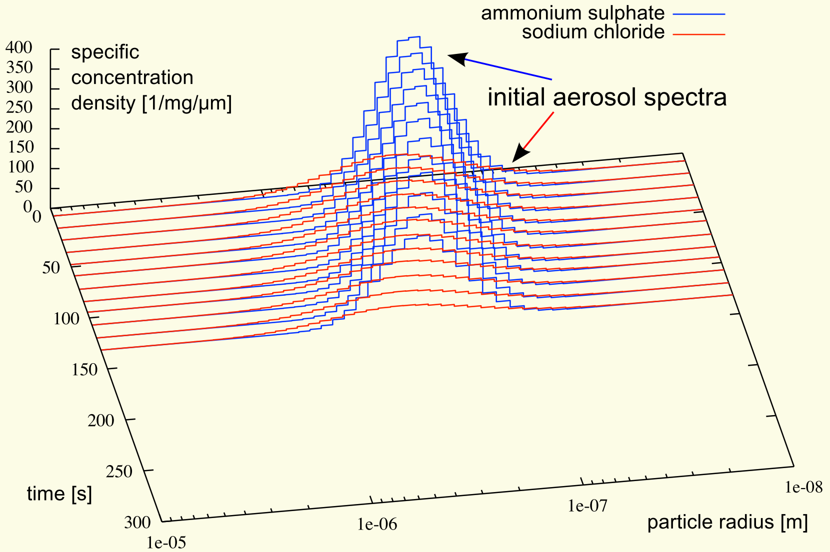

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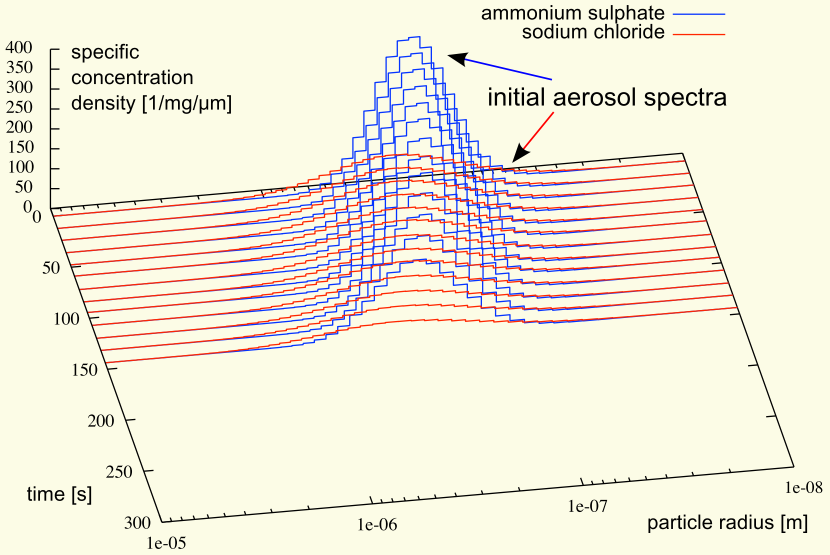

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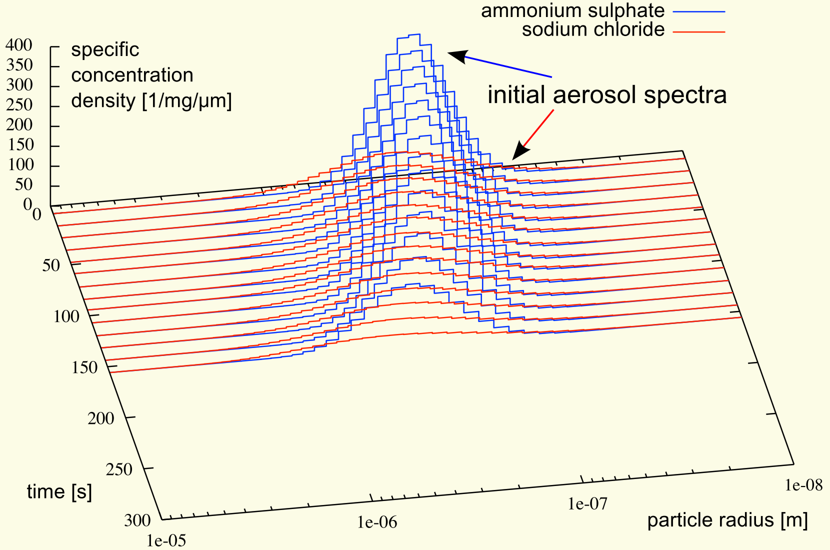

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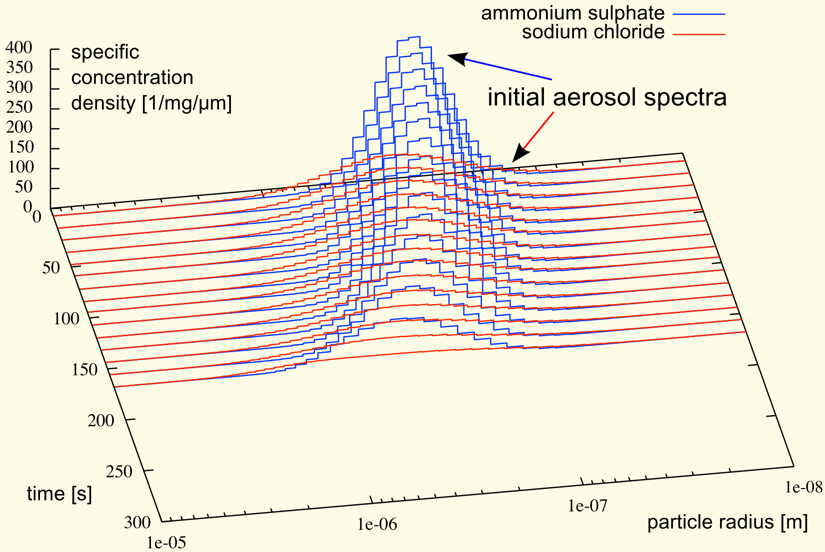

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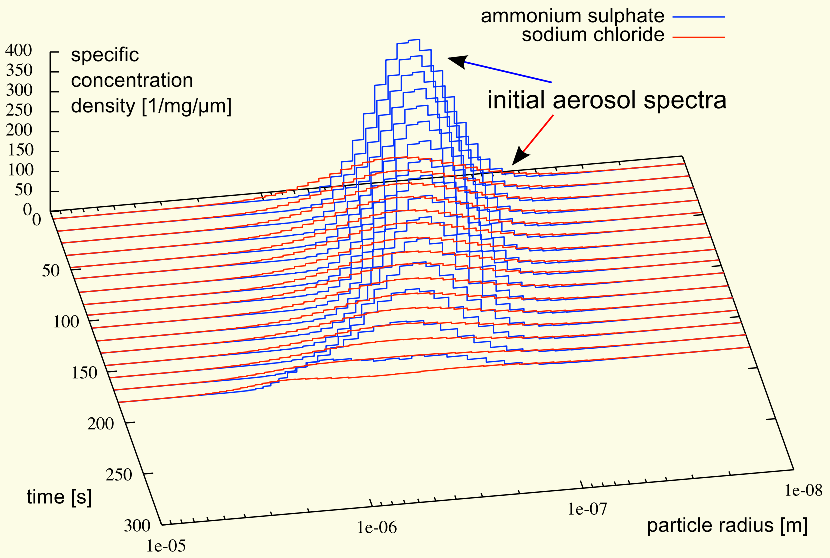

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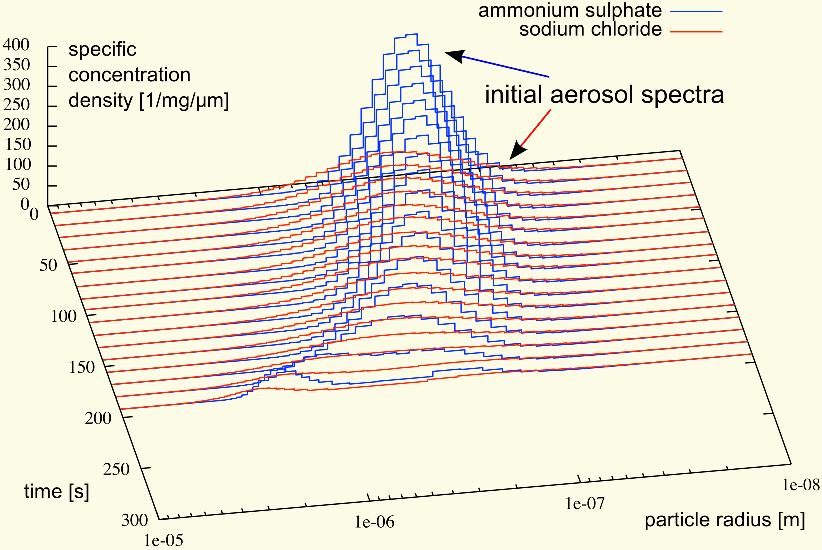

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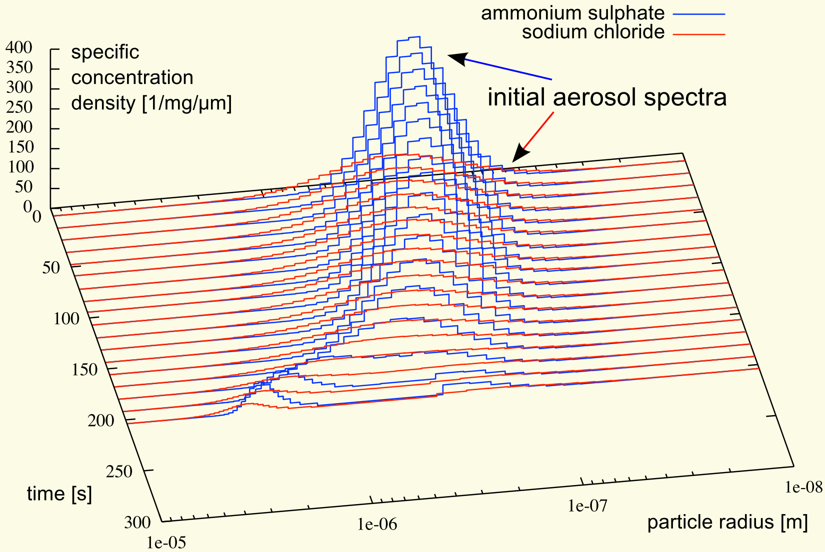

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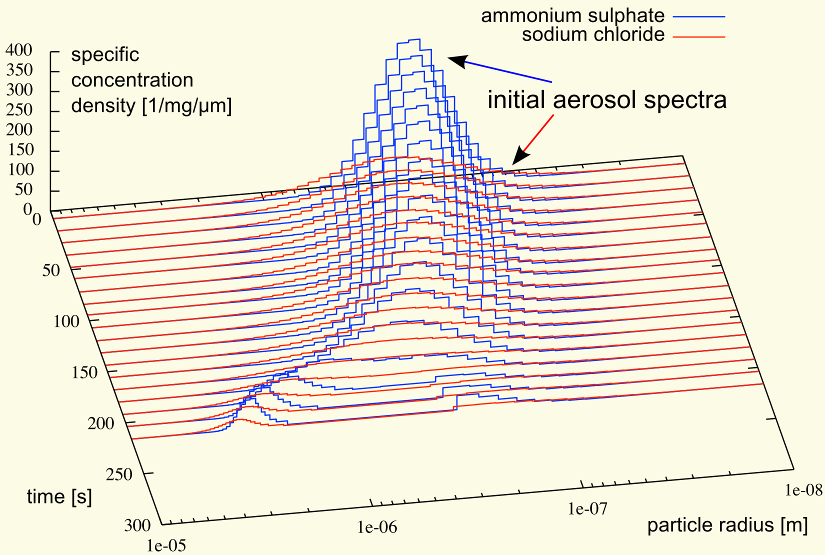

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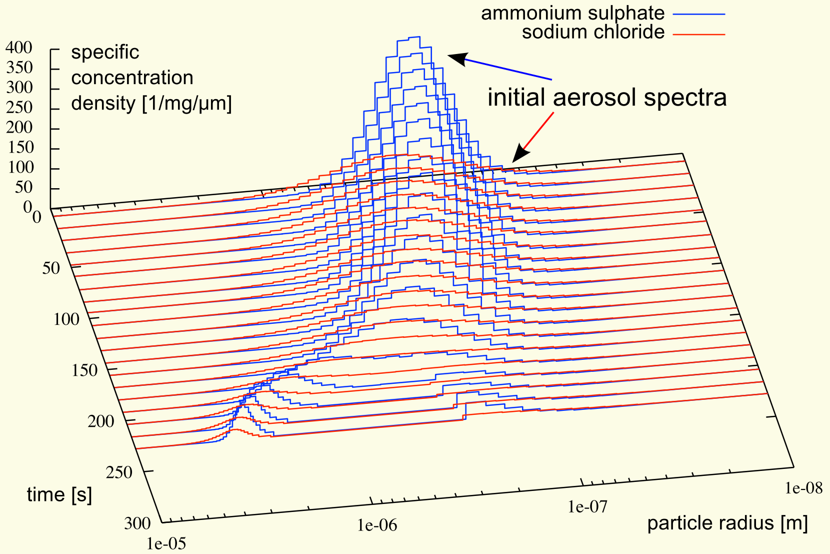

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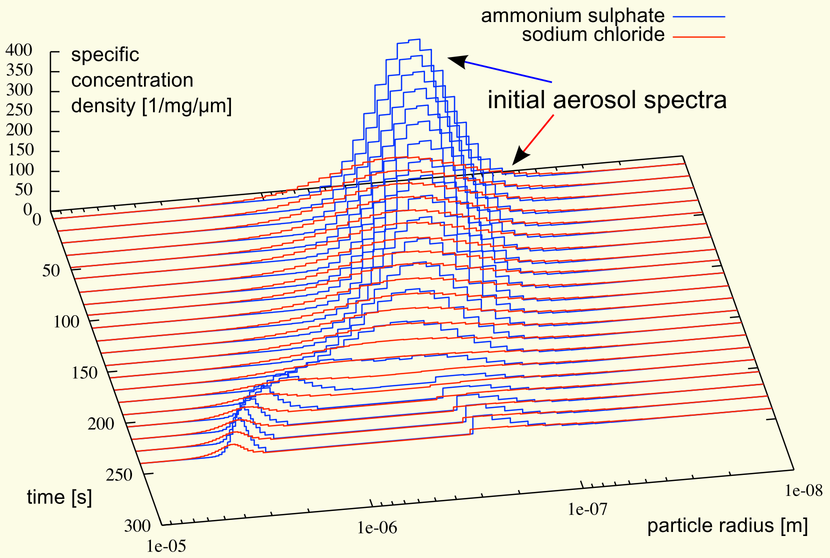

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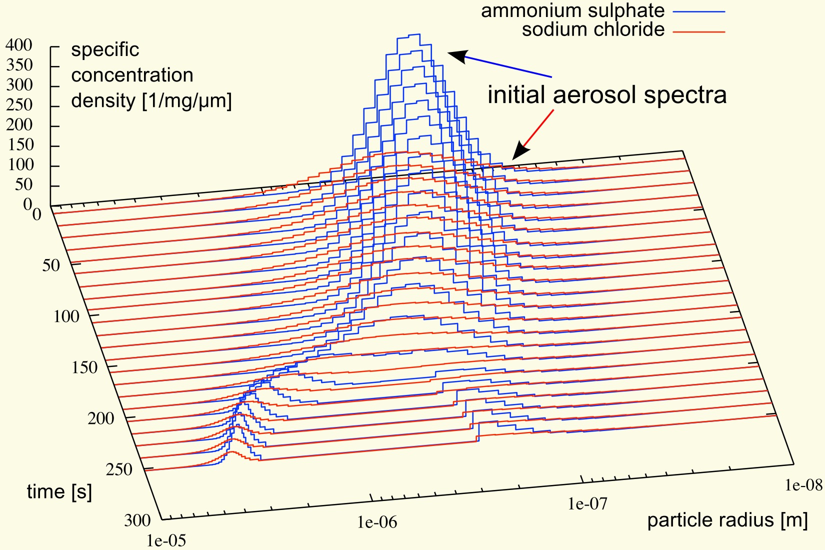

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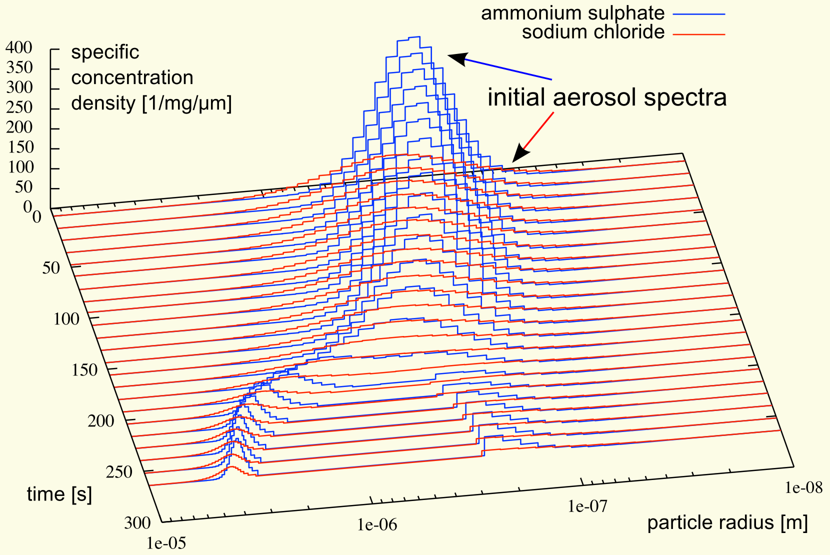

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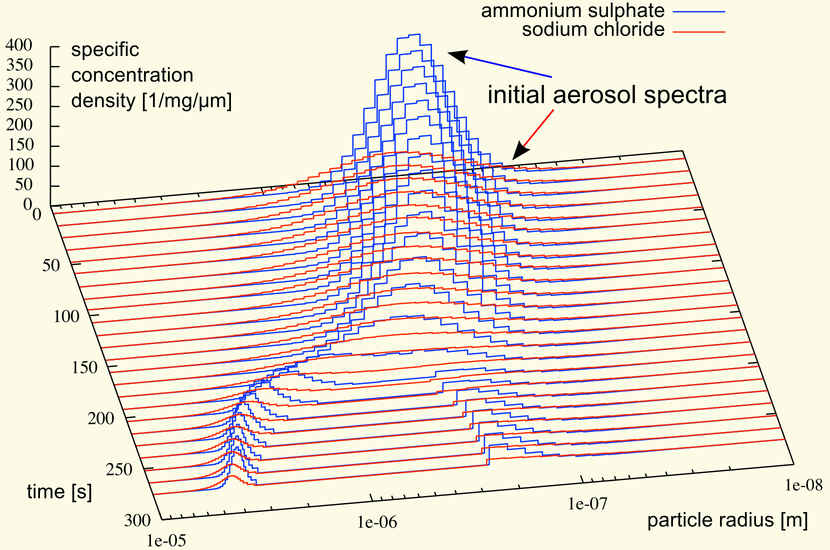

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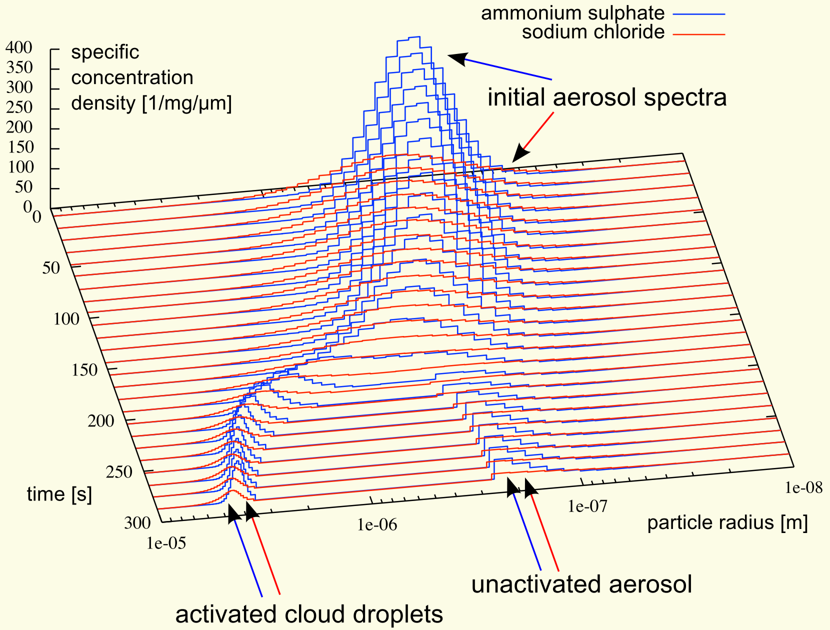

Lagrangian μ-physics in 0D, 2D and 3D

particle attributes:
- multiplicity (**n**),
- "wet" size ($\mathbf{r_w}$),
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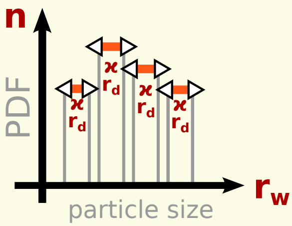
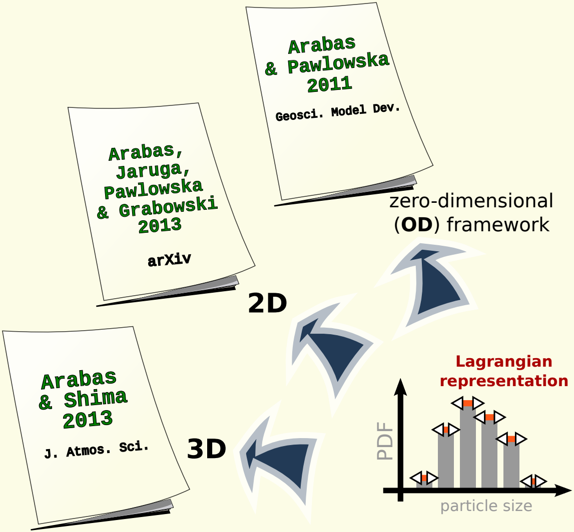
- solute hygroscopicity ($\boldsymbol{\varkappa}$)

processes:
- condensational growth





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- spatial coordinates (**x, y, z**)

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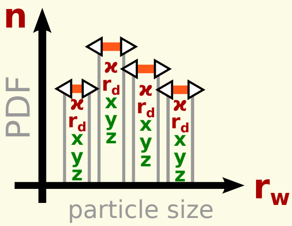

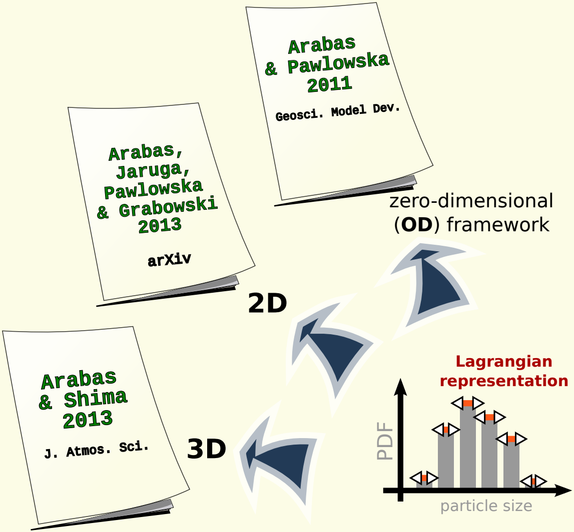

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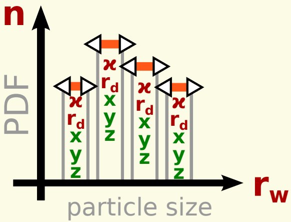
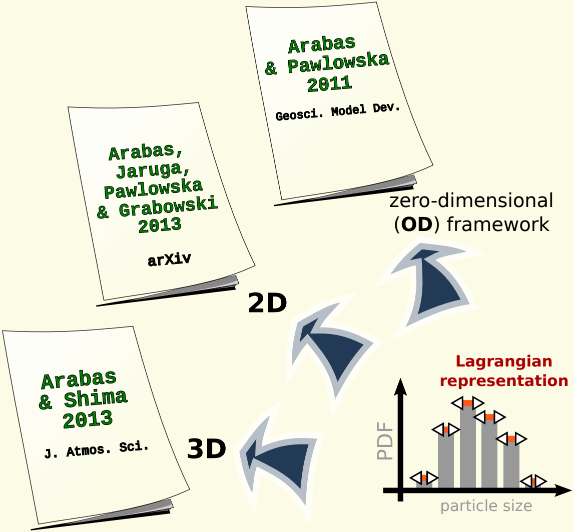
- sedimentation
- collisional growth





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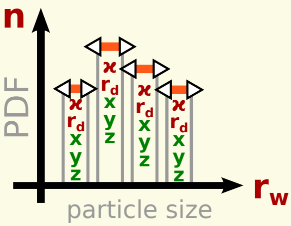
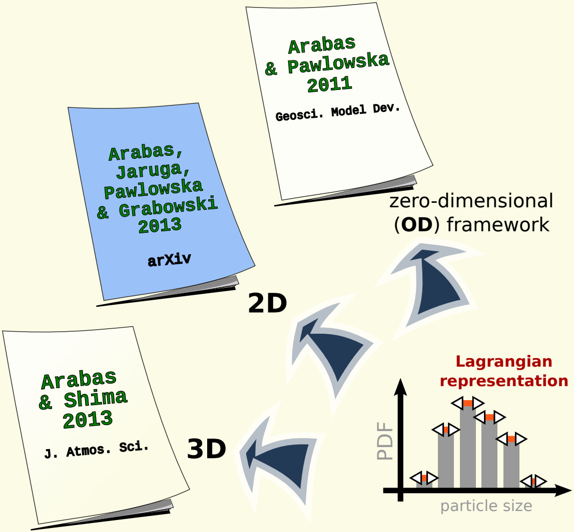
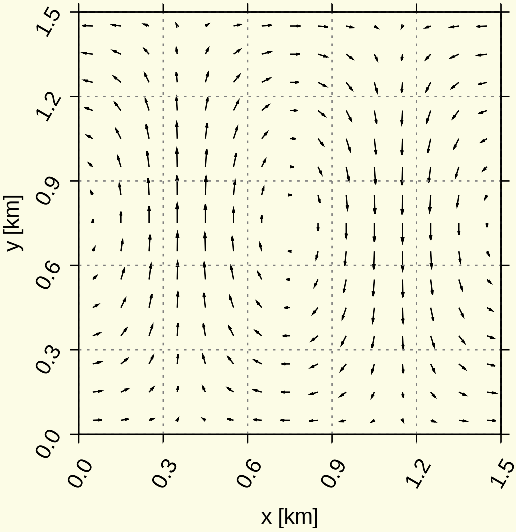




Lagrangian μ-physics in 2D (prescribed-flow model)



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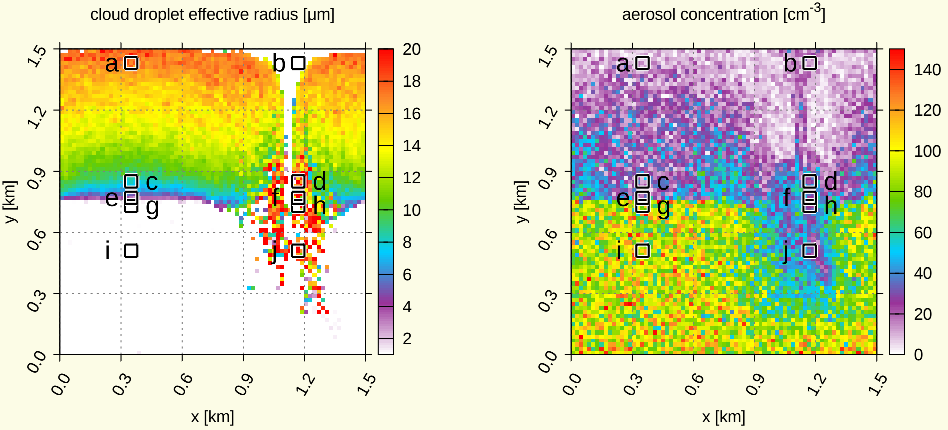

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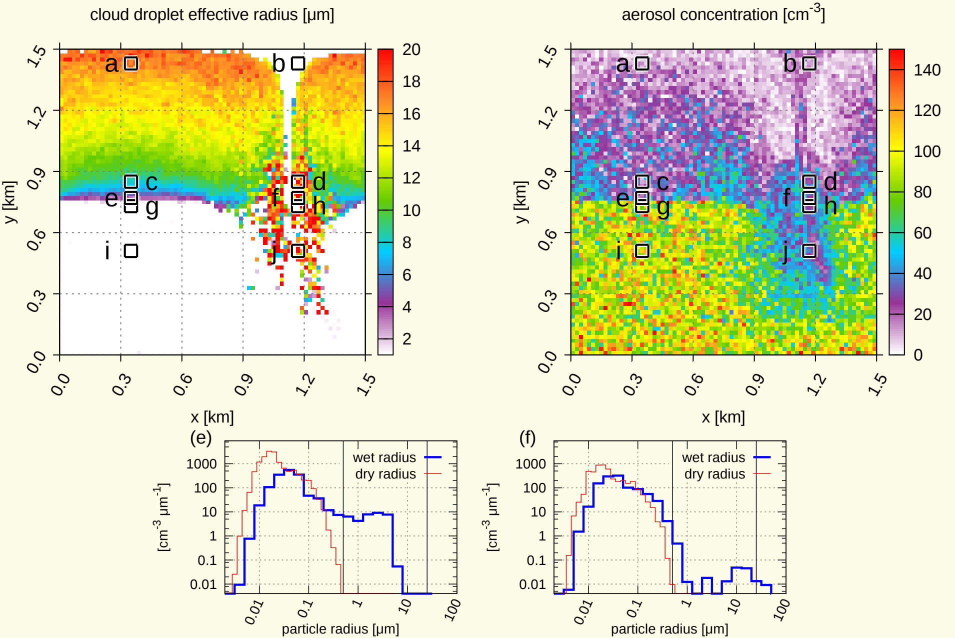

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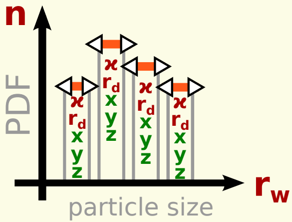
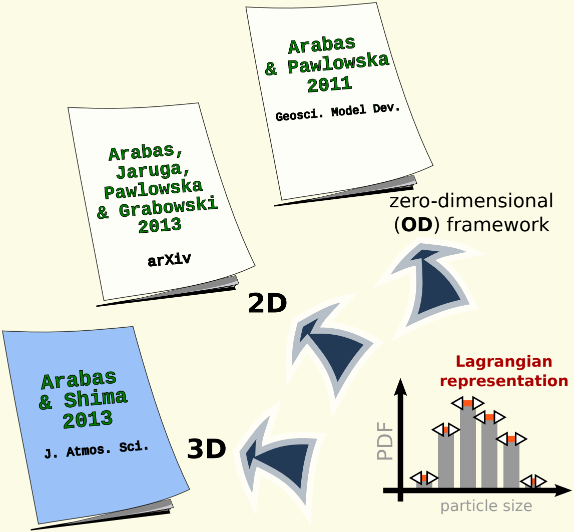
Lagrangian μ-physics in 0D, 2D and 3D

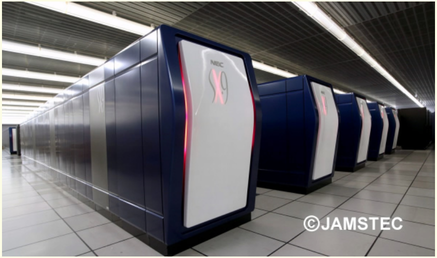
particle attributes:
- multiplicity (**n**),
- "wet" size (**r_w**),
- "dry" size (**r_d**),
- solute hygroscopicity (**$\varkappa$**)
- spatial coordinates (**x, y, z**)

processes:
- condensational growth
- sedimentation
- collisional growth





Lagrangian μ-physics in 3D: simulations vs. aircraft data



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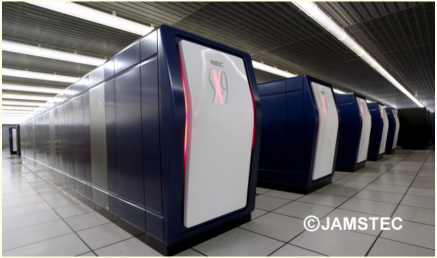

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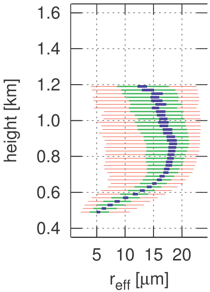

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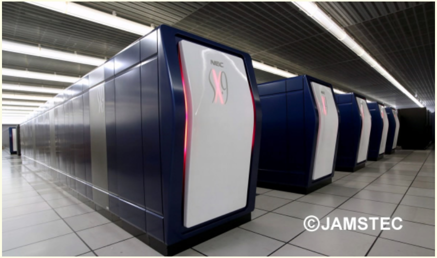

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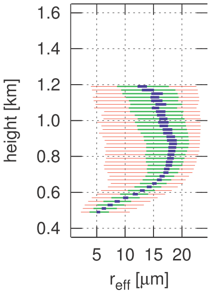
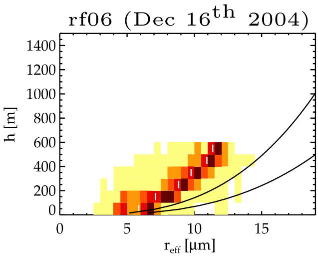


Arabas, Pawlowska, Grabowski 2009, GRL



(h = height - 550 m)

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public/social scientific coding

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- reproduce the results (**free**)

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- reuse the code (**modular, reusable**)

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- continue the work (**extendable, libre**)

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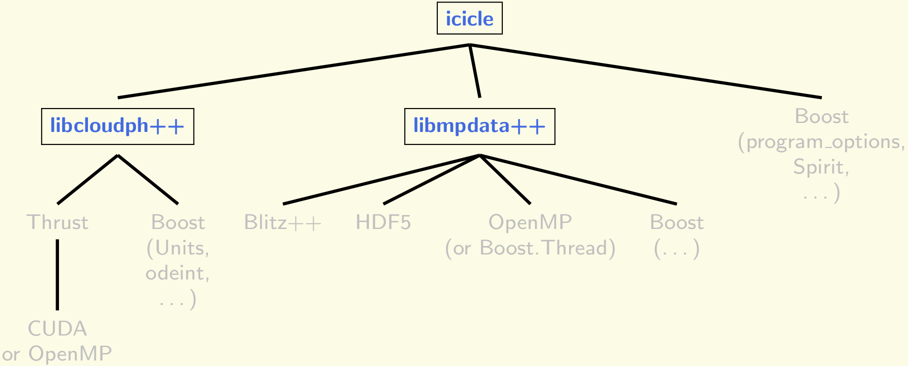

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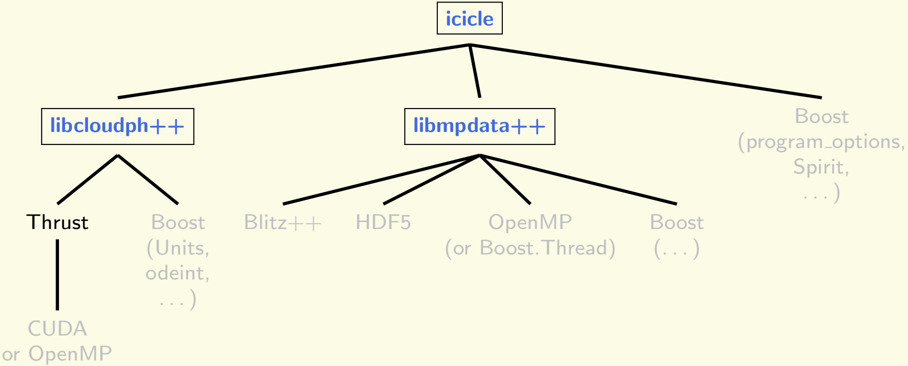

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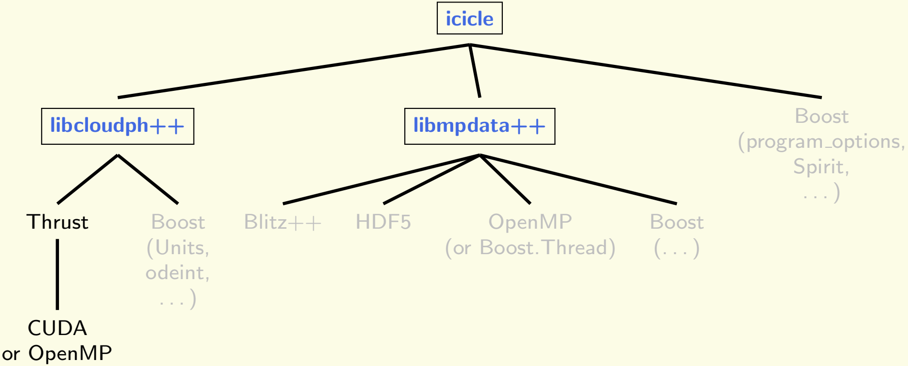

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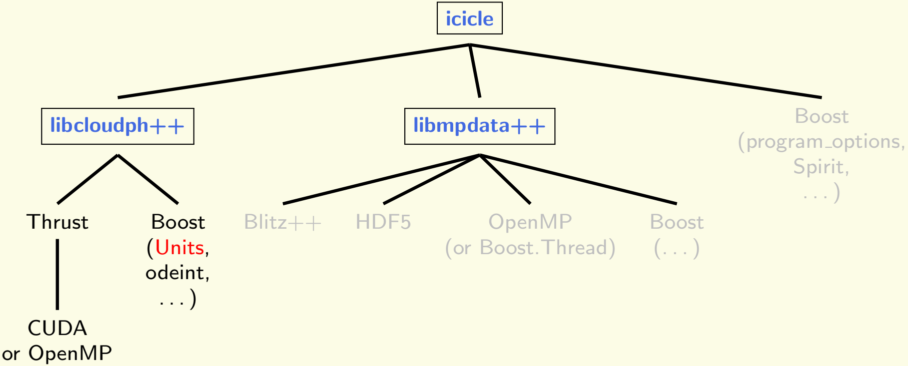

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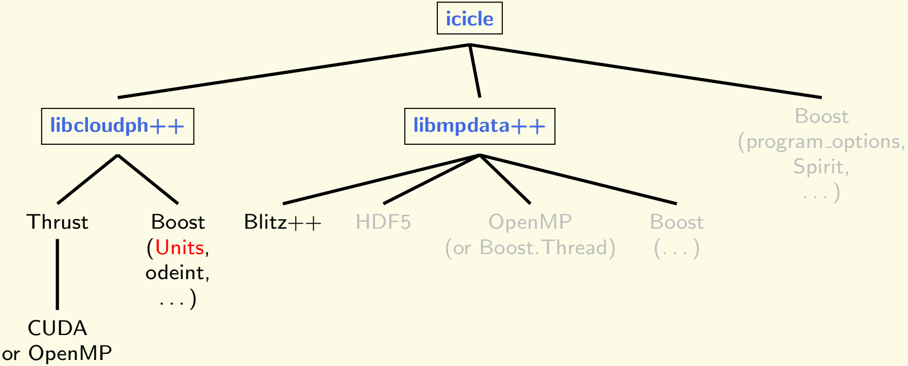

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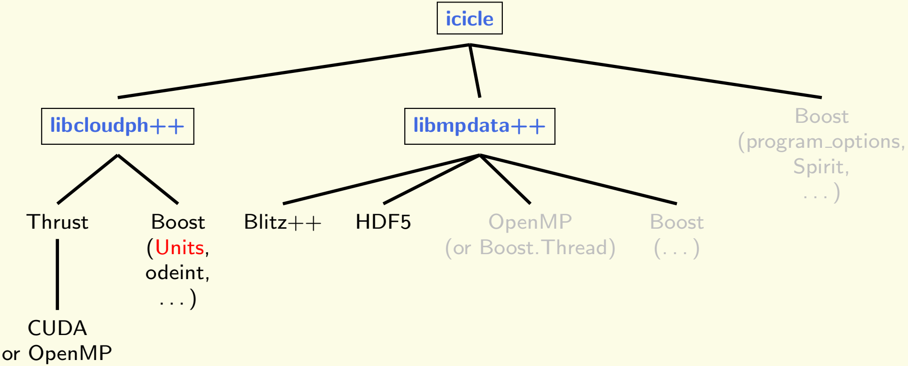

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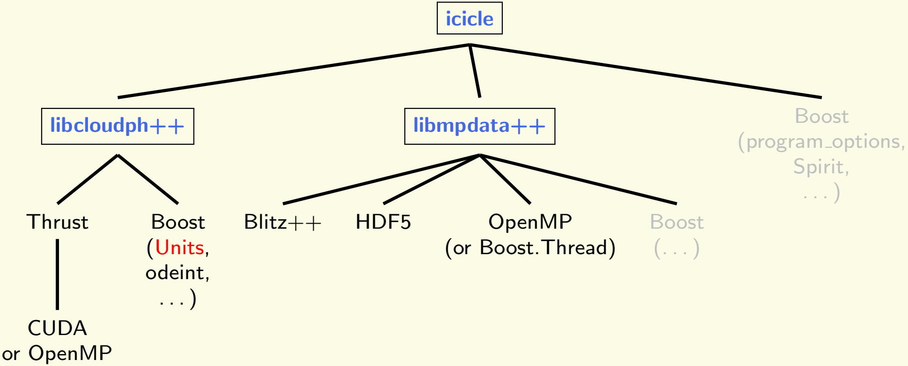

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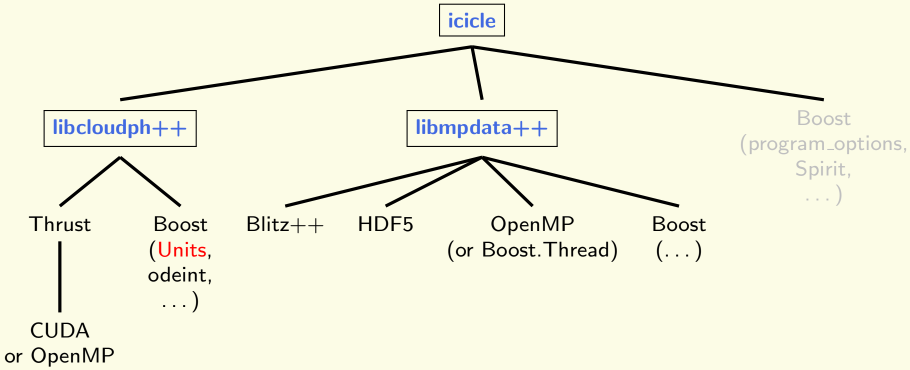

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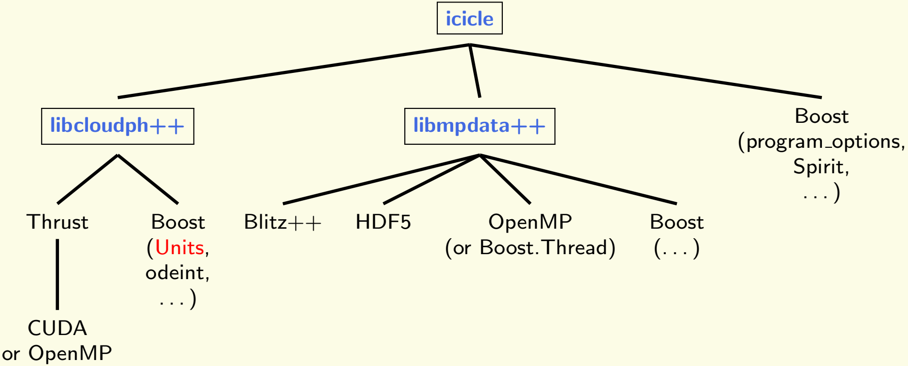

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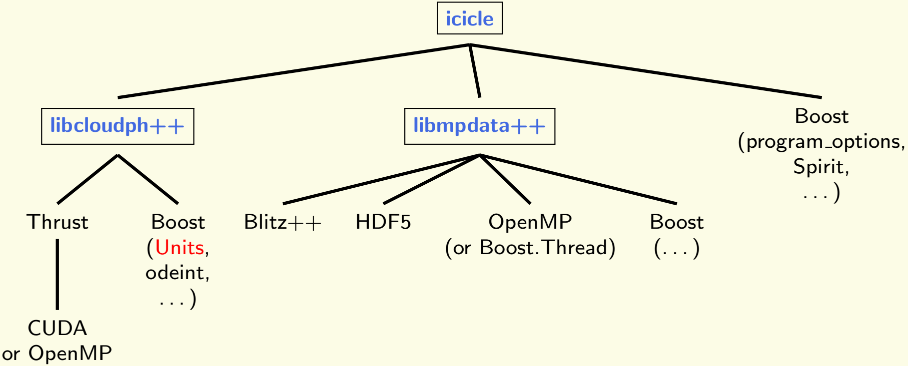

Ongoing work (NCN-funded HARMONIA project):
icicles – an LES system based on libmpdata++ and libcloudph++ developed as a tool for studying **aerosol processing by clouds**

code:

- **libcloudph++**: `github.com/slayoo/libcloudphxx`
- **libmpdata++**: `github.com/slayoo/libmpdataxx`
- **icicle**: `github.com/slayoo/icicle`

papers:

- 0D: **Arabas & Pawlowska 2011** doi:10.5194/gmd-4-15-2011
- 3D: **Arabas & Shima 2013** doi:10.1175/JAS-D-12-0295.1
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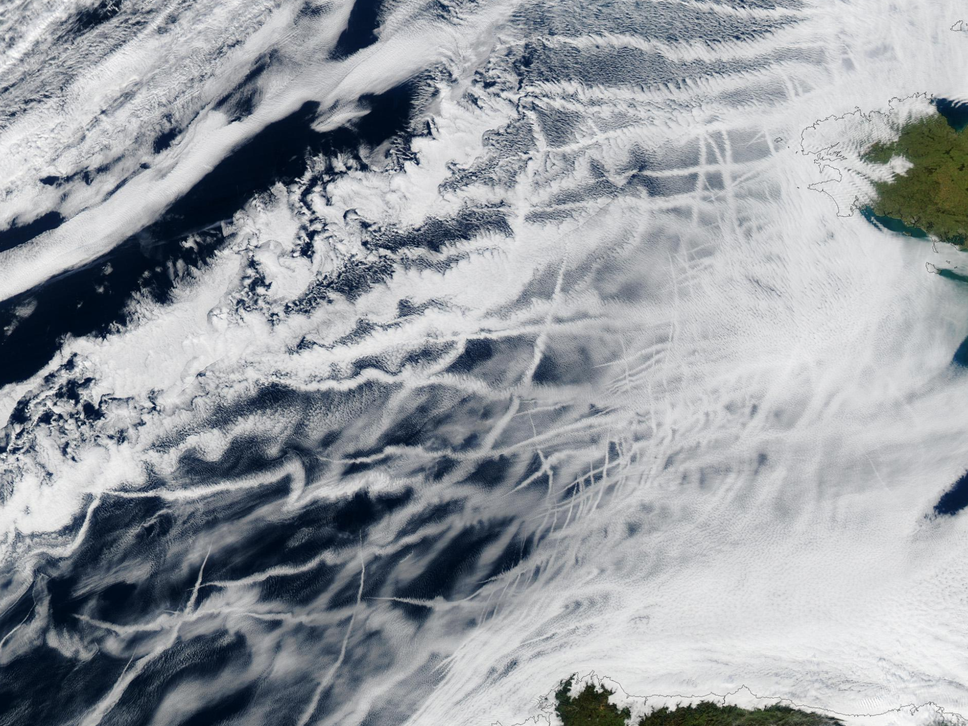
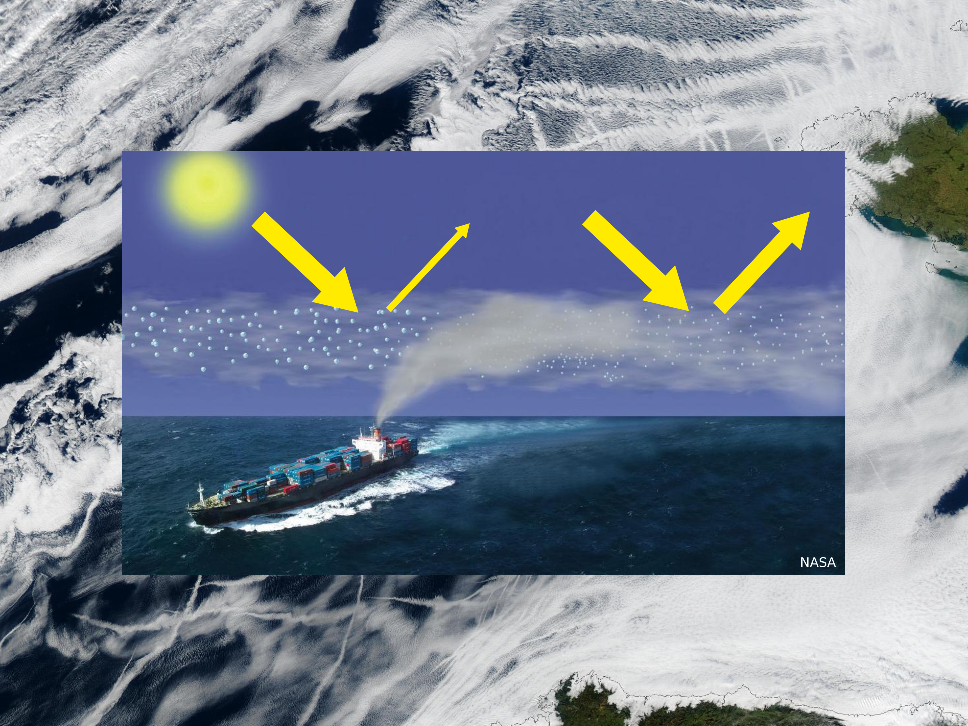
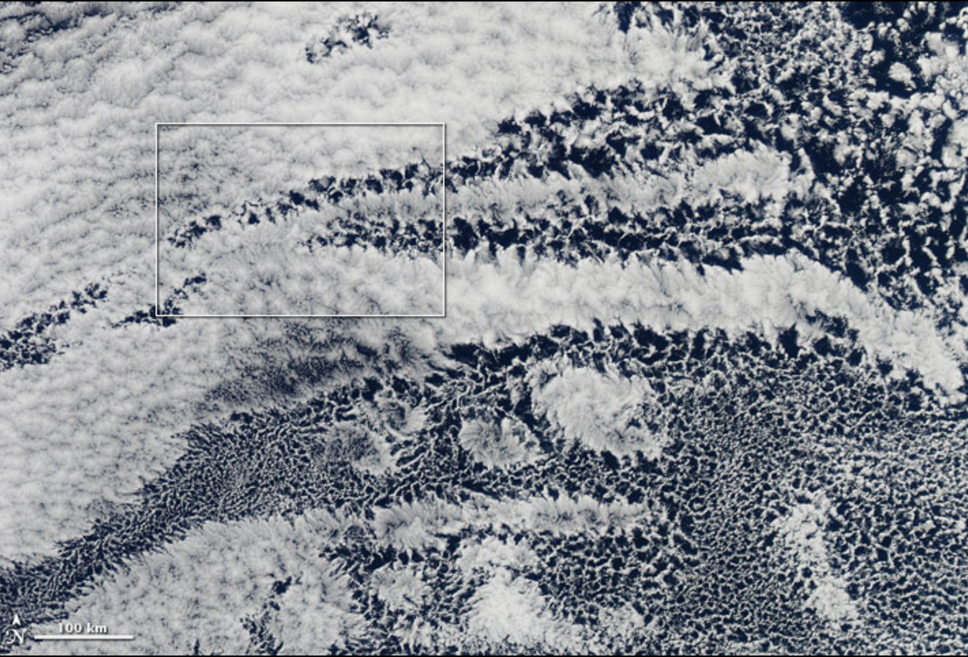
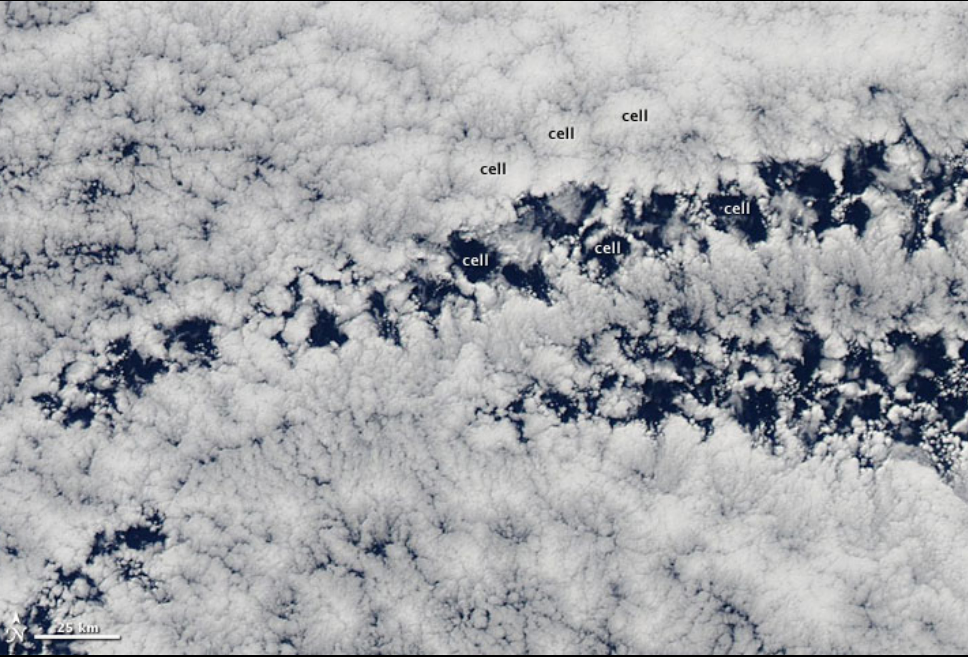
Thank you for your attention




NASA


N
100 km


cell
cell
cell
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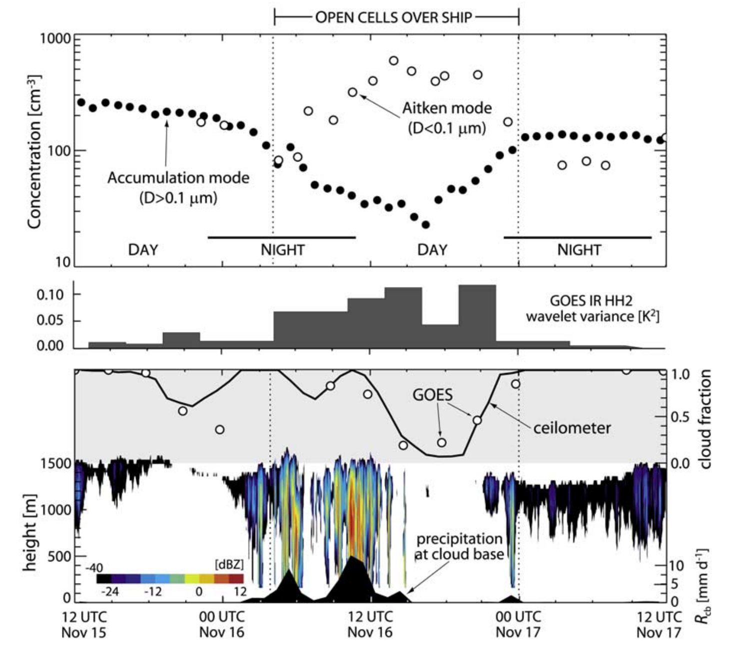
cell
25 km



Wood et al. doi:10.1029/2007JD009371

Morin et al. 2012 doi:10.1126/science.1218263

„the inability to reproduce many published computational results or to perform credible peer review in the absence of program source code has contributed to a perceived "credibility crisis" for research computation"

Ince et al. 2012 doi:10.1038/nature10836

„anything less than the release of source programs is intolerable for results that depend on computation"

GMD 6. Editorial 2013 doi:10.5194/gmd-6-1233-2013

[all papers] "must be accompanied by the code, or means of accessing the code, for the purpose of peer-review", [while the editors] "strongly encourage referees to compile the code, and run test cases supplied by the authors" arxiv.org/abs/1301.1334

[1301.1334] Object-oriented impl...

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arXiv.org > physics > arXiv:1301.1334

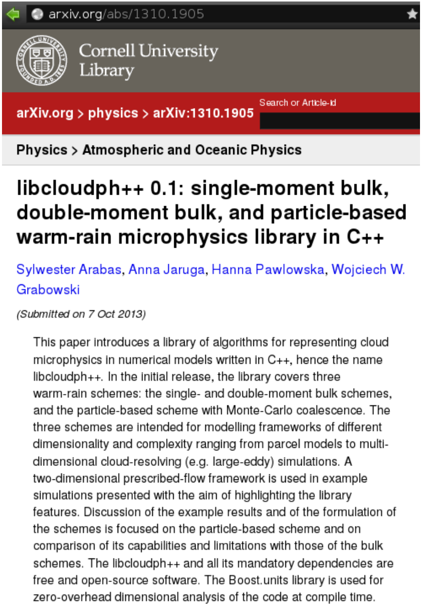
Physics > Computational Physics

Object-oriented implementations of the MPDATA advection equation solver in C++, Python and Fortran

Sylwester Arabas, Dorota Jarecka, Anna Jaruga, Maciej Fijałkowski

(Submitted on 7 Jan 2013 (v1), last revised 19 Mar 2013 (this version, v2))

libcloudph++ API (part of the paper)



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libcloudph++ 0.1: single-moment bulk, double-moment bulk, and particle-based warm-rain microphysics library in C++

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(Submitted on 7 Oct 2013)

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tion, and are grouped into a structure named **lgrngn::opts_init_t** (Listing 5.2). The initial

```
template<typename real_t>
struct opts_init_t
{
  // initial dry sizes of aerosol
  typedef boost::ptr_unordered_map<
    real_t,                   // kappa
    unary_function<real_t> // n(ln(rd)) @ STP
  > dry_distros_t;
  dry_distros_t dry_distros;

  // Eulerian component parameters
  int nx, ny, nz;
  real_t dx, dy, dz, dt;

  // mean no. of super-droplets per cell
  real_t sd_conc_mean;

  // coalescence Kernel type
  kernel_t kernel;

  // ctor with defaults (C++03 compliant) ...
```

Listing 5.2: **lgrngn::opts_init_t** structure definition

dry size spectrum of aerosol is represented with a map associating values of the solubility parameter κ with pointers to functors returning con-

Questions and comments sent by Graham Feingold

Some broad questions and some that might be worth clarifying in unpublished work:

1) Is the particle-based method (Arabas and Shima 2012) moment conserving? If not, how does moment conservation change with the number of superdroplets
2) How would you design a more rigorous comparison of model output with observations?
3) Why C++ when modern fortran compilers are able to use GPUs? Is it mostly the stability of the code (maintainability, compatibility)? C++ code has a reputation of requiring an extremely careful programming style. Might this outweigh the advantages when the new modeling framework proposed here becomes more of a community model?
4) In many aspects of cloud modeling, we lack a basic understanding of the processes themselves (e.g., collection kernels). How do you view the balance in effort expended on modeling methods as opposed to laboratory and theoretical descriptions of the physics?
5) Have you used the particle-based approach (Appendices A.2 and A.3) to investigate where the raindrop embryos first form?
6) How is supersaturation calculated in the particle-based method (Appendices A.2 and A.3)? Thi was not clear from these papers. Is it the semi-analytical method of Clark (1973)?
7) Where do you view the bin microphysical schemes in terms of their future application in the proposed modeling framework?

Q: Is the particle-based method **moment conserving**? If not, how does moment conservation change with the number of superdroplets?

- initialisation: no (the more super droplets, the better)

[a] e.g.: Tzivion, Reisin, Levin 1999, JCP

[b] e.g.: Alfonso, Raga & Baumgardner 2008, 2010, 2013, ACP

Q: Is the particle-based method **moment conserving**? If not, how does moment conservation change with the number of superdroplets?

- initialisation: no (the more super droplets, the better)
- advection: all moments conserved for both dry and wet spectra

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Q: Is the particle-based method **moment conserving**? If not, how does moment conservation change with the number of superdroplets?

- initialisation: no (the more super droplets, the better)
- advection: all moments conserved for both dry and wet spectra
- sedimentation: no (as in reality)
- condensation: particle number conserved (0^{th} moment)
- collisions: mass conserved (3^{rd} moment of dry and wet spectra)
  note: this may not always be the case for Smoluchowski coagulation equation-based methods either due to discretisation issues[a] or due to gelation[b]

[a] e.g.: Tzivion, Reisin, Levin 1999, JCP
[b] e.g.: Alfonso, Raga & Baumgardner 2008, 2010, 2013, ACP

Q: How would you design a more rigorous **comparison of model output with observations**?

- a wider synergy among analyses of macro- & micro-physics

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- a wider synergy among analyses of macro- & micro-physics
- **more error bars**:
  - **simulations**: more realisations (different grids, timesteps, random seeds, ensembles of initial parameters, ensembles of tuning parameters, different parameterisations)
  - **observations**: propagation of instrumental error throughout the data analysis procedures

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  - Fortran is domain-specific language $\rightsquigarrow$ no cross-domain benefits
    (C++: gaming, banking, defense, CAD/CAM, telecom, ...)
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  - High-level libs (where the user don't have to know a single bit of OpenCL/CUDA, and that allow to run the programs with no GPU):
    Boost.compute, VexCL, ViennaCL, nVidia's Thrust, AMD's Bolt, Microsoft's AMP – all in C++

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  - Fortran lacks error handling facility (exceptions in C++)
    ⇝an issue when using multiple libraries
  - Fortran lacks compile-time programming facility (templates in C++)
    ⇝no zero-runtime-overhead mechanisms, e.g. units checking

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    (would aerosol/cloud models pass airworthiness or spaceworthines tests of aerosol/cloud instruments?)
- **a related remark**
  - open data needed as much as open code
    (to foster transfer of knowledge between modellers and observationalists)

Q: Have you used the particle-based approach to investigate where the raindrop embryos first form?

- no, thanks for suggestion

Q: How is supersaturation calculated in the particle-based method? This was not clear from these papers. Is it the semi-analytical method of Clark (1973)?

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- explicitly, from dynamical tendencies alone
- but $\leqslant$ 1s timesteps and marine aerosol were used
- again: thanks for suggestion, will look into it
  (starting off by implementing the scheme of Thouron et. al. 2013[a])

[a] O. Thouron, J.-L. Brenguier, and F. Burnet: Supersaturation calculation in large eddy simulation models for prediction of the droplet number concentration Geosci. Model Dev., 5, 761-772, 2012

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- quantification of some of the limitations of the Lagrangian method (e.g. importance of regions that become void of particles)