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

Sylwester Arabas and Shin-ichiro Shima

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

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  - 2015–2017: Chatham Financial, Cracow (software developer)
  - 2017–2018: AETHON, Athens (H2020 "Innovation Associate")

#### Arabas & Shima 2017



#### On the CCN (de)activation nonlinearities

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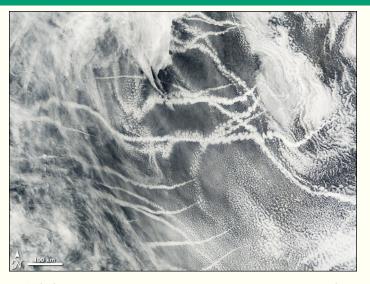




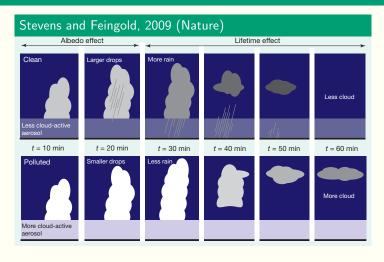


This movie was made onboard the ice breaker "Oden" during the ASCOS 2008 expedition to the Arctic. The high resolution version of the movie is available through Queensland University of Technology. Please email: z.ristovski@qut.edu.au

 $\label{eq:no_particles} \begin{picture}(0,0) \put(0,0){\line(0,0){100}} \put(0,0){\line(0,0){100}}$ 



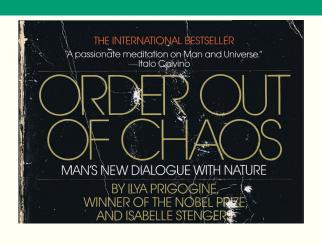
 ${\tt NASA~(https://earthobservatory.nasa.gov/Natural Hazards/view.php?id=20248)}$ 

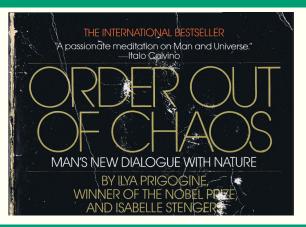




#### Stevens and Boucher, 2012 (Nature)

"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"





#### 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

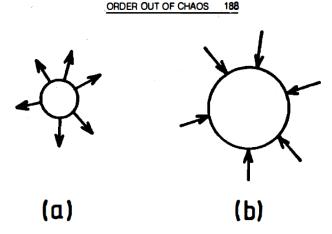
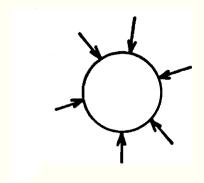
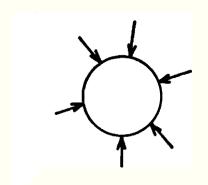
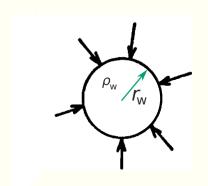


Figure 19. Nucleation of a liquid droplet in a supersaturated vapor. (a) droplet smaller than the critical size; (b) droplet larger than the critical size. The existence of the threshold has been experimentally verified for dissipative structures.

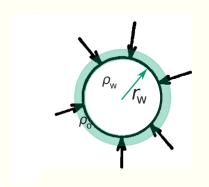




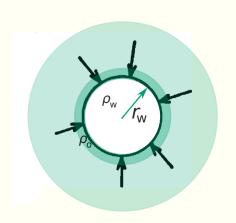
$$\dot{r}_{\mathsf{w}} = rac{1}{r_{\mathsf{w}}} rac{D_{\mathsf{eff}}}{
ho_{\mathsf{w}}} \left( 
ho_{\mathsf{v}} - 
ho_{\circ} 
ight)$$



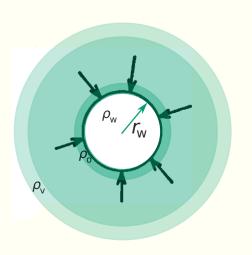
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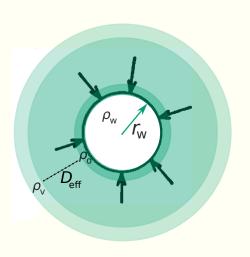
$$\dot{r}_{\mathsf{w}} = \frac{1}{r_{\mathsf{w}}} \frac{D_{\mathsf{eff}}}{\rho_{\mathsf{w}}} (\rho_{\mathsf{v}} - \rho_{\circ})$$



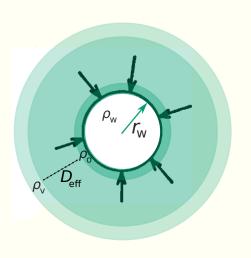
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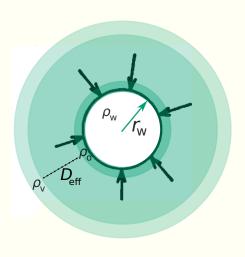


Fick's and Fourier's laws combined spherical geometry

$$\dot{r}_{\mathsf{w}} = rac{1}{r_{\mathsf{w}}} rac{D_{\mathsf{eff}}}{
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non-dimensional numbers:

$$\mathrm{RH} = 
ho_\mathrm{v}/
ho_\mathrm{vs}$$
  $\mathrm{RH}_\mathrm{eq} = 
ho_\mathrm{o}/
ho_\mathrm{vs}$ 



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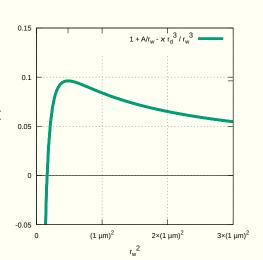
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$$\approx 1 + \frac{A}{r_{\rm w}} - \frac{\kappa r_{\rm d}^3}{r_{\rm w}^3}$$

$$\dot{r}_{w} = \frac{1}{r_{w}} D_{eff} \frac{\rho_{vs}}{\rho_{w}} \left( RH - RH_{eq} \right) \qquad RH_{eq} = \frac{r_{w}^{3} - r_{d}^{3}}{r_{w}^{3} - r_{d}^{3} (1 - \kappa)} \exp \left( \frac{A}{r_{w}} \right)$$

$$\approx 1 + \frac{A}{r_{w}} - \frac{\kappa r_{d}^{3}}{r_{w}^{3}}$$

$$= \frac{1 + \frac{A}{r_{w}} - \frac{\kappa r_{d}^{3}}{r_{w}^{3}}}{(1 - \kappa)} \exp \left( \frac{A}{r_{w}} \right)$$

$$= \frac{1}{r_{w}} \int_{0.15}^{r_{w}} \frac{A}{r_{w}} \left( \frac{A}{r_{w}} \right) \left( \frac{A}{r_{w}} \right) \left( \frac{A}{r_{w}} \right)$$

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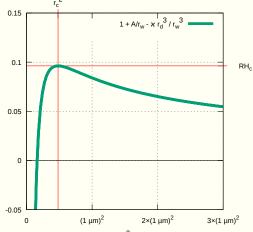
$$= \frac{1}{r_{w}} \int_{0.15}^{r_{w}} \frac{A}{r_{w}} \left( \frac{A}{r_{w}} \right) \left( \frac{A}{r_{w}}$$

RH - 1 [%]

 $\approx 1 + \frac{A}{r_w} - \frac{\kappa r_d^3}{r^3}$ 

$$\dot{r}_{w} = \frac{1}{r_{w}} D_{eff} \frac{\rho_{vs}}{\rho_{w}} \left( RH - RH_{eq} \right) \qquad RH_{eq} = \frac{r_{w}^{3} - r_{d}^{3}}{r_{w}^{3} - r_{d}^{3} (1 - \kappa)} \exp \left( \frac{A}{r_{w}} \right)$$

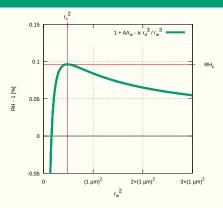
$$\approx 1 + \frac{A}{r_{w}} - \frac{\kappa r_{d}^{3}}{r_{w}^{3}}$$



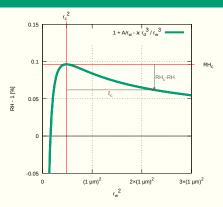
maximum at  $(r_c, RH_c)$ :

$$r_{\rm c} = \sqrt{3\kappa r_{\rm d}^3/A}$$
  
 $RH_{\rm c} = 1 + \frac{2A}{3r_{\rm c}}$ 

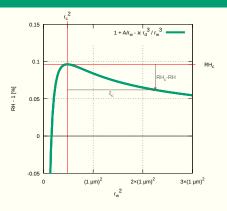
#### phase portrait of the system: flipped Köhler curve



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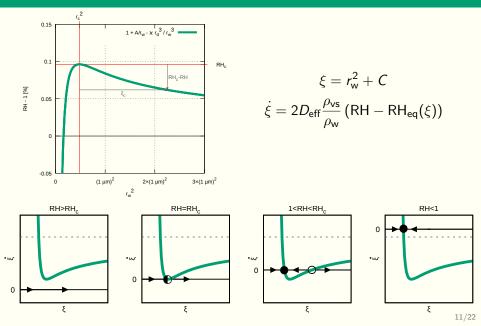


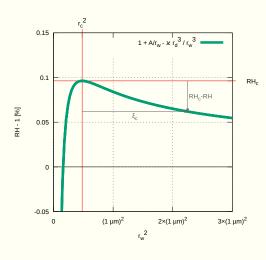
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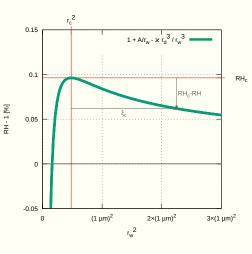
$$\xi = r_{
m w}^2 + C$$
  $\dot{\xi} = 2 D_{
m eff} rac{
ho_{
m vs}}{
ho_{
m w}} \left( {
m RH} - {
m RH}_{
m eq}(\xi) 
ight)$ 

# phase portrait of the system: flipped Köhler curve

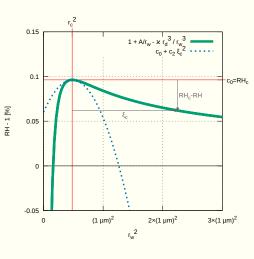




$$RH_{eq}(\xi_c) = c_0 + c_1 \xi_c + c_2 \xi_c^2 + \dots$$

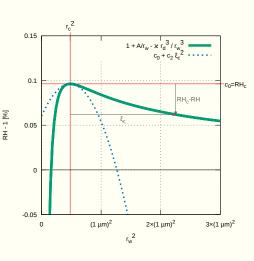


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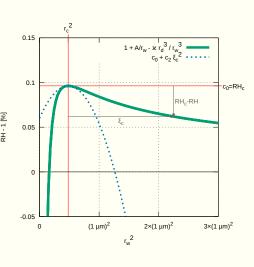
$$\left.\dot{\xi_{c}}\right|_{\xi_{c}\rightarrow0}\sim\frac{\mathsf{RH}-\mathsf{RH}_{c}}{A/(4r_{c}^{5})}+\xi_{c}^{2}$$



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

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

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



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

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$$au_{act} pprox \int_{-\infty}^{+\infty} rac{d\xi_{
m c}}{\dot{\xi}_{
m c}}$$

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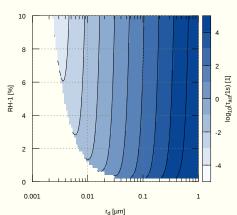
$$\tau_{act} \approx \int_{-\infty}^{+\infty} \frac{d\xi_{\rm c}}{\dot{\xi}_{\rm c}}$$

$$= \frac{r_{\rm c}^{5/2}}{\sqrt{A}} \frac{\rho_{\rm w}/\rho_{\rm vs}}{D_{\rm eff}} \frac{\pi}{\sqrt{\rm RH - RH_c}}$$

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

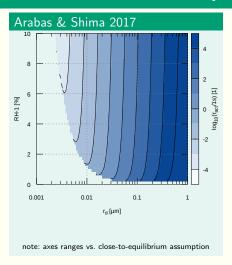
key observation: time of passage through the parabolic *bottleneck* dominates all other timescales

$$au_{act} pprox \int_{-\infty}^{+\infty} rac{d\xi_{
m c}}{\dot{\xi_{
m c}}} \ = rac{r_{
m c}^{5/2}}{\sqrt{A}} rac{
ho_{
m w}/
ho_{
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m RH-RH_c}}$$

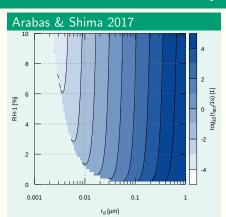


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### activation timescale: analytic vs. numerical



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

#### Hoffmann, 2016 (MWR)

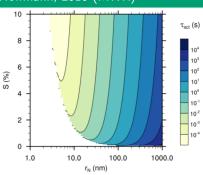


FIG. 2. The activation time scale  $\tau_{\rm act}$  as a function of dry aerosol radius  $r_N$  and supersaturation S. For values of  $S < S_{\rm crit}$  (white areas),  $\tau_{\rm act}$  does not exist.

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

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  $\tau_{\rm act}$  measuring the time needed for a wetted aerosol to grow beyond its critical radius  $r_{\rm crit} = \sqrt{3Br_{\rm b}^3/A}$  are given in Fig. 2 as a function of

simple moisture budget (const T,p):

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

simple moisture budget (const T,p):

$$\dot{RH} pprox rac{\dot{
ho}_{
m v}}{
ho_{
m vs}} = -N \underbrace{rac{4\pi 
ho_{
m w}}{3
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m w}^2 \dot{r}_{
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integrating in time:

$$RH = RH_0 - \alpha N r_w^3$$

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m w}$$

integrating in time:

$$RH = RH_0 - \alpha N r_w^3$$

new phase portrait:

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

### simple moisture budget (const T,p):

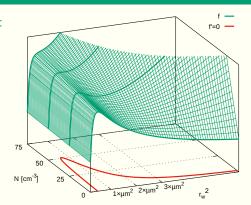
$$\dot{RH} pprox rac{\dot{
ho}_{v}}{
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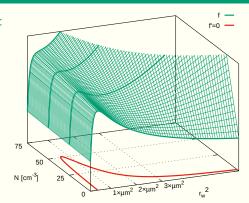
integrating in time:

$$RH = RH_0 - \alpha N r_w^3$$

new phase portrait:

$$\dot{\xi} \sim (\mathsf{RH_0} - 1) - \underbrace{\left(\frac{A}{\xi^{\frac{1}{2}}} - \frac{\kappa r_\mathsf{d}^3}{\xi^{\frac{3}{2}}} + \alpha N \xi^{\frac{3}{2}}\right)}_{f}$$

regime-controlling params: RH, N



simple moisture budget (const T,p):

$$\dot{RH} pprox rac{\dot{
ho}_{
m V}}{
ho_{
m Vs}} = -N \underbrace{rac{4\pi
ho_{
m W}}{3
ho_{
m Vs}}}_{lpha} 3r_{
m W}^2 \dot{r}_{
m W}$$

integrating in time:

$$RH = RH_0 - \alpha N r_w^3$$

new phase portrait:

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

N [cm<sup>-3</sup>] 1×µm² 2×µm² 3×µm²

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

regime-controlling params: RH, N

# bifurcations (and catastrophe) in the RH-coupled system

#### Prigogine & Stengers 1984

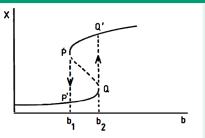


Figure 15. This figure shows how a "hysteresis" phenomenon occurs if we have the value of the bifurcation parameter D first growing and then diminishing. If the system is initially in a stationary state belonging to the lower branch, it will stay there while b grows. But at b= $b_2$ , there will be a 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, 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

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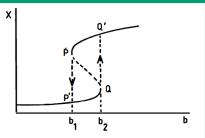
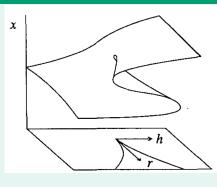


Figure 15. This figure shows how a "hysteresis" phenomenon occurs if we have the value of the bifurcation parameter b first growing and then diminishing. If the system is initially in a stationary state belonging to the lower branch, it will stay there while b grows. But at  $b-b_0$ , there will be a discontinuity. The system jumps from 0 to C, on the higher branch. Inversely, starting from a state on the higher branch, the system will remain there till  $b-b_0$ , 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



# bifurcations (and catastrophe) in the RH-coupled system

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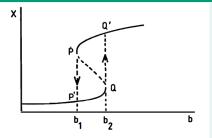
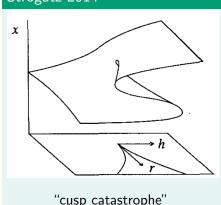


Figure 15. This figure shows how a "hysteresis" phenomenon occurs if we have the value of the bifurcation parameter b first growing and then diminishing. If the system is initially in a stationary state belonging to the lower branch, it will stay there while b grows. But at  $b = b_2$ , there will be 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

#### Strogatz 2014



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

vertically displaced (velocity w, hydrostatic background) adiabatic parcel: (q: mixing ratio,  $p_d$ : bgnd pressure,  $\rho_d$  bgnd density, g,  $l_v$ ,  $c_{pd}$ : constants)

$$\begin{bmatrix} \dot{p}_{d} \\ \dot{T} \\ \dot{r}_{w} \end{bmatrix} = \begin{bmatrix} -\rho_{\mathsf{d}} g w \\ (\dot{p}_{\mathsf{d}}/\rho_{\mathsf{d}} - \dot{q} \mathit{l}_{\mathsf{v}})/c_{\mathsf{pd}} \\ (D_{\mathsf{eff}}/\rho_{\mathsf{w}})(\rho_{\mathsf{v}} - \rho_{\circ})/\mathit{r}_{\mathsf{w}} \end{bmatrix}$$

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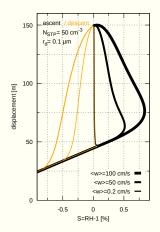
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 $w \to 0$  (and hence  $\dot{p}_{\rm d} \approx 0$ ) i.e., slow, close-to-equilibrium evolution of the system relevant to fixed-point analysis (by some means pertinent to formation of non-convective clouds such as fog)

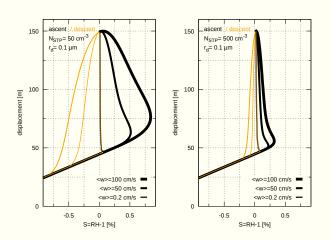
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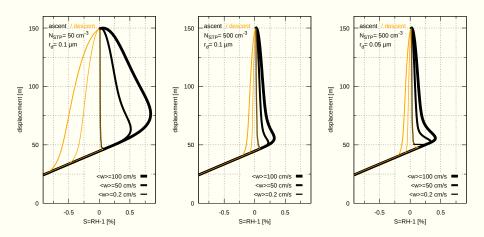
- $w \to 0$  (and hence  $\dot{p}_d \approx 0$ ) i.e., slow, close-to-equilibrium evolution of the system relevant to fixed-point analysis (by some means pertinent to formation of non-convective clouds such as fog)
- $N \to 0$  (and hence  $\dot{q} \approx 0$ ) i.e., weak coupling between particle size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



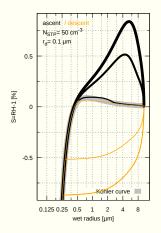
integration using CVODE adaptive solver open source code (based on libcloudph++) as electronic paper supplement



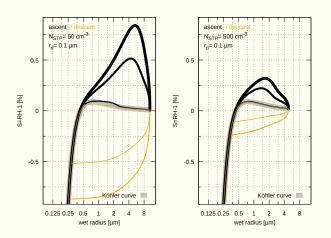
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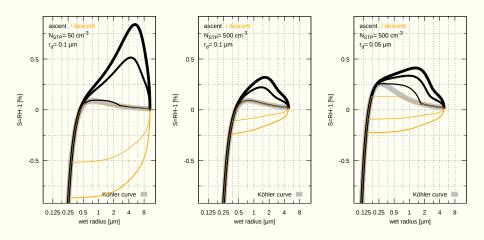
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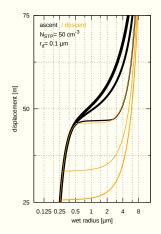
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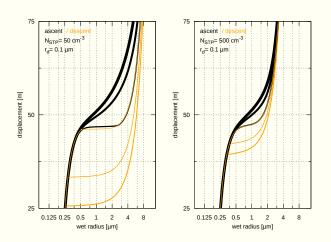


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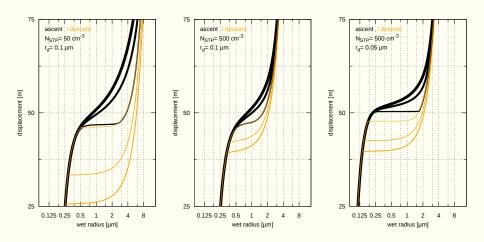
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## parcel model: numerical integration (sinusoidal w)



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nomenclature:





- nomenclature:
  - CCN activation





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



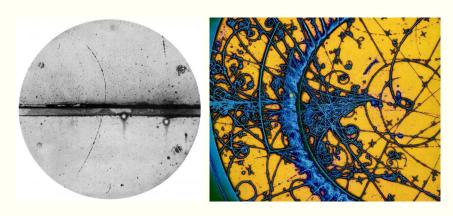


- nomenclature:
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- significance:



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

## applicability beyond cloud physics (hypothesis...)



Wilson & bubble chambers

https://home.cern/about/updates/2015/06/seeing-invisible-event-displays-particle-physics

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  - formation of droplets on aerosol,
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- 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!

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