

# On the CCN (de)activation nonlinearities

Sylwester Arabas and Shin-ichiro Shima

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- ❖ back to academia:
  - ❖ 2018–...: Jagiellonian University, Cracow (Math/CS Dept.)

## Shin-ichiro Shima



兵庫県立大学大学院  
シミュレーション学研究科  
GRADUATE SCHOOL OF SIMULATION STUDIES, UNIVERSITY OF HYOGO

日本語 / English

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### 🏠 ホーム

#### 研究科について

- 研究科長のメッセージ
- 本研究科が目指す研究
- 入学後の研究について
- 教員
- 計算機環境
- 受験や入学を希望される方へ

### SHIN-ICHIRO SHIMA (ASSOCIATE PROFESSOR)



( [Japanese](#) / [English](#) )

Computer simulation is the third methodology of scientific research, complementing theory and experiment. This methodology is new and still developing. In particular, it is still difficult to predict the behavior of complex systems, in which a large number of components are interacting together and various collective behaviors emerge. My research interest is on exploring the full possibility of computer simulation to understand complex systems.

**Keywords:** Nonlinear Science, Complex Systems, Computational Science, Multiscale-Multiphysics Phenomena, Meteorology, Data Assimilation, Synchronization

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## Arabas & Shima 2017

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Nonlinear Processes  
in Geophysics



### On the CCN (de)activation nonlinearities

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<sup>2</sup>Chatham Financial Corporation Europe, Cracow, Poland

<sup>3</sup>Graduate School of Simulation Studies, University of Hyogo, Kobe, Japan

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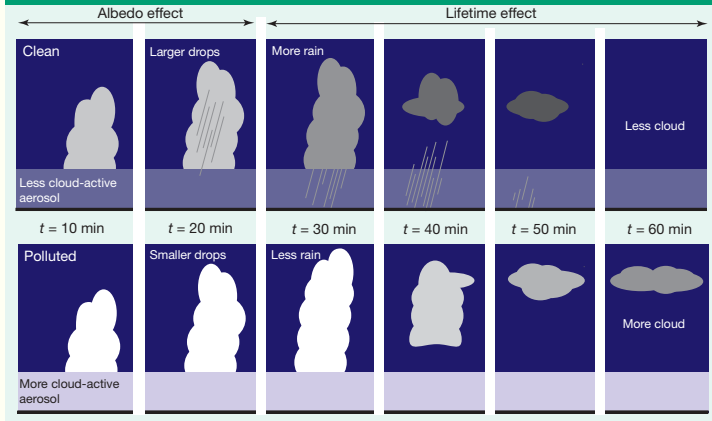
Revised: 23 May 2017 – Accepted: 24 July 2017 – Published: 5 September 2017



# one-slide aerosol-cloud (micro-macro) interaction primer

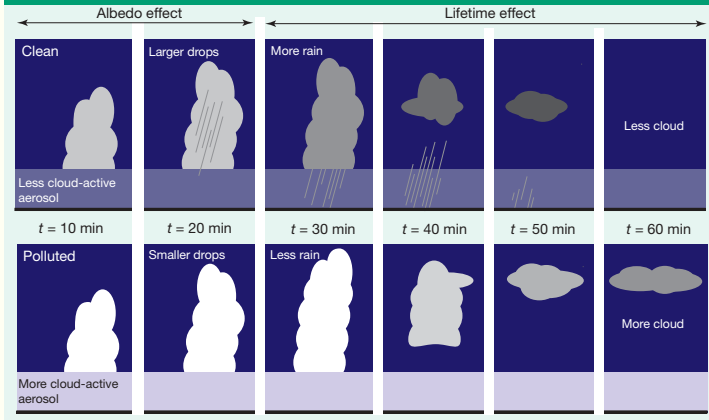
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Stevens and Feingold, 2009 (Nature)



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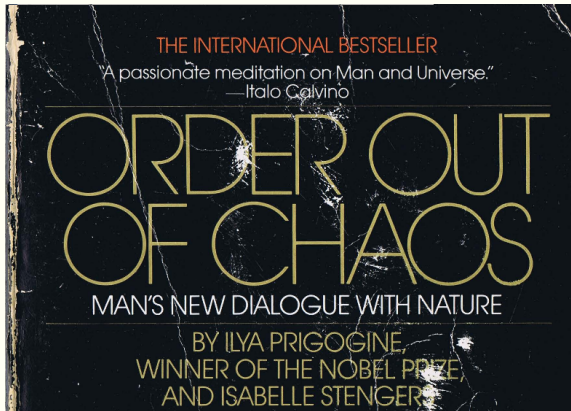


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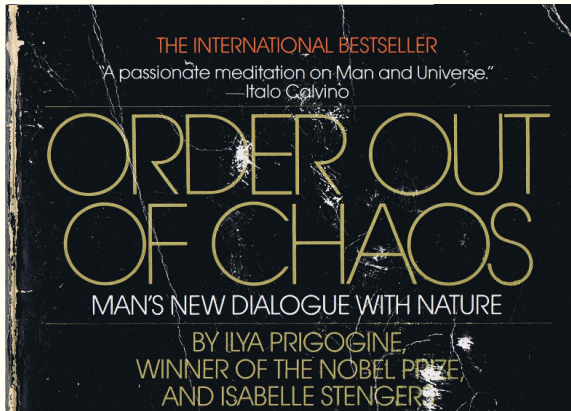
*"there is something captivating about the idea that fine particulate matter, suspended almost invisibly in the atmosphere, holds the key to some of the greatest mysteries of climate science"*

... others captivated by micro-macro interactions

... others captivated by micro-macro interactions



... others captivated by micro-macro interactions



### 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

## ORDER OUT OF CHAOS 188

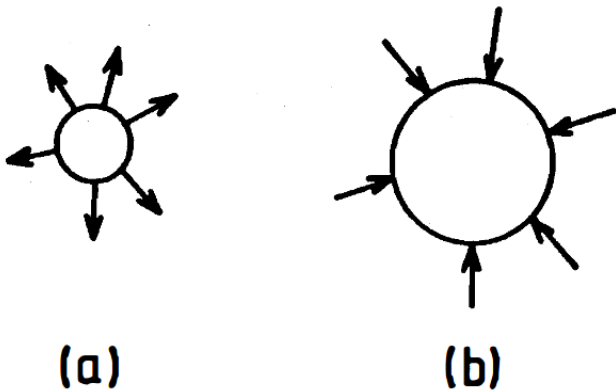


Figure 19. Nucleation of a liquid droplet in a supersaturated vapor. (a) droplet smaller than the critical size; (b) droplet larger than the critical size. The existence of the threshold has been experimentally verified for dissipative structures.



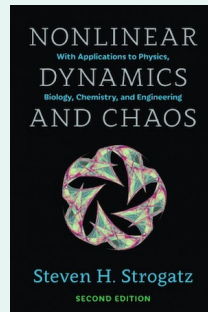
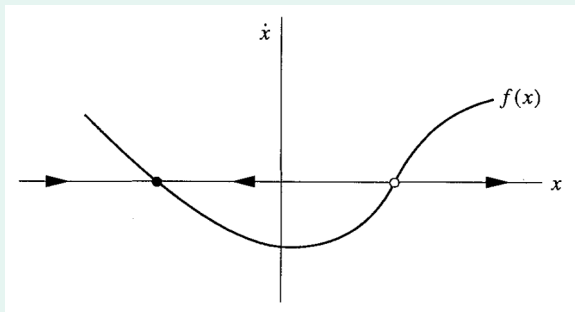
## two-slide bifurcation analysis primer (1/2)

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Strogatz 2014 (sect. 2.2): fixed points and stability

graphical (qualitative) analysis  
of a non-linear one-dimensional dynamical system:

$$\dot{x} = f(x)$$



## two-slide bifurcation analysis primer (2/2)

Strogatz 2014 (sect. 3.1): saddle-node bifurcation

prototypical example of saddle-node bifurcation:

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

$r$ : parameter (distinct regimes if positive, negative or zero)

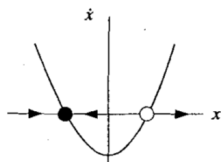
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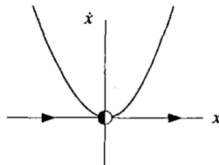
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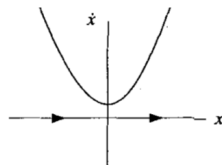
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(a)  $r < 0$



(b)  $r = 0$



(c)  $r > 0$

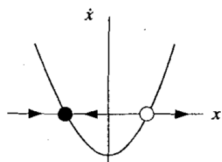
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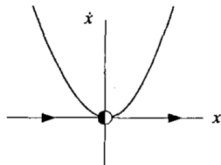
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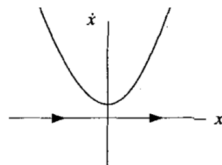
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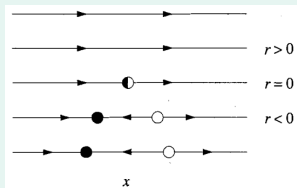
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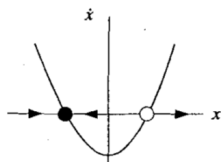
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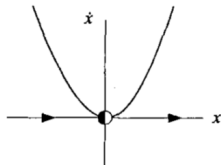
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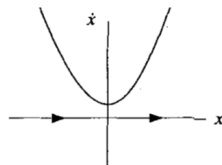
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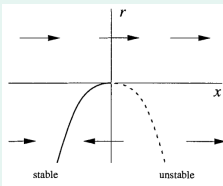
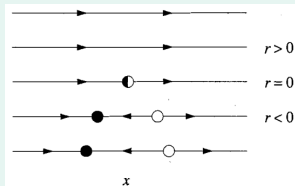
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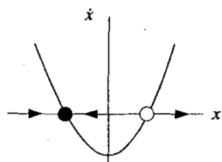
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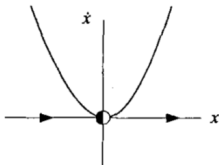
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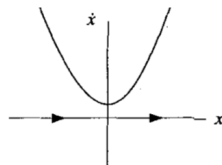
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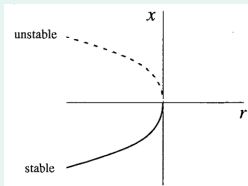
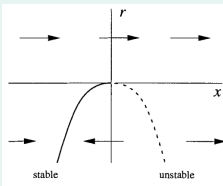
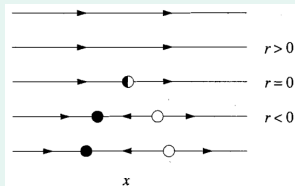
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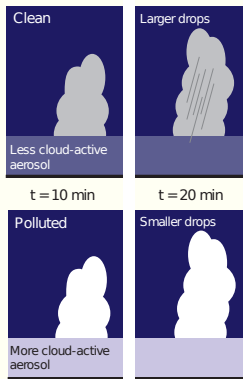
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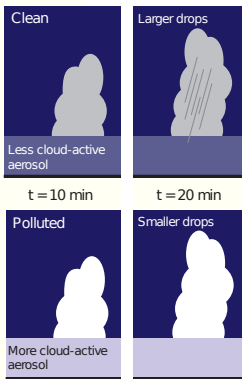
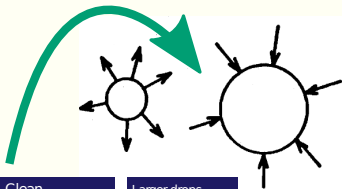




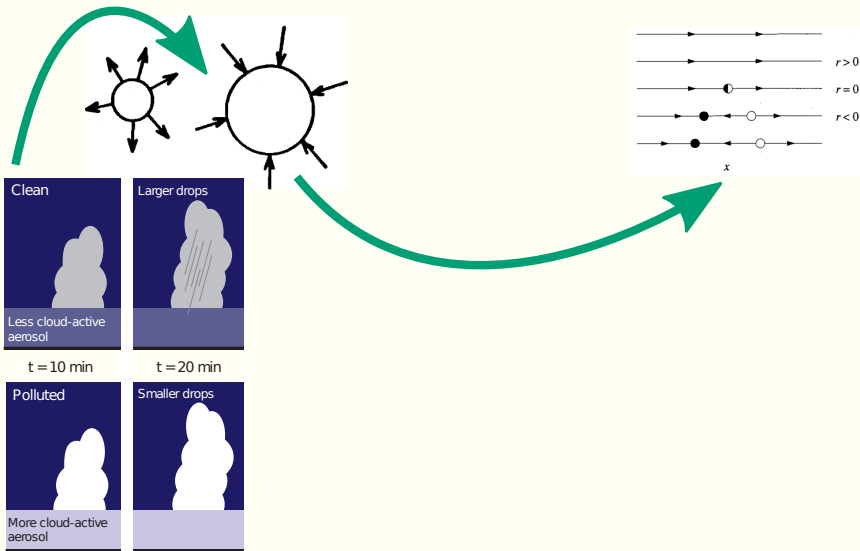
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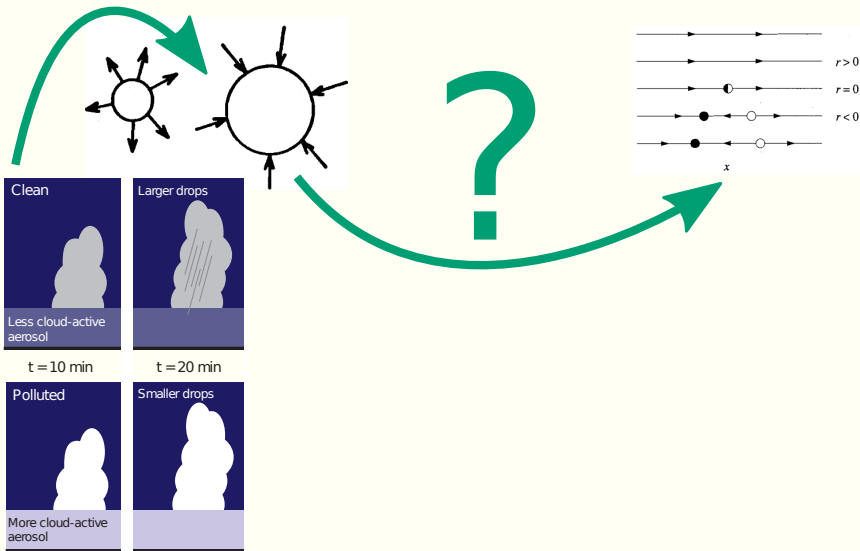
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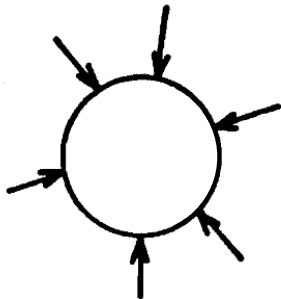
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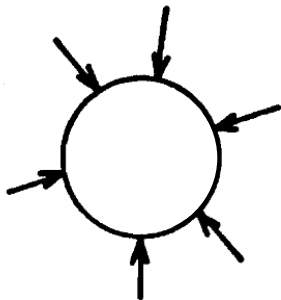


## droplet growth laws in a nutshell: mass and heat diffusion



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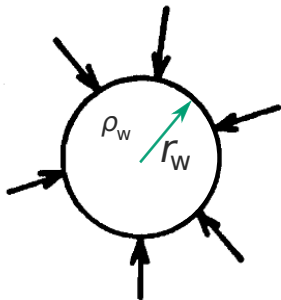
Fick's and Fourier's laws combined  
spherical geometry



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

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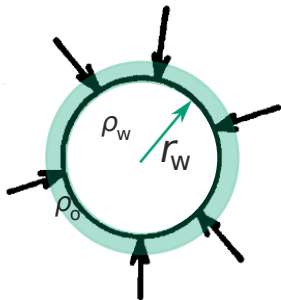
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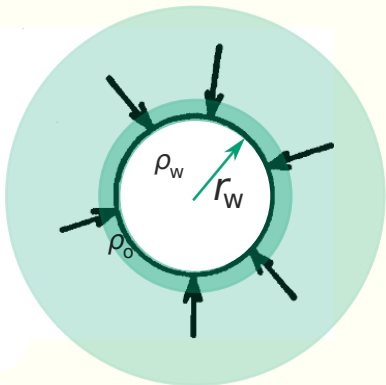
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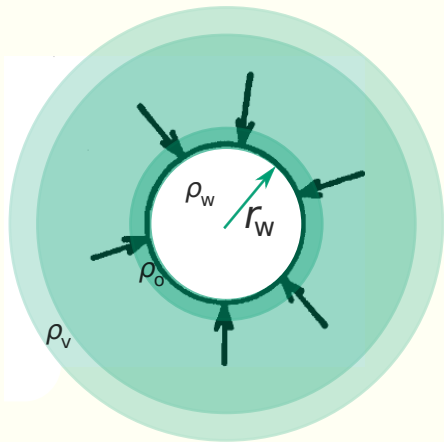
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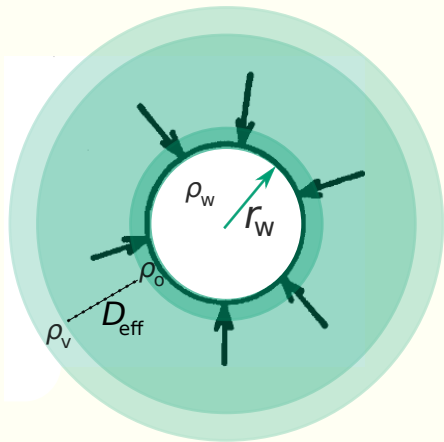
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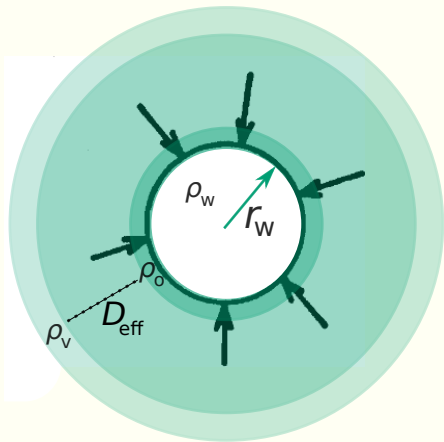
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non-dimensional numbers:

$$\text{RH} = \rho_v / \rho_{vs}$$

$$\text{RH}_{\text{eq}} = \rho_o / \rho_{vs}$$



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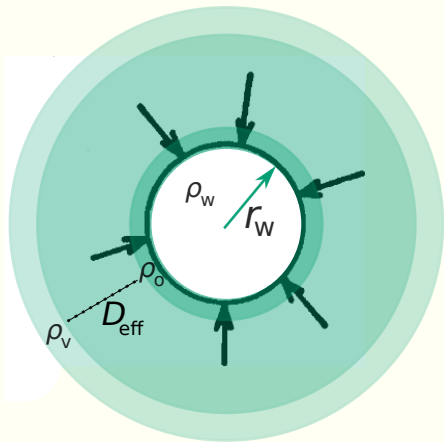
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## droplet growth laws in a nutshell: Köhler curve

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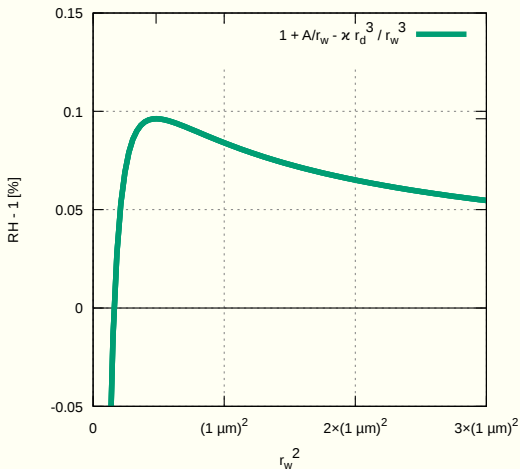
$$\begin{aligned} \text{RH}_{\text{eq}} &= \frac{r_w^3 - r_d^3}{r_w^3 - r_d^3(1 - \kappa)} \exp\left(\frac{A}{r_w}\right) \\ &\approx 1 + \frac{A}{r_w} - \frac{\kappa r_d^3}{r_w^3} \end{aligned}$$

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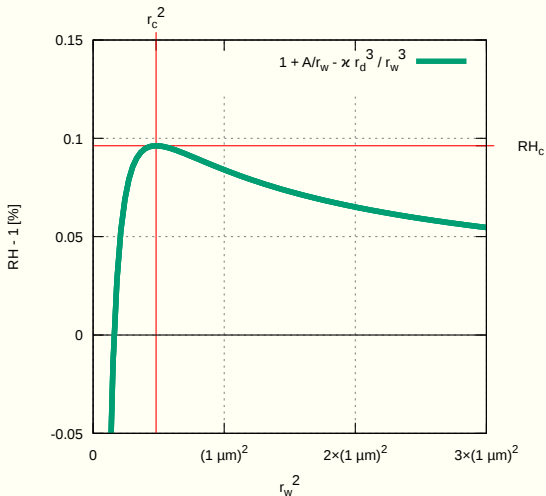


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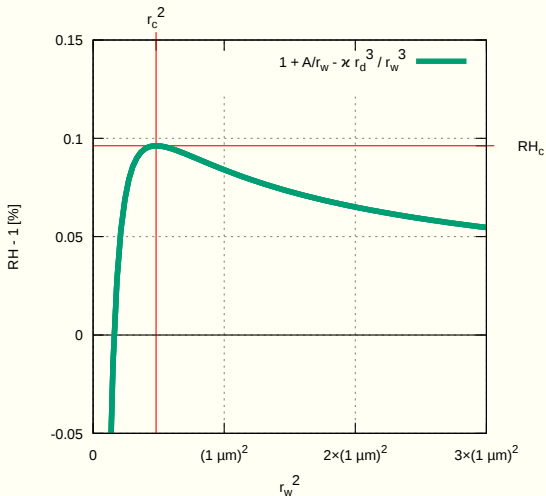


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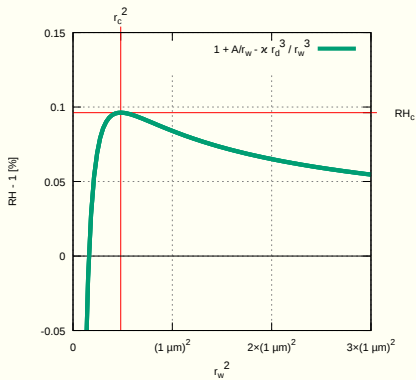


maximum at  $(r_c, RH_c)$ :

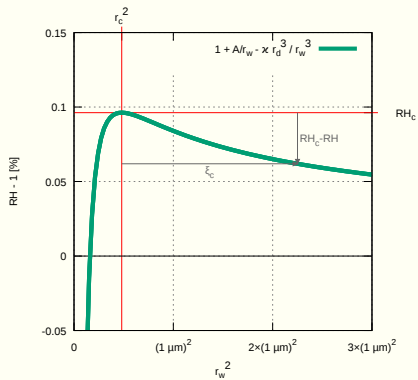
$$r_c = \sqrt{3\kappa r_d^3 / A}$$

$$RH_c = 1 + \frac{2A}{3r_c}$$

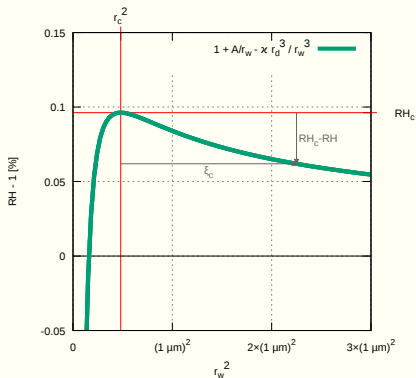
# phase portrait of the system: flipped Köhler curve



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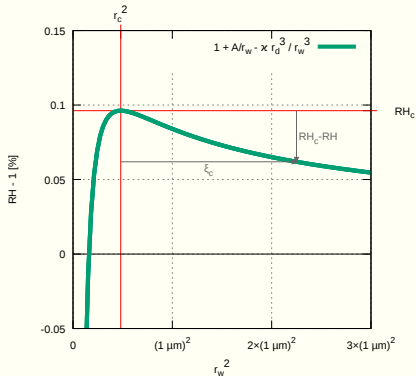
# phase portrait of the system: flipped Köhler curve



$$\xi = r_w^2 + C$$

$$\dot{\xi} = 2D_{\text{eff}} \frac{\rho_{vs}}{\rho_w} (RH - RH_{\text{eq}}(\xi))$$

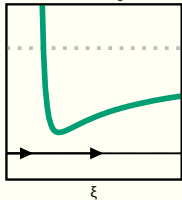
# phase portrait of the system: flipped Köhler curve



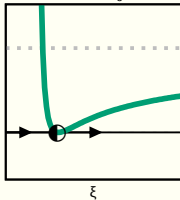
$$\xi = r_w^2 + C$$

$$\dot{\xi} = 2D_{\text{eff}} \frac{\rho_{vs}}{\rho_w} (RH - RH_{\text{eq}}(\xi))$$

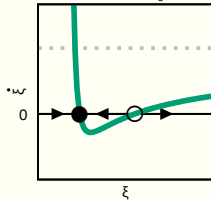
$RH > RH_c$



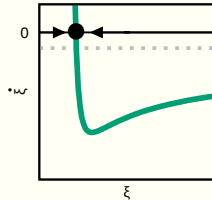
$RH = RH_c$



$1 < RH < RH_c$

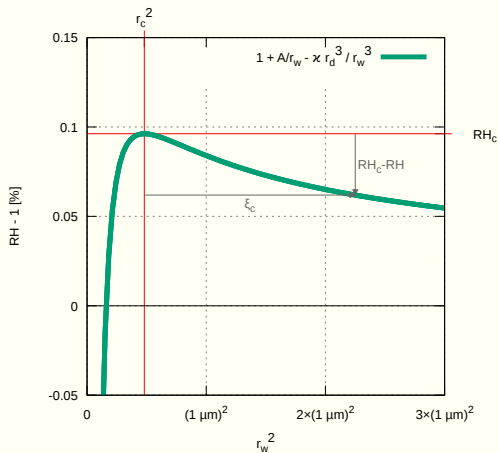


$RH < 1$



# saddle-node bifurcation at Köhler curve maximum

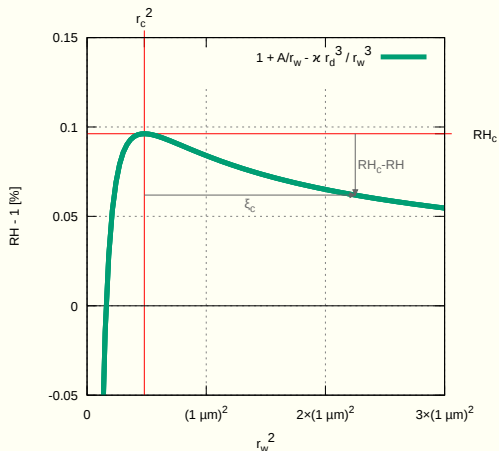
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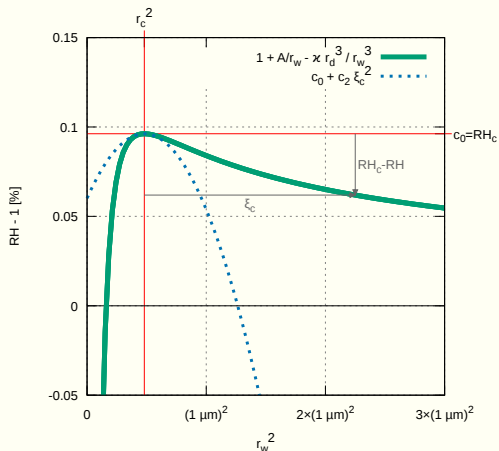
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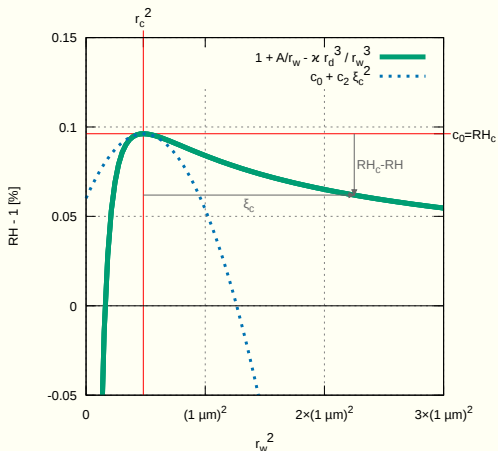
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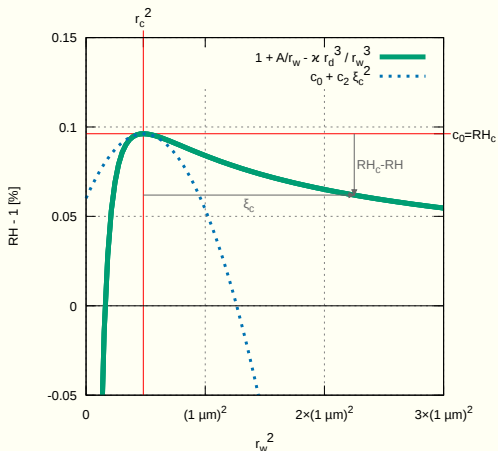


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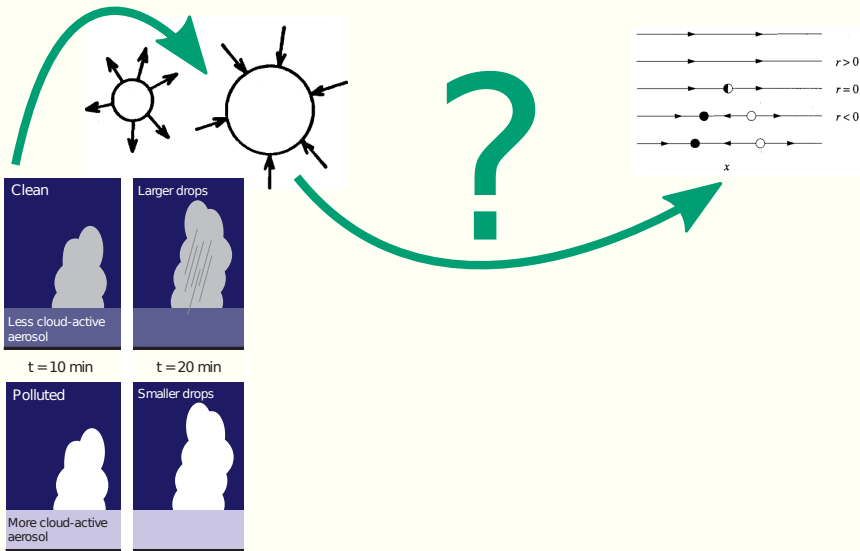
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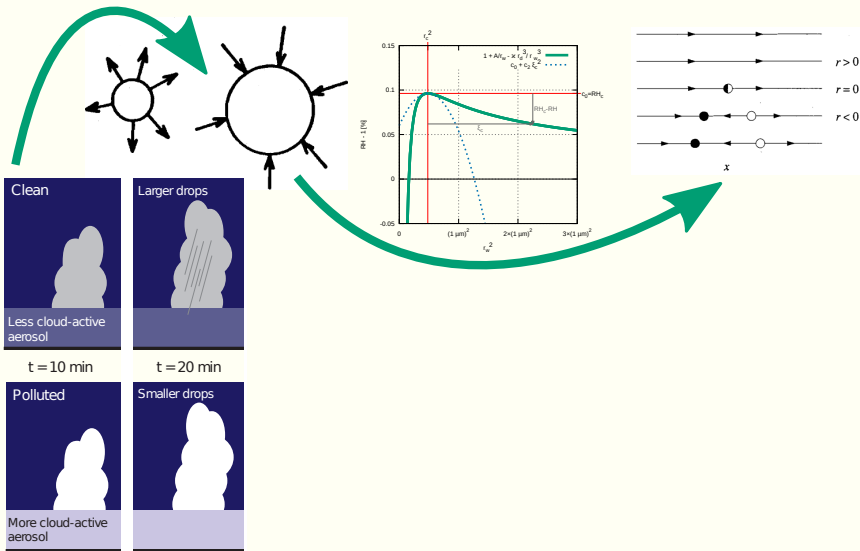
$$\dot{x} = r + x^2$$



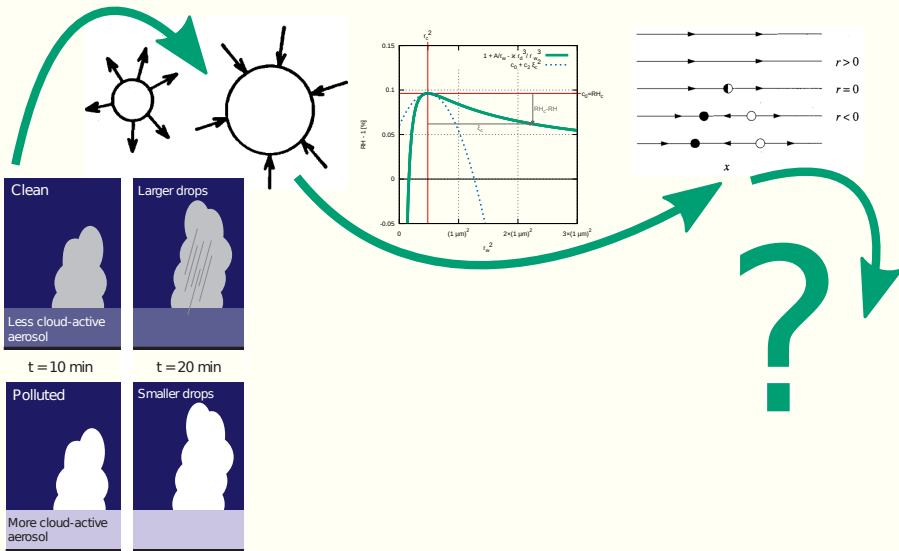
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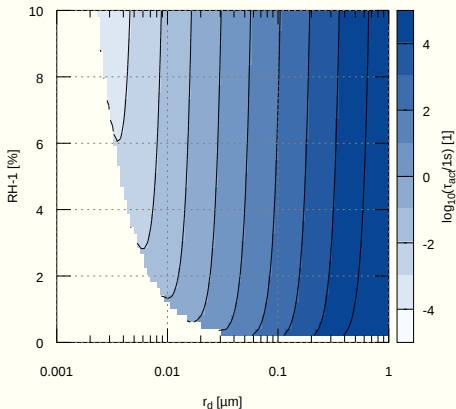
$$\begin{aligned}\tau_{\text{act}} &\approx \int_{-\infty}^{+\infty} \frac{d\xi_c}{\dot{\xi}_c} \\ &= \frac{r_c^{5/2}}{\sqrt{A}} \frac{\rho_w/\rho_{vs}}{D_{\text{eff}}} \frac{\pi}{\sqrt{RH - RH_c}}\end{aligned}$$

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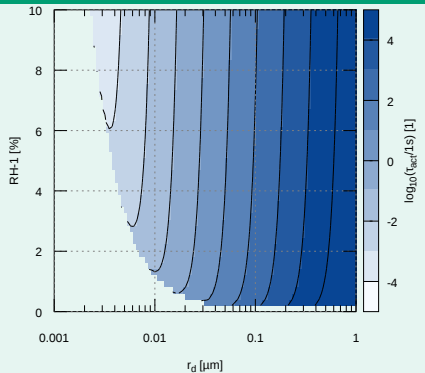
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# activation timescale: analytic vs. numerical

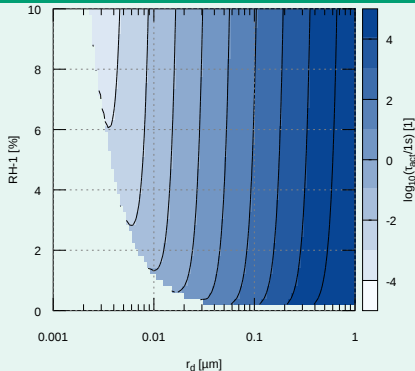
Arabas & Shima 2017



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

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## Arabas & Shima 2017



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## Hoffmann, 2016 (MWR)

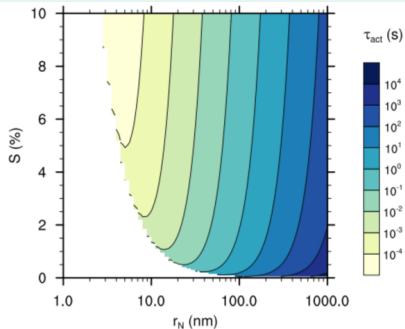
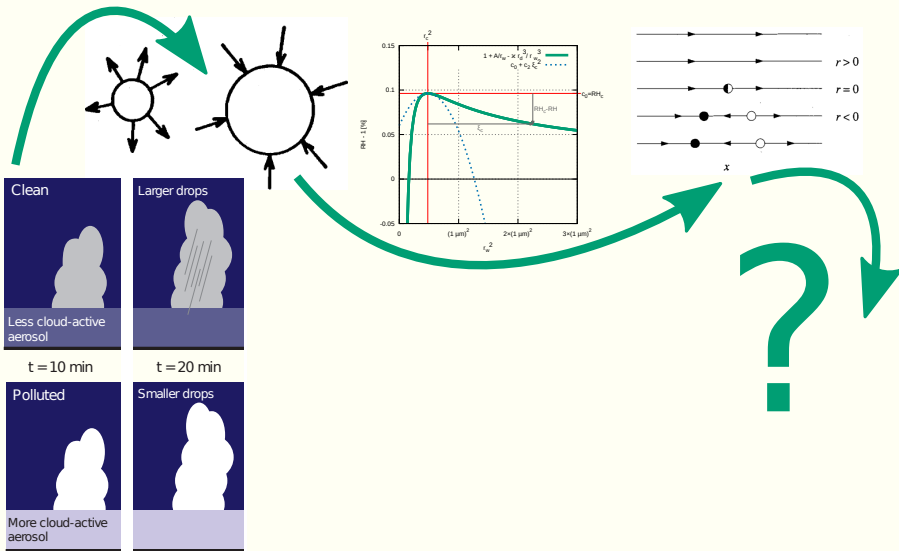


FIG. 2. The activation time scale  $\tau_{\text{act}}$  as a function of dry aerosol radius  $r_N$  and supersaturation  $S$ . For values of  $S < S_{\text{crit}}$  (white areas),  $\tau_{\text{act}}$  does not exist.

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

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

# connecting the dots ...





# RH-coupled system & particle concentration as parameter

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simple moisture budget (const T,p):

$$\text{RH} \approx \frac{\dot{\rho}_v}{\rho_{vs}} = -N \underbrace{\frac{4\pi\rho_w}{3\rho_{vs}}}_{\alpha} 3r_w^2 \dot{r}_w$$

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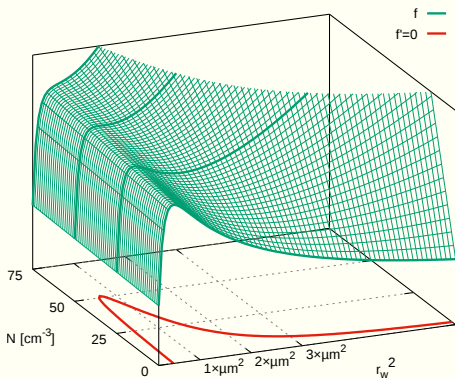
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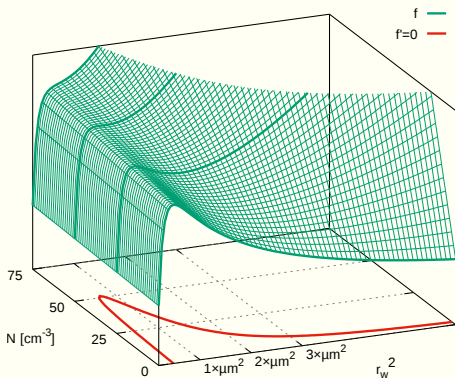
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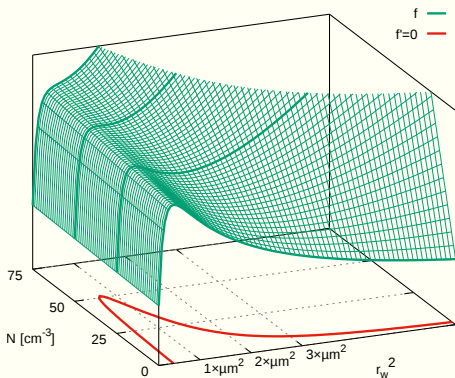
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# bifurcations (and catastrophe) in the RH-coupled system

Prigogine & Stengers 1984

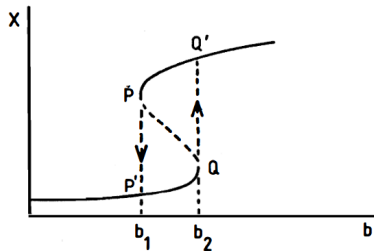


Figure 15. This figure shows how a "hysteresis" phenomenon occurs if we have the value of the bifurcation parameter  $b$  first growing and then diminishing. If the system is initially in a stationary state belonging to the lower branch, it will stay there while  $b$  grows. But at  $b=b_2$ , there will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



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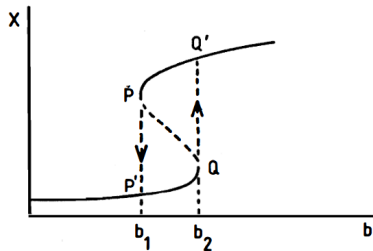
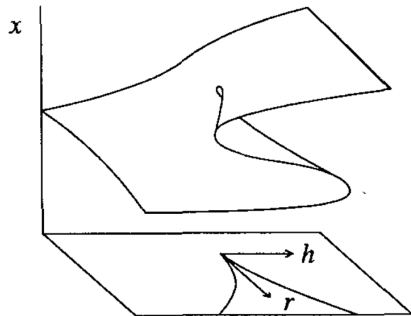


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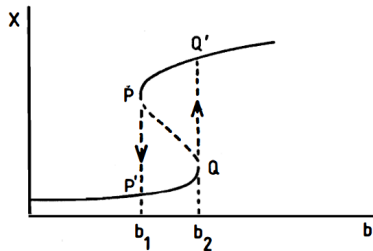
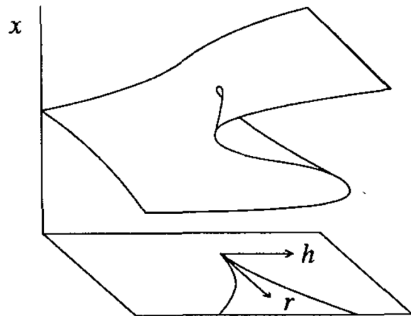


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↪ "jumps", hysteretic behaviour ( $r_w$ , RH) for small enough  $N$ , close to equilibrium (slow process)

## hysteresis: activation/deactivation cycle



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vertically displaced (velocity  $w$ , hydrostatic background) adiabatic parcel:  
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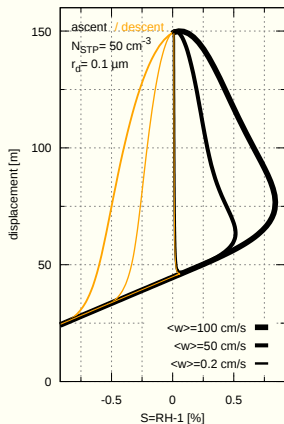
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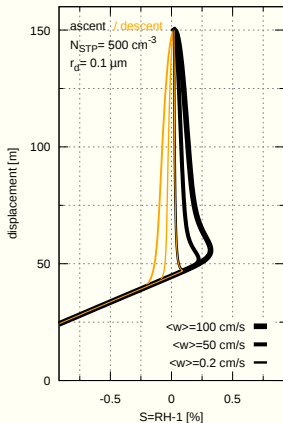
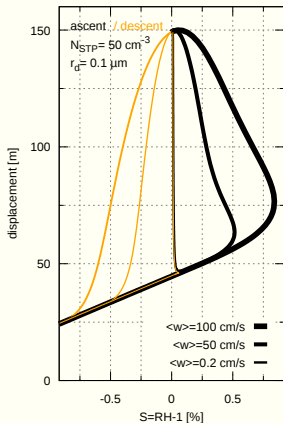
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- ❖  $N \rightarrow 0$  (and hence  $\dot{q} \approx 0$ ) i.e., weak coupling between particle size evolution and ambient thermodynamics (pertinent to the case of low particle concentration).

# parcel model: numerical integration (sinusoidal $w$ )



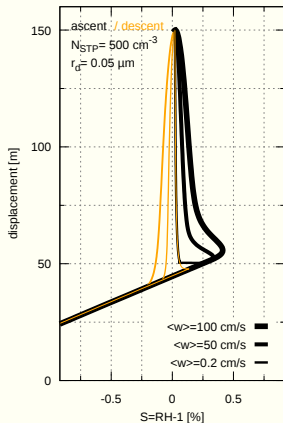
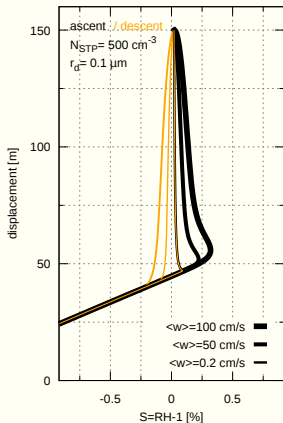
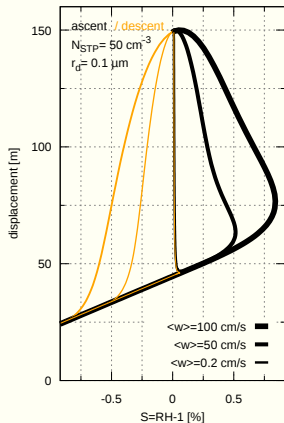
integration using CVODE adaptive solver  
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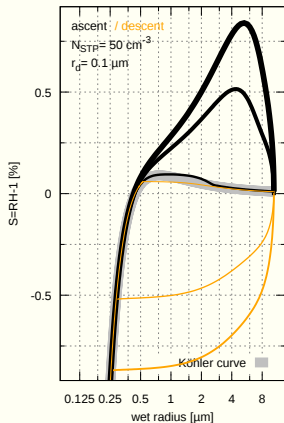
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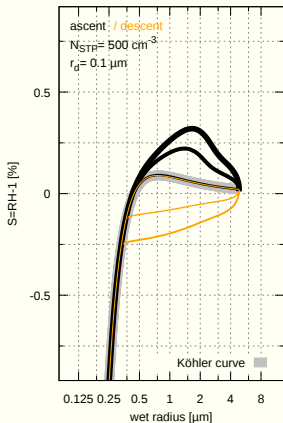
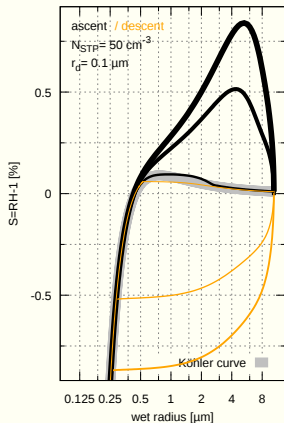


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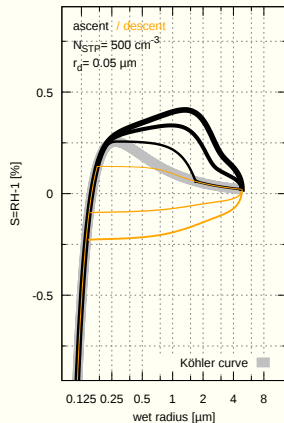
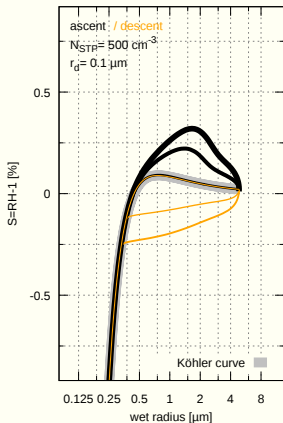
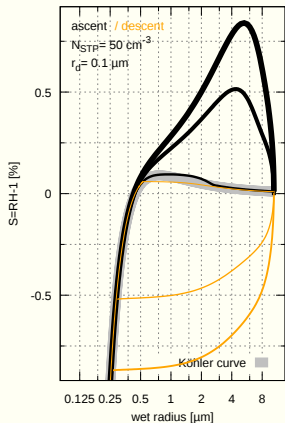
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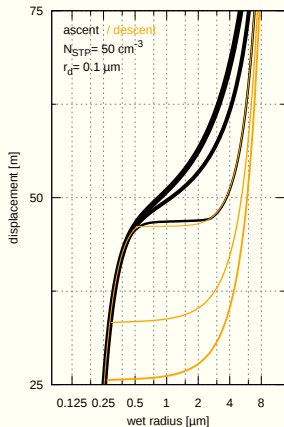
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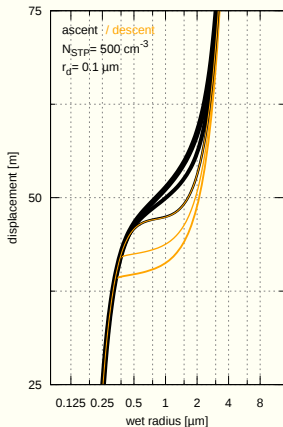
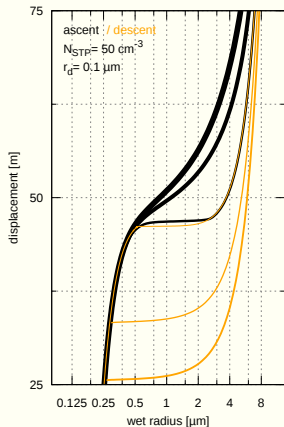
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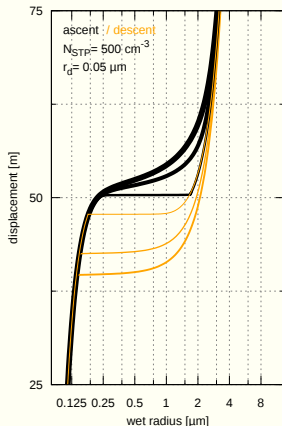
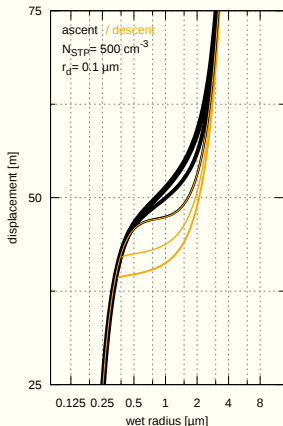
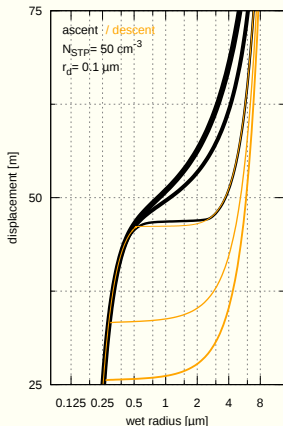
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# parcel model: numerical integration (sinusoidal $w$ )



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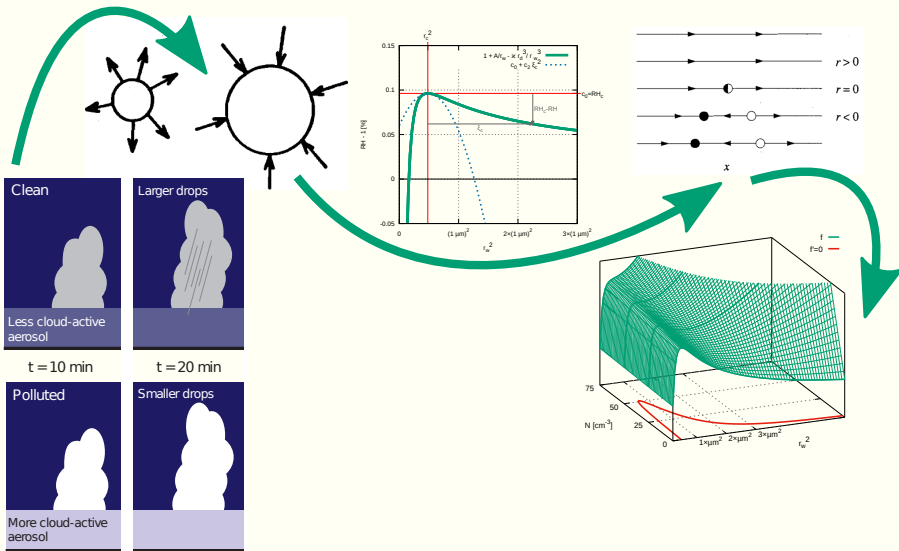
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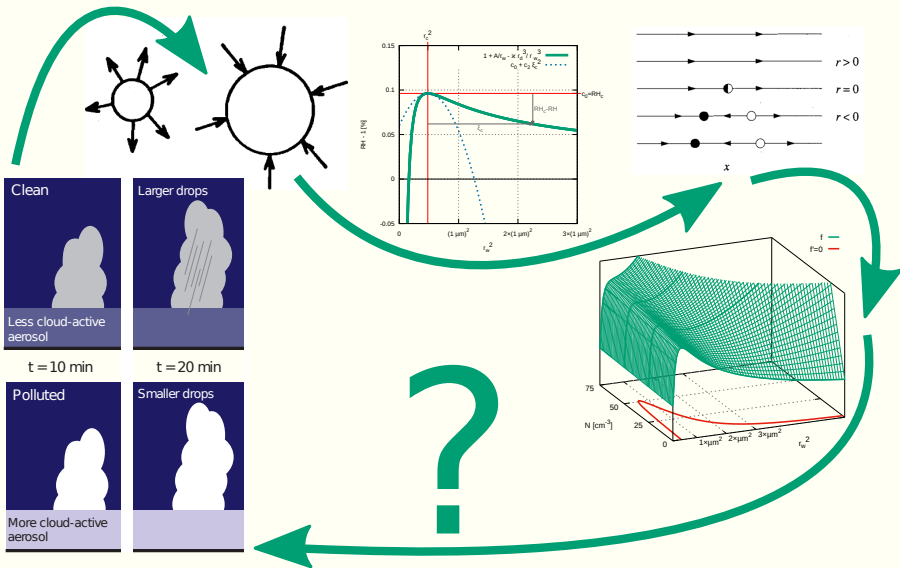


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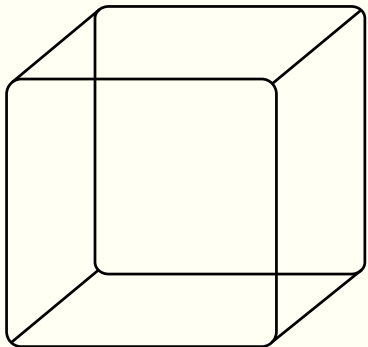
## ... applicability?

**particle-based  $\mu$ -physics schemes for LES!**  
(Lagrangian Cloud Models / Super-Droplet Models)

- “information carriers” in LES domain



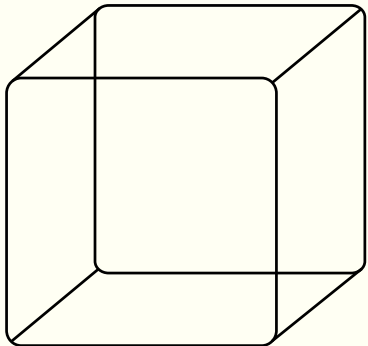
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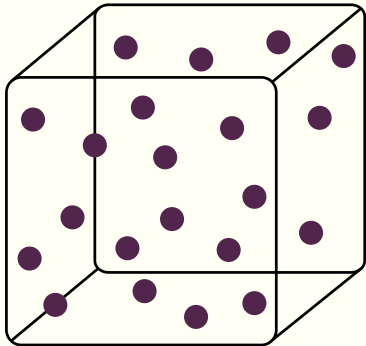
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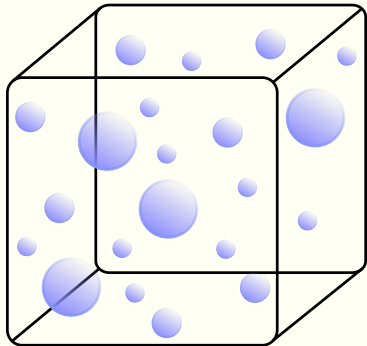


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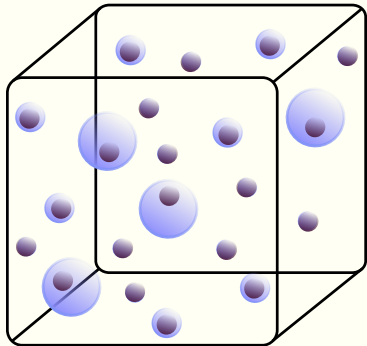
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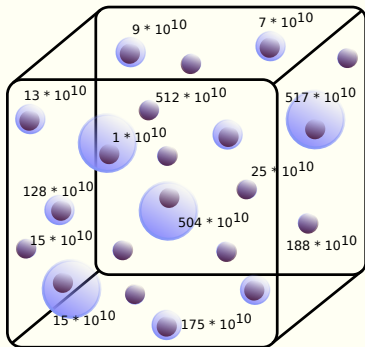
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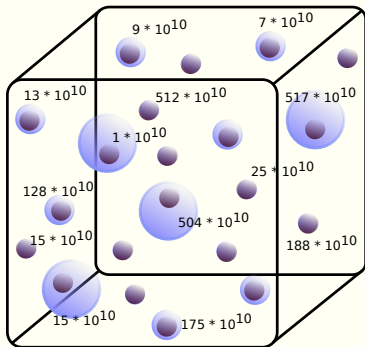
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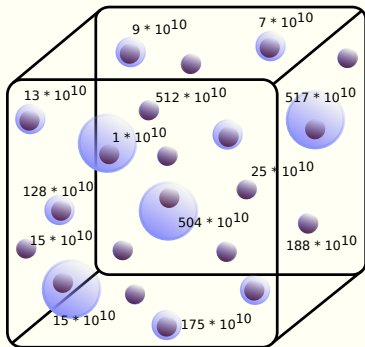
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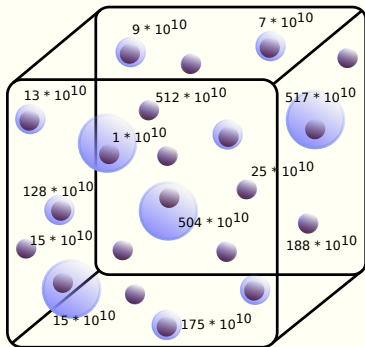
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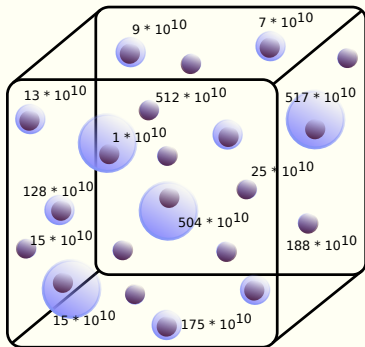


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- ❖ each particle: **monodisperse!**
- ❖ each timestep: **constant RH!**

# particle-based $\mu$ -physics for LES

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

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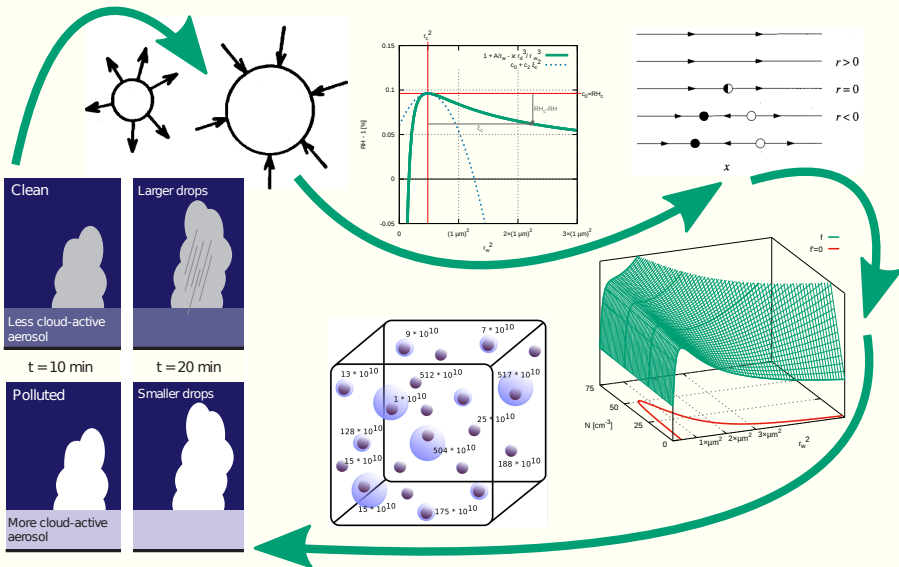
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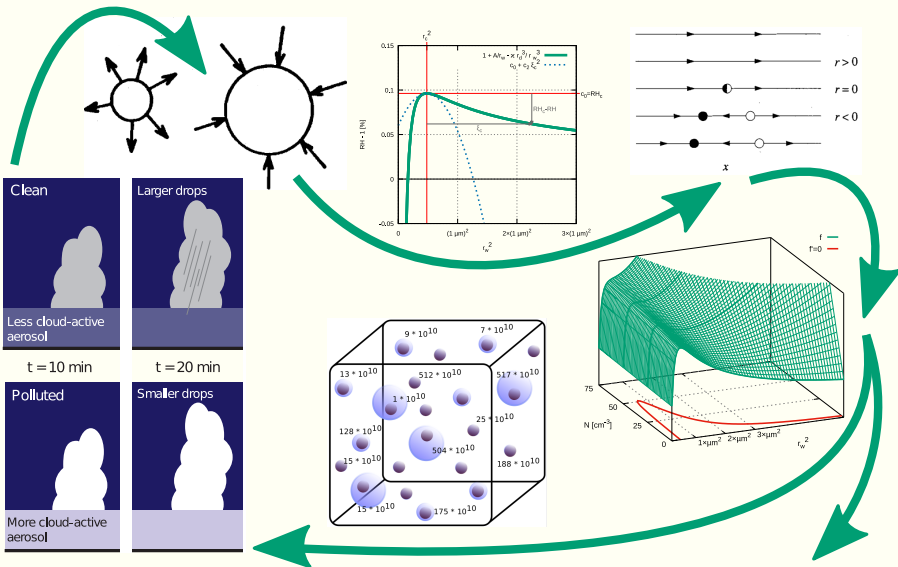
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connecting the dots ...

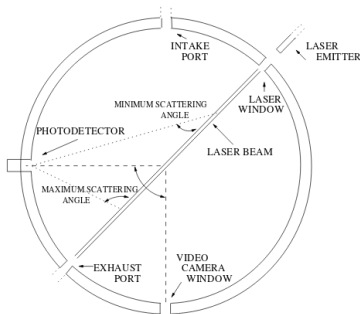
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# model applicability: CCN instruments? (hypothesis...)

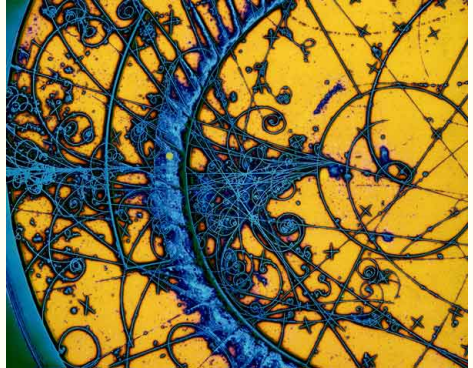
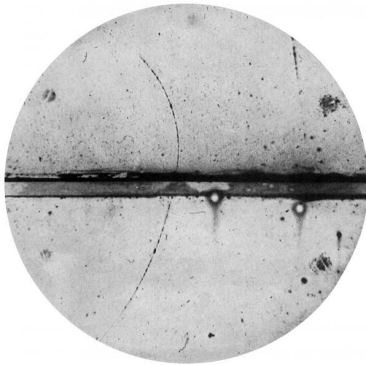


pictured: UWyoming WyoCCN instrument

(photo from DYCOMS-II CCN data report by Jeff Snider et al.)

[https://www.eol.ucar.edu/projects/dycoms/dm/archive/docs/snider\\_ccnreadme.pdf](https://www.eol.ucar.edu/projects/dycoms/dm/archive/docs/snider_ccnreadme.pdf)

# applicability beyond cloud physics (hypothesis...)



## Wilson & bubble chambers

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



conclusions, takeaways, prospects

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- ❖ applications: CCN instrumentation modelling, non-cloud appl...



last slide

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Thank you for your attention!

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