Bifurcations in a dynamical system describing formation of cloud droplets on atmospheric particulate matter

Sylwester Arabas

Sylwester Arabas

Sylwester Arabas

- alma mater: University of Warsaw (group of Hanna Pawłowska)

Sylwester Arabas

- alma mater: University of Warsaw (group of Hanna Pawłowska)
  - MSc (2008) in observational cloud μ-physics (EUCAARI)

Sylwester Arabas

- alma mater: University of Warsaw (group of Hanna Pawłowska)
  - MSc (2008) in observational cloud μ-physics (EUCAARI)
  - PhD (2013) in computational cloud μ-physics

Sylwester Arabas

- alma mater: University of Warsaw (group of Hanna Pawłowska)
  - MSc (2008) in observational cloud μ-physics (EUCAARI)
  - PhD (2013) in computational cloud μ-physics
  - postdoc (till 2015): research software development

Sylwester Arabas

- alma mater: University of Warsaw (group of Hanna Pawłowska)
  - MSc (2008) in observational cloud μ-physics (EUCAARI)
  - PhD (2013) in computational cloud μ-physics
  - postdoc (till 2015): research software development
- outside of academia:

Sylwester Arabas

- alma mater: University of Warsaw (group of Hanna Pawłowska)
  - MSc (2008) in observational cloud μ-physics (EUCAARI)
  - PhD (2013) in computational cloud μ-physics
  - postdoc (till 2015): research software development
- outside of academia:
  - 2015–2017: Chatham Financial, Cracow (software developer)

Sylwester Arabas

- alma mater: University of Warsaw (group of Hanna Pawłowska)
  - MSc (2008) in observational cloud μ-physics (EUCAARI)
  - PhD (2013) in computational cloud μ-physics
  - postdoc (till 2015): research software development
- outside of academia:
  - 2015–2017: Chatham Financial, Cracow (software developer)
  - 2017–2018: AETHON, Athens (H2020 "Innovation Associate")

Arabas & Shima 2017

Nonlin. Processes Geophys., 24, 535–542, 2017
https://doi.org/10.5194/npg-24-535-2017

Nonlinear Processes
in Geophysics
Open Access

On the CCN (de)activation nonlinearities

Sylwester Arabas[1,2] **and Shin-ichiro Shima**[3]

[1]Institute of Geophysics, Faculty of Physics, University of Warsaw, Warsaw, Poland
[2]Chatham Financial Corporation Europe, Cracow, Poland
[3]Graduate School of Simulation Studies, University of Hyogo, Kobe, Japan

Correspondence to: Sylwester Arabas (sarabas@chathamfinancial.eu) and Shin-ichiro Shima (s_shima@sim.u-hyogo.ac.jp)

Received: 9 September 2016 – Discussion started: 4 October 2016
Revised: 23 May 2017 – Accepted: 24 July 2017 – Published: 5 September 2017

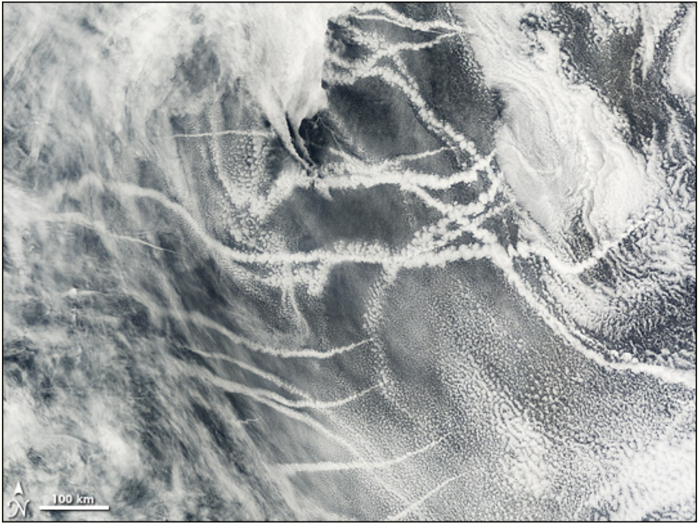
atmospheric particulate matter (PM) and clouds

atmospheric particulate matter (PM) and clouds

no particles $\rightsquigarrow$ no clouds

`https://www.youtube.com/watch?v=EneDwu0HrVg`

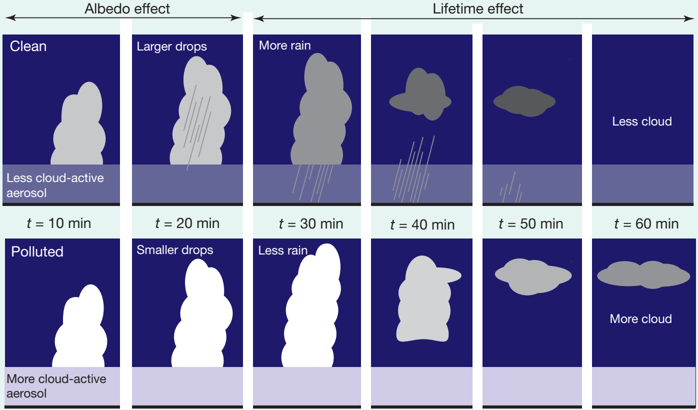
atmospheric particulate matter (PM) and clouds



NASA (https://earthobservatory.nasa.gov/NaturalHazards/view.php?id=20248)

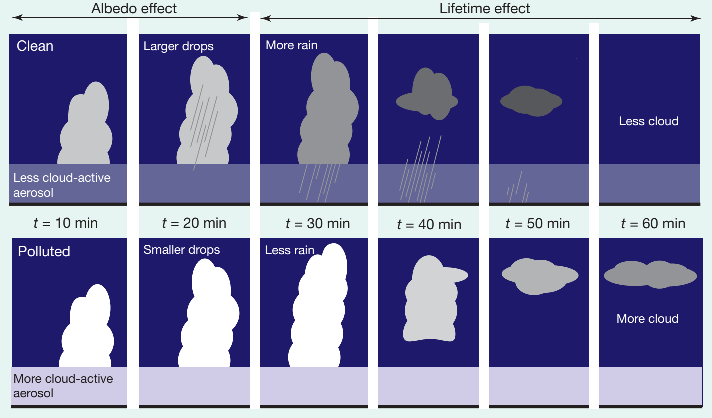
atmospheric particulate matter (PM) and clouds

Stevens and Feingold, 2009 (Nature)



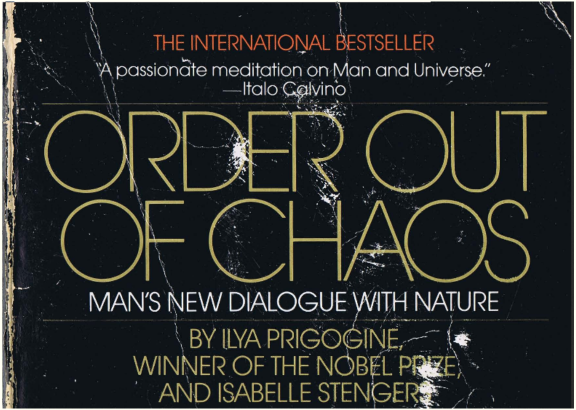
atmospheric particulate matter (PM) and clouds

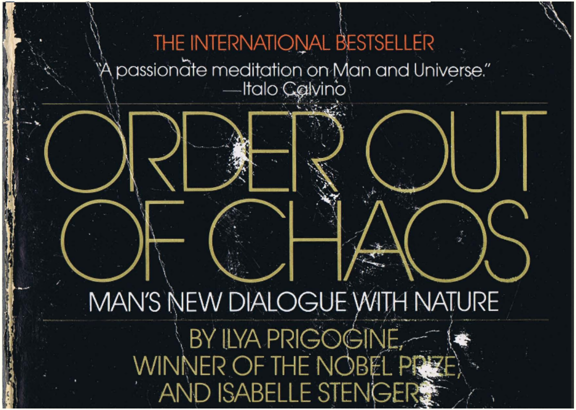
Stevens and Feingold, 2009 (Nature)



Stevens and Boucher, 2012 (Nature)

"there is something captivating about the idea that fine particulate matter, suspended almost invisibly in the atmosphere, holds the key to some of the greatest mysteries of climate science"


THE INTERNATIONAL BESTSELLER
"A passionate meditation on Man and Universe."
—Italo Calvino
ORDER OUT OF CHAOS
MAN'S NEW DIALOGUE WITH NATURE
BY ILYA PRIGOGINE,
WINNER OF THE NOBEL PRIZE,
AND ISABELLE STENGERS



Prigogine and Stengers 1984

"Much of this book has centered around the relation between the microscopic and the macroscopic. One of the most important problems in evolutionary theory is the eventual feedback between macroscopic structures and microscopic events: macroscopic structures emerging from microscopic events would in turn lead to a modification of the microscopic mechanisms."

regime-transition (bifurcation) example from P&S 1984

regime-transition (bifurcation) example from P&S 1984

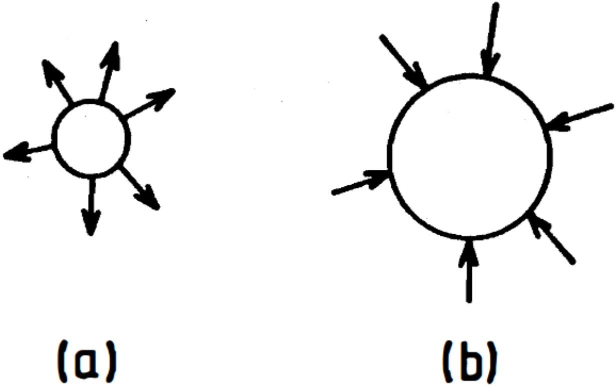
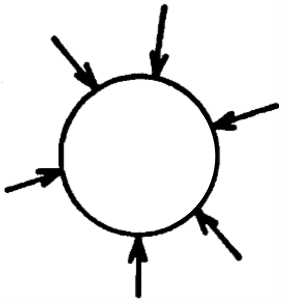
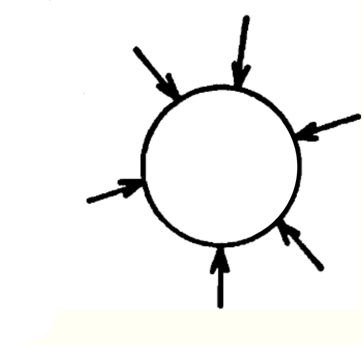


Figure 19. Nucleation of a liquid droplet in a supersaturated vapor. (a) droplet smaller than the critical size; (b) droplet larger than the critical size. The existence of the threshold has been experimentally verified for dissipative structures.

droplet growth laws in a nutshell: mass and heat diffusion



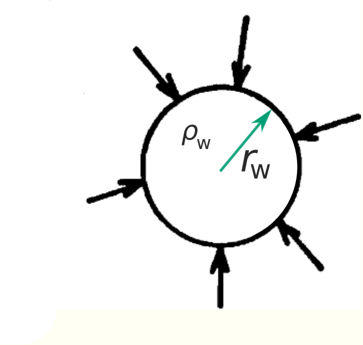
droplet growth laws in a nutshell: mass and heat diffusion



Fick's and Fourier's laws combined

spherical geometry

$$\dot{r}_{\mathsf{w}} = \frac{1}{r_{\mathsf{w}}} \frac{D_{\mathsf{eff}}}{\rho_{\mathsf{w}}} (\rho_{\mathsf{v}} - \rho_{\circ})$$

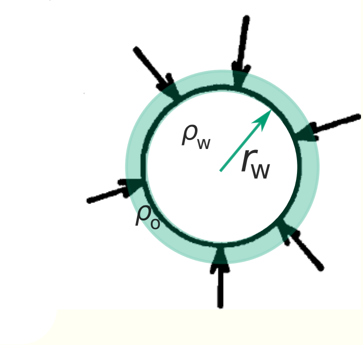


Fick's and Fourier's laws combined

spherical geometry

$$\dot{r}_w = \frac{1}{r_w}\frac{D_{\text{eff}}}{\rho_w}(\rho_v - \rho_\circ)$$

droplet growth laws in a nutshell: mass and heat diffusion

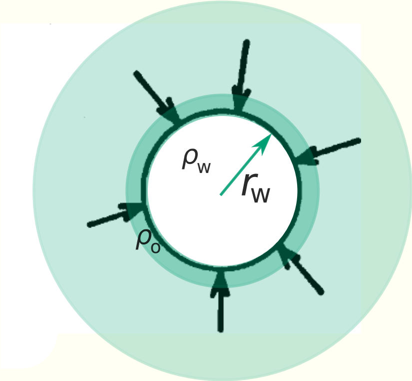


Fick's and Fourier's laws combined

spherical geometry

$$\dot{r}_w = \frac{1}{r_w}\frac{D_{\text{eff}}}{\rho_w}\left(\rho_v - \rho_\circ\right)$$

droplet growth laws in a nutshell: mass and heat diffusion

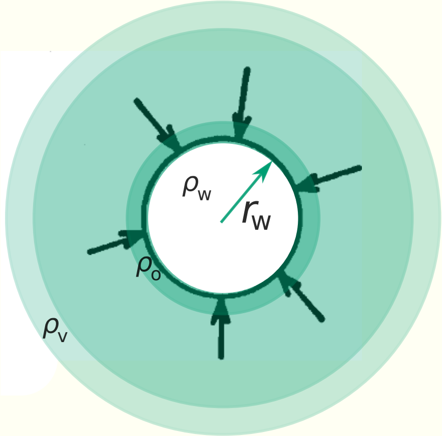


Fick's and Fourier's laws combined

spherical geometry

$$\dot{r}_w = \frac{1}{r_w} \frac{D_{eff}}{\rho_w} (\rho_v - \rho_\circ)$$

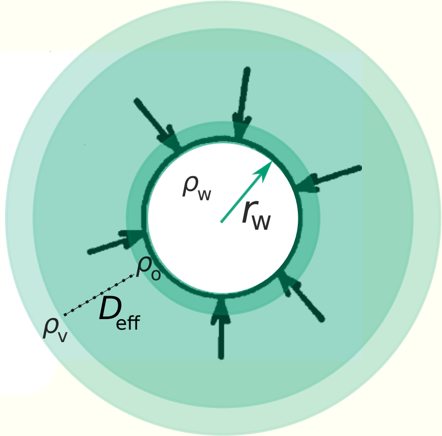
droplet growth laws in a nutshell: mass and heat diffusion



Fick's and Fourier's laws combined

spherical geometry

$$\dot{r}_w = \frac{1}{r_w}\frac{D_{\text{eff}}}{\rho_w}\left(\rho_v - \rho_\circ\right)$$

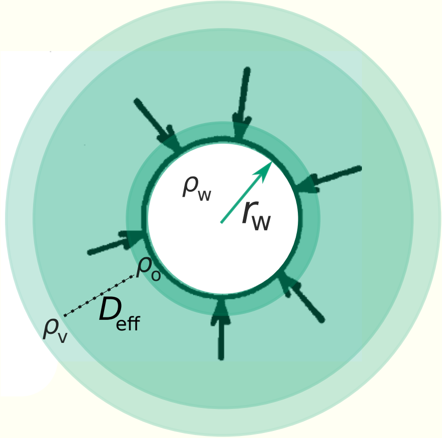


Fick's and Fourier's laws combined

spherical geometry

$$\dot{r}_w = \frac{1}{r_w}\frac{D_{\text{eff}}}{\rho_w}(\rho_v - \rho_\circ)$$

droplet growth laws in a nutshell: mass and heat diffusion



Fick's and Fourier's laws combined

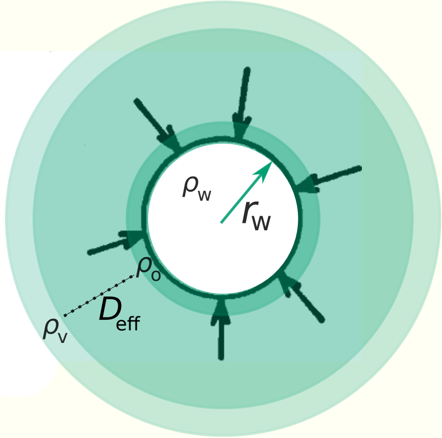
spherical geometry

$$\dot{r}_w = \frac{1}{r_w}\frac{D_{eff}}{\rho_w}\left(\rho_v - \rho_\circ\right)$$

non-dimensional numbers:

$$\mathrm{RH} = \rho_v/\rho_{vs}$$
$$\mathrm{RH}_{eq} = \rho_\circ/\rho_{vs}$$

droplet growth laws in a nutshell: mass and heat diffusion



Fick's and Fourier's laws combined

spherical geometry

$$\dot{r}_w = \frac{1}{r_w}\frac{D_{eff}}{\rho_w}(\rho_v - \rho_\circ)$$

non-dimensional numbers:

$$\mathrm{RH} = \rho_v/\rho_{vs}$$
$$\mathrm{RH}_{eq} = \rho_\circ/\rho_{vs}$$

$$\dot{r}_w = \frac{1}{r_w}D_{eff}\frac{\rho_{vs}}{\rho_w}\left(\mathrm{RH} - \mathrm{RH}_{eq}\right)$$

droplet growth laws in a nutshell: Köhler curve

$$\dot{r}_{\mathrm{w}} = \frac{1}{r_{\mathrm{w}}} D_{\mathrm{eff}} \frac{\rho_{\mathrm{vs}}}{\rho_{\mathrm{w}}} \left(\mathrm{RH} - \mathrm{RH}_{\mathrm{eq}}\right)$$

droplet growth laws in a nutshell: Köhler curve

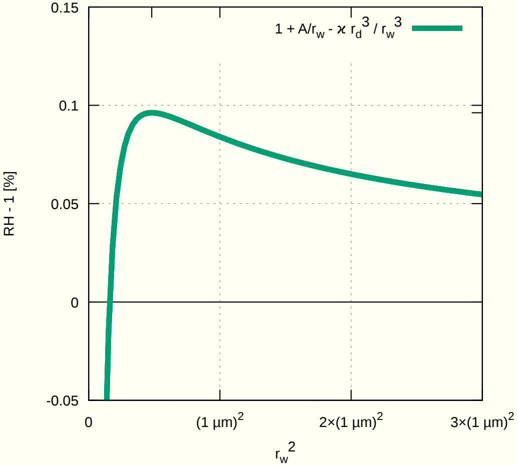
$$\dot{r}_\mathrm{w} = \frac{1}{r_\mathrm{w}} D_\mathrm{eff} \frac{\rho_\mathrm{vs}}{\rho_\mathrm{w}} \left(\mathrm{RH} - \mathrm{RH}_\mathrm{eq}\right)$$

$$\begin{aligned}\mathrm{RH}_\mathrm{eq} &= \frac{r_w^3 - r_d^3}{r_w^3 - r_d^3(1-\kappa)} \exp\left(\frac{A}{r_w}\right) \\ &\approx 1 + \frac{A}{r_\mathrm{w}} - \frac{\kappa r_\mathrm{d}^3}{r_\mathrm{w}^3}\end{aligned}$$

droplet growth laws in a nutshell: Köhler curve

$$\dot{r}_w = \frac{1}{r_w} D_{eff} \frac{\rho_{vs}}{\rho_w} (RH - RH_{eq})$$

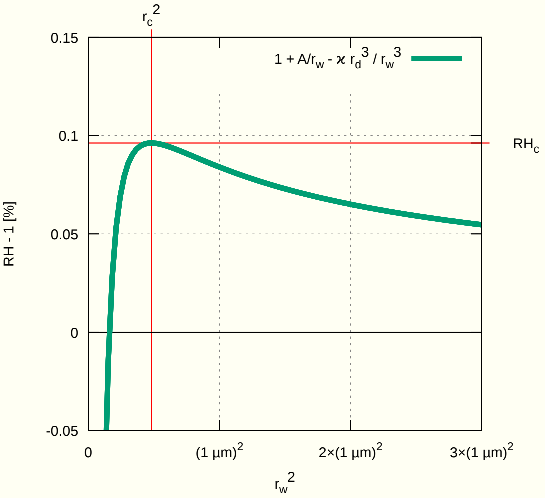
$$RH_{eq} = \frac{r_w^3 - r_d^3}{r_w^3 - r_d^3(1-\kappa)} \exp\left(\frac{A}{r_w}\right) \approx 1 + \frac{A}{r_w} - \frac{\kappa r_d^3}{r_w^3}$$



droplet growth laws in a nutshell: Köhler curve

$$\dot{r}_{\text{w}} = \frac{1}{r_{\text{w}}} D_{\text{eff}} \frac{\rho_{\text{vs}}}{\rho_{\text{w}}} \left(\text{RH} - \text{RH}_{\text{eq}}\right)$$

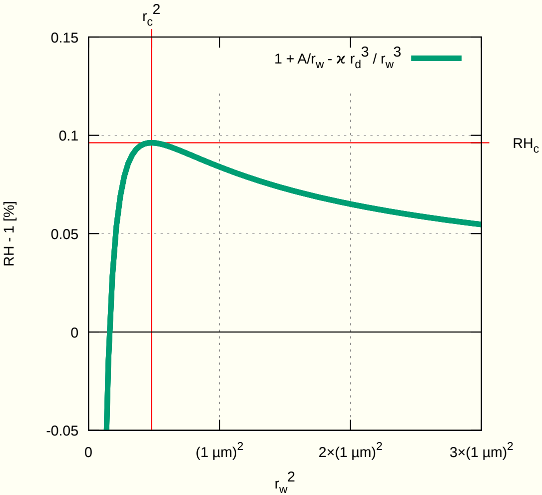
$$\text{RH}_{\text{eq}} = \frac{r_w^3 - r_d^3}{r_w^3 - r_d^3(1-\kappa)} \exp\left(\frac{A}{r_w}\right) \approx 1 + \frac{A}{r_{\text{w}}} - \frac{\kappa r_{\text{d}}^3}{r_{\text{w}}^3}$$



droplet growth laws in a nutshell: Köhler curve

$$\dot{r}_\mathrm{w} = \frac{1}{r_\mathrm{w}} D_\mathrm{eff} \frac{\rho_\mathrm{vs}}{\rho_\mathrm{w}} \left(\mathrm{RH} - \mathrm{RH}_\mathrm{eq}\right)$$

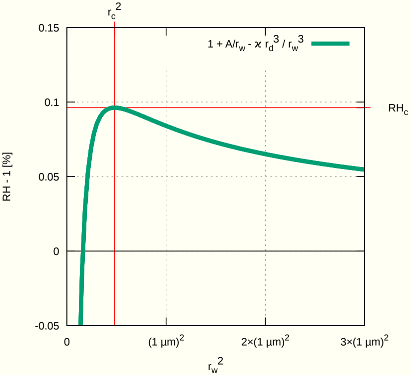
$$\mathrm{RH}_\mathrm{eq} = \frac{r_w^3 - r_d^3}{r_w^3 - r_d^3(1-\kappa)} \exp\left(\frac{A}{r_w}\right) \approx 1 + \frac{A}{r_\mathrm{w}} - \frac{\kappa r_\mathrm{d}^3}{r_\mathrm{w}^3}$$



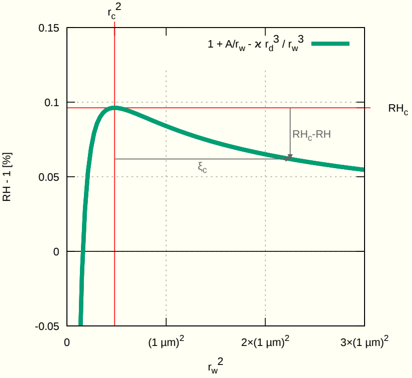
maximum at $(r_\mathrm{c}, \mathrm{RH}_\mathrm{c})$:

$$r_\mathrm{c} = \sqrt{3\kappa r_\mathrm{d}^3/A}$$
$$\mathrm{RH}_\mathrm{c} = 1 + \tfrac{2A}{3r_\mathrm{c}}$$

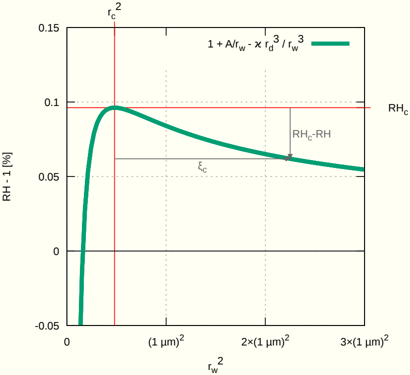
phase portrait of the system: flipped Köhler curve



phase portrait of the system: flipped Köhler curve



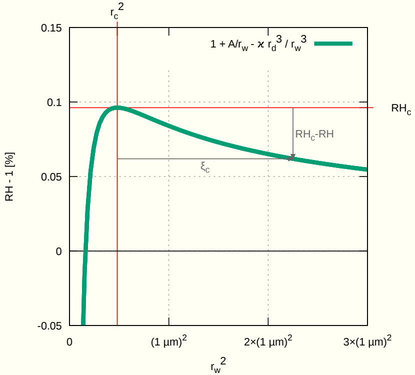
phase portrait of the system: flipped Köhler curve



$$\xi = r_{\mathsf{w}}^2 + C$$

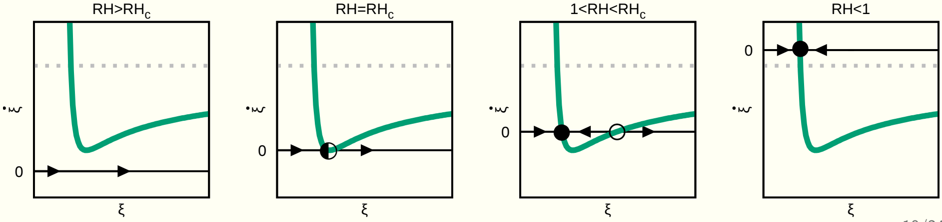
$$\dot{\xi} = 2D_{\mathsf{eff}}\frac{\rho_{\mathsf{vs}}}{\rho_{\mathsf{w}}}\left(\mathsf{RH} - \mathsf{RH}_{\mathsf{eq}}(\xi)\right)$$

phase portrait of the system: flipped Köhler curve



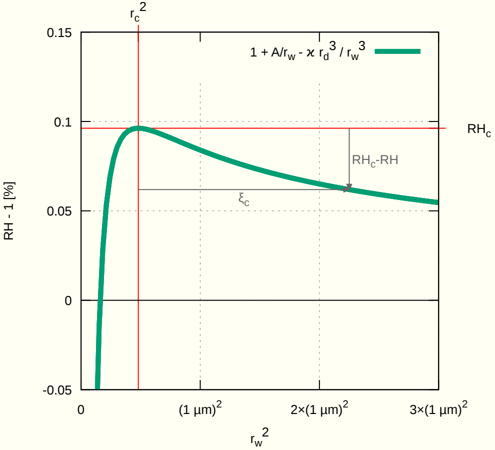
$$\xi = r_\mathrm{w}^2 + C$$

$$\dot{\xi} = 2D_\mathrm{eff}\frac{\rho_\mathrm{vs}}{\rho_\mathrm{w}}\left(\mathrm{RH} - \mathrm{RH}_\mathrm{eq}(\xi)\right)$$



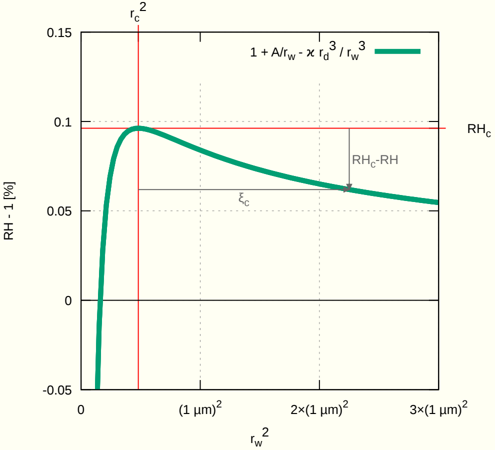
saddle-node bifurcation at Köhler curve maximum

saddle-node bifurcation at Köhler curve maximum



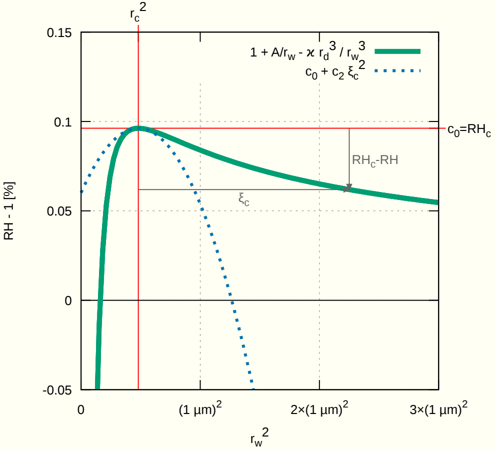
saddle-node bifurcation at Köhler curve maximum

$$\mathrm{RH_{eq}}(\xi_c) = c_0 + \cancel{c_1\xi_c} + c_2\xi_c^2 + \ldots$$



saddle-node bifurcation at Köhler curve maximum

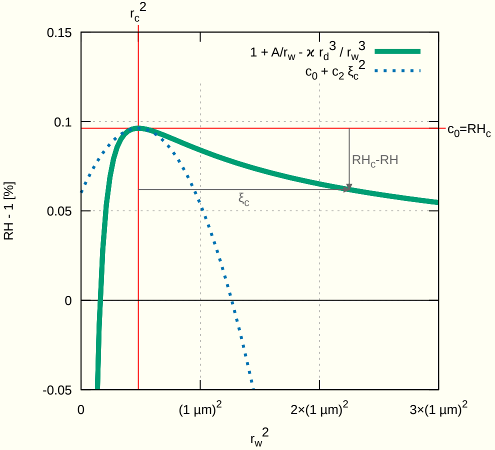
$$\mathrm{RH_{eq}}(\xi_c) = c_0 + \cancel{c_1 \xi_c} + c_2 \xi_c^2 + \ldots$$



saddle-node bifurcation at Köhler curve maximum

$$\mathrm{RH_{eq}}(\xi_c) = c_0 + \cancel{c_1 \xi_c} + c_2 \xi_c^2 + \ldots$$

$$\dot{\xi}_c \Big|_{\xi_c \to 0} \sim \frac{\mathrm{RH} - \mathrm{RH_c}}{A/(4 r_c^5)} + \xi_c^2$$

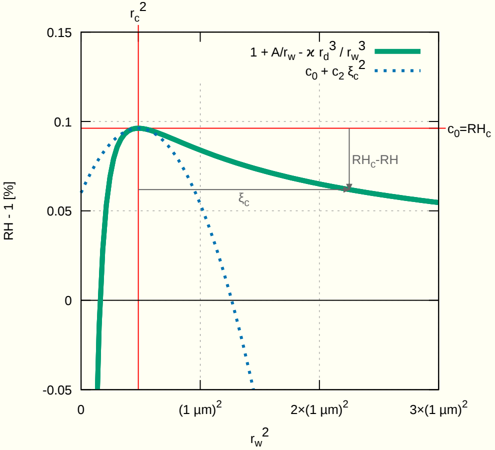


saddle-node bifurcation at Köhler curve maximum

$$\mathrm{RH}_{\mathrm{eq}}(\xi_\mathrm{c}) = c_0 + \cancel{c_1 \xi_\mathrm{c}} + c_2 \xi_\mathrm{c}^2 + \dots$$

$$\dot{\xi}_\mathrm{c}\Big|_{\xi_\mathrm{c}\to 0} \sim \frac{\mathrm{RH} - \mathrm{RH}_\mathrm{c}}{A/(4 r_\mathrm{c}^5)} + \xi_\mathrm{c}^2$$

$$\dot{x} = r + x^2$$



coalescence in the saddle-node bottleneck

coalescence in the saddle-node bottleneck

coalescence of the fixed points is associated with a passage through a *bottleneck* (e.g., Strogatz 2014),

key observation: time of passage through the parabolic *bottleneck* dominates all other timescales

coalescence in the saddle-node bottleneck

coalescence of the fixed points is associated with a passage through a *bottleneck* (e.g., Strogatz 2014),

key observation: time of passage through the parabolic *bottleneck* dominates all other timescales

coalescence in the saddle-node bottleneck

coalescence of the fixed points is associated with a passage through a *bottleneck* (e.g., Strogatz 2014),

key observation: time of passage through the parabolic *bottleneck* dominates all other timescales

$$\tau_{act} \approx \int_{-\infty}^{+\infty} \frac{d\xi_c}{\dot{\xi}_c}$$

coalescence in the saddle-node bottleneck

coalescence of the fixed points is associated with a passage through a *bottleneck* (e.g., Strogatz 2014),

key observation: time of passage through the parabolic *bottleneck* dominates all other timescales

$$\tau_{act} \approx \int_{-\infty}^{+\infty} \frac{d\xi_c}{\dot{\xi}_c}$$

$$= \frac{r_c^{5/2}}{\sqrt{A}} \frac{\rho_w/\rho_{vs}}{D_{eff}} \frac{\pi}{\sqrt{RH - RH_c}}$$

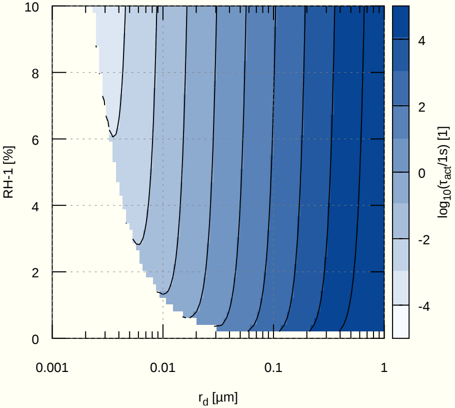
coalescence in the saddle-node bottleneck

coalescence of the fixed points is associated with a passage through a *bottleneck* (e.g., Strogatz 2014),

key observation: time of passage through the parabolic *bottleneck* dominates all other timescales

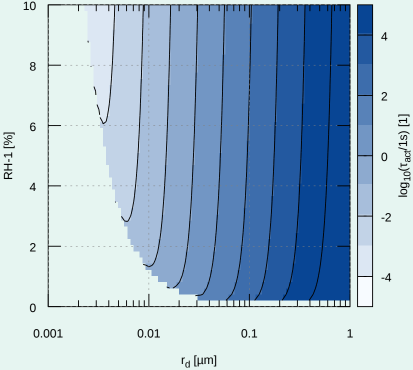
$$\tau_{act} \approx \int_{-\infty}^{+\infty} \frac{d\xi_c}{\dot{\xi}_c}$$

$$= \frac{r_c^{5/2}}{\sqrt{A}} \frac{\rho_w/\rho_{vs}}{D_{eff}} \frac{\pi}{\sqrt{RH - RH_c}}$$



activation timescale: analytic vs. numerical

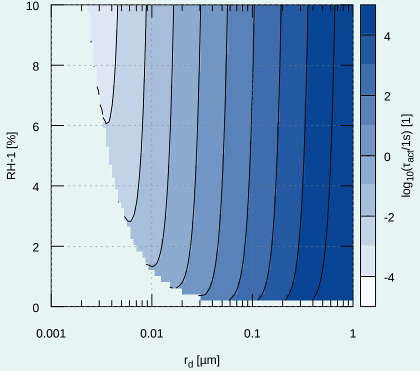
Arabas & Shima 2017



note: axes ranges vs. close-to-equilibrium assumption

activation timescale: analytic vs. numerical

Arabas & Shima 2017



note: axes ranges vs. close-to-equilibrium assumption

Hoffmann, 2016 (MWR)

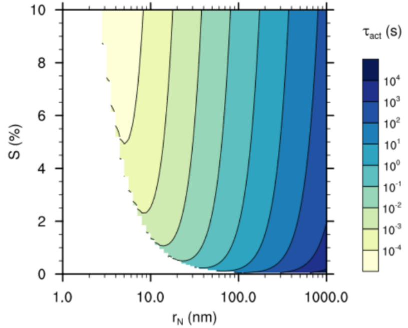


FIG. 2. The activation time scale τ_{act} as a function of dry aerosol radius r_N and supersaturation S. For values of $S < S_{crit}$ (white areas), τ_{act} does not exist.

$$r\frac{dr}{dt} = \left(S - \frac{A}{r} + \frac{Br_N^3}{r^3}\right) \Big/ (F_k + F_D), \qquad (10)$$

The second time scale is associated with the activation of particles, for which Köhler theory is essential. This makes an analytic solution for (10) impossible. Numerically calculated values of τ_{act} measuring the time needed for a wetted aerosol to grow beyond its critical radius $r_{crit} = \sqrt{3Br_N^3/A}$ are given in Fig. 2 as a function of

RH-coupled system & particle concentration as parameter

RH-coupled system & particle concentration as parameter

simple moisture budget (const T,p):

$$\dot{\mathrm{RH}} \approx \frac{\dot{\rho}_\mathrm{v}}{\rho_\mathrm{vs}} = -N \underbrace{\frac{4\pi\rho_\mathrm{w}}{3\rho_\mathrm{vs}}}_{\alpha} 3 r_\mathrm{w}^2 \dot{r}_\mathrm{w}$$

RH-coupled system & particle concentration as parameter

simple moisture budget (const T,p):

$$\dot{\mathrm{RH}} \approx \frac{\dot{\rho}_{\mathrm{v}}}{\rho_{\mathrm{vs}}} = -N \underbrace{\frac{4\pi\rho_{\mathrm{w}}}{3\rho_{\mathrm{vs}}}}_{\alpha} 3r_{\mathrm{w}}^2\dot{r}_{\mathrm{w}}$$

integrating in time:

$$\mathrm{RH} = \mathrm{RH}_0 - \alpha N r_{\mathrm{w}}^3$$

RH-coupled system & particle concentration as parameter

simple moisture budget (const T,p):

$$\dot{\mathrm{RH}} \approx \frac{\dot{\rho}_{\mathrm{v}}}{\rho_{\mathrm{vs}}} = -N \underbrace{\frac{4\pi\rho_{\mathrm{w}}}{3\rho_{\mathrm{vs}}}}_{\alpha} 3r_{\mathrm{w}}^2 \dot{r}_{\mathrm{w}}$$

integrating in time:

$$\mathrm{RH} = \mathrm{RH}_0 - \alpha N r_{\mathrm{w}}^3$$

new phase portrait:

$$\dot{\xi} \sim (\mathrm{RH}_0 - 1) - \underbrace{\left(\frac{A}{\xi^{\frac{1}{2}}} - \frac{\kappa r_{\mathrm{d}}^3}{\xi^{\frac{3}{2}}} + \alpha N \xi^{\frac{3}{2}} \right)}_{f}$$

RH-coupled system & particle concentration as parameter

simple moisture budget (const T,p):

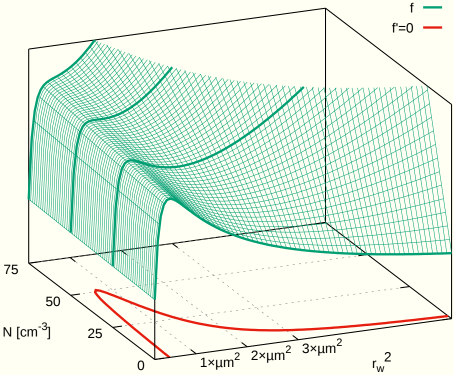
$$\dot{\mathrm{RH}} \approx \frac{\dot{\rho}_\mathrm{v}}{\rho_\mathrm{vs}} = -N \underbrace{\frac{4\pi\rho_\mathrm{w}}{3\rho_\mathrm{vs}}}_{\alpha} 3r_\mathrm{w}^2 \dot{r}_\mathrm{w}$$

integrating in time:

$$\mathrm{RH} = \mathrm{RH}_0 - \alpha N r_\mathrm{w}^3$$

new phase portrait:

$$\dot{\xi} \sim (\mathrm{RH}_0 - 1) - \underbrace{\left(\frac{A}{\xi^{\frac{1}{2}}} - \frac{\kappa r_\mathrm{d}^3}{\xi^{\frac{3}{2}}} + \alpha N \xi^{\frac{3}{2}} \right)}_{f}$$



RH-coupled system & particle concentration as parameter

simple moisture budget (const T,p):

$$\dot{\mathrm{RH}} \approx \frac{\dot{\rho}_\mathrm{v}}{\rho_\mathrm{vs}} = -N \underbrace{\frac{4\pi\rho_\mathrm{w}}{3\rho_\mathrm{vs}}}_{\alpha} 3r_\mathrm{w}^2 \dot{r}_\mathrm{w}$$

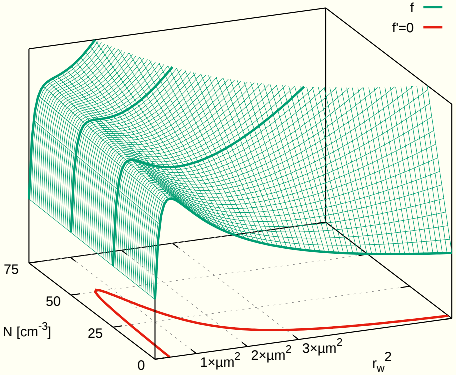
integrating in time:

$$\mathrm{RH} = \mathrm{RH}_0 - \alpha N r_\mathrm{w}^3$$

new phase portrait:

$$\dot{\xi} \sim (\mathrm{RH}_0 - 1) - \underbrace{\left(\frac{A}{\xi^{\frac{1}{2}}} - \frac{\kappa r_\mathrm{d}^3}{\xi^{\frac{3}{2}}} + \alpha N \xi^{\frac{3}{2}}\right)}_{f}$$

regime-controlling params: RH, N



RH-coupled system & particle concentration as parameter

simple moisture budget (const T,p):

$$\dot{\mathrm{RH}} \approx \frac{\dot{\rho}_\mathrm{v}}{\rho_\mathrm{vs}} = -N \underbrace{\frac{4\pi\rho_\mathrm{w}}{3\rho_\mathrm{vs}}}_{\alpha} 3r_\mathrm{w}^2\dot{r}_\mathrm{w}$$

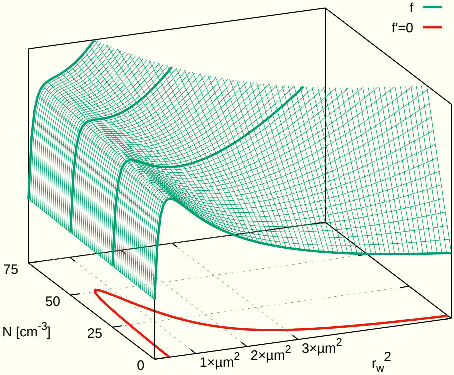
integrating in time:

$$\mathrm{RH} = \mathrm{RH}_0 - \alpha N r_\mathrm{w}^3$$

new phase portrait:

$$\dot{\xi} \sim (\mathrm{RH}_0 - 1) - \underbrace{\left(\frac{A}{\xi^{\frac{1}{2}}} - \frac{\kappa r_\mathrm{d}^3}{\xi^{\frac{3}{2}}} + \alpha N \xi^{\frac{3}{2}}\right)}_{f}$$

regime-controlling params: RH, N



$$\mathrm{sgn}(f') = \mathrm{sgn}\left(\kappa r_d^3 - \frac{A}{3} r_w + \alpha N r_w^3\right)$$

bifurcations (and catastrophe) in the RH-coupled system

Prigogine & Stengers 1984

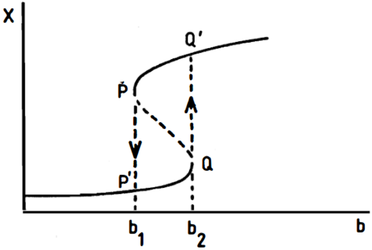


Figure 15. This figure shows how a "hysteresis" phenomenon occurs if we have the value of the bifurcation parameter *b* first growing and then diminishing. If the system is initially in a stationary state belonging to the lower branch, it will stay there while *b* grows. But at $b = b_2$, there will be a discontinuity: The system jumps from *Q* to *Q′*, on the higher branch. Inversely, starting from a state on the higher branch, the system will remain there till $b = b_1$, when it will jump down to *P′*. Such types of bistable behavior are observed in many fields, such as lasers, chemical reactions or biological membranes.

bifurcations (and catastrophe) in the RH-coupled system

Prigogine & Stengers 1984

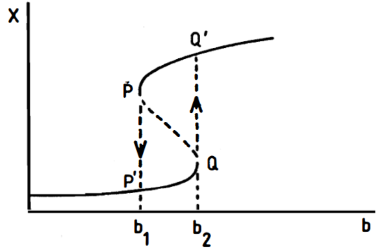
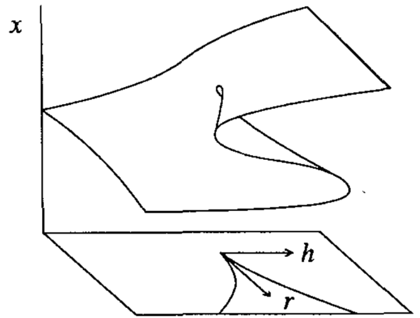


Figure 15. This figure shows how a "hysteresis" phenomenon occurs if we have the value of the bifurcation parameter *b* first growing and then diminishing. If the system is initially in a stationary state belonging to the lower branch, it will stay there while *b* grows. But at $b = b_2$, there will be a discontinuity: The system jumps from *Q* to *Q'*, on the higher branch. Inversely, starting from a state on the higher branch, the system will remain there till $b = b_1$, when it will jump down to *P'*. Such types of bistable behavior are observed in many fields, such as lasers, chemical reactions or biological membranes.

Strogatz 2014



"cusp catastrophe"

bifurcations (and catastrophe) in the RH-coupled system

Prigogine & Stengers 1984

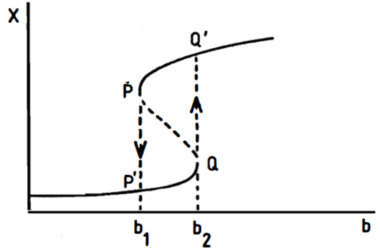
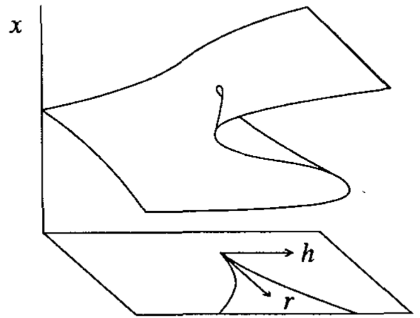


Figure 15. This figure shows how a "hysteresis" phenomenon occurs if we have the value of the bifurcation parameter b first growing and then diminishing. If the system is initially in a stationary state belonging to the lower branch, it will stay there while b grows. But at $b = b_2$, there will be a discontinuity: The system jumps from Q to Q', on the higher branch. Inversely, starting from a state on the higher branch, the system will remain there till $b = b_1$, when it will jump down to P'. Such types of bistable behavior are observed in many fields, such as lasers, chemical reactions or biological membranes.

Strogatz 2014



"cusp catastrophe"

$\rightsquigarrow$ "jumps", hysteretic behaviour (r_w, RH) for small enough N, close to equilibrium (slow process)

hysteresis: activation/deactivation cycle

hysteresis: activation/deactivation cycle

- nomenclature:

- nomenclature:
  - CCN activation
  - (heterogeneous) nucleation

hysteresis: activation/deactivation cycle

- nomenclature:
  - CCN activation
  - (heterogeneous) nucleation

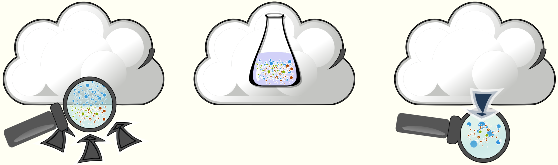
  - CCN deactivation
  - aerosol regeneration / resuspension / recycling
  - drop-to-particle conversion
  - droplet evaporation

hysteresis: activation/deactivation cycle

- nomenclature:
  - CCN activation
  - (heterogeneous) nucleation

  - CCN deactivation
  - aerosol regeneration / resuspension / recycling
  - drop-to-particle conversion
  - droplet evaporation
- significance:

hysteresis: activation/deactivation cycle



- nomenclature:
  - CCN activation
  - (heterogeneous) nucleation

  - CCN deactivation
  - aerosol regeneration / resuspension / recycling
  - drop-to-particle conversion
  - droplet evaporation
- significance:
  - aerosol processing by clouds (aqueous chemistry, coalescence)

lifting the constant T-p assumptions: parcel model

lifting the constant T-p assumptions: parcel model

vertically displaced (velocity w, hydrostatic background) adiabatic parcel:
(q: mixing ratio, p_d: bgnd pressure, ρ_d bgnd density, g,l_v,c_pd: constants)

$$\begin{bmatrix} \dot{p}_d \\ \dot{T} \\ \dot{r}_w \end{bmatrix} = \begin{bmatrix} -\rho_\mathrm{d} g w \\ (\dot{p}_\mathrm{d}/\rho_\mathrm{d} - \dot{q} l_\mathrm{v})/c_\mathrm{pd} \\ (D_\mathrm{eff}/\rho_\mathrm{w})(\rho_\mathrm{v} - \rho_\circ)/r_\mathrm{w} \end{bmatrix}$$

lifting the constant T-p assumptions: parcel model

vertically displaced (velocity w, hydrostatic background) adiabatic parcel:
(q: mixing ratio, p_d: bgnd pressure, ρ_d bgnd density, g,l_v,c_pd: constants)

$$\begin{bmatrix} \dot{p}_d \\ \dot{T} \\ \dot{r}_w \end{bmatrix} = \begin{bmatrix} -\rho_\mathrm{d} g w \\ (\dot{p}_\mathrm{d}/\rho_\mathrm{d} - \dot{q} l_\mathrm{v})/c_\mathrm{pd} \\ (D_\mathrm{eff}/\rho_\mathrm{w})(\rho_\mathrm{v} - \rho_\circ)/r_\mathrm{w} \end{bmatrix}$$

- $w \rightarrow 0$ (and hence $\dot{p}_\mathrm{d} \approx 0$) i.e., slow, close-to-equilibrium evolution of the system relevant to fixed-point analysis (by some means pertinent to formation of non-convective clouds such as fog)

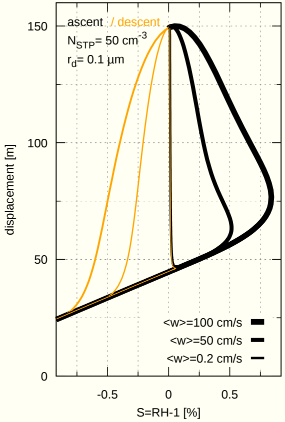
lifting the constant T-p assumptions: parcel model

vertically displaced (velocity w, hydrostatic background) adiabatic parcel:
(q: mixing ratio, p_d: bgnd pressure, ρ_d bgnd density, g,l_v,c_pd: constants)

$$\begin{bmatrix} \dot{p}_d \\ \dot{T} \\ \dot{r}_w \end{bmatrix} = \begin{bmatrix} -\rho_\mathrm{d} g w \\ (\dot{p}_\mathrm{d}/\rho_\mathrm{d} - \dot{q} l_\mathrm{v})/c_\mathrm{pd} \\ (D_\mathrm{eff}/\rho_\mathrm{w})(\rho_\mathrm{v} - \rho_\circ)/r_\mathrm{w} \end{bmatrix}$$

- $w \rightarrow 0$ (and hence $\dot{p}_\mathrm{d} \approx 0$) i.e., slow, close-to-equilibrium evolution of the system relevant to fixed-point analysis (by some means pertinent to formation of non-convective clouds such as fog)
- $N \rightarrow 0$ (and hence $\dot{q} \approx 0$) i.e., weak coupling between particle size evolution and ambient thermodynamics (pertinent to the case of low particle concentration).

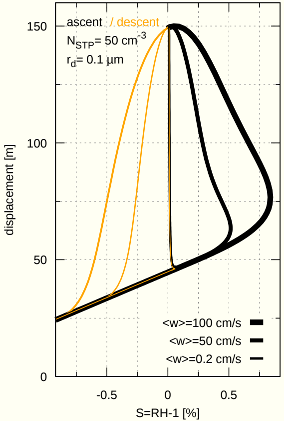
parcel model: numerical integration (sinusoidal w)

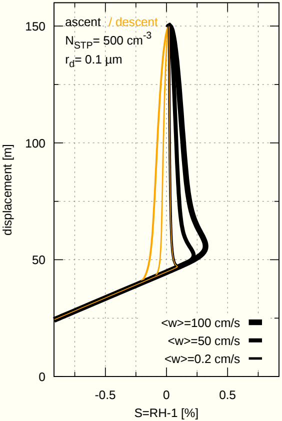


integration using CVODE adaptive solver

open source code (based on libcloudph++) as electronic paper supplement

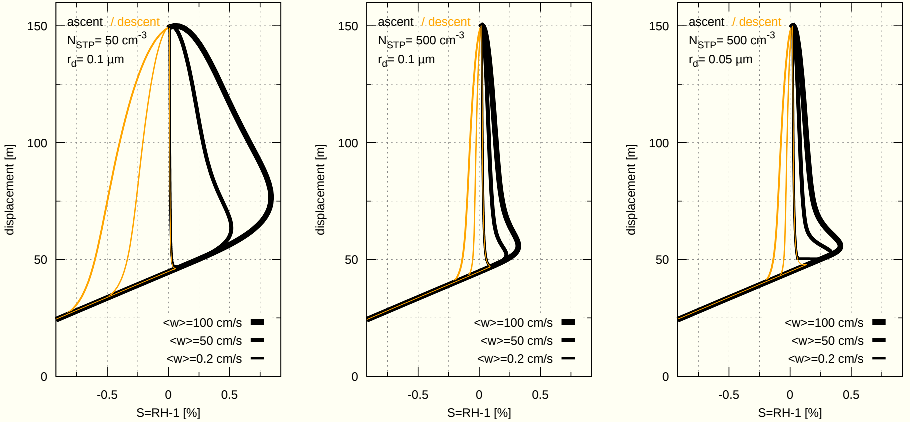
parcel model: numerical integration (sinusoidal w)





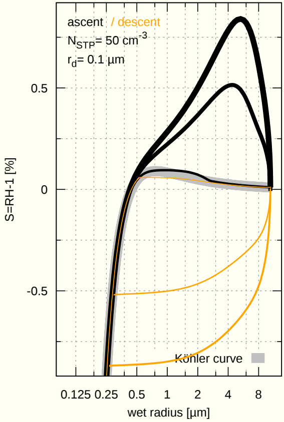
integration using CVODE adaptive solver
open source code (based on libcloudph++) as electronic paper supplement

parcel model: numerical integration (sinusoidal w)



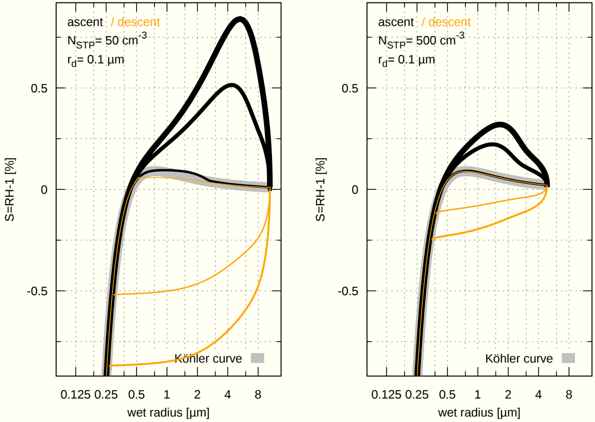
integration using CVODE adaptive solver
open source code (based on libcloudph++) as electronic paper supplement

parcel model: numerical integration (sinusoidal w)



integration using CVODE adaptive solver
open source code (based on libcloudph++) as electronic paper supplement

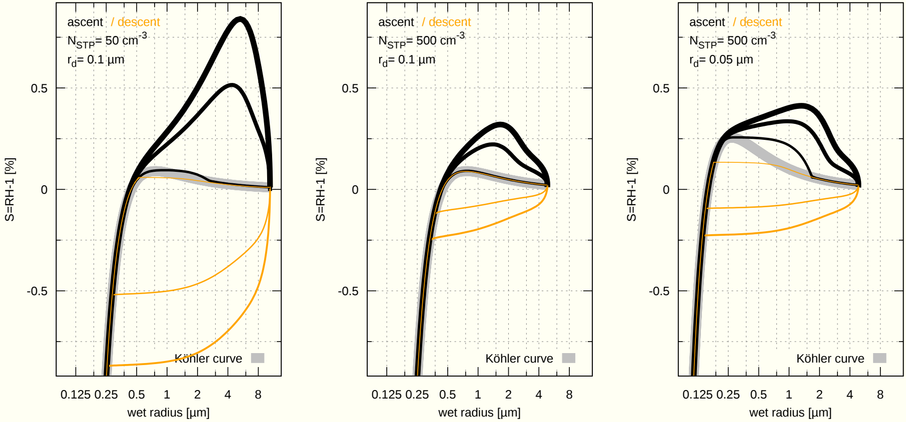
parcel model: numerical integration (sinusoidal w)



integration using CVODE adaptive solver

open source code (based on libcloudph++) as electronic paper supplement

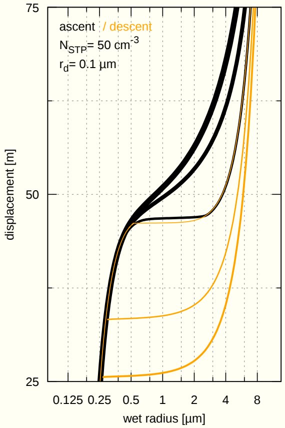
parcel model: numerical integration (sinusoidal w)



integration using CVODE adaptive solver

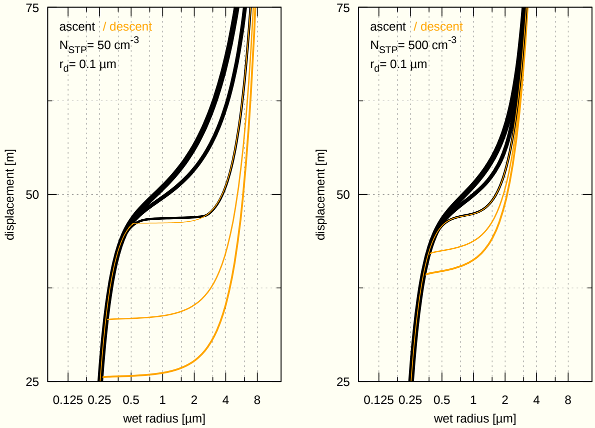
open source code (based on libcloudph++) as electronic paper supplement

parcel model: numerical integration (sinusoidal w)



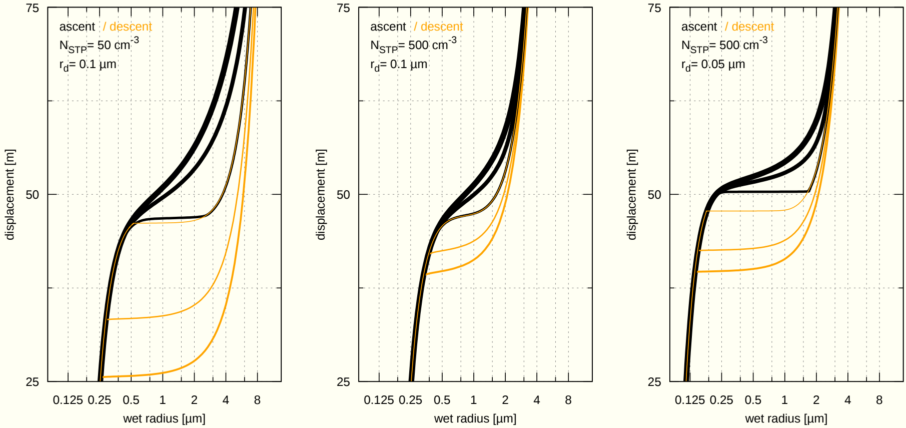
integration using CVODE adaptive solver
open source code (based on libcloudph++) as electronic paper supplement

parcel model: numerical integration (sinusoidal w)



integration using CVODE adaptive solver
open source code (based on libcloudph++) as electronic paper supplement

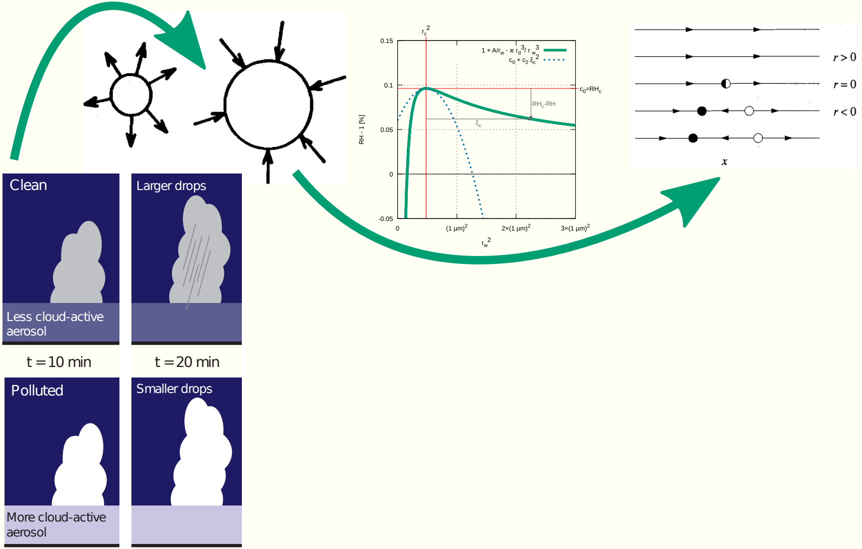
parcel model: numerical integration (sinusoidal w)



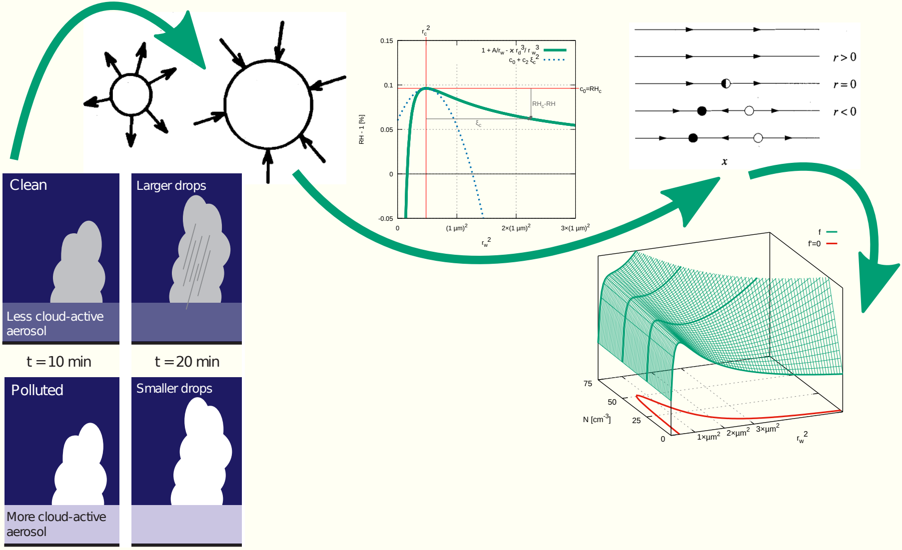
integration using CVODE adaptive solver
open source code (based on libcloudph++) as electronic paper supplement

connecting the dots ...

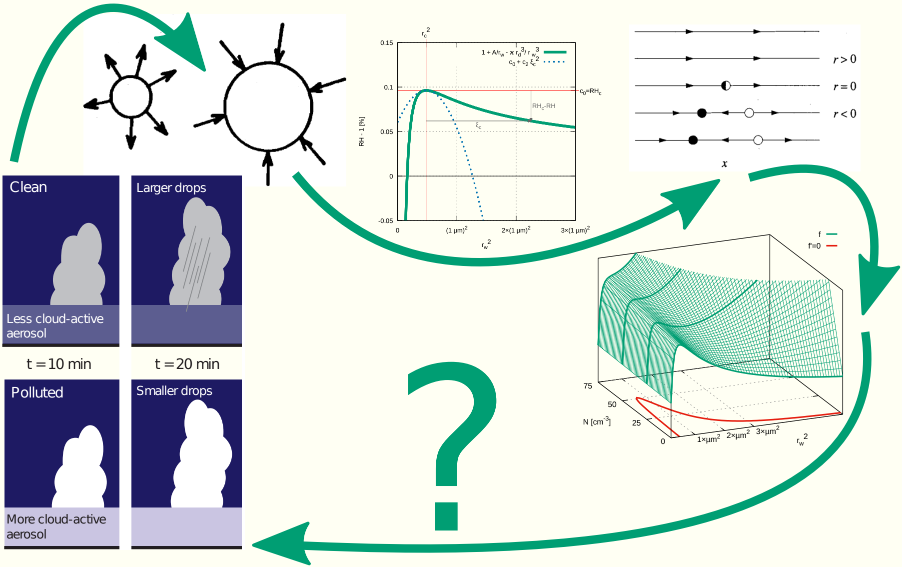
connecting the dots ...



connecting the dots ...



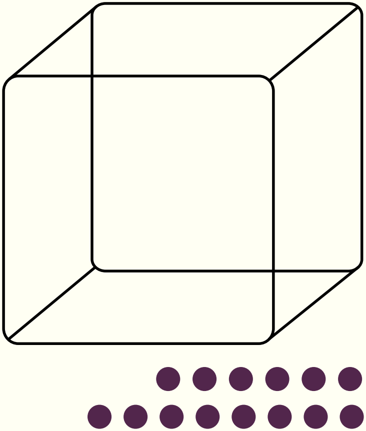
connecting the dots ...



particle-based μ-physics for LES

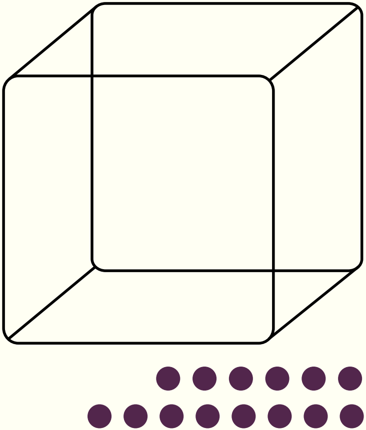
- “information carriers” in LES domain

particle-based μ-physics for LES



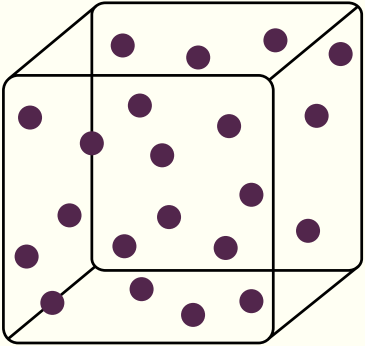
- “information carriers” in LES domain
- ab-initio approach:
  particle=aerosol/cloud/rain

particle-based μ-physics for LES



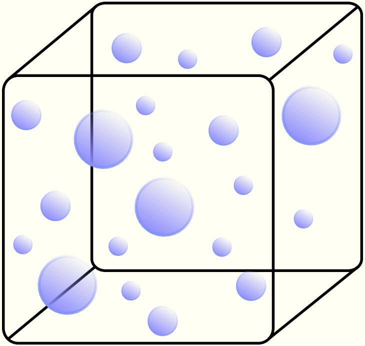
- "information carriers" in LES domain
- ab-initio approach:
  particle=aerosol/cloud/rain
- attributes:

particle-based μ-physics for LES



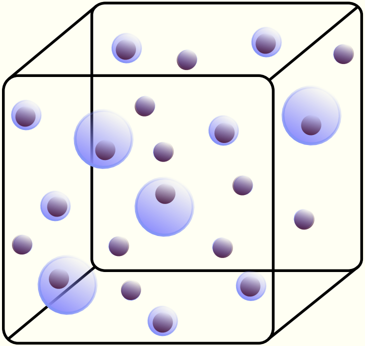
- "information carriers" in LES domain
- ab-initio approach:
  particle=aerosol/cloud/rain
- attributes:
  - spatial coordinates

particle-based μ-physics for LES



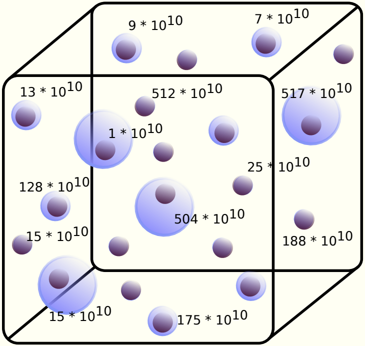
- "information carriers" in LES domain
- ab-initio approach:
  particle=aerosol/cloud/rain
- attributes:
  - spatial coordinates
  - wet radius

particle-based μ-physics for LES



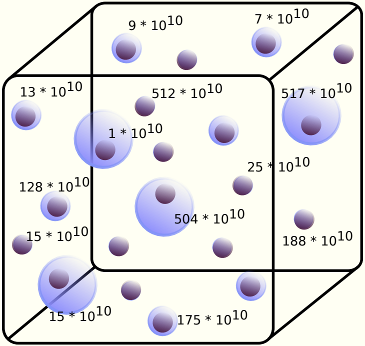
- "information carriers" in LES domain
- ab-initio approach:
  particle=aerosol/cloud/rain
- attributes:
  - spatial coordinates
  - wet radius
  - dry radius

particle-based μ-physics for LES



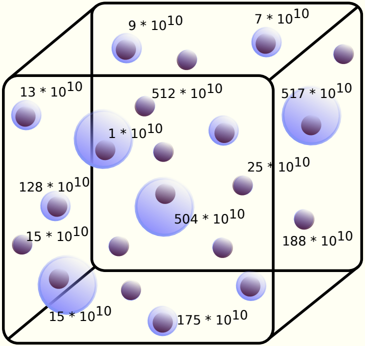
- "information carriers" in LES domain
- ab-initio approach:
  particle=aerosol/cloud/rain
- attributes:
  - spatial coordinates
  - wet radius
  - dry radius
  - multiplicity

particle-based μ-physics for LES



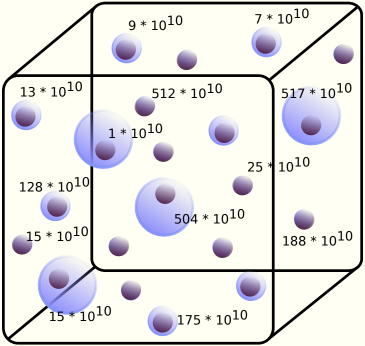
- "information carriers" in LES domain
- ab-initio approach:
  particle=aerosol/cloud/rain
- attributes:
  - spatial coordinates
  - wet radius
  - dry radius
  - multiplicity
  - ...

particle-based μ-physics for LES



- "information carriers" in LES domain
- ab-initio approach:
  particle=aerosol/cloud/rain
- attributes:
  - spatial coordinates
  - wet radius
  - dry radius
  - multiplicity
  - ...
- scalability in no. of attributes
  (aqueous chemistry!)

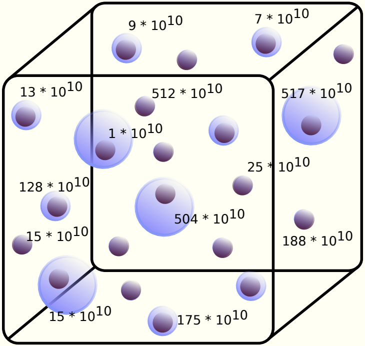
particle-based μ-physics for LES



- "information carriers" in LES domain
- ab-initio approach:
  particle=aerosol/cloud/rain
- attributes:
  - spatial coordinates
  - wet radius
  - dry radius
  - multiplicity
  - ...
- scalability in no. of attributes (aqueous chemistry!)

- each particle: **monodisperse**!

particle-based μ-physics for LES



- "information carriers" in LES domain
- ab-initio approach:
  particle=aerosol/cloud/rain
- attributes:
  - spatial coordinates
  - wet radius
  - dry radius
  - multiplicity
  - ...
- scalability in no. of attributes (aqueous chemistry!)

- each particle: **monodisperse**!
- each timestep: **constant RH**!

Seminal works: Shima et al. 2009, Andrejczuk et al. 2010
(3D simulations of atmospheric aerosol-cloud-precipitation system)

1
2
3
4
5
6
7

particle-based μ-physics for LES

Seminal works: Shima et al. 2009, Andrejczuk et al. 2010
(3D simulations of atmospheric aerosol-cloud-precipitation system)

recent research software (re)developments:

1
2
3
4
5
6
7

particle-based μ-physics for LES

Seminal works: Shima et al. 2009, Andrejczuk et al. 2010
(3D simulations of atmospheric aerosol-cloud-precipitation system)

recent research software (re)developments:

- EULAG-LCM[1] from NCAR/DLR (Soelch and Kaercher 2010),

[1] http://www.mmm.ucar.edu/eulag/
2
3
4
5
6
7

particle-based μ-physics for LES

Seminal works: Shima et al. 2009, Andrejczuk et al. 2010
(3D simulations of atmospheric aerosol-cloud-precipitation system)

recent research software (re)developments:

- EULAG-LCM[1] from NCAR/DLR (Soelch and Kaercher 2010),
- PALM-LES[2] from Univ. Hannover (Riechelmann et al. 2012),

[1] http://www.mmm.ucar.edu/eulag/
[2] http://palm.muk.uni-hannover.de/
3
4
5
6
7

particle-based μ-physics for LES

Seminal works: Shima et al. 2009, Andrejczuk et al. 2010
(3D simulations of atmospheric aerosol-cloud-precipitation system)

recent research software (re)developments:

- EULAG-LCM[1] from NCAR/DLR (Soelch and Kaercher 2010),
- PALM-LES[2] from Univ. Hannover (Riechelmann et al. 2012),
- CReSS[3] from Univ. Nagoya (Arabas and Shima 2013),

[1] http://www.mmm.ucar.edu/eulag/
[2] http://palm.muk.uni-hannover.de/
[3] http://www.rain.hyarc.nagoya-u.ac.jp/
4
5
6
7

particle-based μ-physics for LES

Seminal works: Shima et al. 2009, Andrejczuk et al. 2010
(3D simulations of atmospheric aerosol-cloud-precipitation system)

recent research software (re)developments:

- EULAG-LCM[1] from NCAR/DLR (Soelch and Kaercher 2010),
- PALM-LES[2] from Univ. Hannover (Riechelmann et al. 2012),
- CReSS[3] from Univ. Nagoya (Arabas and Shima 2013),
- UCLA-LES[4] from UCLA/Max-Planck (Naumann and Seifert 2015),

[1] http://www.mmm.ucar.edu/eulag/
[2] http://palm.muk.uni-hannover.de/
[3] http://www.rain.hyarc.nagoya-u.ac.jp/
[4] http://github.com/uclales
5
6
7

particle-based μ-physics for LES

Seminal works: Shima et al. 2009, Andrejczuk et al. 2010
(3D simulations of atmospheric aerosol-cloud-precipitation system)

recent research software (re)developments:

- EULAG-LCM[1] from NCAR/DLR (Soelch and Kaercher 2010),
- PALM-LES[2] from Univ. Hannover (Riechelmann et al. 2012),
- CReSS[3] from Univ. Nagoya (Arabas and Shima 2013),
- UCLA-LES[4] from UCLA/Max-Planck (Naumann and Seifert 2015),
- Pencil-Code[5] from Nordita (Li et al. 2017),

[1] http://www.mmm.ucar.edu/eulag/
[2] http://palm.muk.uni-hannover.de/
[3] http://www.rain.hyarc.nagoya-u.ac.jp/
[4] http://github.com/uclales
[5] http://pencil-code.nordita.org
6
7

particle-based μ-physics for LES

Seminal works: Shima et al. 2009, Andrejczuk et al. 2010
(3D simulations of atmospheric aerosol-cloud-precipitation system)

recent research software (re)developments:

- EULAG-LCM[1] from NCAR/DLR (Soelch and Kaercher 2010),
- PALM-LES[2] from Univ. Hannover (Riechelmann et al. 2012),
- CReSS[3] from Univ. Nagoya (Arabas and Shima 2013),
- UCLA-LES[4] from UCLA/Max-Planck (Naumann and Seifert 2015),
- Pencil-Code[5] from Nordita (Li et al. 2017),
- SCALE[6] from RIKEN (Sato et al. 2017),

---

[1] http://www.mmm.ucar.edu/eulag/
[2] http://palm.muk.uni-hannover.de/
[3] http://www.rain.hyarc.nagoya-u.ac.jp/
[4] http://github.com/uclales
[5] http://pencil-code.nordita.org
[6] http://scale.aics.riken.jp/
[7]

particle-based μ-physics for LES

Seminal works: Shima et al. 2009, Andrejczuk et al. 2010
(3D simulations of atmospheric aerosol-cloud-precipitation system)

recent research software (re)developments:

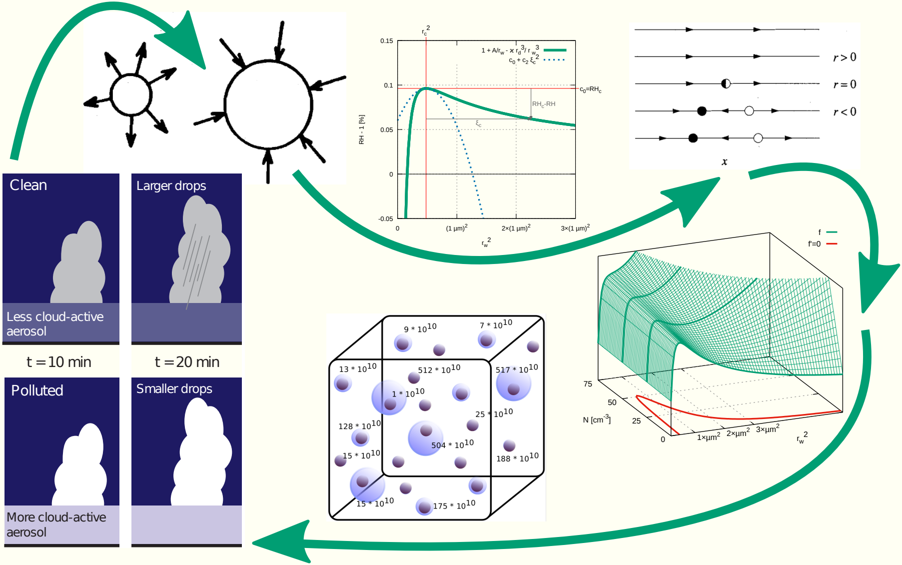
- EULAG-LCM[1] from NCAR/DLR (Soelch and Kaercher 2010),
- PALM-LES[2] from Univ. Hannover (Riechelmann et al. 2012),
- CReSS[3] from Univ. Nagoya (Arabas and Shima 2013),
- UCLA-LES[4] from UCLA/Max-Planck (Naumann and Seifert 2015),
- Pencil-Code[5] from Nordita (Li et al. 2017),
- SCALE[6] from RIKEN (Sato et al. 2017),
- UWLCM[7] from Univ. Warsaw (Grabowski et al. 2018).

---

[1] http://www.mmm.ucar.edu/eulag/
[2] http://palm.muk.uni-hannover.de/
[3] http://www.rain.hyarc.nagoya-u.ac.jp/
[4] http://github.com/uclales
[5] http://pencil-code.nordita.org
[6] http://scale.aics.riken.jp/
[7] http://github.com/igfuw/UWLCM

connecting the dots ...

connecting the dots ...



conclusions, takeaways, prospects

conclusions, takeaways, prospects

- aerosol-cloud interactions:
  – formation of droplets on aerosol,
  – cloud processing of aerosol,
  – wet deposition

conclusions, takeaways, prospects

- aerosol-cloud interactions:
  – formation of droplets on aerosol,
  – cloud processing of aerosol,
  – wet deposition

- CCN (de)activation as a bifurcating dynamical system:
  – analytical results: conditions for hysteretic behaviour, timescales
  – guidance for numerical scheme design (particle-based μ-physics)

conclusions, takeaways, prospects

- aerosol-cloud interactions:
  – formation of droplets on aerosol,
  – cloud processing of aerosol,
  – wet deposition
- CCN (de)activation as a bifurcating dynamical system:
  – analytical results: conditions for hysteretic behaviour, timescales
  – guidance for numerical scheme design (particle-based μ-physics)
- applicability beyond cloud physics:
  – e.g., charge-induced activation ($\rightsquigarrow$ Wilson chamber),
  – modelling operation of air-pollution monitoring instruments

conclusions, takeaways, prospects

- aerosol-cloud interactions:
  – formation of droplets on aerosol,
  – cloud processing of aerosol,
  – wet deposition
- CCN (de)activation as a bifurcating dynamical system:
  – analytical results: conditions for hysteretic behaviour, timescales
  – guidance for numerical scheme design (particle-based μ-physics)
- applicability beyond cloud physics:
  – e.g., charge-induced activation ($\rightsquigarrow$ Wilson chamber),
  – modelling operation of air-pollution monitoring instruments
- extensions:
  – bi-/poly- modal/disperse spectra (spectrum width!),
  – activated/unactivated partitioning (excitable behaviour!),
  – beyond Köhler curve (charge, surfactants, non-soluble aerosol, ...)

Thank you for your attention!

https://doi.org/10.5194/npg-24-535-2017