The Lagrangian ice microphysics code LCM within EULAG: Applications and current developments

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Outline

Introduction to LCM: overview, physics, strategy, benefits

Applications: contrails and natural cirrus

Recent improvements

LCM module: overview

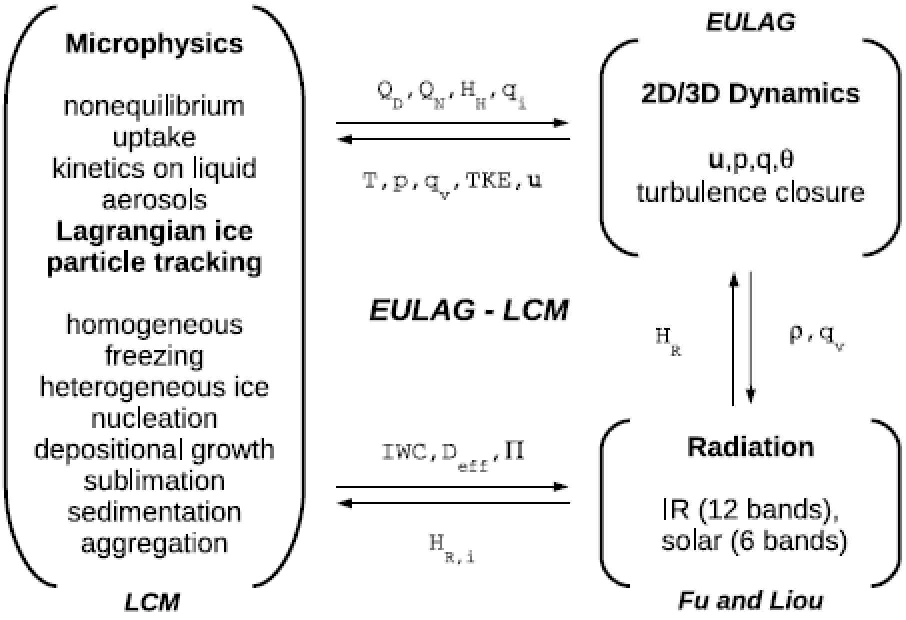

Figure 1. Schematic overview of the DLR EULAG-LCM model system. The LCM (Lagrangian Cirrus Module) can also be coupled to other dynamical core and radiation models, provided the interfaces for the exchange of model variables are similar.

Sölch & Kärcher, 2010, QJRMS

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LCM module: physics

explicit aerosol and ice microphysics:

- non-equlibrium growth of supercooled aerosol particles (sulphuric acid H2S04 + H20) + their homogeneous freezing
- heterogeneous ice nucleation of ice nuclei (immersion/deposition mode)
- deposition/sublimation including ventilation, Kelvin and kinetic regime corrections and optionally radiative surface fluxes

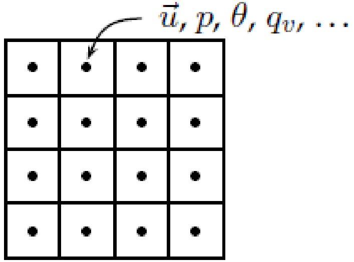
LCM module: physics

explicit aerosol and ice microphysics:

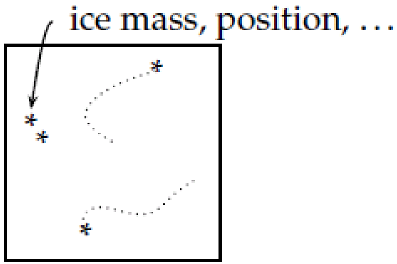
- sedimentation
- aggregation by gravitational settling
- advection including subgrid scale turbulence
- several ice crystal habit options

LCM module: strategy

- Lagrangian approach for ice phase: each simulation particle (SIP) represents m_{sim} identical ice crystals.



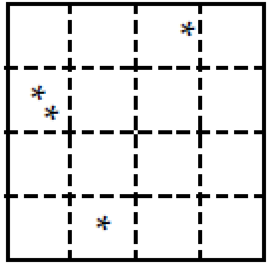
- Eulerian approach for all other quantities: water vapor, aerosol concentrations (spectrally resolved)



- SIPs have discrete position xp, yp, zp

LCM module: strategy

- Attribution of SIPs to grid box for coupling with EULAG:
    - 1 to 1 relation
    - Any SIP affects one GB
    - SIPs use grid point values of EULAG (interpolation optionally)
    - so far only Cartesian grid supported
- Coupling
    - water vapor, latent heat, aerosol for nucleation
    - density potential temperature (ice mass + water vapour corrected air density)



LCM module: strategy

- Nucleation
  - subcycling of timestep
  - a SIP is generated if more than m_{min} real ice crystal form ($m_{sim} > m_{min}$).

- Advection
  - EULAG wind
  - sedimentation fall speed
  - auto-correlated subgrid scale turbulent fluctuations

LCM module: strategy

- Deposition and sedimentation
    - solved individually for each SIP

- Aggregation
    - only by differential sedimentation
    - no „lateral“ collisions, turbulence enhancement
    - pairwise collision testing of nearby SIPs (sort SIPs by zp; costs O(N log N))

LCM module: benefits

Lagrangian advection treatment

Deposition: Ice crystal size distributions evolve freely

Sedimentation: Straight-forward inclusion in advection equation

Aggregation: collisions explicitly resolved; SIPs carry information on collision history

Analysis of ice crystal trajectories

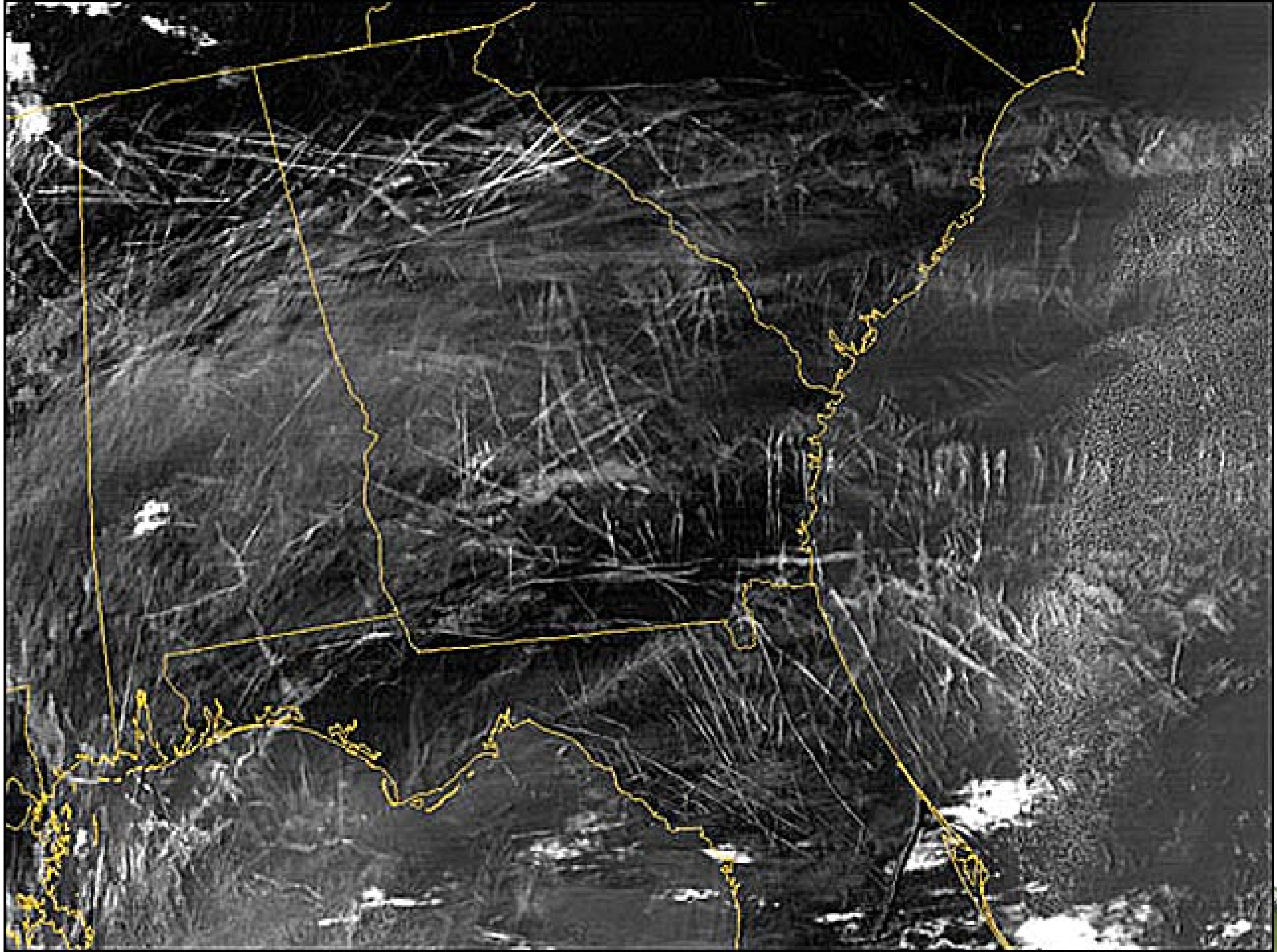
Application

At DLR Oberpfaffenhofen climate impact of aviation is assessed.

Focus on contrail research (but also natural cirrus)

Application: contrail basics

- The climate impact of contrail-cirrus only vaguely known
  (Lee et al., 2009; Sausen et al., 2005; IPCC, 2007)
  Radiative Forcing of contrail-cirrus probably larger than that of accumulated aviation CO2 emissions (Burkhardt & Kärcher, 2011)
- Discrimination from natural cirrus difficult (in-situ and in satellite imagery)
- Formation of contrails is temperature-, not humidity-controlled!
  Below ~225K contrails form irrespective of humidity
- Causes additional cloud coverage in supersaturated areas where natural cirrus formation is still inhibited.




Application – Temporal evolution of a Contrail

The contrail evolution can be divided into 3 temporal phases:

Jet Phase	Vortex Phase	Dispersion Phase
5 - 10s	2 - 4 minutes	Minutes to hours

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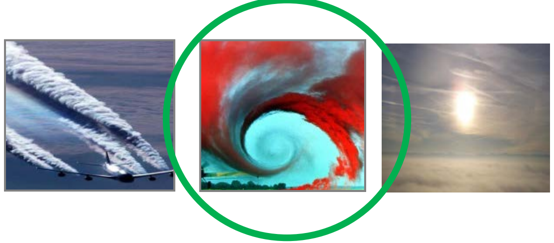
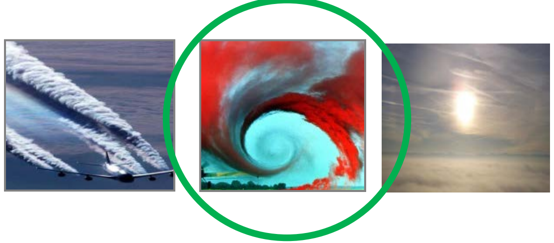
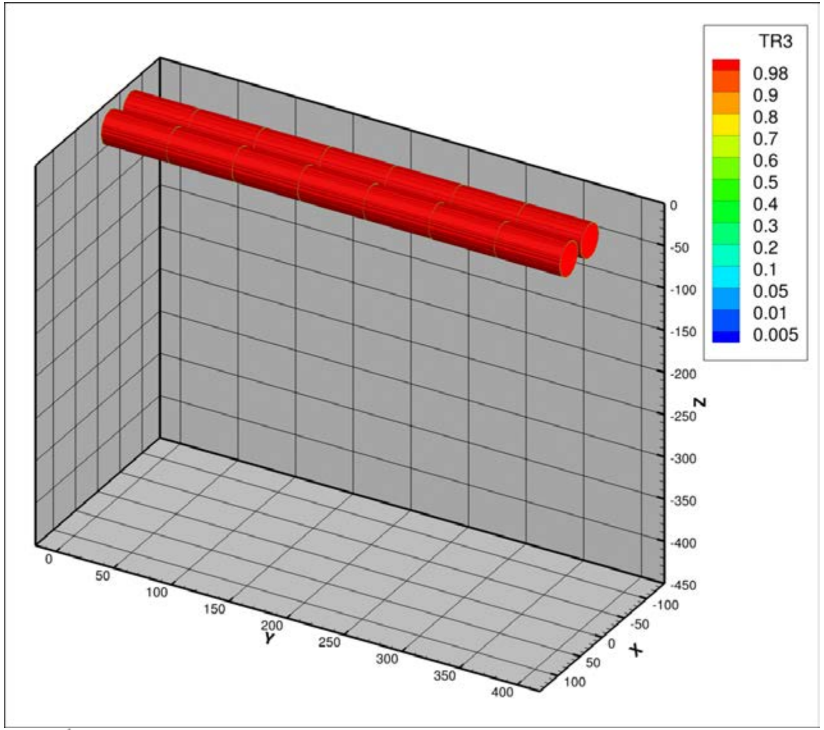


Application: contrail vortex phase

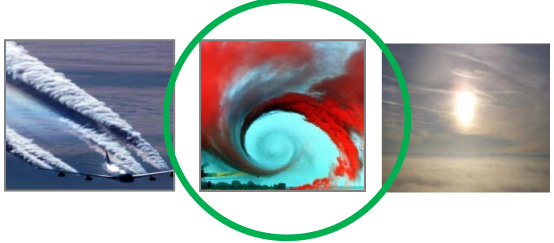
- Dimension of aircraft plumes and contrails are affected by vortex dynamics
- Adiabatic heating in downward sinking vortex system leads to ice crystal loss



Application: contrail vortex phase



- 3D simulation with 80e6 grid points and 160e6 SIPs
- covers first 5 minutes behind aircraft

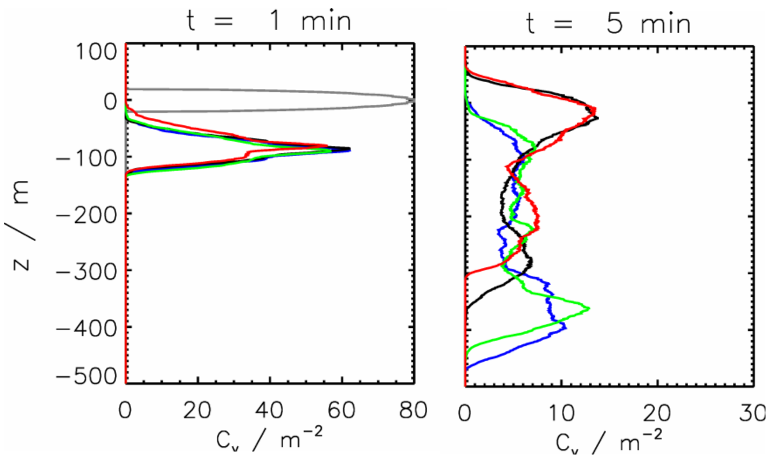


Application: contrail vortex phase

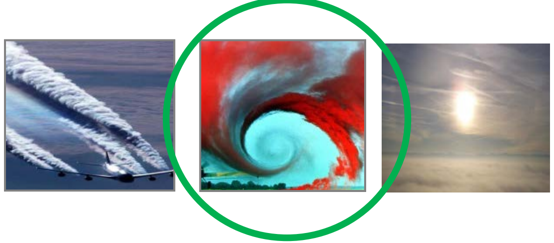
Examine spatial distribution of aircraft emissions (passive tracer):

- Variation of thermal stratification and/or ambient turbulence

Vertical tracer profile



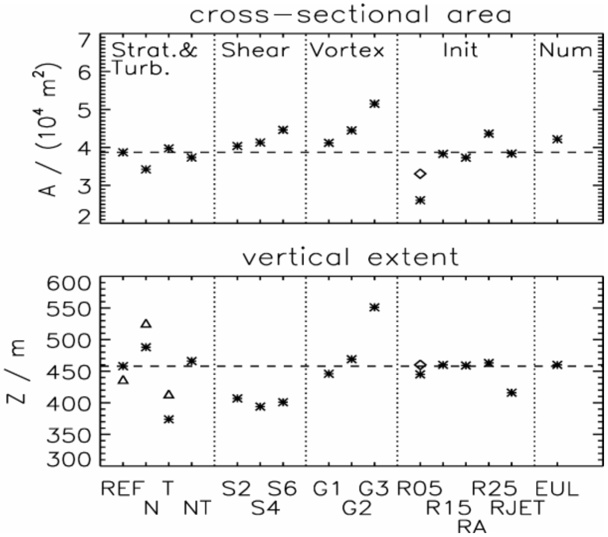
Dimension of aircraft exhaust plumes at cruise conditions: effect of wake vortices.
S.Unterstrasser, R. Paoli, I. Sölch, C. Kühnlein, T. Gerz, subm to ACP



Application: contrail vortex phase

Examine spatial distribution of aircraft emissions (passive tracer):

- Summary of sensitivity analyses



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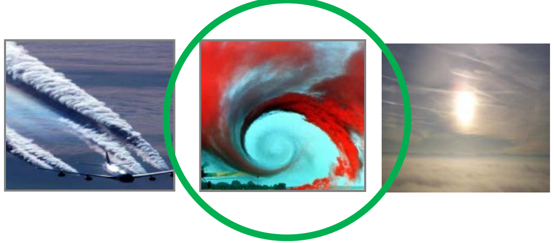
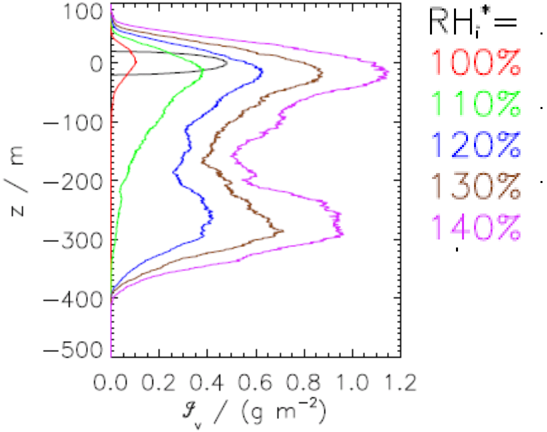
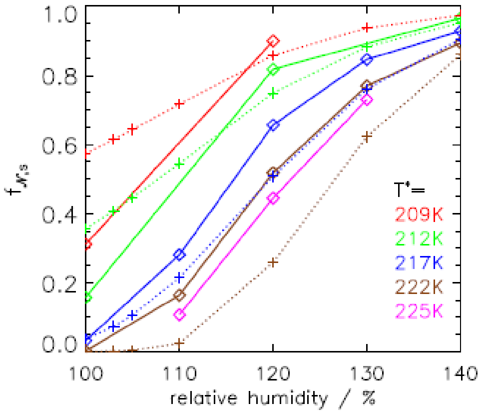


Application: contrail vortex phase

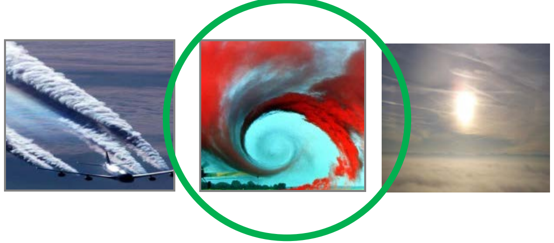
Contrail ice mass profile



Crystal loss



Large eddy simulation study of contrail microphysics and geometry during the vortex phase and consequences on contrail-to-cirrus transition. *S.Unterstrasser*, in prep.



Application: contrail vortex phase

EULAG-LCM “efficient” tool for extensive parameter studies!

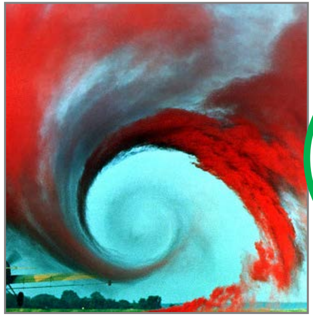
~50 sensitivity simulations cp. to 5 - 10 simulations in *Naiman et al, 2011* or *Paugam et al, 2009*

Stanford code: unstructured grid LES solver (Mahesh et al, 2004; Ham et al, 2007)

NTMIX, CERFACS: compressible code

Application: contrail to cirrus transition

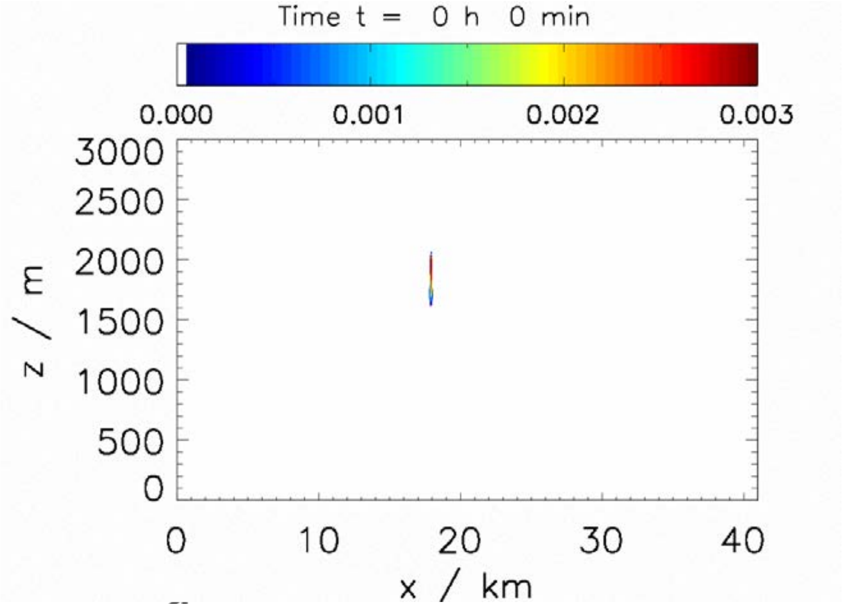
Study long-term evolution contrails





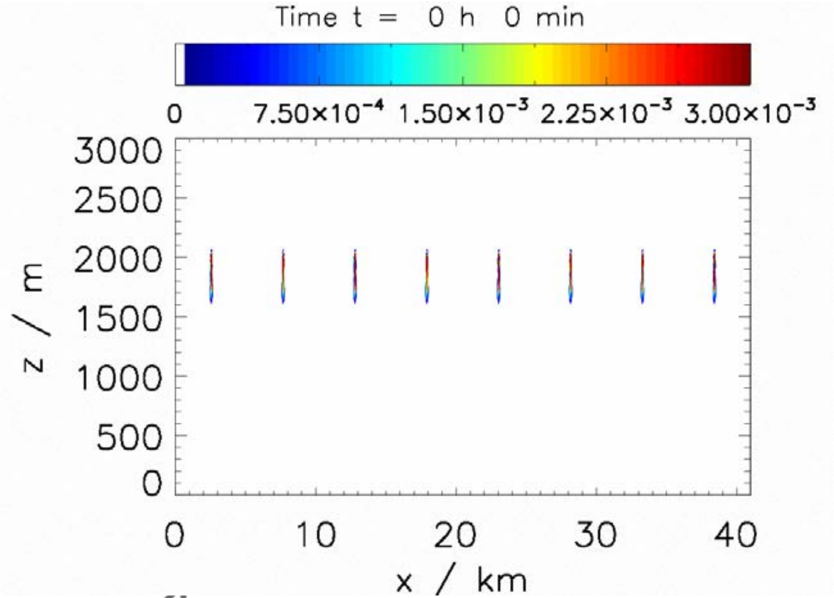
Application: contrail to cirrus transition

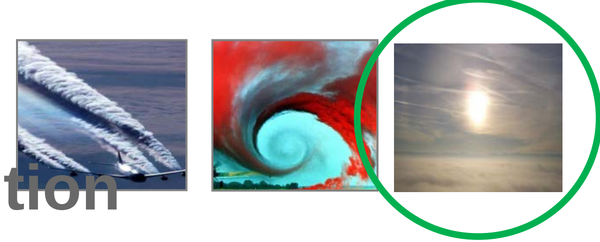
Evolution of a single contrail in a supersaturated layer with background vertical wind shear over 4 hours.



Application: contrail to cirrus transition

Evolution of eight contrails in a supersaturated layer with background vertical wind shear over 4 hours.





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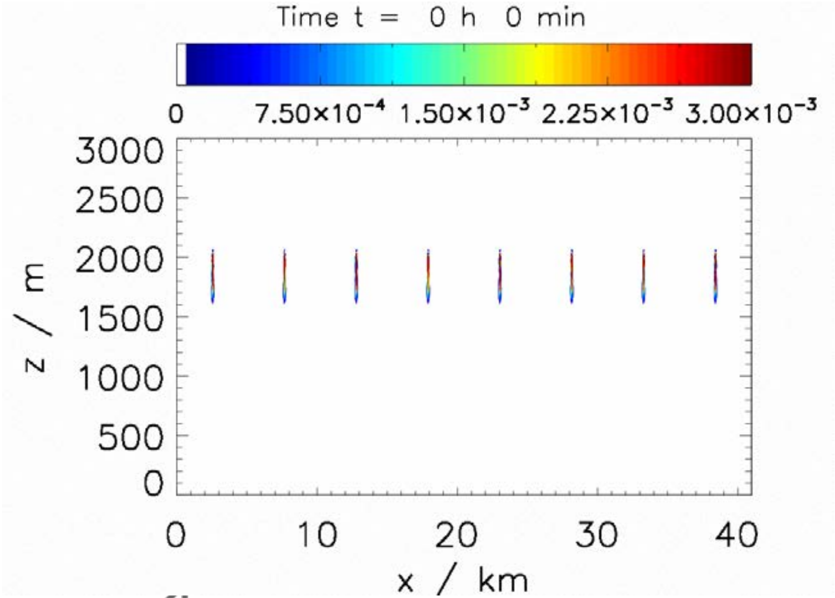
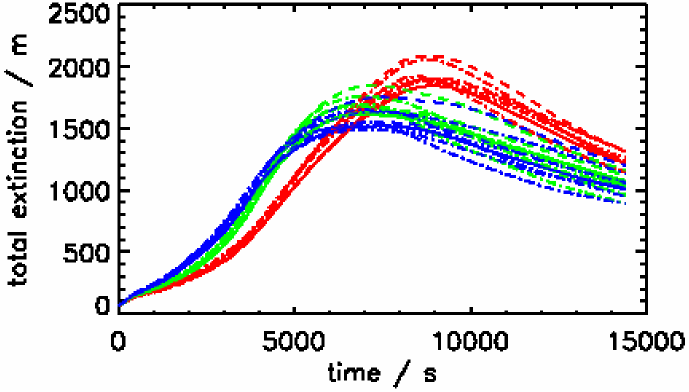




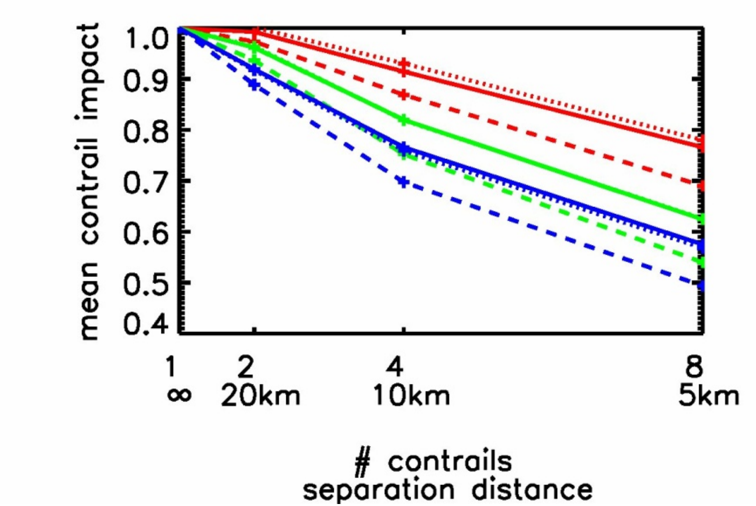
Analyse each contrail instance separately by introducing a memory-efficient flag variable



Application: contrail to cirrus transition

Formation of contrail cluster: Saturation effects in regions with dense air traffic

Non-linear scaling of contrail climate with airtraffic density



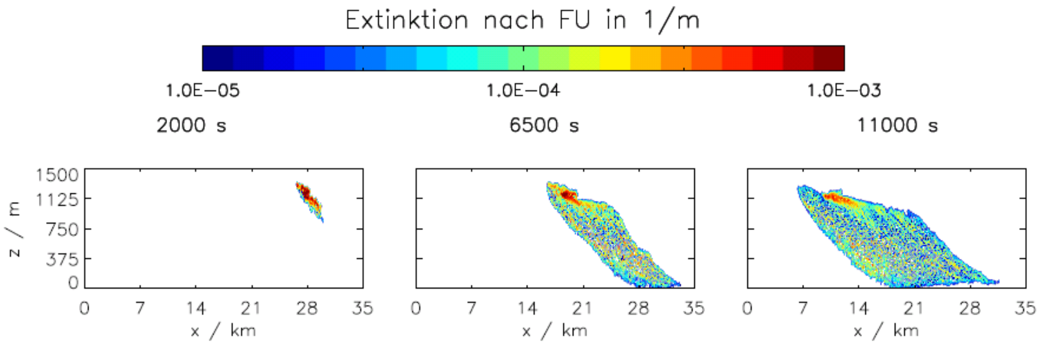
Numerical Modeling of contrail cluster formation. *S.Unterstrasser & I Sölch*, Proceedings of TAC-3 Conference on Transport, Atmosphere and Climate



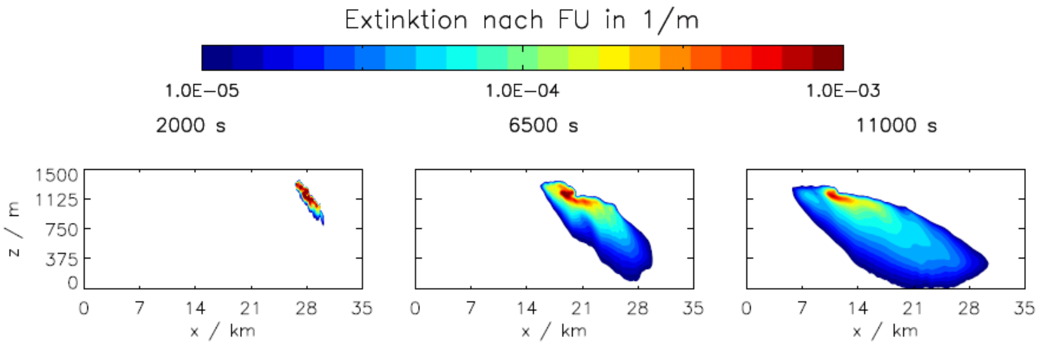
Application: contrail to cirrus transition

Comparison of

LCM



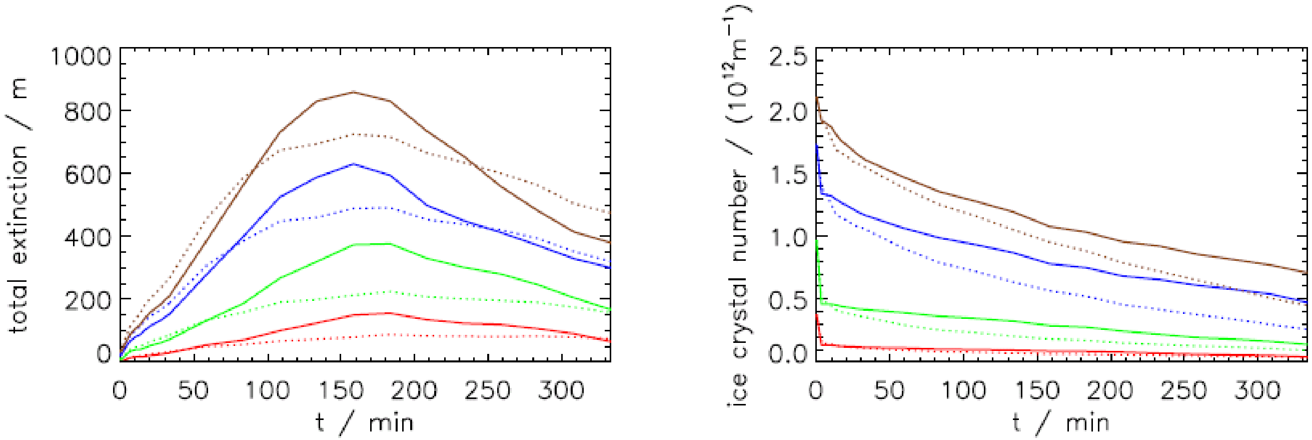
BULK
(Spichtinger & Gierens)





Application: contrail to cirrus transition

Comparison of LCM (solid) and BULK (dotted)



Total extinction agrees very well.
Ice crystal loss due to Kelvin effect (Lewellen, 2012) in LCM.
In BULK, ice crystal loss numerical artefact (Gierens & Bretl, 2009)

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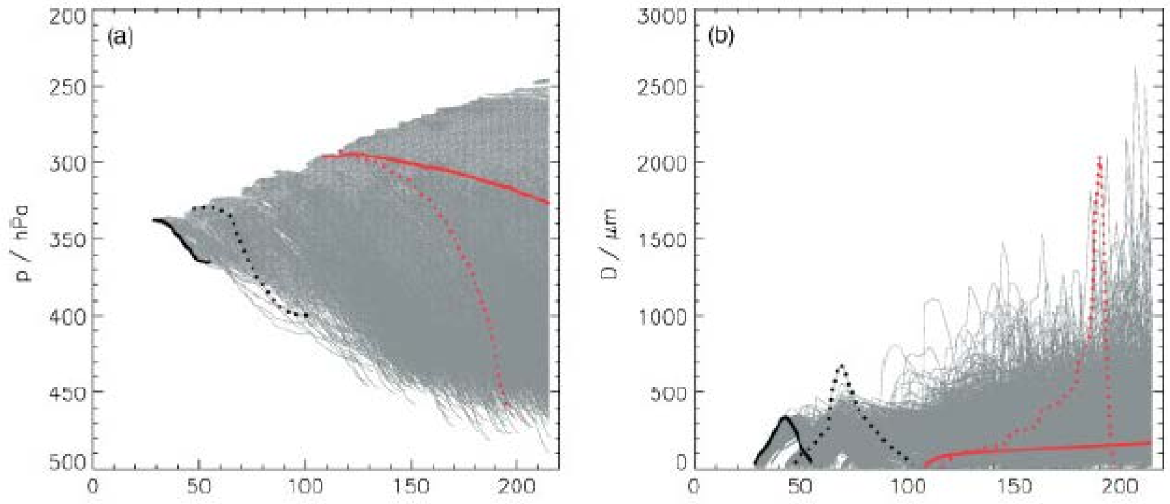
Application: Trajectory-based analyses

Simulation of a midlatitude cirrus cloud system based on observations (Sölch & Kärcher, 2011)



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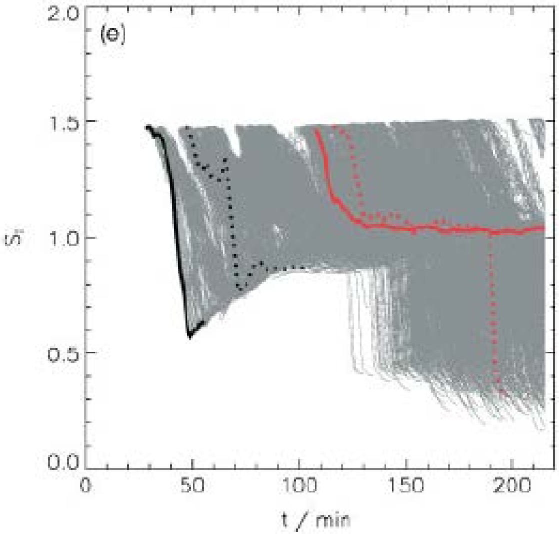

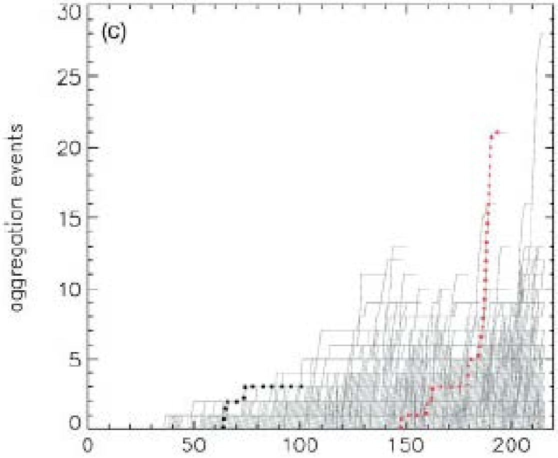

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Recent improvements

Memory and computing time scales linearly with number of SIPs.
How many SIPs do we need to reach physical convergence?

1. Stochastic nucleation implementation
2. Adaptation of SIP number
3. Technical implementation

Stochastic nucleation implementation

Number of nucleated ice crystals m_{nuc} :

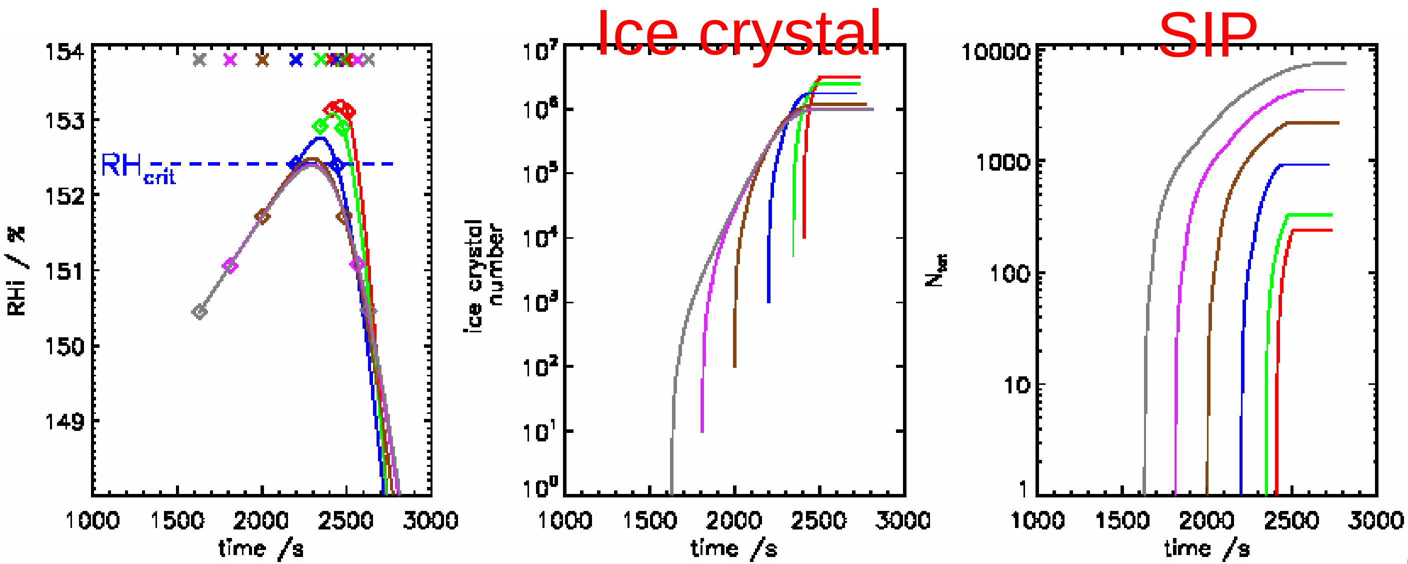
$$m_{nuc} = J_f(a_w)\ V_{a,i}\ n_{a,i}\ \Delta t_{nuc}\ V_{GB}$$

- Nucleation rate $J_f(a_w)$
- $V_{a,i}$ and $n_{a,i}$ volume and number of aerosols in bin i
- Nucleation timestep Δt_{nuc}
- Grid box volume V_{GB}

SIP generation condition $m_{nuc} > m_{min}$

Stochastic nucleation implementation

SIP generation condition $m_{nuc} > m_{min}$ retards ice crystal formation
Variation of m_{min} in box model simulations



Stochastic nucleation implementation

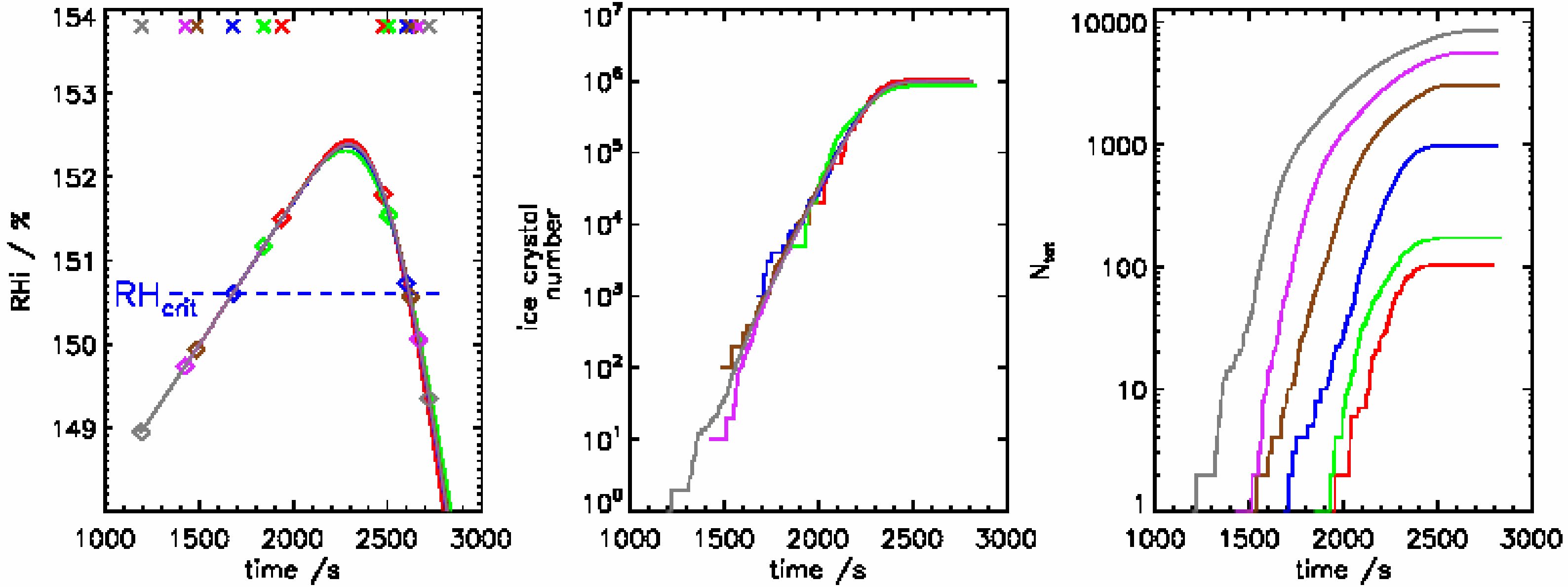
SOLUTION:
As before generate SIP if $m_{nuc} > m_{min}$ with $m_{sim} = m_{nuc}$

New stochastic component, if $m_{nuc} < m_{min}$:
generate SIP with $m_{sim} = m_{min}$ with probability $P_{SIP} = m_{nuc} / m_{min}$

Stochastic nucleation implementation

Ice crystal

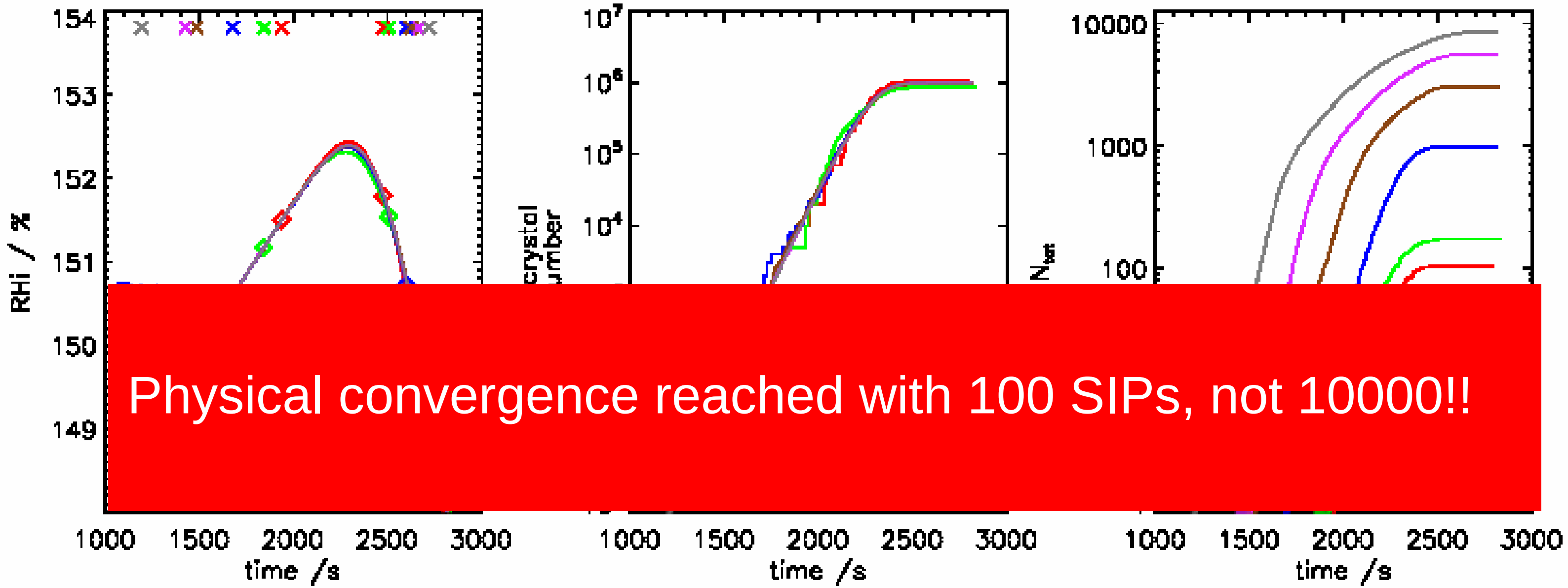
SIP



Stochastic nucleation implementation

Ice crystal

SIP



Physical convergence reached with 100 SIPs, not 10000!!

SIP number adaptation

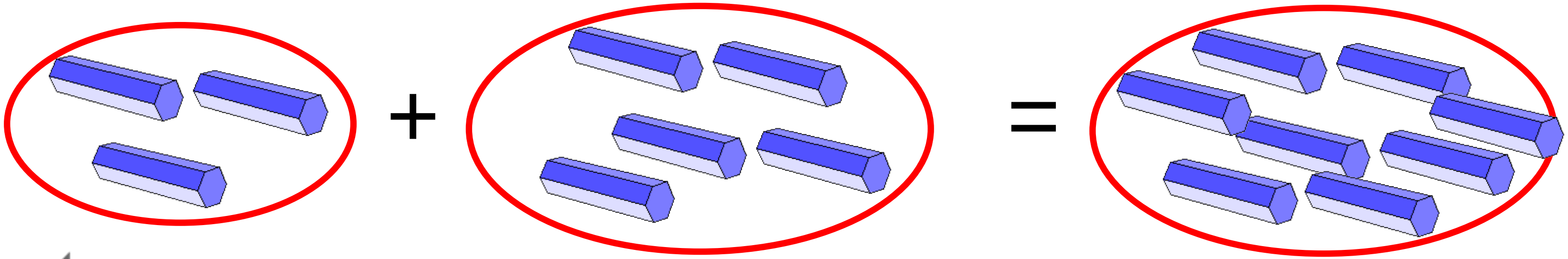
Deposition/sublimation and sedimentation are well resolved with few SIPs.

Operation SIPMERGE:
Merge two similar SIPs (position, radius) into one SIP with

SIP1 $m_{sim,1}$ = 3 ice crystals

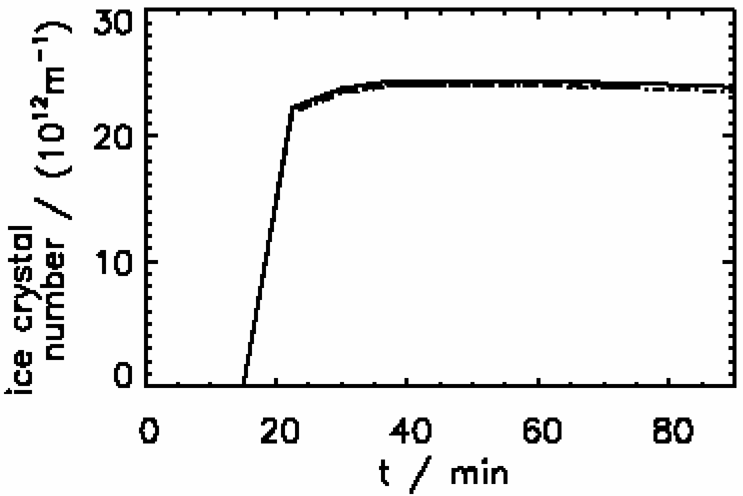
SIP2 $m_{sim,2}$ = 5

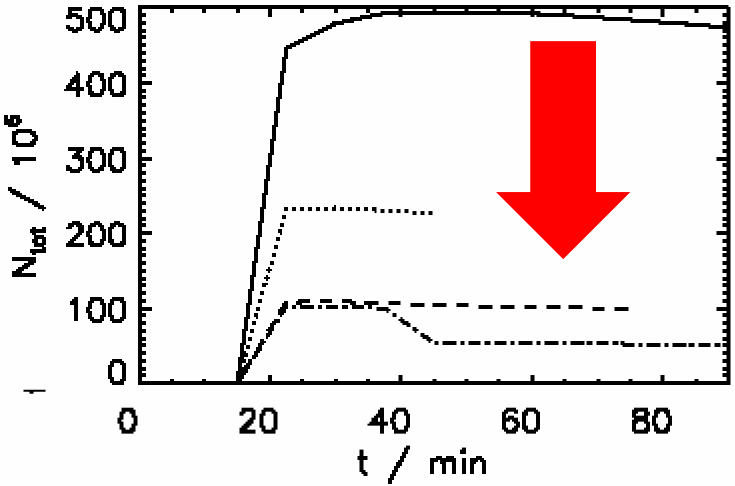
SIPnew $m_{sim,new} = m_{sim,1} + m_{sim,2}$



SIP number adaptation

Application of SIPMERGE further reduces SIP number





Stochastic nucleation implementation SIP number adaptation

Described in

Unterstrasser, S. and Sölch, I.: *Speeding up a Lagrangian ice microphysics code*, Geosci. Model Dev. Discuss., 6, 3787-3817, doi:10.5194/gmdd-6-3787-2013, 2013

LCM implementation

Original LCM version in F77 style (fixed format + memory management).
Static memory allocation of SIP data very memory-inefficient!!

- A-priori guess for maximum number of SIPs per processor and per grid box.
- Inefficient data structure to keep track to which grid box a SIP belongs.

LCM implementation

1. Code reorganisation

- Extract LCM code from .csh file

- Split in several files (around 20)
- Convert to F90

- Reduce LCM-codes in eulag.csh

- Communication with EULAG via few interface routines LCM_init, LCM_timestep, LCM_outp and LCM_finalize (AND common blocks)

LCM implementation

2. Dynamic SIP memory allocation using singly linked lists

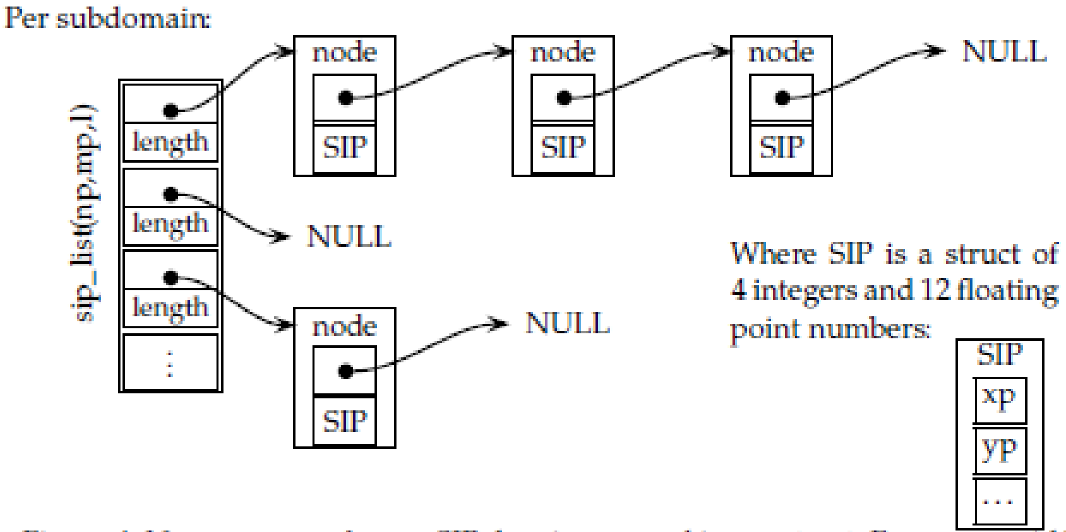
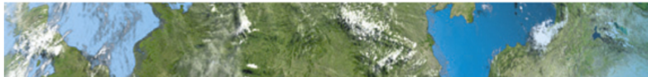


Figure 4: New storage scheme: SIP data is grouped into a *struct*. For every grid box there is a separate linked list which stores those SIP *structs*. The *sip_list* array contains a pointer to the head of each linked list.

B. Stegmaier, Oct 2013, master thesis CompSci



LCM implementation

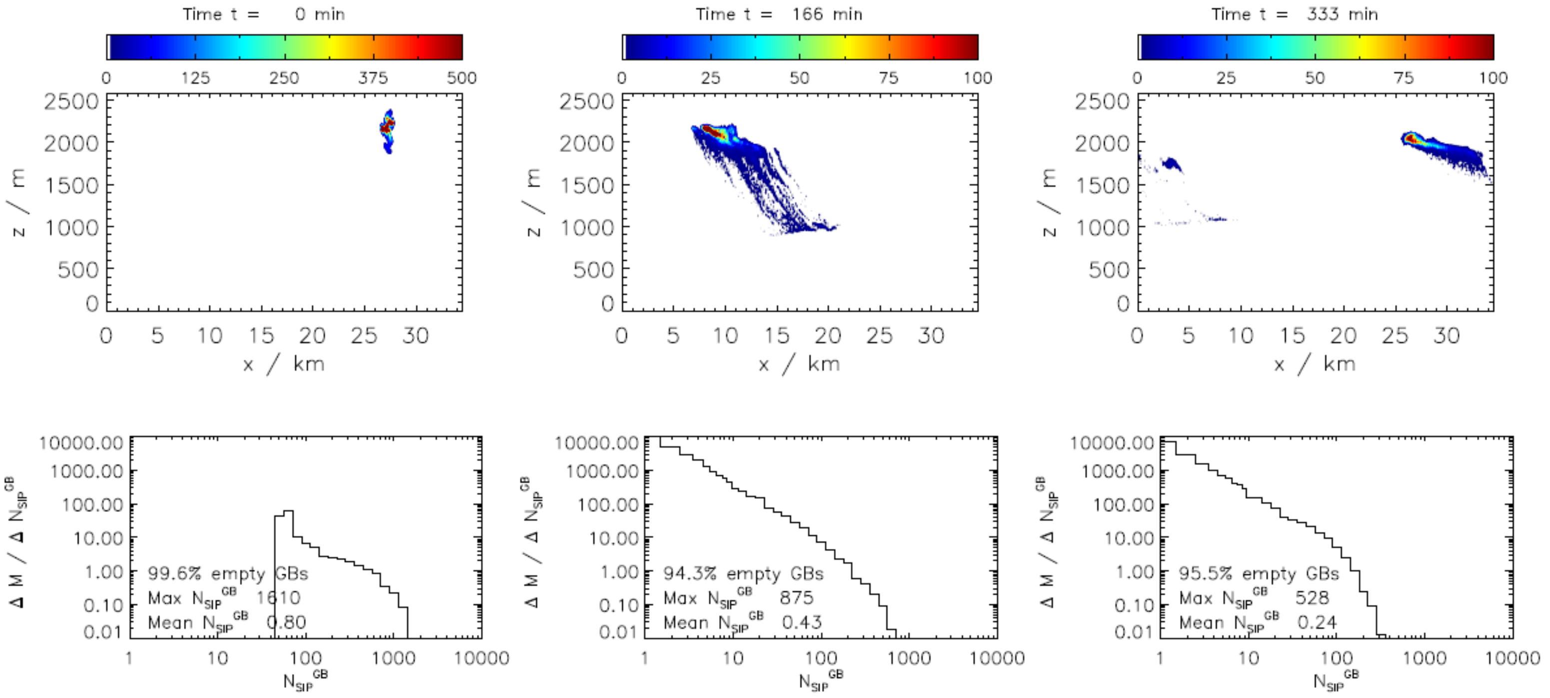
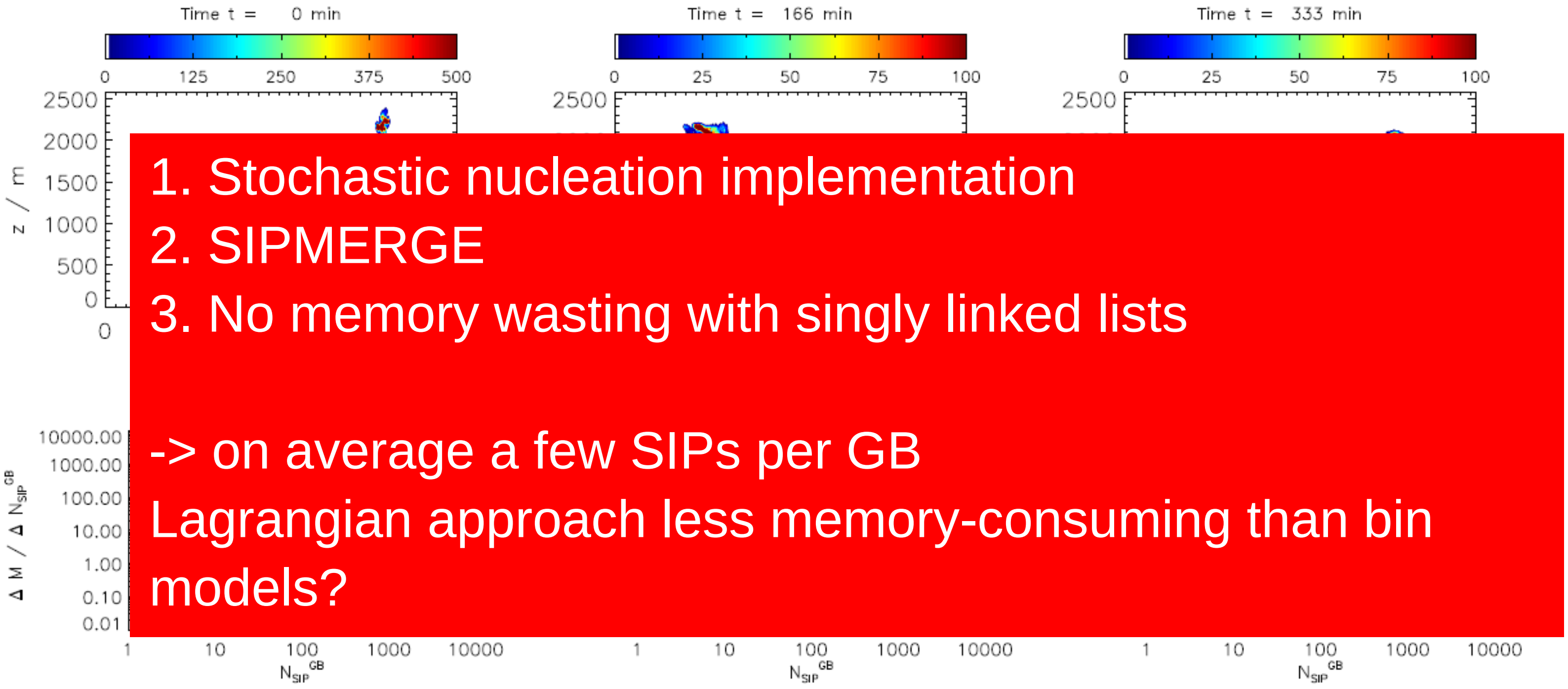


Figure 2: A simulated contrail cirrus cloud after 0 min, 166 min and 333 min. The upper panel shows the number of SIPs per grid box $N_{\mathrm{SIP}}^{\mathrm{GB}}$ over a 2D cross-section. Colorbars do not extend to the maximum $N_{\mathrm{SIP}}^{\mathrm{GB}}$ value. The frequency of occurence of a certain $N_{\mathrm{SIP}}^{\mathrm{GB}}$ value can be read from the histograms in the lower panel. Only non-empty grid boxes are taken into account, as $N_{\mathrm{SIP}}^{\mathrm{GB}}$ is zero for over 94% of all grid boxes.

LCM implementation



1. Stochastic nucleation implementation
2. SIPMERGE
3. No memory wasting with singly linked lists

-> on average a few SIPs per GB

Lagrangian approach less memory-consuming than bin models?

Figure 2: A simulated contrail cirrus cloud after 0 min, 166 min and 333 min. The upper panel shows the number of SIPs per grid box $N_{\mathrm{SIP}}^{\mathrm{GB}}$ over a 2D cross-section. Colorbars do not extend to the maximum $N_{\mathrm{SIP}}^{\mathrm{GB}}$ value. The frequency of occurence of a certain $N_{\mathrm{SIP}}^{\mathrm{GB}}$ value can be read from the histograms in the lower panel. Only non-empty grid boxes are taken into account, as $N_{\mathrm{SIP}}^{\mathrm{GB}}$ is zero for over 94% of all grid boxes.

Future plans & points for discussion

Related to LCM implementation

- LCM still coupled with old EULAG version (the one without the common block files)
- Couple to EULAG2p and finally to EULAG3p (SIP transfer routines have to be adapted)
- LCM supports only Cartesian grids.
  Curvilinear grids: attribution of SIPs to GB not straighforward

Future plans & points for discussion



Contrail formation:

Jet phase modeling with pseudocompressible equations?

- Mixing of hot aircraft exhaust with cold ambient air
- Strong axial velocity of jet
- usually studied with 0D-box models, recently 3D-study with compressible code (Paoli et al, 2013, Phys. Fluids)

Acknowledgement

The simulations were carried out at the high performance computing facilities of the DKRZ in Hamburg.

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CONCLUSION=CONtrailCLUsterSimulatION

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