The Lagrangian ice microphysics code LCM: Introduction, current developments and benefits

S. Unterstrasser (DLR Oberpfaffenhofen)

Contribution D3624 | EGU2020-2307
in session AS5.9

Introduction

In the original format, this solicited contribution should have an extended introduction to Lagrangian cloud modelling.
I decided to keep those slides with basic facts of Lagrangian cloud models.
Due to time limitations, however, I will have to go quickly over all slides.

Introduction:

- Lagrangian cloud models (LCMs) are considered the future of cloud microphysical modeling, though they are computationally expensive.
- Particle-based methods can be applied in 0D and 1D.
- This presentation, however, focuses on LCMs coupled to a LES model and used in 2D and 3D simulations.
- Most upcoming statements are relevant for LCMs irrespective of the cloud type (pure ice, warm clouds, mixed-phase).
- But a few aspects in the ice microphysical model are differently treated than in all present liquid cloud LCMs.

Terminology

- Lagrangian cloud model (LCM) = particle-based microphysics = super-droplet method.
- Simulation particle (SIP) = computational droplet = super-droplet.

  Usually, each SIP represents a certain number of identical hydrometeors or CCNs.
- Weighting factor = multiplicity
- In my case of ice microphysics, LCM = Lagrangian <u>Cirrus</u> Model

Design concept

General design concepts of (current) LCMs:

- Information about hydrometeors is carried in simulation particles (SIPs), not in field variables.
- These SIPs carry information on: location, size, weighting factor and other attributes (e.g. ice crystal habit, aerosol properties, tags, chemical composition)
- Separation of transport and microphysical processes unlike to Eulerian methods.
- Transport: Solve $\partial x_{particle}/\partial t = u_{particle}$
- Treatment of Microphysical Processes is intuitive as the evolution of single hydrometeors is of relevance.
- All other variables like velocity, temperature, pressure, water vapour concentration are field variables of the coupled LES model.
- All SIPs that lie inside a grid box volume are associated with this grid box.

Features of ice LCM

- Described in Sölch & Kärcher, 2010 with technical improvements from Unterstrasser & Sölch, 2014
- Spectrally resolved aerosol physics: non-equlibrium growth of supercooled aerosol particles (solution droplets of sulphuric acid H_2S0_4 and water H_20 (and optionally HNO3)) + their homogeneous freezing; starts at RH_i around 150%
- Heterogeneous ice nucleation of ice nuclei (immersion/deposition mode); Threshold RH_i depends on IN, but usually smaller than for homogeneous freezing.
- Deposition/sublimation including ventilation, Kelvin and kinetic regime corrections and optionally radiative surface fluxes
- Transport including sedimentation and the effect of subgrid scale turbulence
- Aggregation with collision history
- Several ice crystal habit options (plates, bullet rosettes, spheres, hexagonal columns, aggregates), but no habit prediction
- **Stochastic nucleation implementation**
- SIP Merging and Splitting

Benefits

- **Comparison between two moment bulk scheme and LCM**
- **Tagging feature inexpensive**
- **Numerical diffusion: interaction of contrail cirrus and natural cirrus**
- Trajectory analysis
- Etc.

Further benefits are discussed in Grabowski et al, 2019.

The benefits discussed there are mainly complimentary to ones picked here.

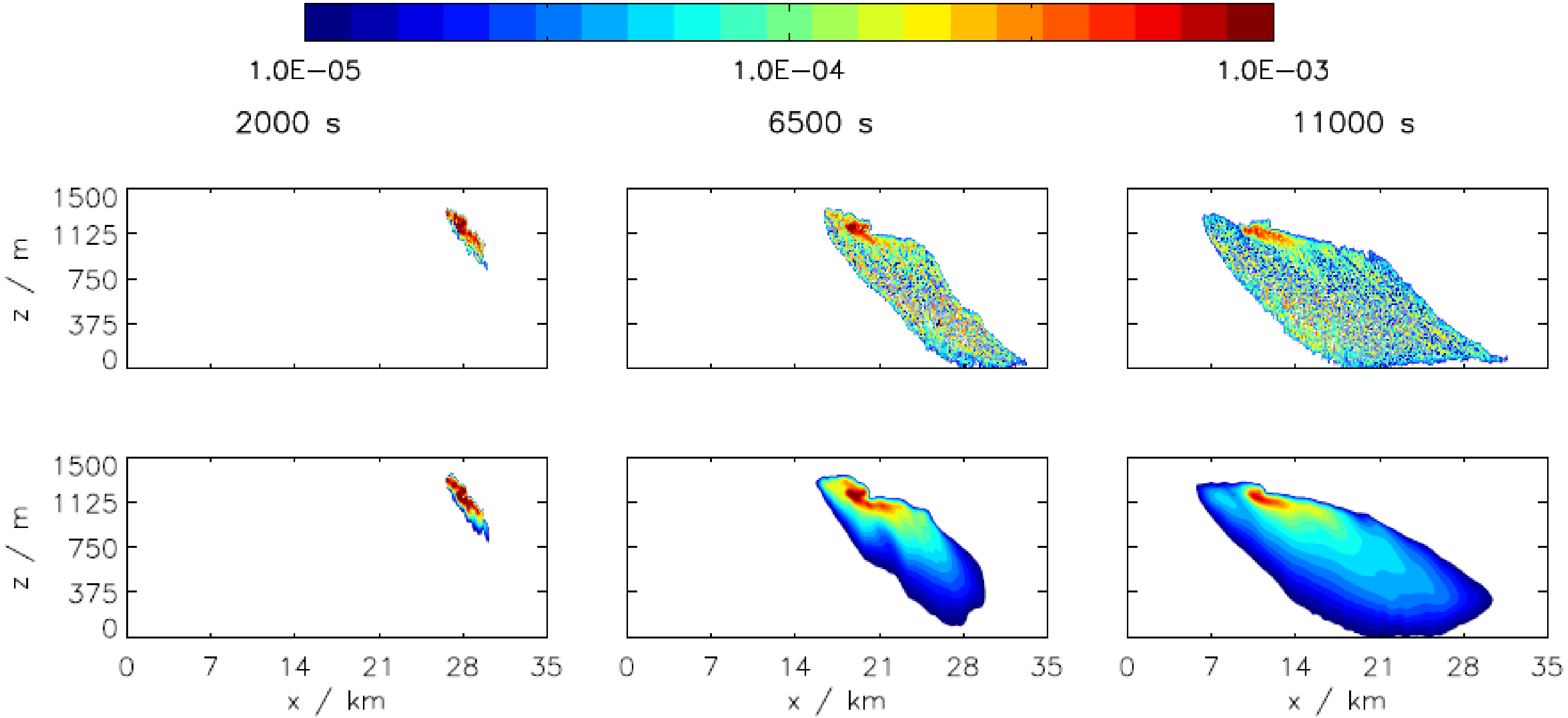
LCM vs. Eulerian bulk scheme

Simulation example: Spreading contrail in the upper troposphere

Extinction coefficient χ in m^{-1}

LCM

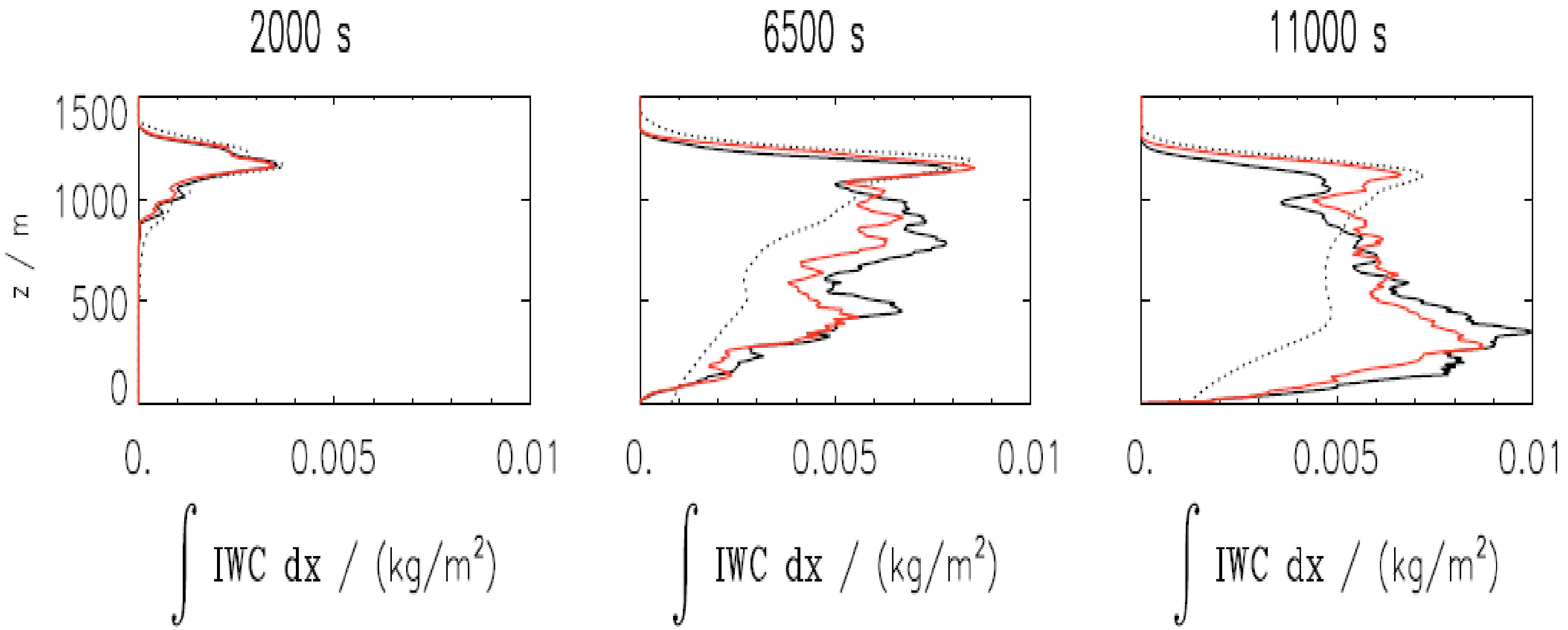
BULK; two moments (Spichtinger & Gierens, 2009)



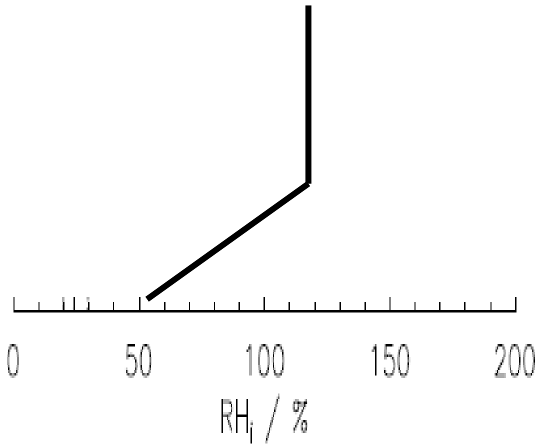
LCMs feature fine-scale structures/fluctuations.

LCM vs. Eulerian bulk scheme

Comparison of **LCM** (solid) and **BULK** (dotted): Vertical distribution



Humidity profile



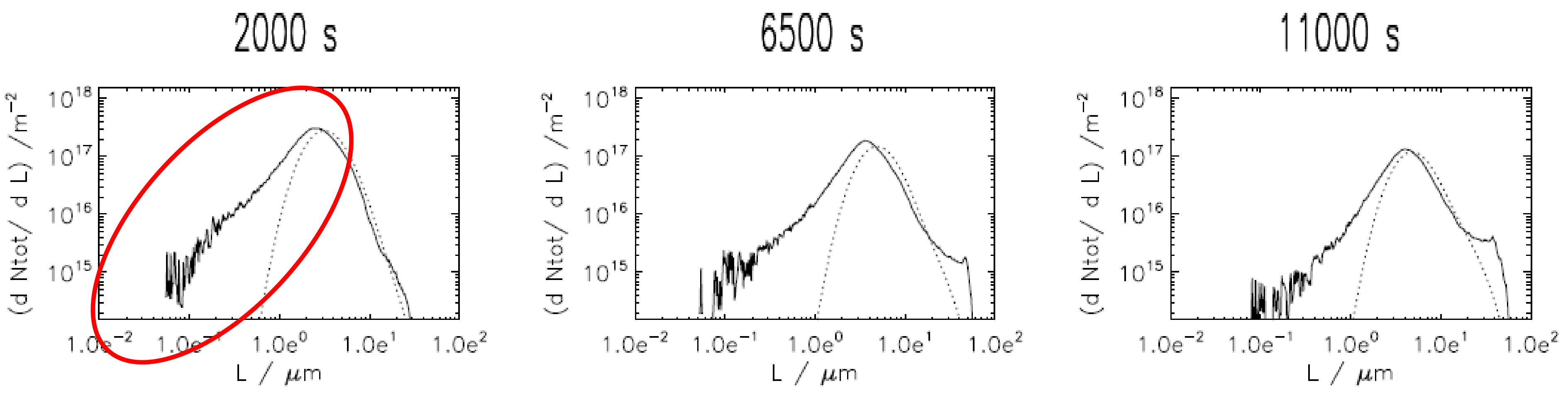
Solid black: original LCM implementation;

Solid red: LCM implementation with sedimentation parametrization as in BULK

Numerical treatment of sedimentation more important than physical parametrisation of settling velocity.

LCM vs. Eulerian bulk scheme

Comparison of **LCM** (solid) and **BULK** (dotted): size distribution



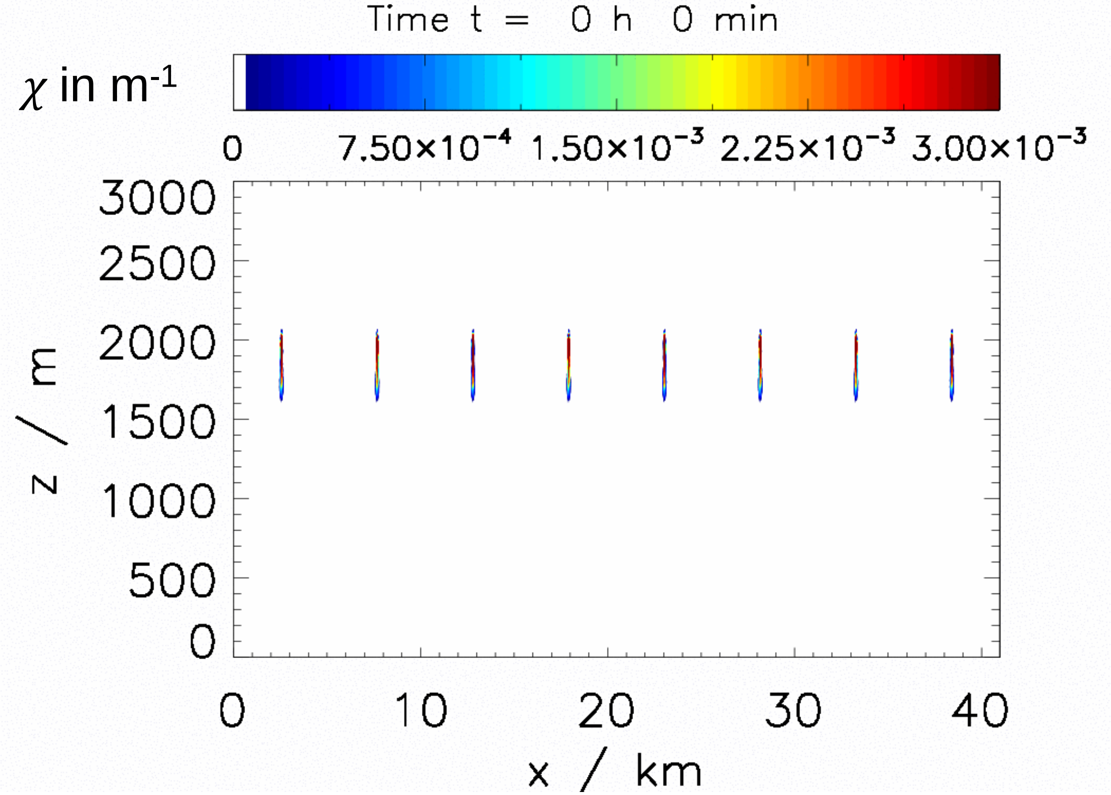
Broadening of size distribution due to Kelvin effect (Lewellen, JAS, 2012).
In (contrail-)cirrus, "spectral ripening" occurs in slowly ascending air and ice crystals get lost (Unterstrasser et al, 2017a).

Adopted from Fig. 9 of Unterstrasser et al, 2017a

Tagging feature

Eight contrails in a supersaturated layer with background vertical wind shear over 4 hours.

Analysis important for quantities for nonlinear dependence of air traffic impact on contrail climate impact.

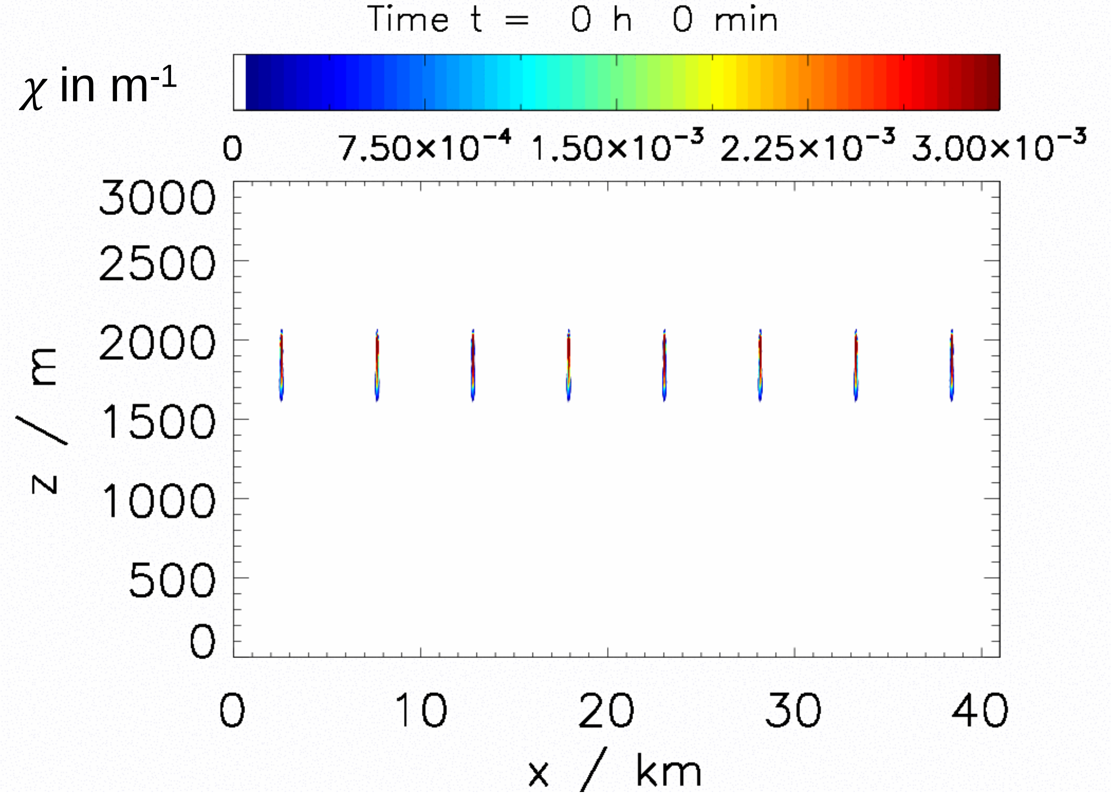


Unterstrasser & Sölch, 2012

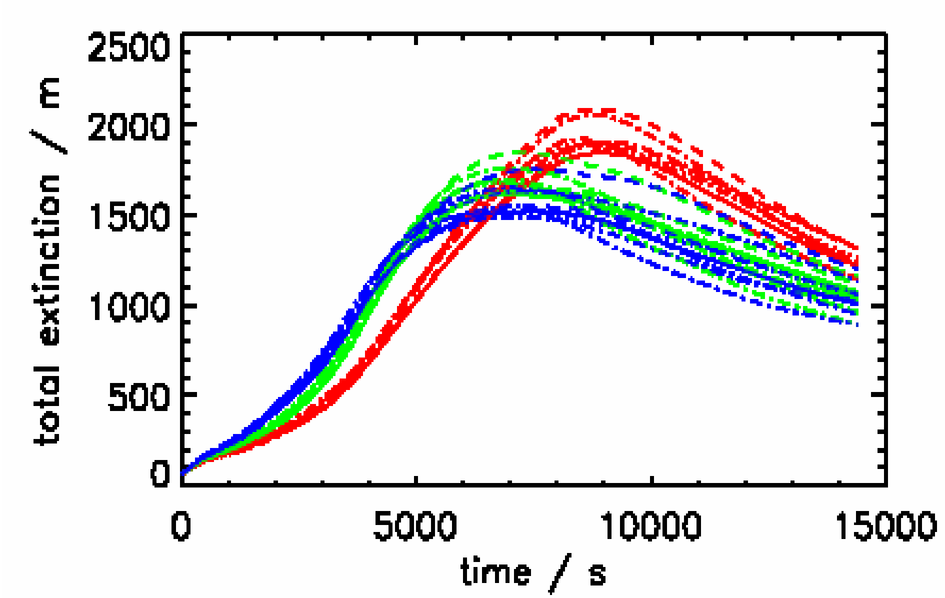
Tagging feature

Eight contrails in a supersaturated layer with background vertical wind shear over 4 hours.

Analysis important for quantities for nonlinear dependence of air traffic impact on contrail climate impact.



Analyse each contrail instance separately by introducing a memory-efficient flag variable

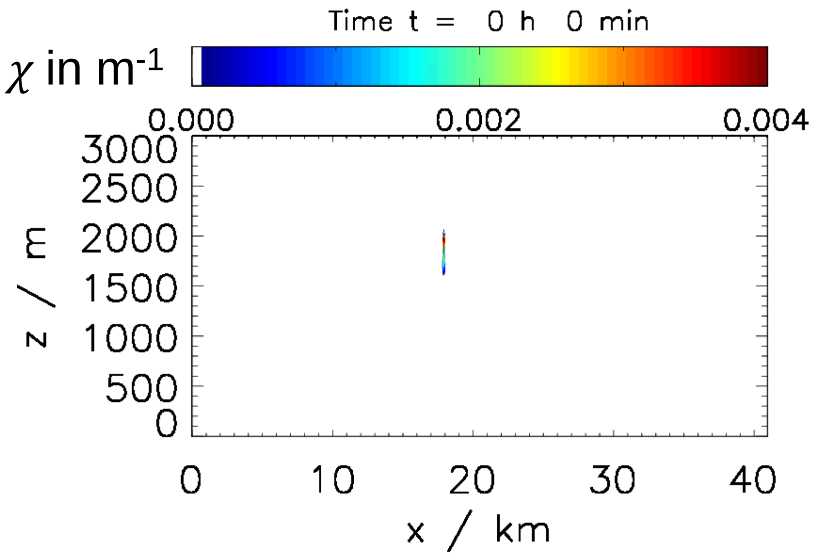


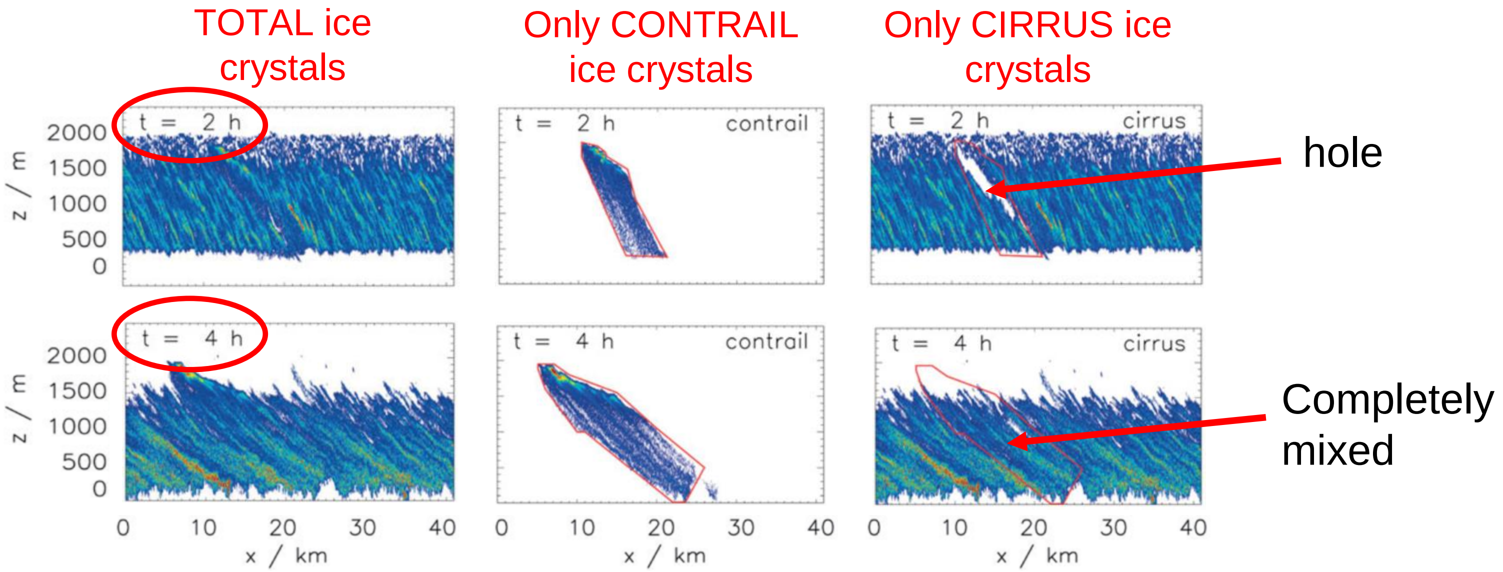
Unterstrasser & Sölch, 2012

For the same analysis in a Eulerian model, one had to establish eight sets of prognostic micro-physics equations. In an LCM, it comes basically for free. No additional computations are required.

Numerical diffusion

In rising air, contrail-cirrus becomes surrounded by natural cirrus once RH_{nuc} is surpassed in the vicinity. Ice crystals of natural cirrus can only form outside of existing contrail-cirrus. Identification of anthropogenic „contamination“ in naturally formed cirrus is important for assessing climate impact of aviation.





After four hours, „natural“ ice crystals are present everywhere inside the contrail-cirrus below z=1500m.

In Eulerian models, this effect could be a spurious one due to numerical diffusion.

There is no numerical diffusion in LCMs and one can be sure that the local co-existence of both cloud types is due to physical reasons. In this example, it is mainly due to differential sedimentation.

Adopted from Figs. 3 & 11 of Unterstrasser et al, 2017b

Formation of hydrometeors in LCMs

In **liquid cloud** LCMs: SIPs are usually initialized in the whole domain and represent CCNs. After activation, the SIP changes its status from aerosol particle to cloud droplet. No new simulation particles are generated during cloud formation.

In **ice** LCM: Strong dependence of number of formed ice crystals on updraught speed w_{syn}. Use spectral bin for solution droplets and generate SIPs with variable weighting factors during ice formation.

Physics: Number of nucleated ice crystals n_{nuc} in a grid box:

$$n_{nuc} = J_f(a_w) \; * \; V_{a,i} \; * \; n_{a,i} \; * \; \Delta t_{nuc} \; * \; V_{GB}$$

- Nucleation rate $J_f(a_w)$: depends **very sensitively** on relative humidity, i.e updraught speed
- $V_{a,i}$ volume of one aerosol in bin i
- $n_{a,i}$ number concentration of aerosols in bin i
- Nucleation timestep Δt_{nuc}
- Grid box volume V_{GB}

Depends on number of bins

Numerical parameters

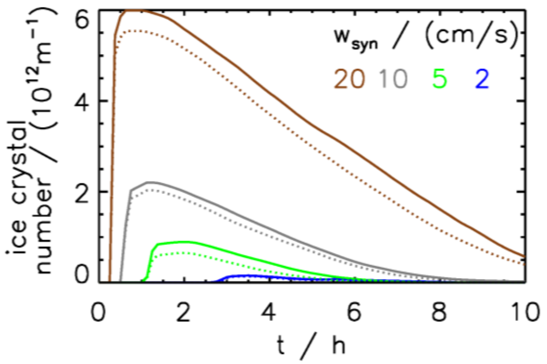
Increase resolution => n_{nuc} is smaller

Implementation with strong threshold:

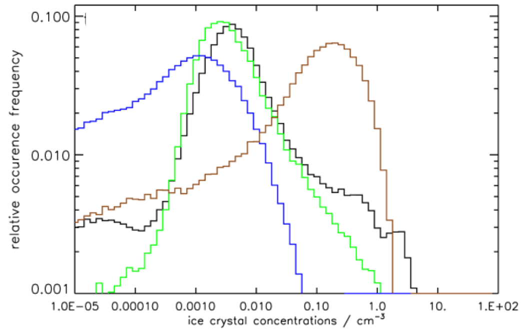
SIP generation condition $n_{nuc} > n_{min}$ (avoids generation of too many SIPs).

Not necessary in Eulerian models, where n can be continuously increased.

Total ice crystal number evolution



PDF of ice crystal number concentrations



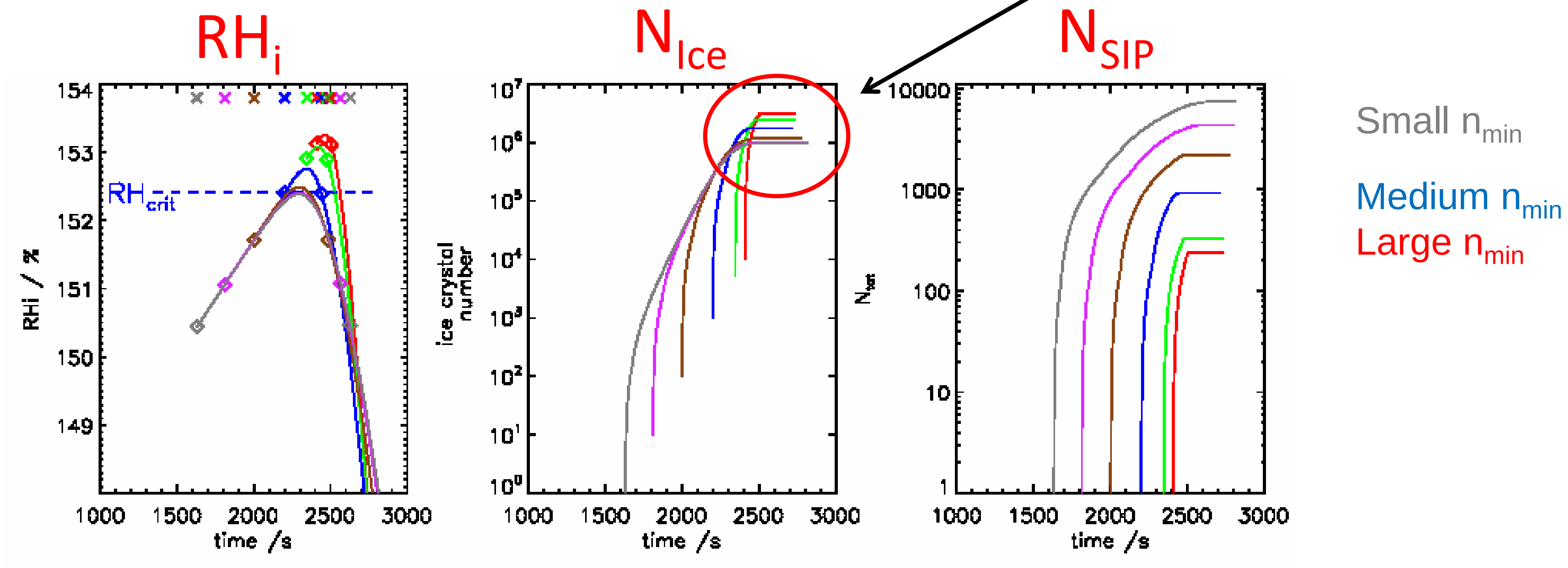
$0.01 L^{-1}$ ....$10 cm^{-3}$

Adopted from Figs. 4 & 8 of Unterstrasser et al, 2017a

Nucleation implementation with strong threshold

Variation of strong threshold n_{min} in box model simulations

No convergence in N_{ice} with N_{SIP}



SIP generation condition $n_{nuc} > n_{min}$ with large n_{min} retards ice crystal formation and number of formed ice crystals is eventually too high!!

Adopted from Fig. 9 of Unterstrasser & Sölch, 2014

Stochastic nucleation implementation

Use a weak threshold:

If $n_{nuc} > n_{min}$: generate SIP with $n_{sim} = n_{nuc}$ (as before)

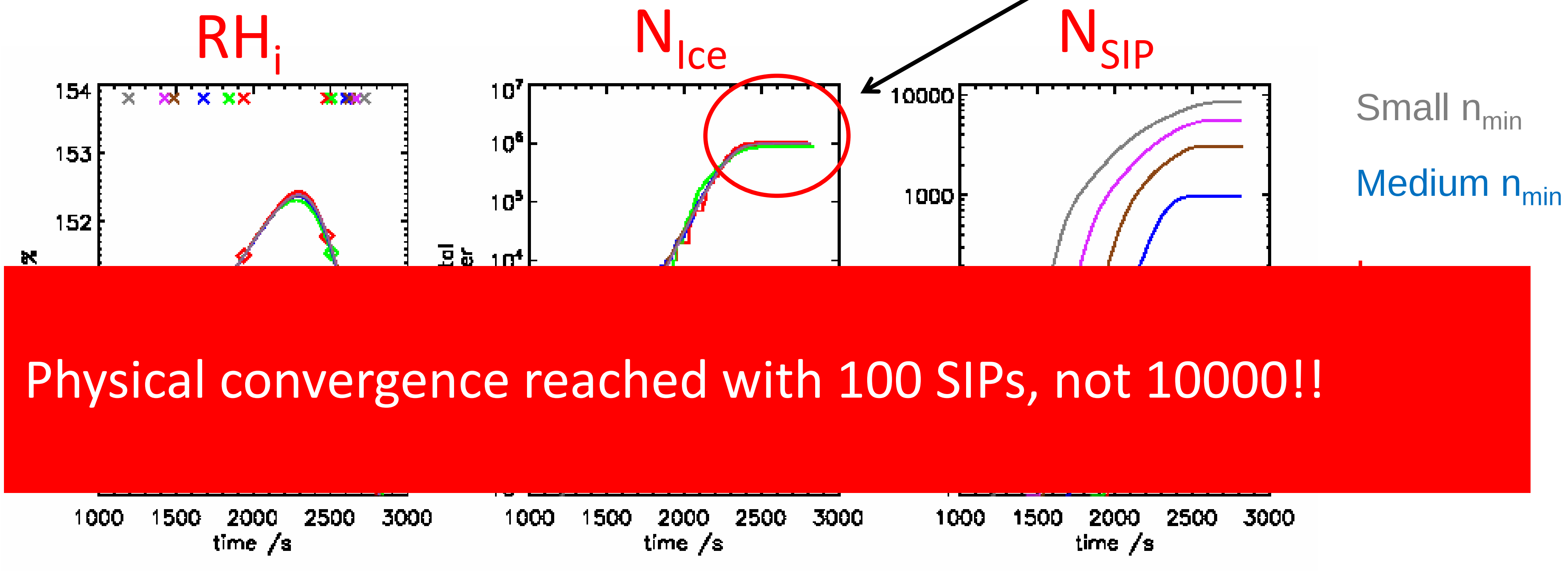
If $n_{nuc} < n_{min}$:
generate a SIP with $n_{sim} = n_{min}$ with probability $P_{SIP} = n_{nuc} / n_{min}$

Add stochastic component to nucleation implementation

Stochastic nucleation implementation

Variation of weak threshold n_{min} in box model simulations

Convergence in N_{Ice}



Stochastic component removes sensitivity to numerical parameter n_{min} !!

Adopted from Fig. 9 of Unterstrasser & Sölch, 2014

Summary

General design concept introduced

A few benefits of the LCM approach

- Spectral ripening due to Kelvin effect illustrated.
- Numerical treatment of sedimentation more important than physical parametrisation of settling velocity.
- Tagging feature illustrated.
- LCMs with no numerical diffusion => better interpretable simulation results.

Stochastic nucleation implementation with a weak threshold.

=> Avoid strong thresholds in discrete LCMs (an aspect absent in continuous Eulerian approaches).

Figure sources

Unterstrasser, S., and I. Sölch, 2012: Numerical modeling of contrail cluster formation. Proceedings of the 3rd International Conference on Transport, Atmosphere and Climate (TAC-3) R. Sausen, S. Unterstrasser, and A. Blum, Eds.,114-119

Unterstrasser, S. , I. Sölch, 2014: Optimisation of the simulation particle number in a Lagrangian ice microphysical model, *Geosci. Model Dev.*, 7, 695-709

Unterstrasser, S., K. Gierens, I. Sölch, M. Lainer, 2017a: Numerical simulations of homogeneously nucleated natural cirrus and contrail-cirrus. Part 1: How different are they?, *Meteorol. Z.*, 26, 621-642

Unterstrasser, S., K. Gierens, I. Sölch, M. Wirth, 2017b: Numerical simulations of homogeneously nucleated natural cirrus and contrail-cirrus. Part 2: Interaction on local scale, *Meteorol. Z.*, 26, 643-661