



**Pacific  
Northwest**  
NATIONAL LABORATORY

# Numerical and Physical Sensitivities in Large Eddy Simulations of Plume Lofting and Spread

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University of Washington

**Warm Boundary Layer Process**

October 27, 2022

U.S. DEPARTMENT OF  
**ENERGY** **BATTELLE**

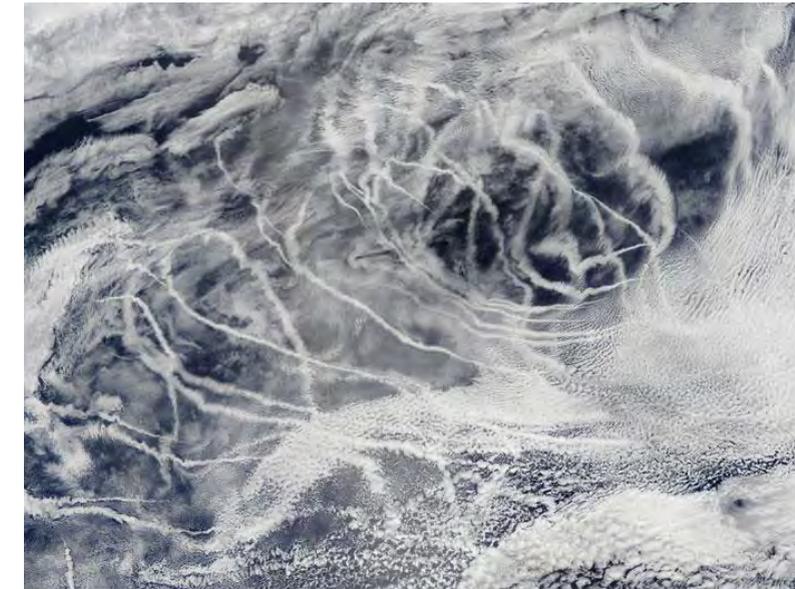
PNNL is operated by Battelle for the U.S. Department of Energy

A visualization of a vertical velocity field, showing a series of diagonal, wavy bands of color (red, orange, yellow, green, blue) against a dark background, representing plume tracers overlaid on the velocity field.

**Near-surface PINACLES  
plume tracers overlaid on  
vertical velocity field**

# Motivation

- Inject salt-water plumes at the ocean surface
  - Droplets evaporate to leave sea salt aerosol
  - Turbulent mixing lofts the aerosol to cloud base
  - Increase cloud albedo and longevity
- Limited opportunities for controlled field experiments
  - **Numerical Experiments**
- PINACLES: Predicting Interactions of Aerosol and Clouds in Large Eddy Simulation
- Similar simulations of stratocumulus cloud test case for sensitivity studies
- 3 plumes injected a few km apart just above the surface with identical properties



“Ship tracks” are brightened cloud areas that result from aerosol particles in ship exhaust. They are an inadvertent example of the same cloud responses MCB seeks to use.  
Credit: NASA

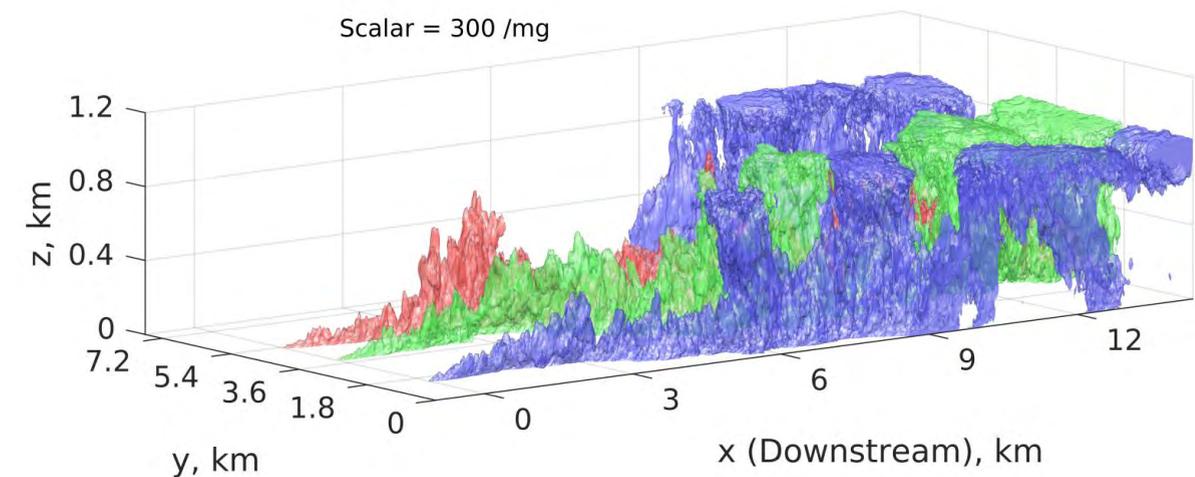
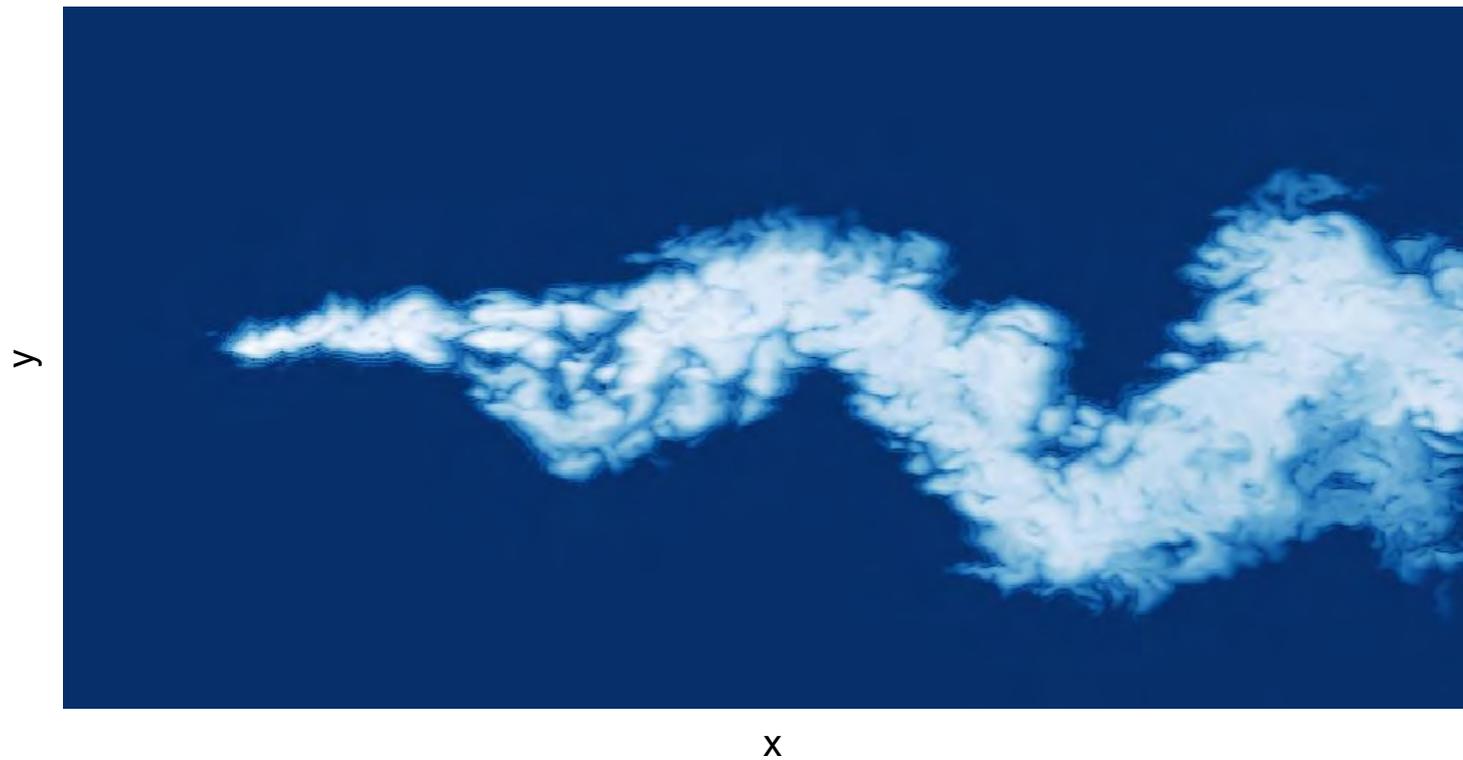


Image credits: Peter Blossey

# Results – Microphysics schemes

- P3 vs Morrison<sup>1,2</sup> microphysics schemes

z = 100 m

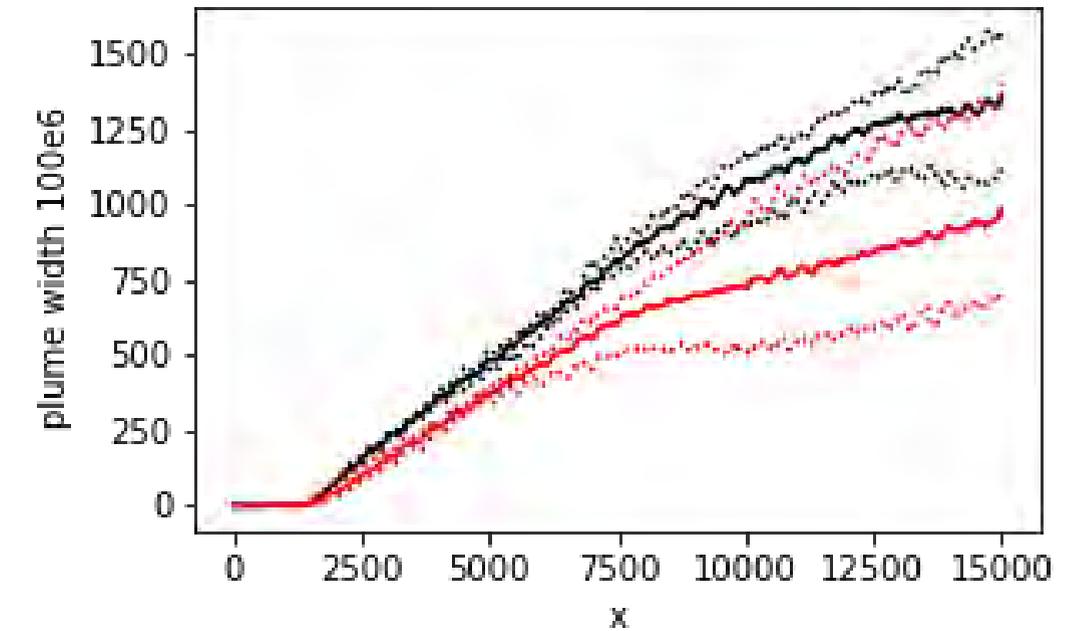


Plume tracer contours from simulation using Morrison (black) microphysics scheme, z = 100 m

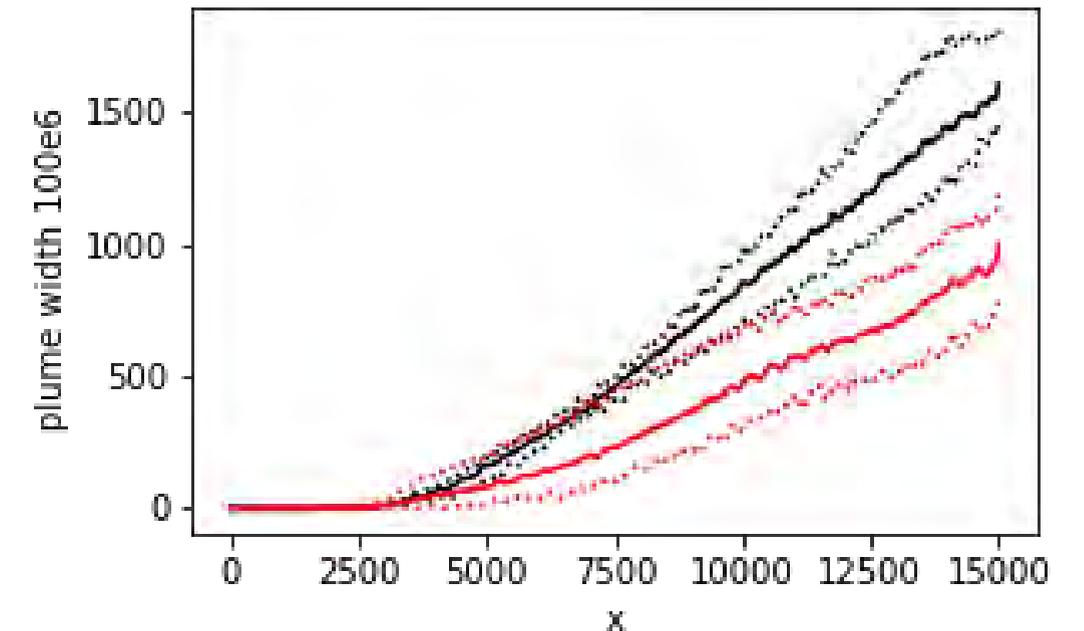
<sup>1</sup> Morrison et al., *Journal of the Atmospheric Sciences* (2005)

<sup>2</sup> Wyant et al., *Journal of Advances in Modeling Earth Systems* (2022)

z = 100 m



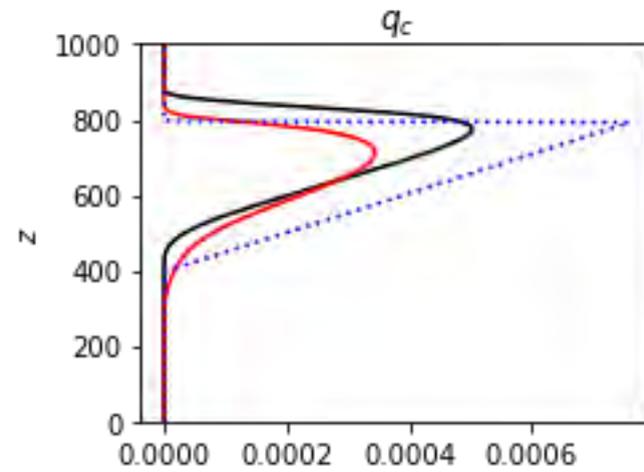
z = 400 m



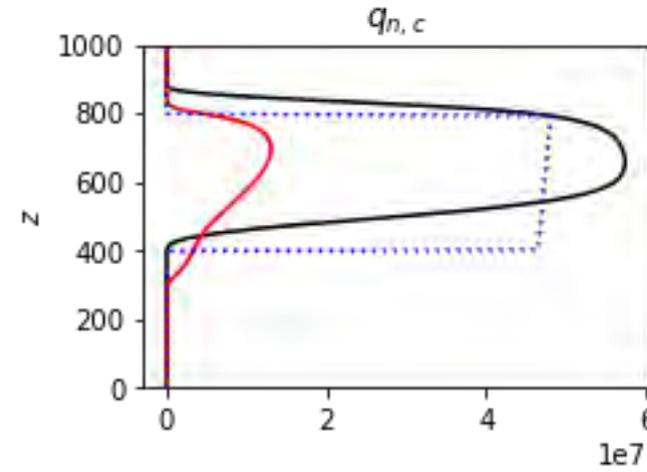
Plume width calculated from simulations in PINACLES using P3 (red) and Morrison (black) microphysics schemes

# Results – Microphysics schemes

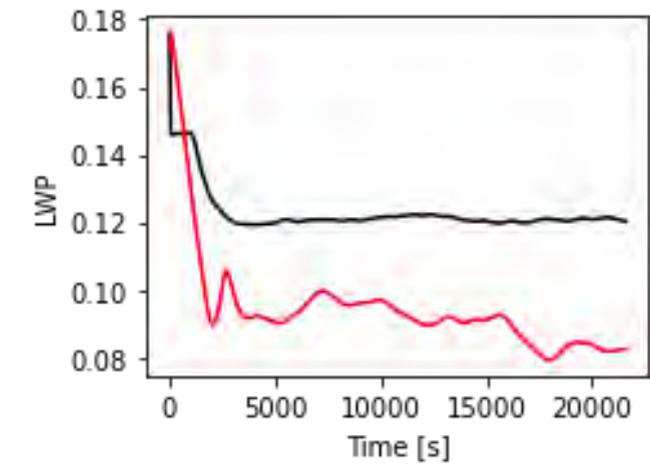
Cloud water mixing ratio



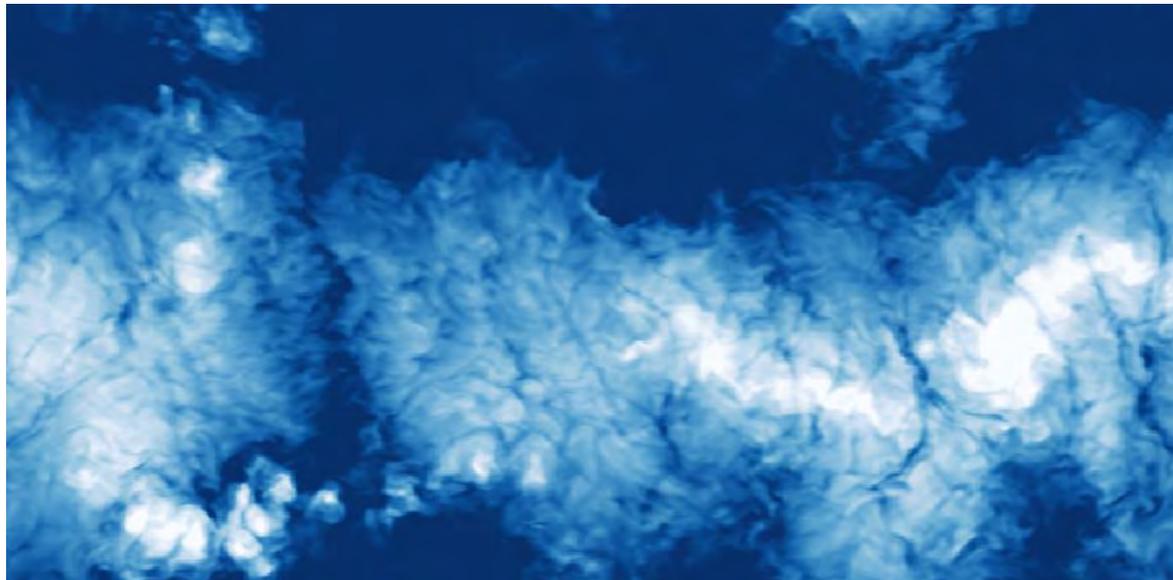
Cloud number concentration



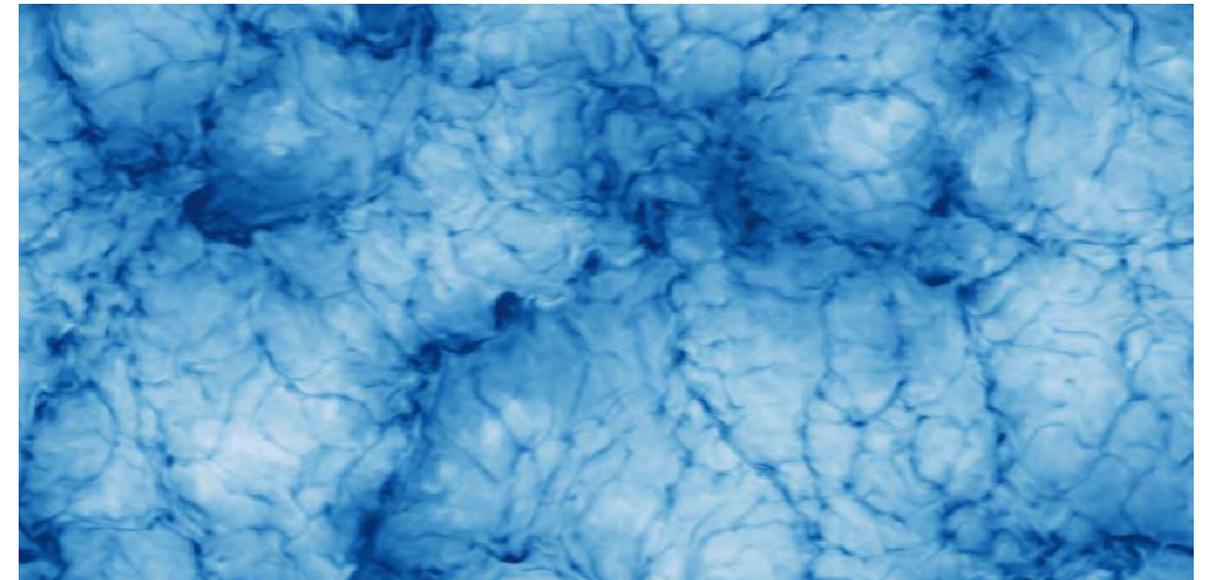
Liquid Water Path



Mean vertical profiles and time evolution calculated from simulations using P3 (red) and Morrison (black) microphysics schemes



P3 (red)

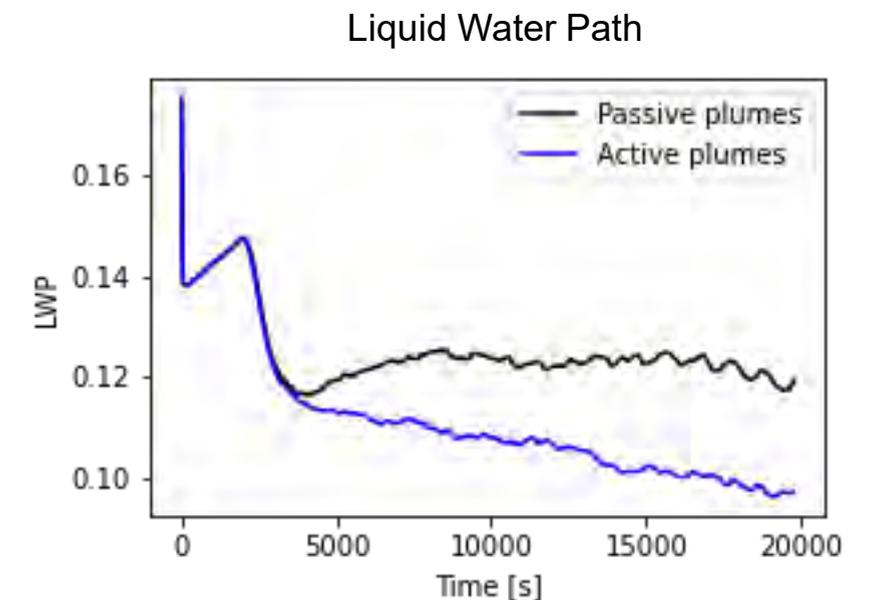
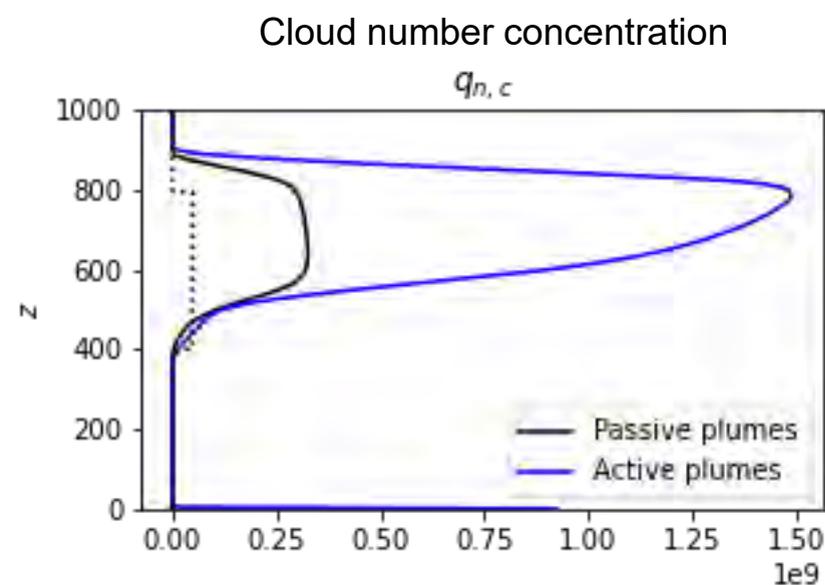
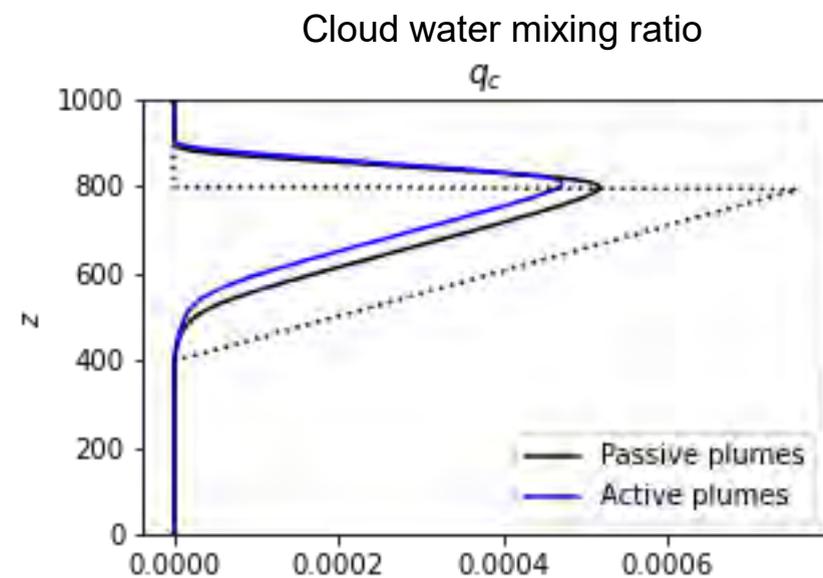
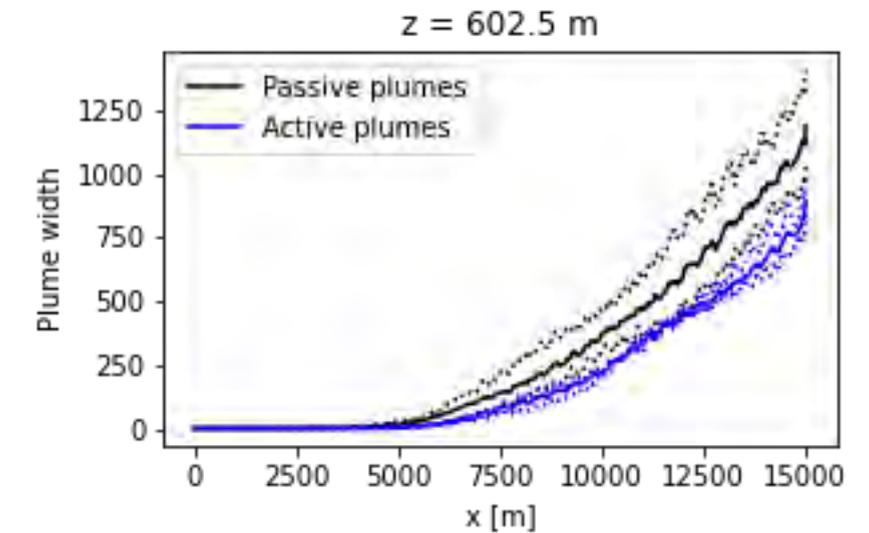
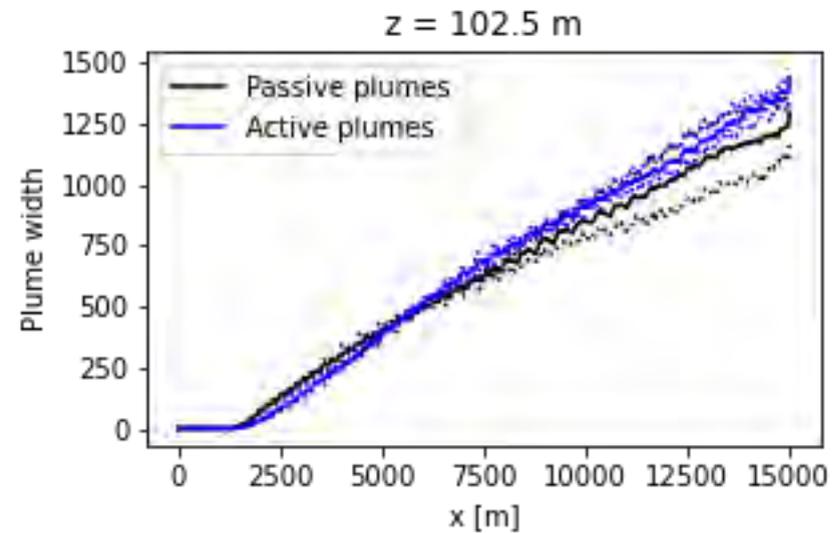


Morrison (black)

# Results – Passive and active plumes

- Passive vs active plumes
- Little difference in plume lofting, with our current resolution
- Aerosol in the plumes result in much smaller cloud droplets
- Aerosol in the plumes lower liquid water path

Plume width calculated from simulations in PINACLES using passive (black) and active (blue) plumes



Mean vertical profiles and time evolution calculated from simulations using passive (black) and active (blue) plumes



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# Conclusions

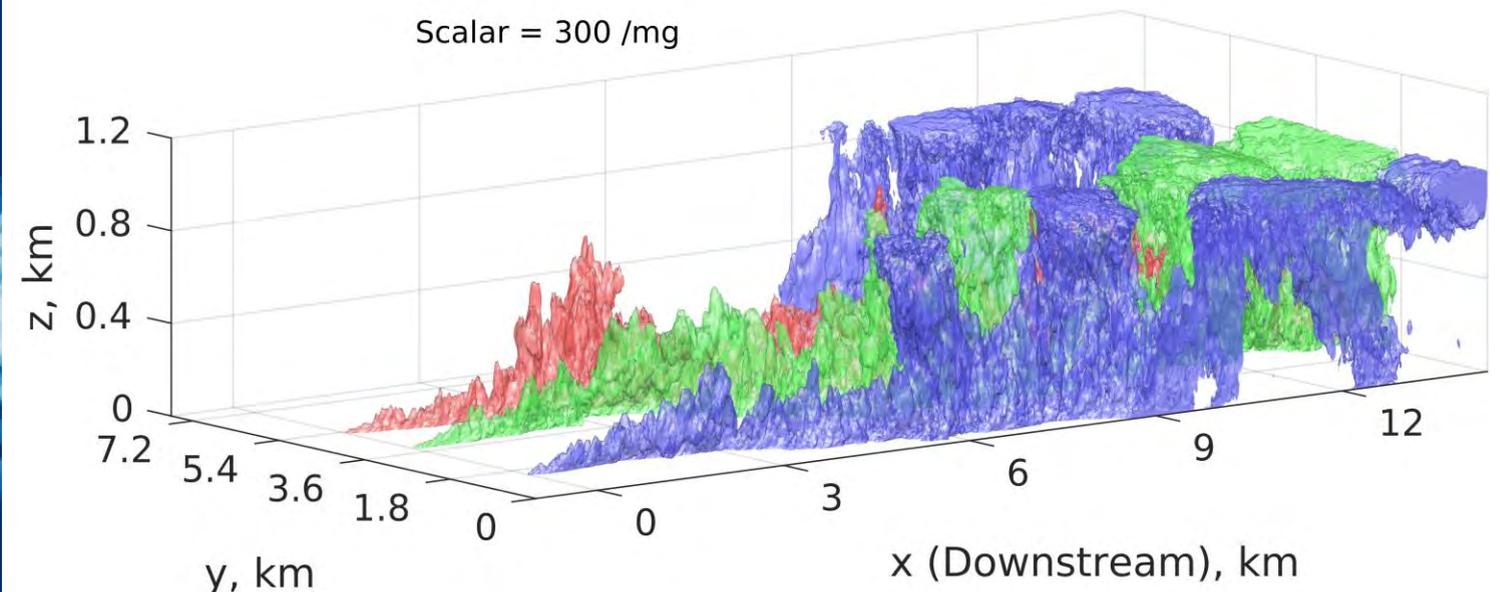
- Sea salt plumes introduced at the ocean surface spread and loft to the clouds
- Microphysics schemes have significant impact on the clouds and plume spread
- Active plumes modify cloud coverage, but have little effect on plume spread
- Different scalar and momentum advection schemes also result in differences of the same order

## Future Work

- Simulations with higher grid resolution
- Simulations of different types of stratocumulus cloud setups



## More info: Poster session 3, number 45



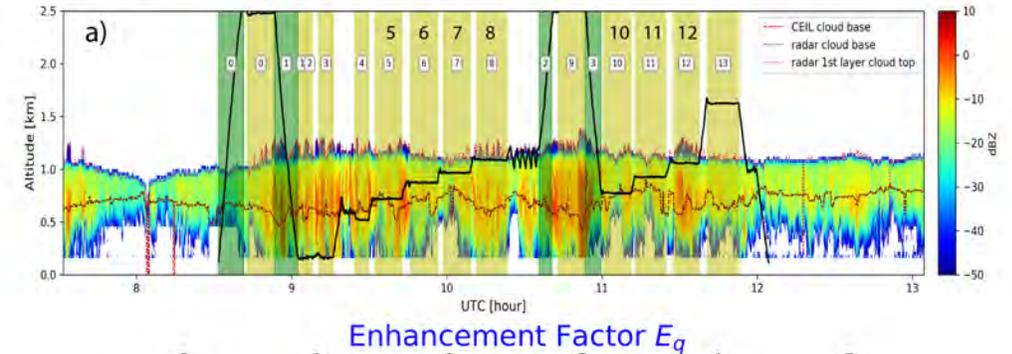
# The impact joint variability of liquid water and droplet concentration on grid-mean autoconversion and enhancement factor

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J. A. Covert<sup>1</sup>, D. B. Mechem<sup>1</sup>, and Z. Zhang<sup>2</sup>

<sup>1</sup>Department of Geography and Atmospheric Science, University of Kansas

<sup>2</sup>Department of Physics, University of Maryland, Baltimore County (UMBC)



Warm Boundary Layer Process Working Group Breakout  
2022 Joint ARM User Facility and ASR PI Meeting  
27 October 2022

We gratefully acknowledge support from the Department of Energy Office of Science.

# Impact of subgrid-scale variability on grid-mean process rates

- Neglect of SGS variability can produce biases in microphysical process rates
- Some ESMs account for via a simple “enhancement factor” multiplier  $E$

For a bivariate lognormal distribution  $P(q_c, N_c)$ ,  $E$  can be written as

$$E = \underbrace{E_q(\nu_{q_c}, \beta_q)}_{(1)} \cdot \underbrace{E_N(\nu_{N_c}, \beta_N)}_{(2)} \cdot \underbrace{E_{\text{COV}}(\rho_L, \beta_q, \beta_N, \nu_{q_c}, \nu_{N_c})}_{(3)}$$

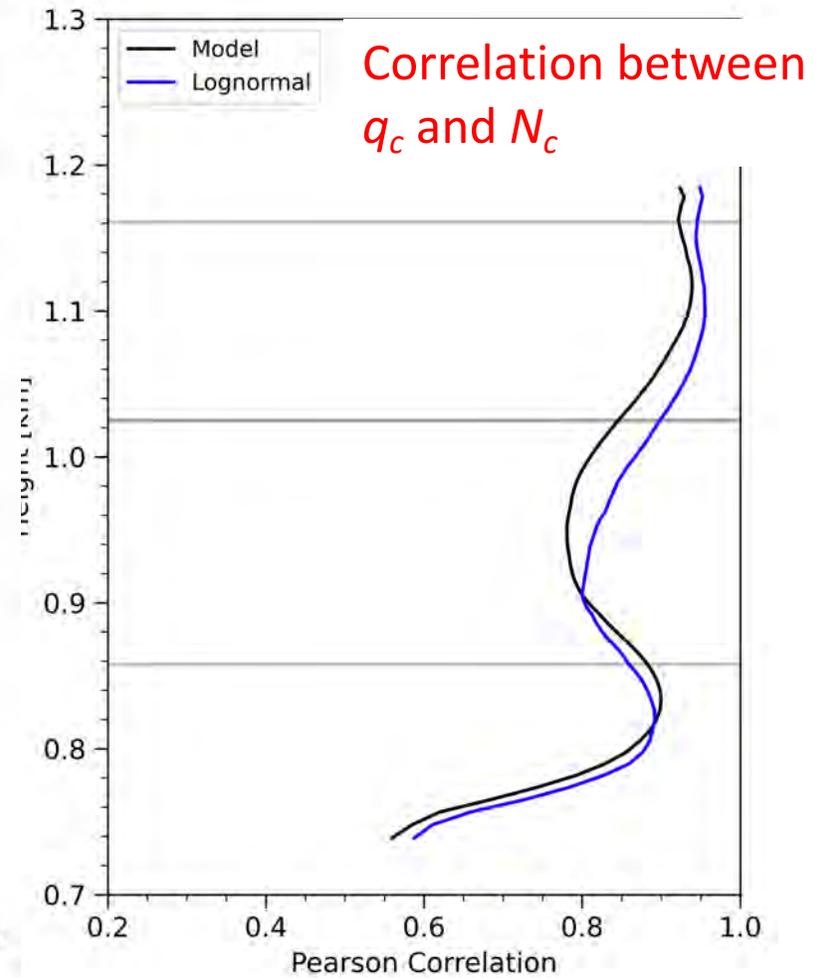
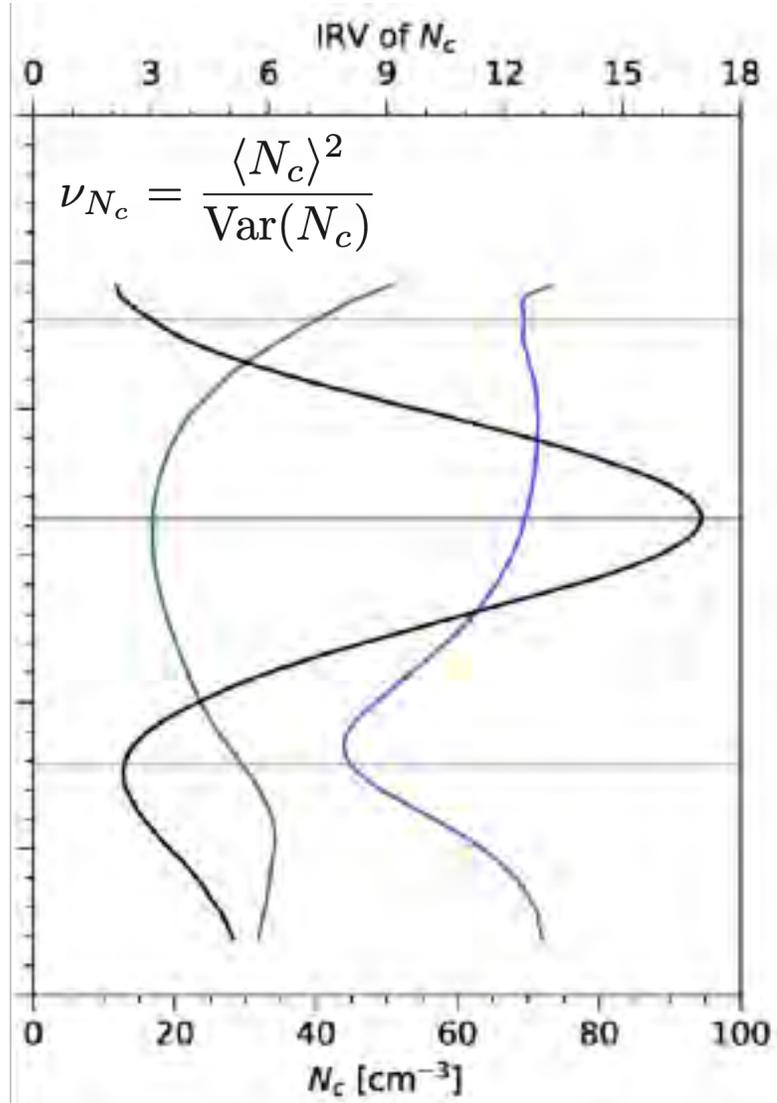
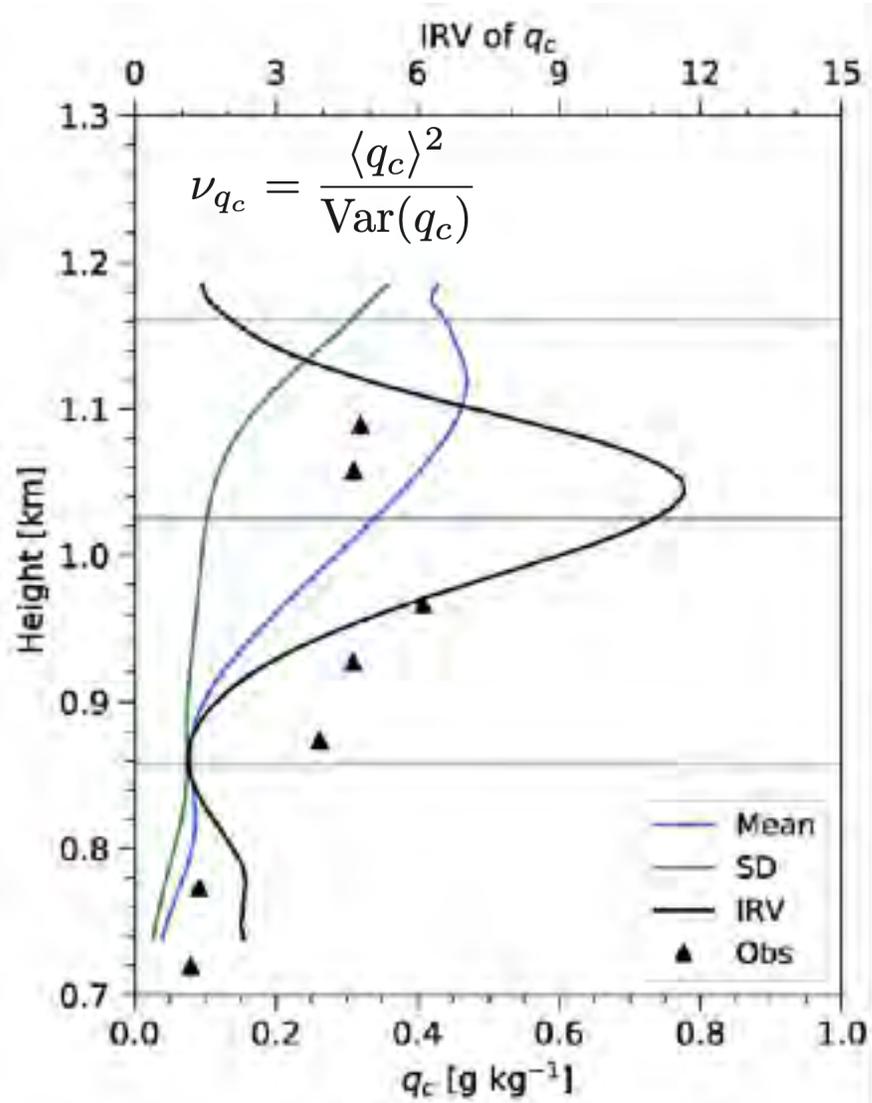
(1) Contribution to  $E$  from variability of cloud water mixing ratio ( $q_c$ )

(2) Contribution to  $E$  from variability of cloud droplet concentration ( $N_c$ )

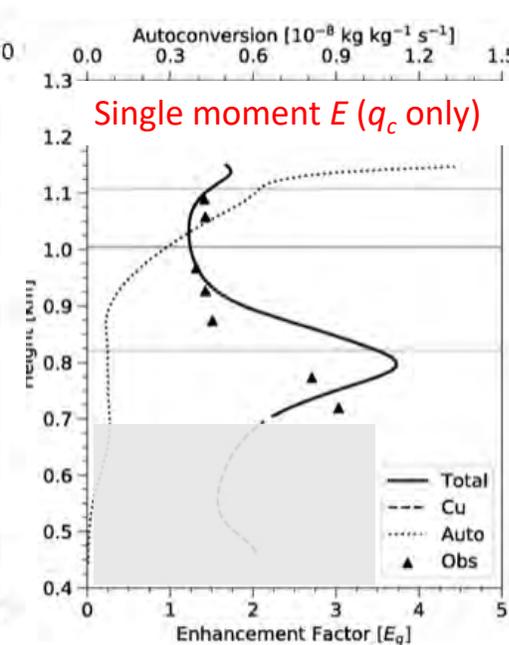
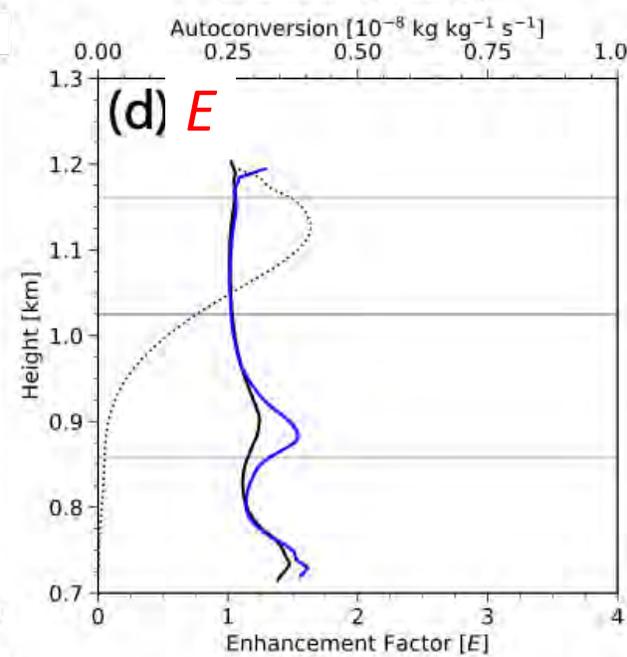
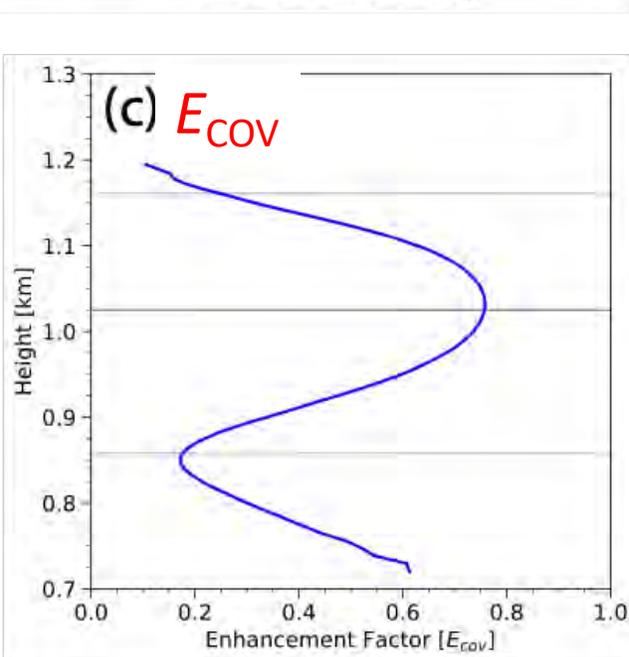
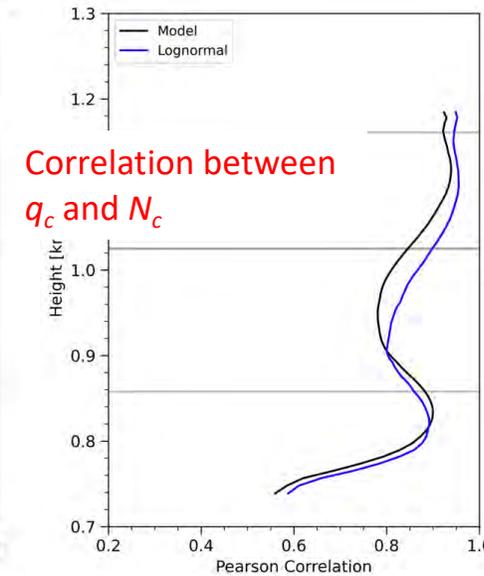
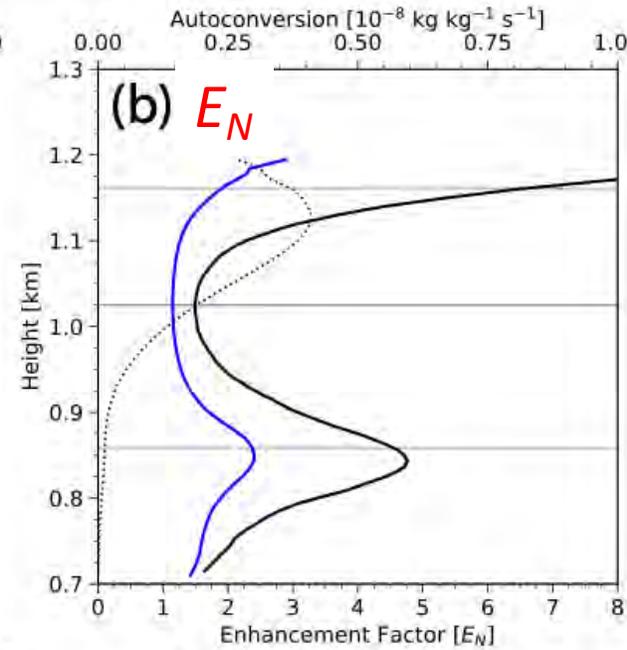
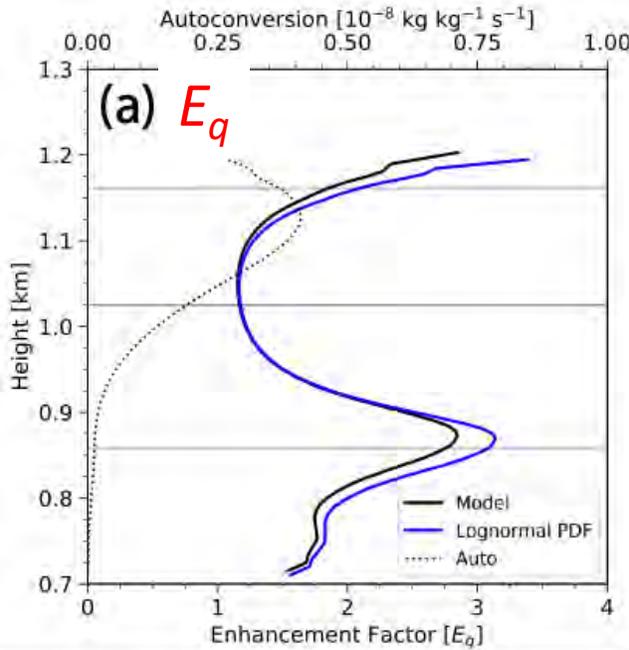
(3) Contribution to  $E$  from the covariance between  $q_c$  and  $N_c$

- Here we present results from large-eddy simulation (LES) with bin microphysics to analyze the impact of the co-variation of cloud water  $q_c$  and cloud droplet concentration  $N_c$  on SGS variability and enhancement factor  $E$

# Impact of subgrid-scale variability on grid-mean process rates



# Contributions to $E$ from variability in $q_c$ , $N_c$ , and $\text{COV}(q_c, N_c)$



## Conclusions

- Both bulk and bin simulations suggest that  $E$  should be lower than the 3.2 value commonly used
- Covariance between  $q_c$  and  $N_c$  responsible for the reduction in  $E$
- Large correlation between  $q_c$  and  $N_c$  near cloud top suggests inhomogeneous mixing

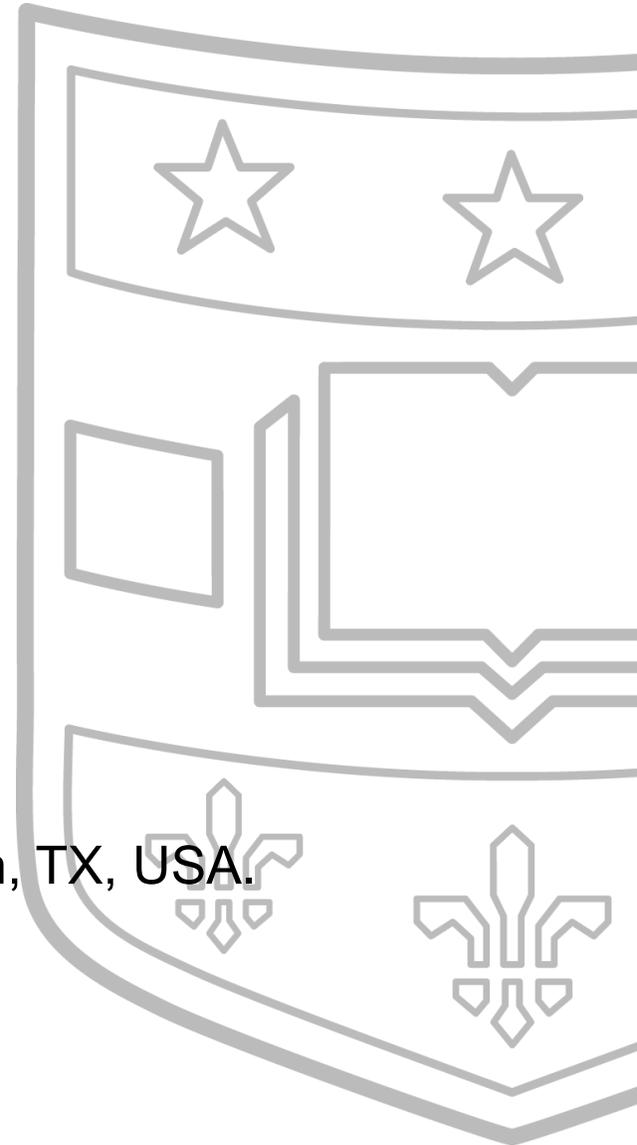
# Maximum Supersaturation in the Marine Boundary Layer Clouds Over the Eastern North Atlantic

**Xianda Gong<sup>1</sup>, Yang Wang<sup>1</sup>, Hua Xie<sup>2</sup>, Jiaoshi Zhang<sup>1</sup>, Zheng Lu<sup>2</sup>, Frank Stratmann<sup>3</sup>, Heike Wex<sup>3</sup>, Xiaohong Liu<sup>2</sup>, Jian Wang<sup>1,\*</sup>**

<sup>1</sup>*Washington University in St. Louis, St. Louis, MO, USA*

<sup>2</sup>*Department of Atmospheric Sciences, Texas A&M University, College Station, TX, USA.*

<sup>3</sup>*Leibniz Institute for Tropospheric Research, Leipzig, Germany*



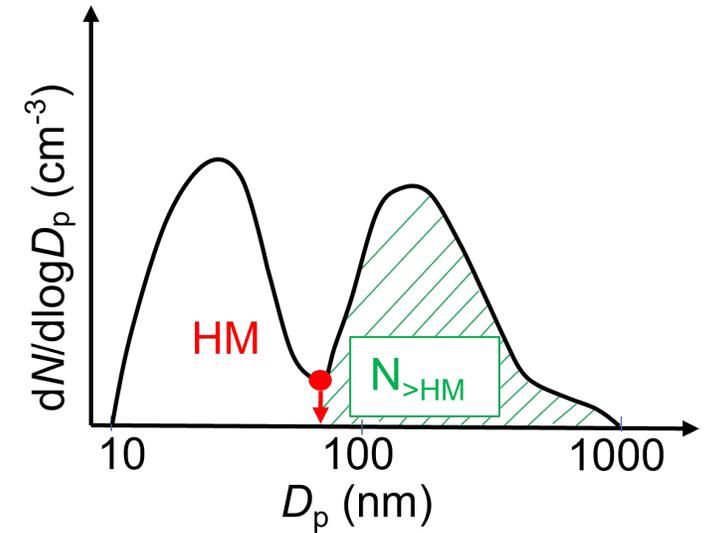
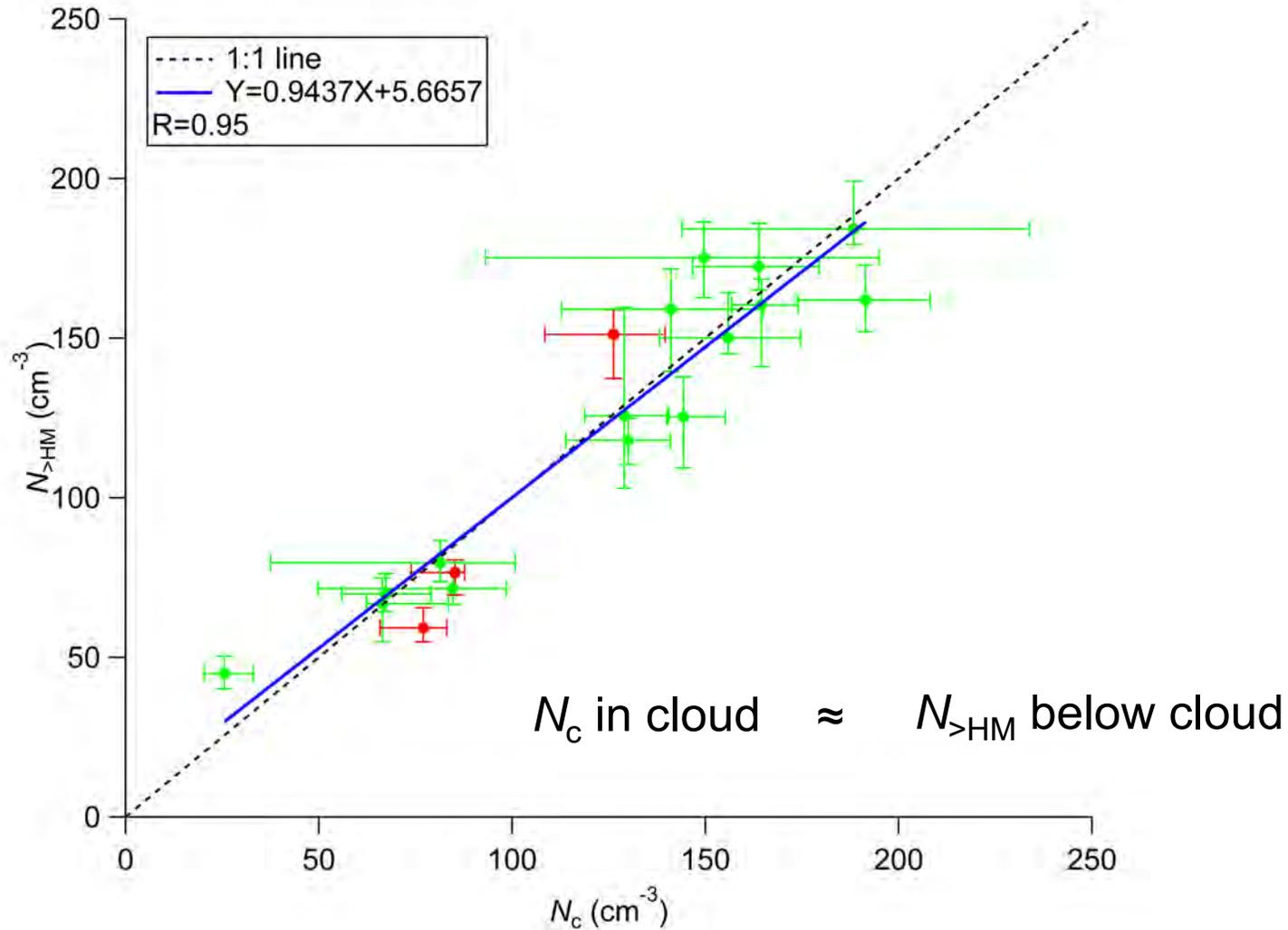
# Aerosol and Cloud Experiment in Eastern North Atlantic (ACE-ENA)



**ENA site:** Particle number size distribution, CN,  $N_{CCN}$ , particle hygroscopicity ( $\kappa_{CCN}$ )

**Aircraft measurements:** aerosol properties and cloud microphysics

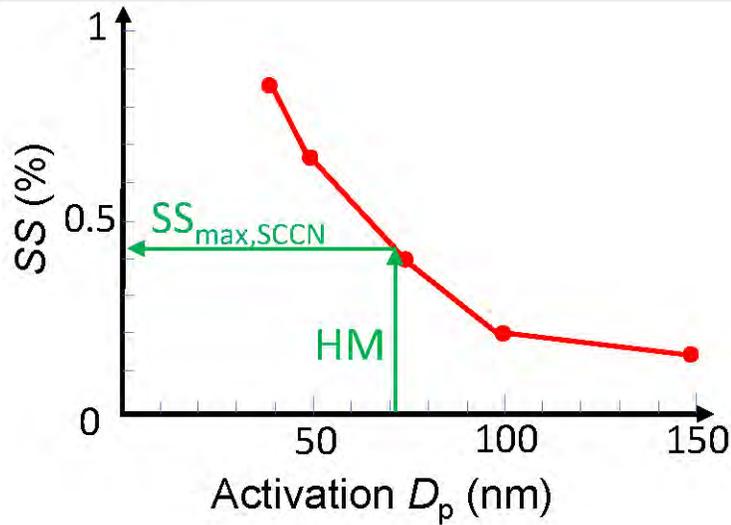
# Hoppel Minimum and Maximum Supersaturation



$N_{>HM}$ : particle number concentration in the size larger than HM

$N_c$ : cloud droplet number concentration

# Maximum Supersaturation in the Clouds

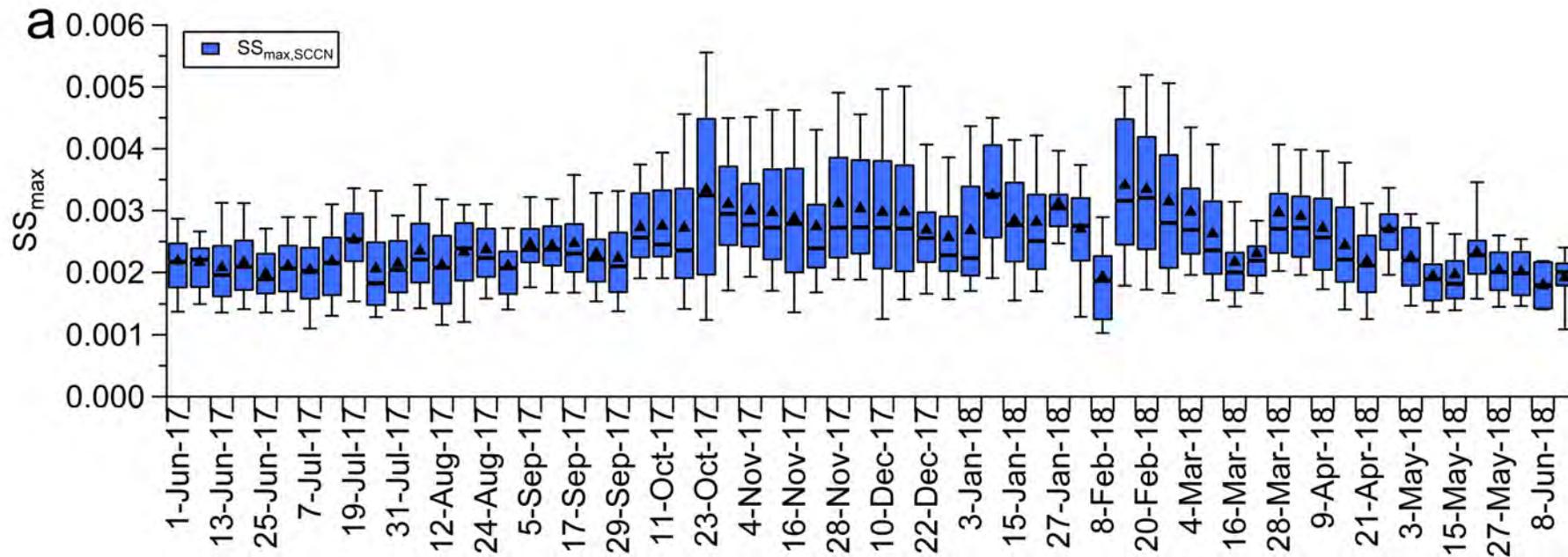


SCCN measured  
particle activation  
spectrum

+ Hoppel  
Minimum

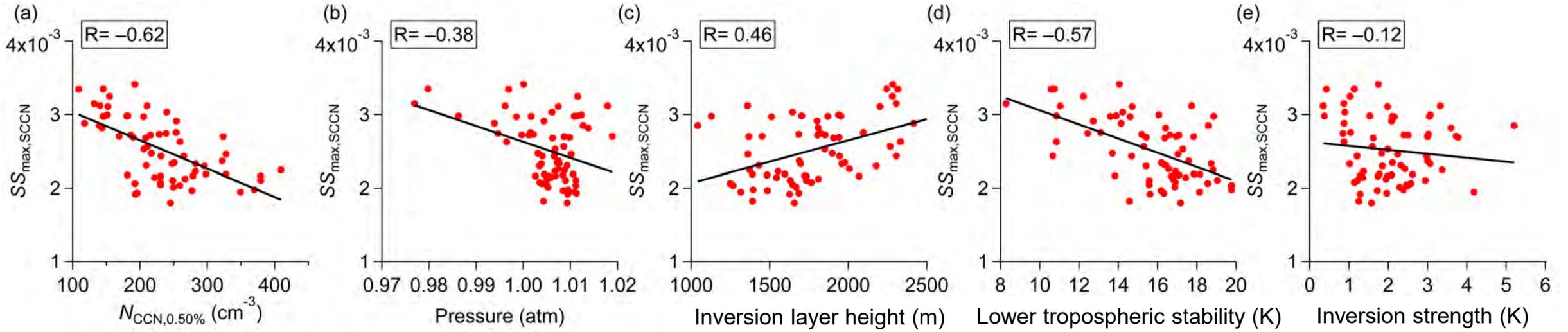


$SS_{max,SCCN}$



Clear seasonal  
variations with high  
values in winter

# Dependence on CCN Concentration and Meteorological Parameters



Suppression of  $SS_{\max}$  by increased condensation sink of water vapor at high  $N_{\text{CCN}}$ .

Stronger convection as cold air advects over warm ocean following the passage of fronts

The strong updrafts are associated with strong radiative cooling on cloud top, and stronger latent heat release, which scales with the cloud thickness. Thicker clouds are often formed in deeper MBL. Lower static stability allows for deeper MBL, as does reduced subsidence.

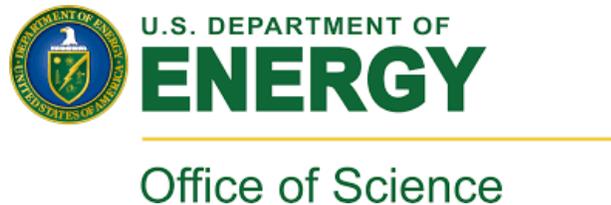
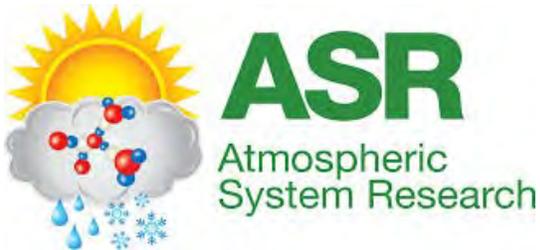
**MLR**  
 **$R^2=0.57$**



# Summary

- Hoppel Minimum in the marine boundary layer is the result of processing by non-precipitation clouds.
- $SS_{\max}$  in the cloud is derived from Hoppel Minimum and aerosol activation measurements at the ENA site.
- $SS_{\max}$  over the Eastern North Atlantic shows a clear seasonal variation.
- $SS_{\max}$  variation is related to CCN number concentration, pressure, lower tropospheric stability, and inversion layer height.

## Acknowledgements



# ENA Warm Boundary Layer Clouds from ARM Observations and Geostationary Satellite Cloud Retrievals

Xue Zheng, Shaoyue Qiu

Lawrence Livermore National Laboratory

David Painemal

NASA Langley Research Center

Science Systems and Applications Inc.

2022 ARM/ASR Joint User Facility and PI Meeting

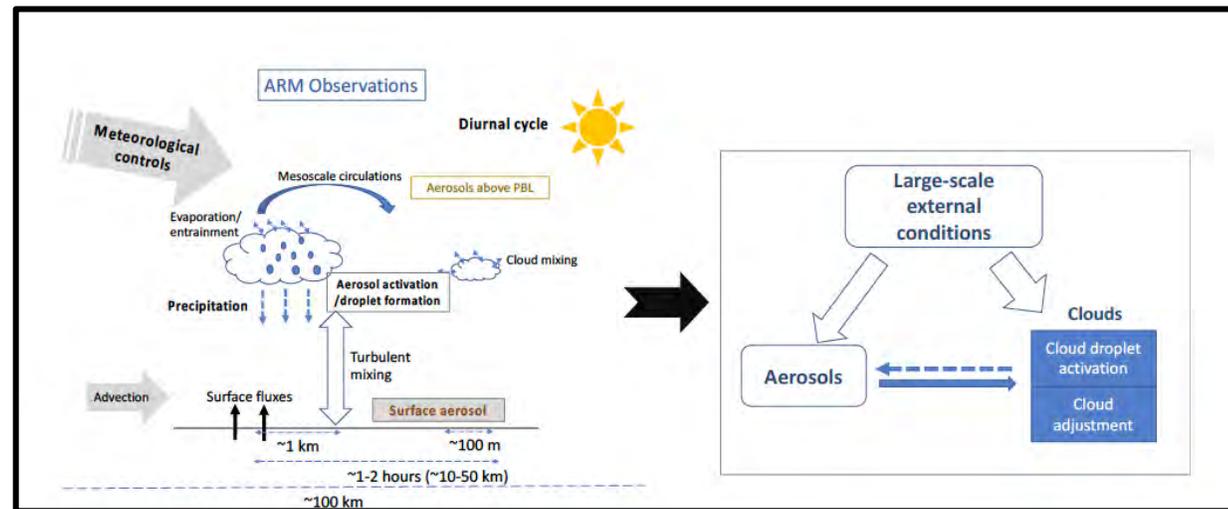
Rockville, MD

Oct. 26, 2022



# Scientific Objectives

- Better detect and understand the liquid-phase cloud response to aerosol perturbations in observations through constraining large-scale meteorological factors
- Reduce the related uncertainty in the DOE Energy Exascale Earth System Model with an emphasis on the process-level understanding

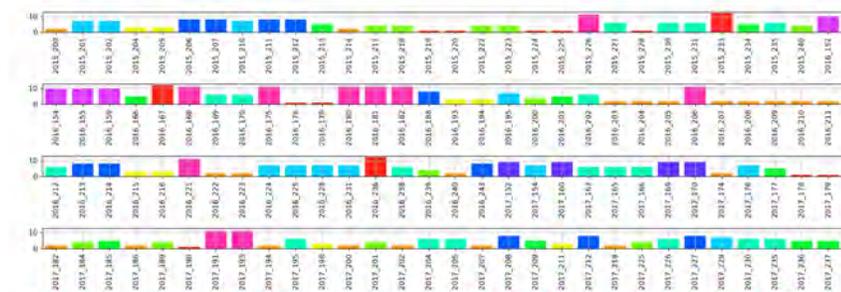


*We started this project with the marine boundary layer clouds over the ENA region*

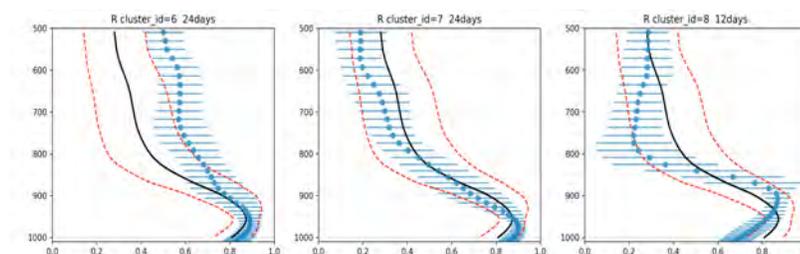
# Constrain meteorological controlling factors

- Multiple meteorological variables clustering
  - Daily U, V, T, Q, Relative humidity profiles (7 pressure levels for now)
  - ECMWF analysis for the ARM ENA site: 2015-2020 JJA. **276** no-deep-convection days in total
  - Unsupervised clustering algorithms (MiniBatchKMeans, DBSCAN, Spectral Clustering)
- Analyze ARM observed cloud and surface CCN for each cluster
  - Daily LWP and surface CCN (SS0.2%): 2016-2019 JJA, **111** days from ARM Best Estimate Data Products (ARMBE)
- Advantages and challenges
  - The approach is applicable to model analyses
  - Limited observed variables and data samples
- Future work
  - Optimize the clustering process
  - Expand the sample size through including different ARM sites
  - Case study based on the clustering result

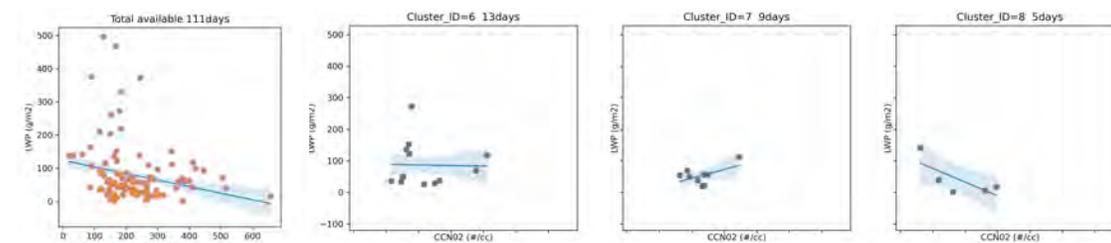
Calendar of clusters

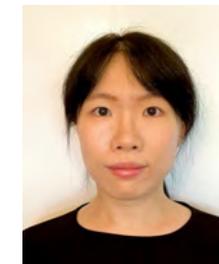
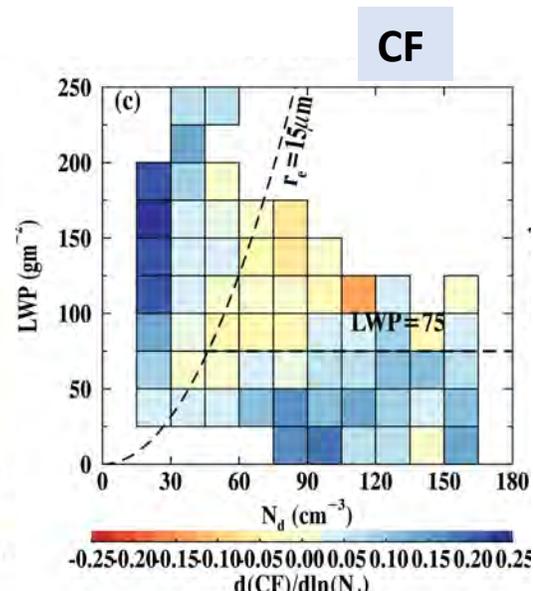
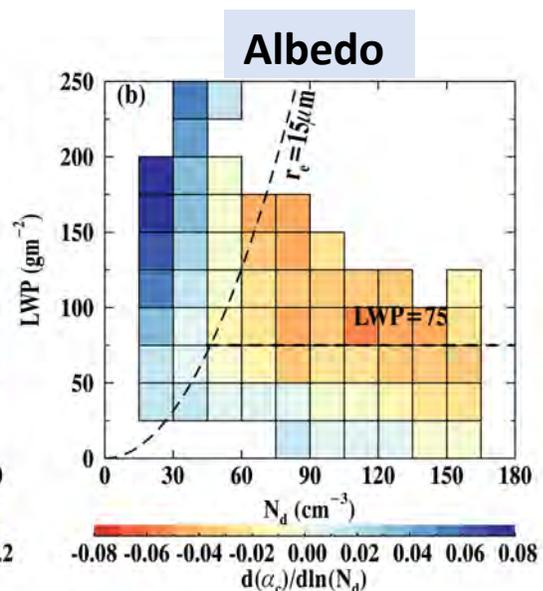
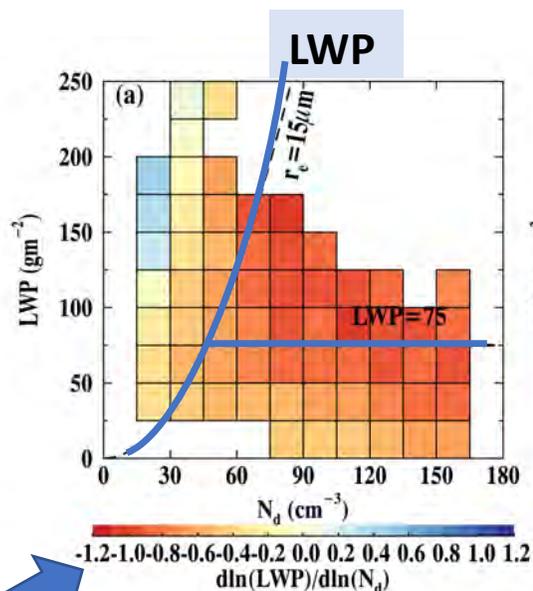
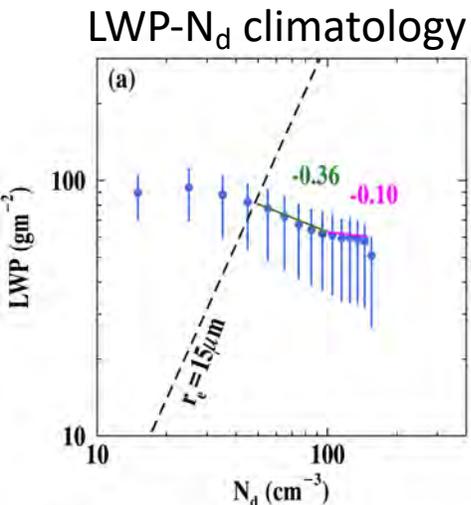


Relative humidity in three clusters as an example



ENA Obs CCN<sub>surf</sub> SS0.2% vs. LWP





Shaoyue Qiu  
LLNL

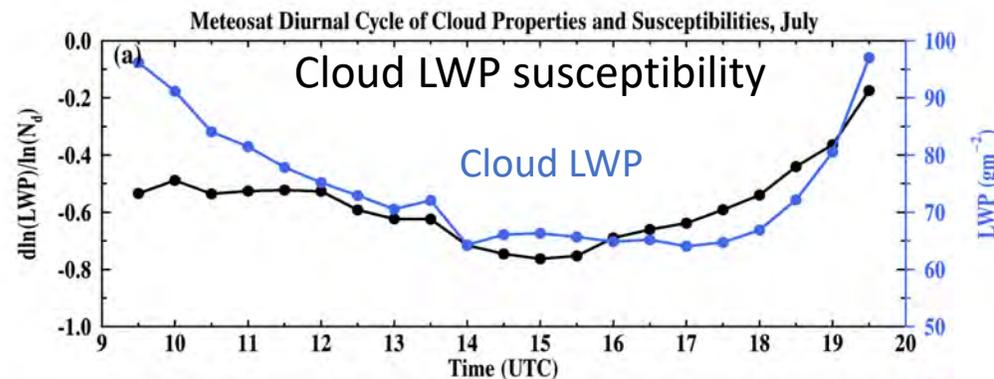
Shaoyue Qiu's virtual poster for more information

Meteorological conditions are **better constrained** in the instantaneous spatial correlation within each  $1^\circ \times 1^\circ$  grid

Different cloud regimes including broken clouds

Daytime half-hourly data during July 2018-2021:  $\sim 8 \times 10^4$  samples for the region ( $33-43^\circ\text{N}$ ,  $23-33^\circ\text{W}$ )

## Diurnal variability



# Understanding the microphysical control and spatial-temporal variability of **warm rain probability** using CloudSat and MODIS observations

Zhibo Zhang (UMBC)

Lazaros Oreopoulos (NASA GSFC), Matthew D. Lebsock (NASA JPL),  
David B. Mechem (Univ. of Kansas), Justin Covert (Univ. of Kansas)

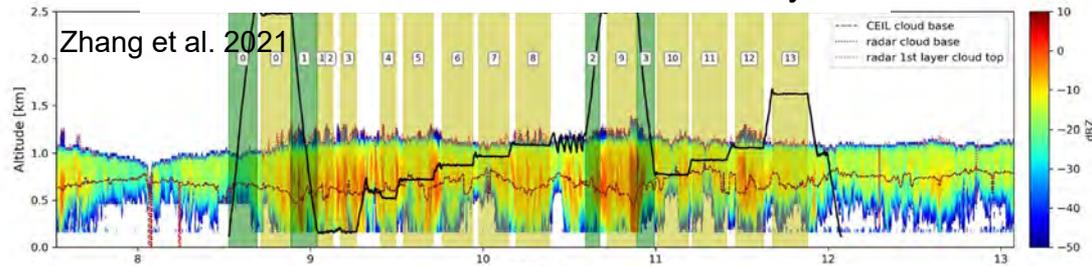
# Warm rain in marine low clouds (MLC)

- Warm rain is generated by the collision coalescence process and prevalent in MLC
- Warm rain is important for
  - Water budget in MLC (important sink of water)
  - Lifetime of MLC
  - Radiative effects of MLC
  - Aerosol-cloud interactions (lifetime effects)
- Measurements of warm rain
  - Intensity/precipitation rate
  - Fraction/probability (e.g., PoP)

Precipitation rate is difficult to quantify from remote sensing observations

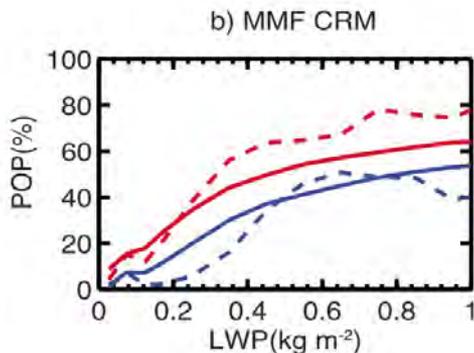
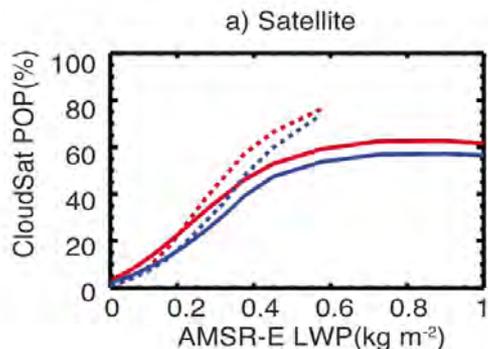
Many previous studies used the PoP to study warm rain. ( Lebsack et al. (2008) and L'Ecuyer et al. (2009) Wang et al. 2012; Mann et al. 2014; Song et al. 2018, Mülmenstädt et al. 2020)

Ground-based w-band radar reflectivity

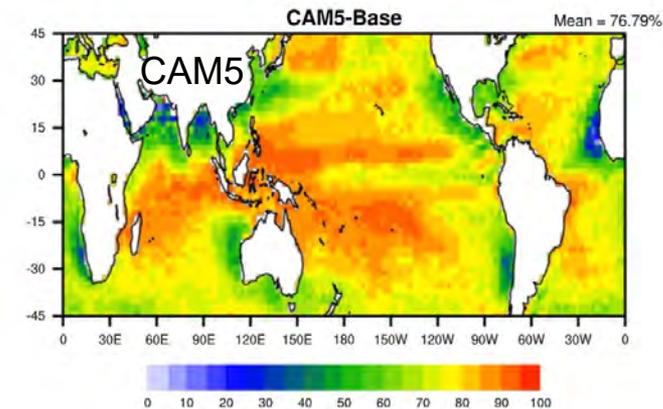
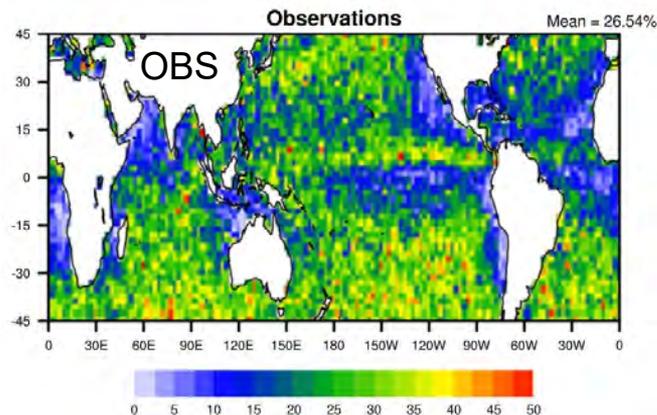
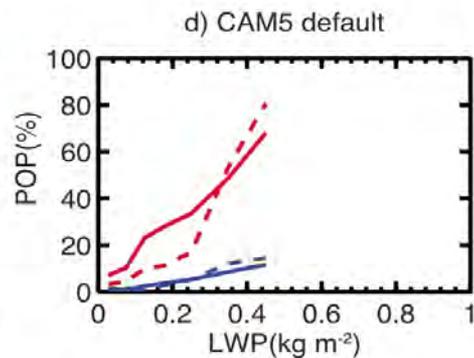
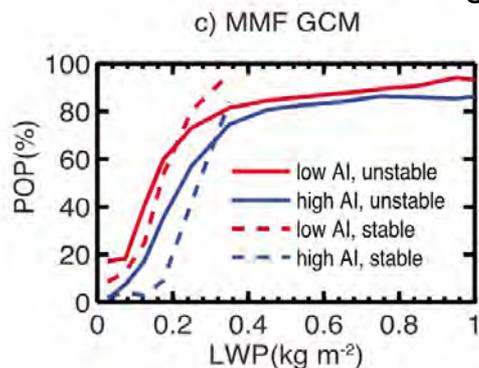


# PoP is important and useful

Song et al. 2018



Wang et al. 2012

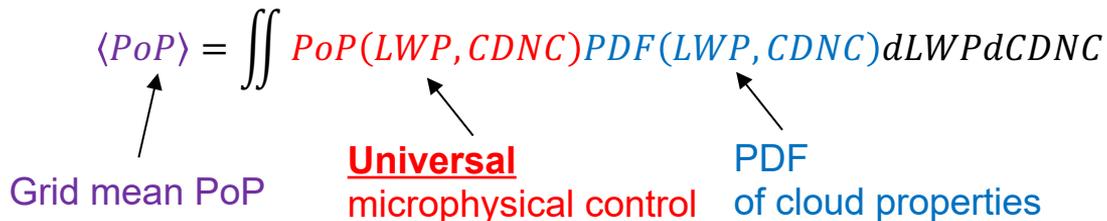


# Motivation and Objectives

- Derive the warm rain probability (i.e., PoP) from the observation (MODIS+CloudSat)
- Investigate the dependence on PoP on cloud properties
  - Cloud liquid water path (LWP)
  - Cloud Droplet Number Concentration (CDNC)
- Understand the spatial-temporal variability of PoP
  - Transition of PoP from stratocumulus to cumulus cloud regimes
  - Seasonal variation of PoP in stratocumulus cloud regions

## Key Hypothesis

$$\langle PoP \rangle = \iint PoP(LWP, CDNC) PDF(LWP, CDNC) dLWP dCDNC$$

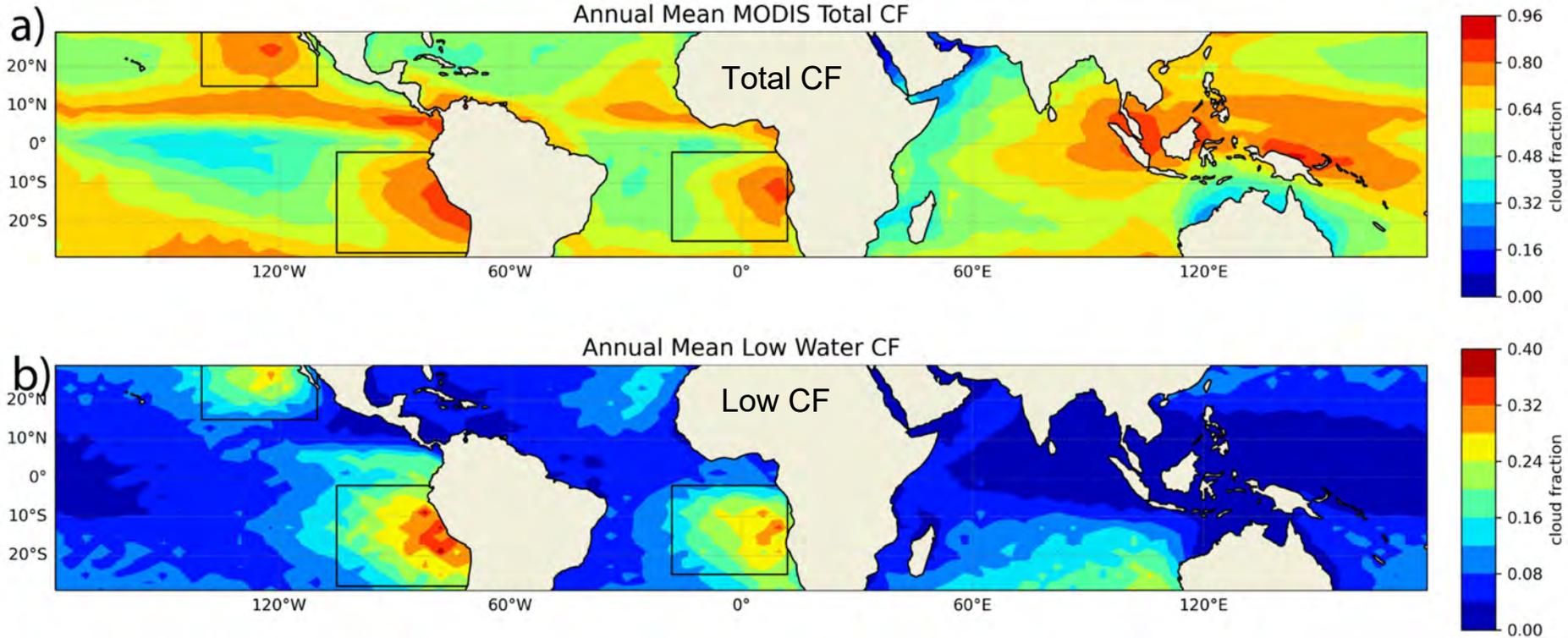


Grid mean PoP      Universal microphysical control      PDF of cloud properties

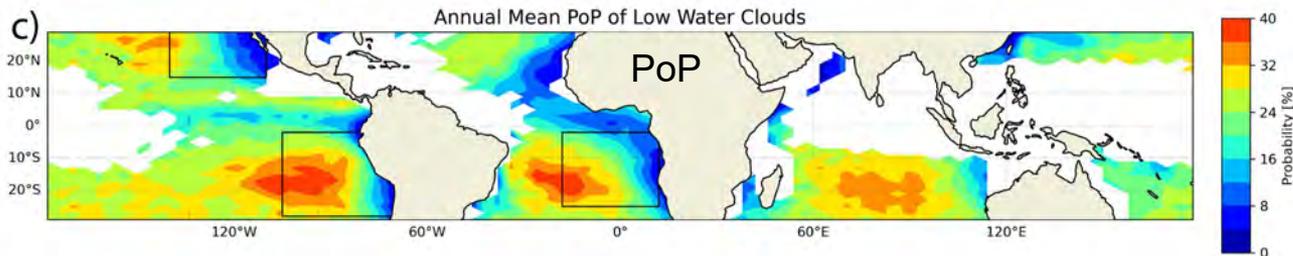
# Data and Methodology

- MODIS-CloudSat collocated product
  - **Identify MLC** from MODIS and CloudSat data
    - “Cloudy” and “Liquid-phase” based on MODIS observation
    - Cloud top < 3km based on CloudSat/CALIOP
  - **Identify precipitation from** CloudSat data
    - Maximum radar reflectivity in the column dBZ\_max > -15
- Definition of PoP
  - **PoP = Number of precipitation MLC clouds / Number MLC clouds** in an area (grid, region) and over certain period (monthly, seasonal, annual)

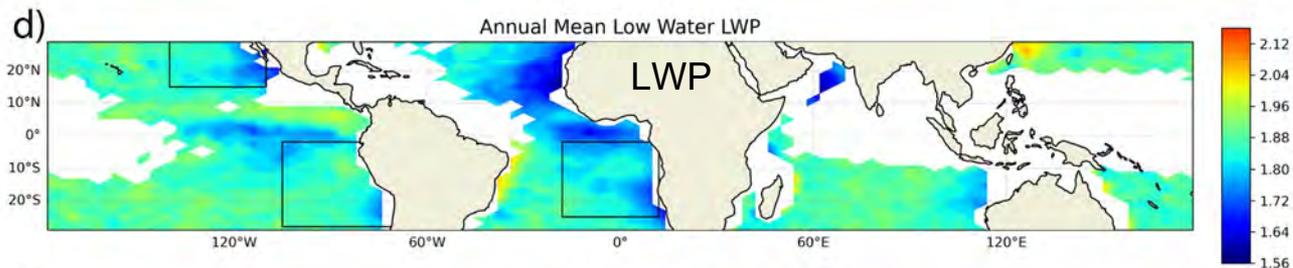
# Properties of MLC in Tropics



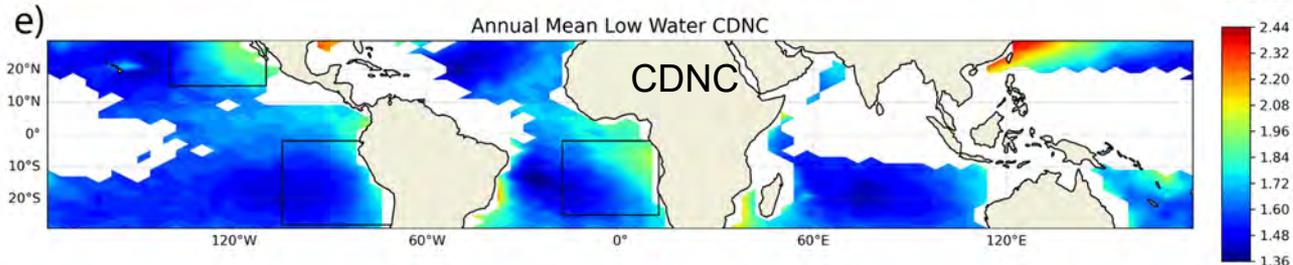
# Properties of MLC in Tropics



PoP = Number of precipitation MLC clouds / Number MLC clouds

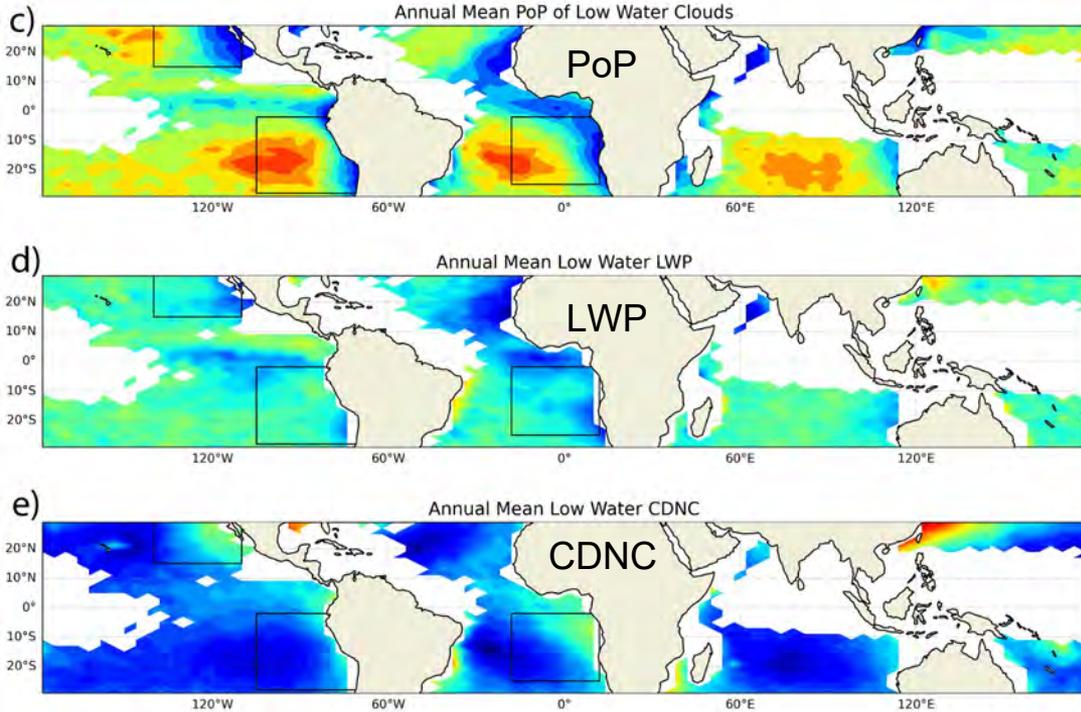


LWP: integrated total water in clouds

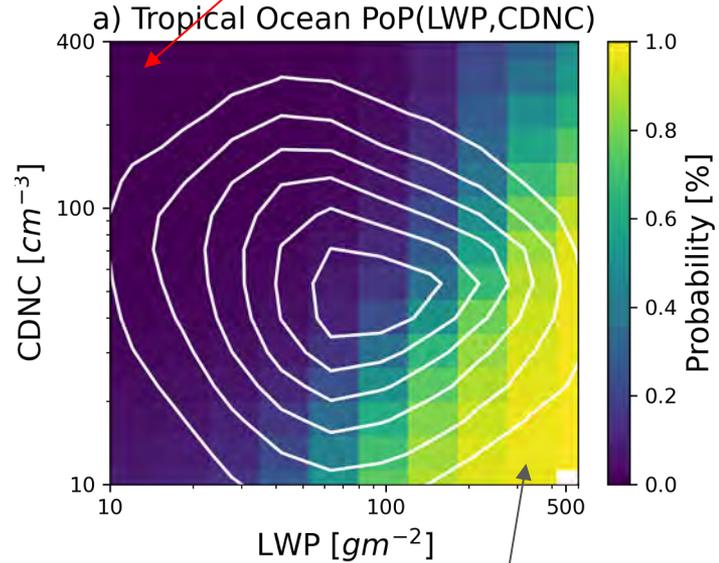


CDNC: Number of droplet in clouds

# Properties of MLC in Tropics



small LWP + large CDNC  $\rightarrow$  small PoP



Large LWP + small CDNC  $\rightarrow$  large PoP

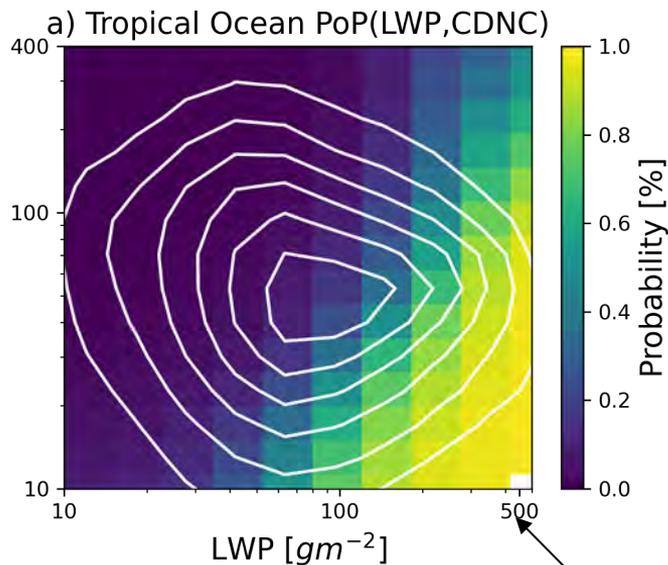
# Parameterization of PoP

## Logistic function

$$PoP(x, y) = \frac{1}{1 + \exp[-(c_0 + c_1x + c_2y)]}$$

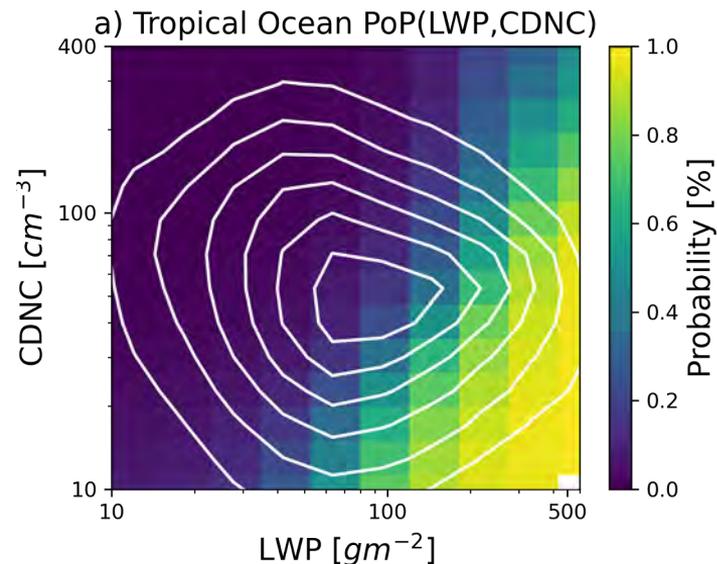
$$x = \log_{10} \left( \frac{LWP}{1gcm^{-2}} \right) \text{ and } y = \log_{10} \left( \frac{CDNC}{1cm^{-3}} \right)$$

$$c_0 = -6.9, c_1 = 5.7, c_2 = -3.2$$



$$\langle PoP \rangle = \iint PoP(LWP, CDNC) PDF(LWP, CDNC) dLWP dCDNC$$

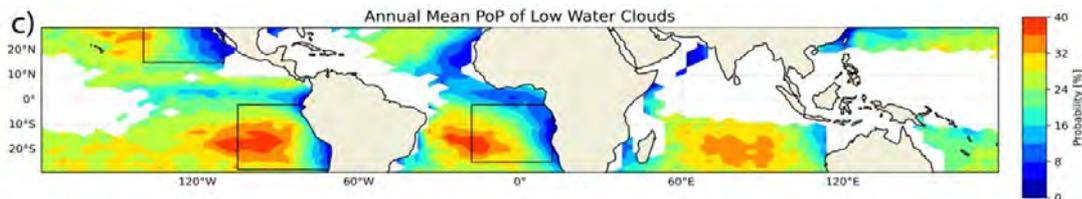
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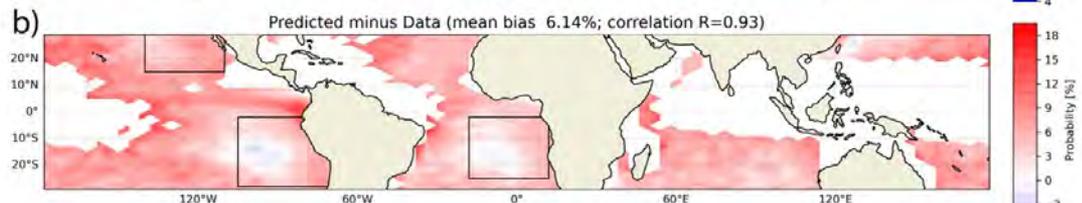
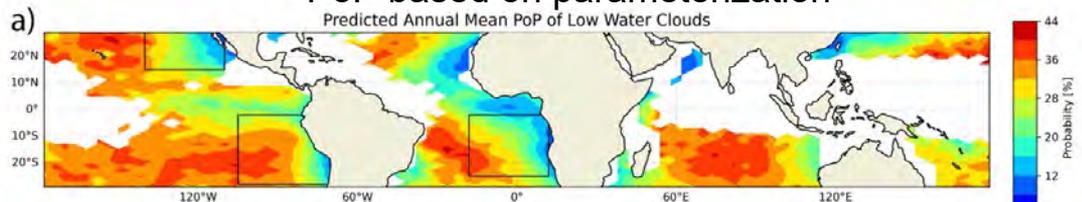
✓ Universal microphysical control

$$\langle PoP \rangle = \iint PoP(LWP, CDNC) PDF(LWP, CDNC) dLWP dCDNC$$

PoP based on observation

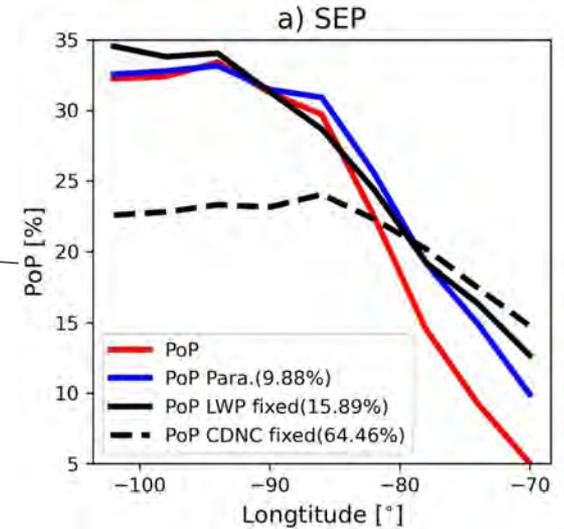
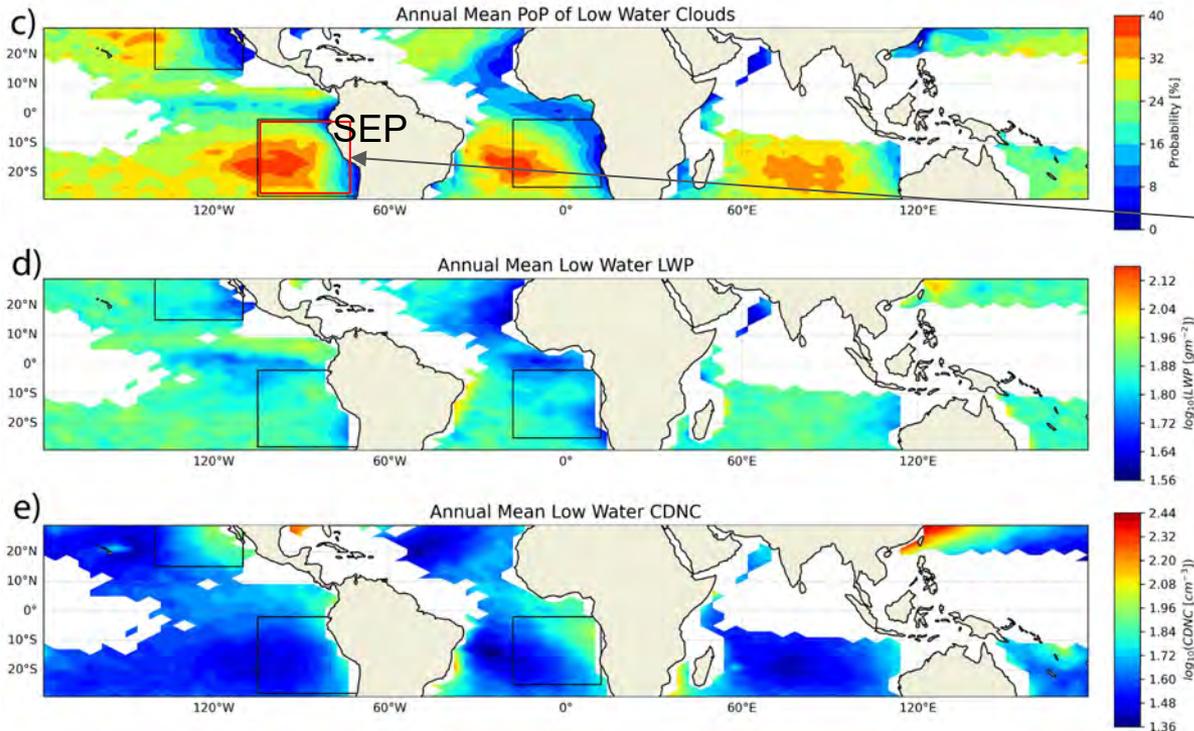


PoP based on parameterization



Error between parameterization and observation

# Understanding the St to Cu transition of PoP



**What is the main reason for the increase of PoP from Sc to Cu?**

# What is the main reason for the PoP transition?

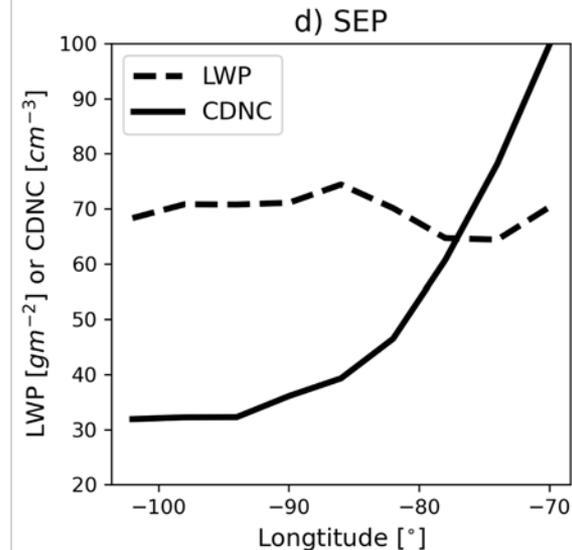
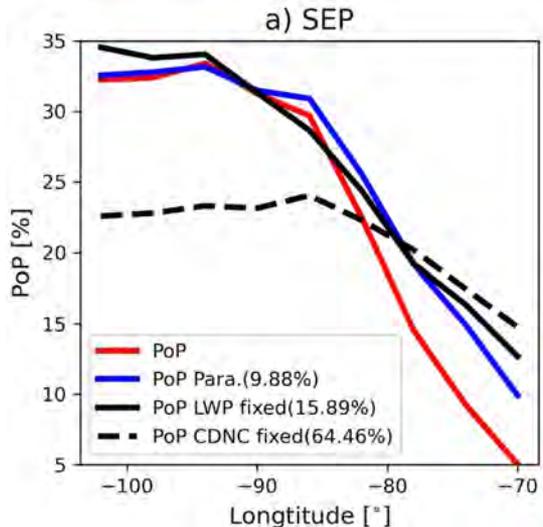
- PoP increases from Sc to Cu region
- LWP increases slightly and CDNC decreases significantly

To understand the relative role of LWP and CDNC, we did the following test

We derived the following two sets of  $\langle \text{PoP} \rangle$

- LWP fixed PDF( $\langle \text{LWP} \rangle$ , CDNC)
- CDNC fixed PDF(LWP,  $\langle \text{CDNC} \rangle$ )

The idea is to keep one factor fixed and allow the other to vary from Sc to Cu

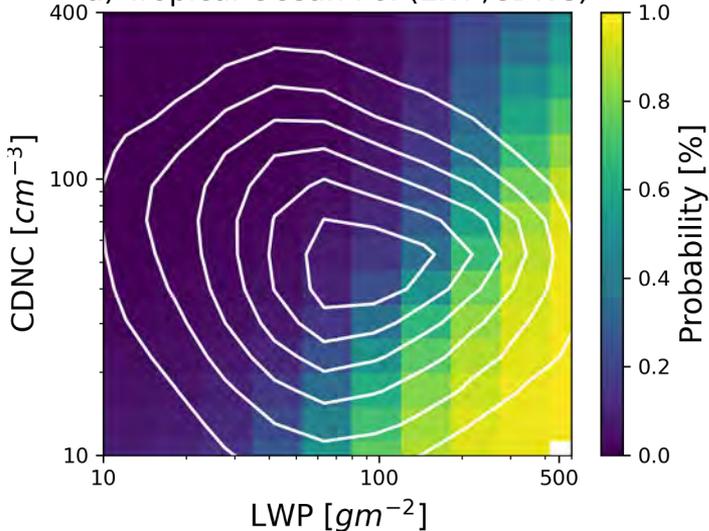


$$\langle \text{PoP} \rangle = \iint \text{PoP}(\text{LWP}, \text{CDNC}) \text{PDF}(\text{LWP}, \text{CDNC}) d\text{LWP} d\text{CDNC}$$

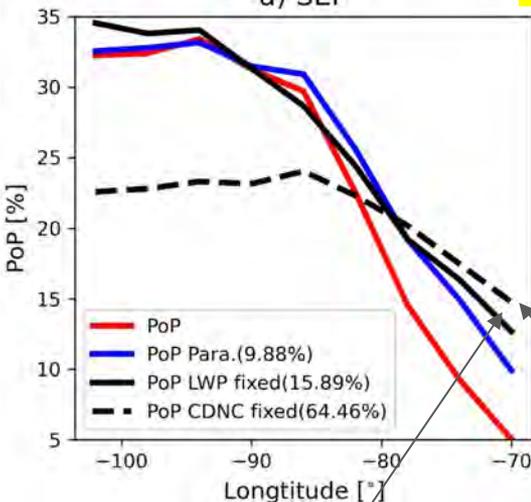
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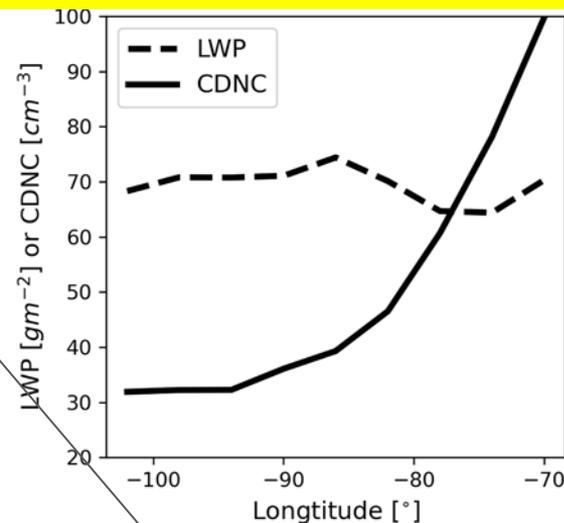
a) Tropical Ocean PoP(LWP, CDNC)



a) SEP

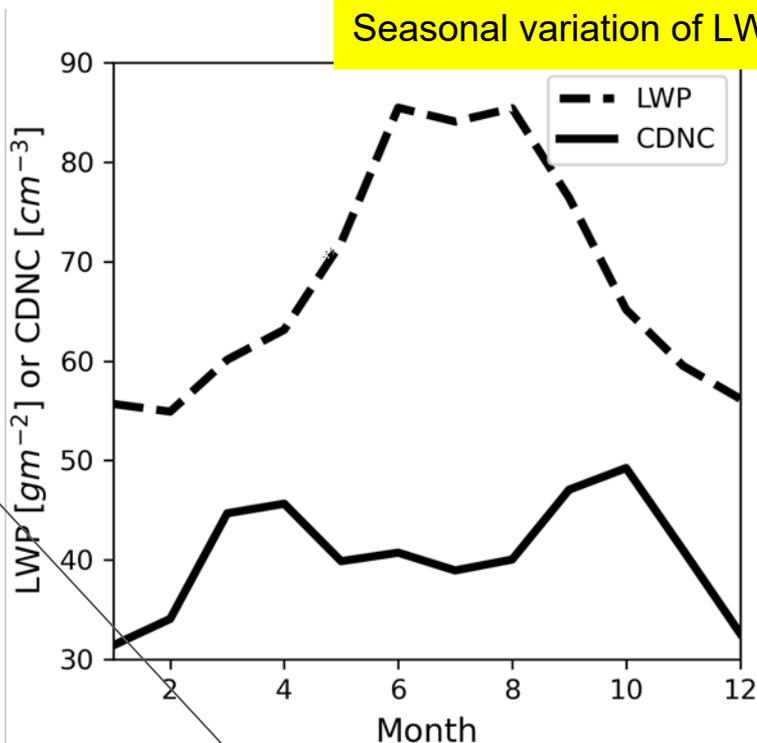
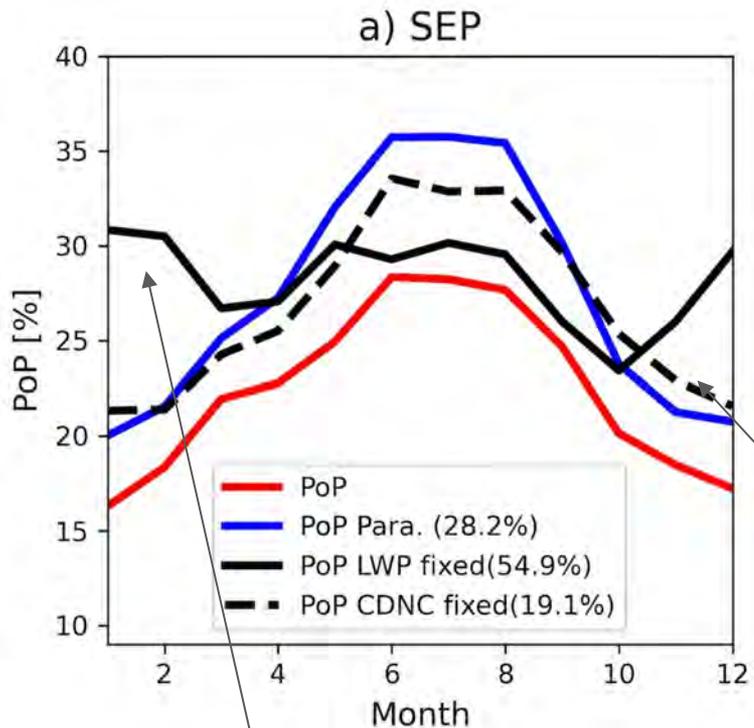


Decreases of CDNC dominates



LWP fixed PDF( $\langle LWP \rangle$ , CDNC)    CDNC fixed PDF(LWP,  $\langle CDNC \rangle$ )

# Understanding the Seasonal variation of PoP



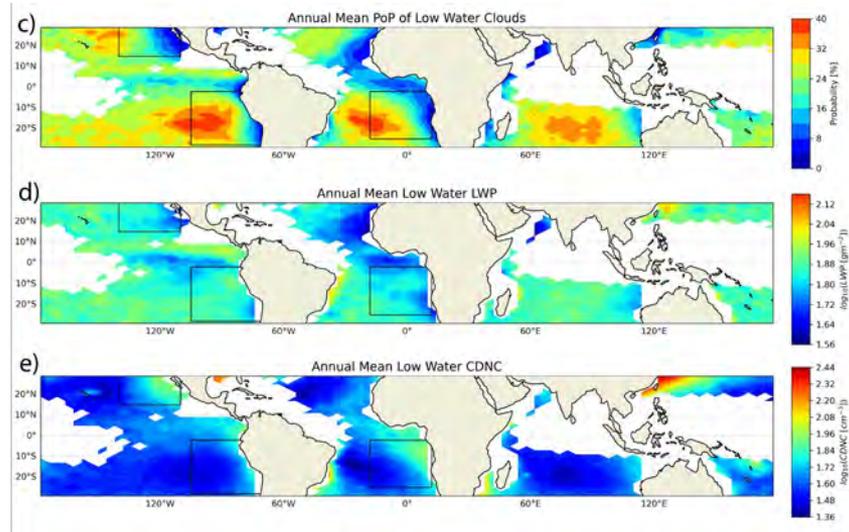
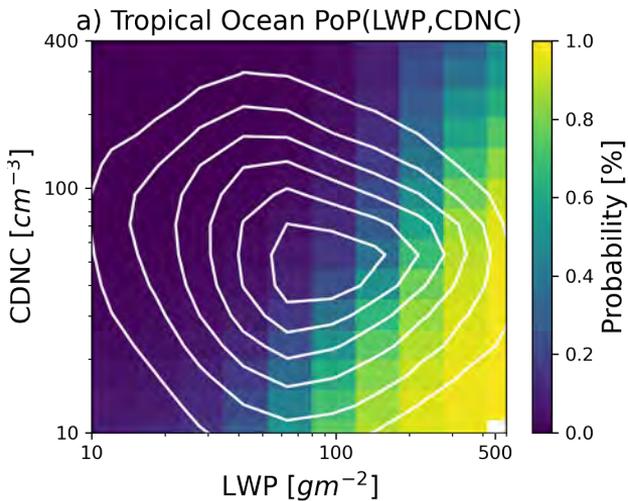
LWP fixed PDF( $\langle \text{LWP} \rangle$ , CDNC)    CDNC fixed PDF(LWP,  $\langle \text{CDNC} \rangle$ )

# Summary

- PoP of MLC over tropical oceans is derived from the collocated MODIS and CloudSat products
- A logistic function based parameterization scheme is developed to quantify the dependence of PoP on LWP and CDNC
- The parameterization can be used to understand the the spatial-temporal variation of PoP
  - Sc to Cu transition is mainly caused by the decrease of CDNC.
  - The seasonal variation of PoP is mainly caused by the seasonality of LWP.

# Outlook

- The PoP parameterization scheme can be used to evaluate the warm rain simulations on the GCMs
  - The PoP(LWP, CDNC) (color) can be used to evaluate the warm rain scheme
  - The PDF(LWP, CDNC) (line) can be used to evaluate the cloud scheme



# Addressing structural errors in warm-rain microphysics with BOSS, a Bayesian data-driven physically-based bulk scheme

Marcus van Lier Walqui — CCSR Columbia University @ NASA/GISS

[mv2525@columbia.edu](mailto:mv2525@columbia.edu)

Sean Patrick Santos — Pacific Northwest National Laboratories

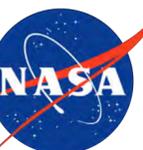
Hugh Morrison — National Center for Atmospheric Research

Karly Reimel — (prev.) Penn State University

Adele Igel — University of California Davis



ASR PI Meeting — Oct 27th 2022



**Bulk parameterization of microphysics remains challenging:**

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- Significant advances have been made in **detailed process modeling** (e.g. Lagrangian microphysics) but there is **uncertainty** in how this can be used to develop *simplified/reduced order* approaches for bulk schemes.

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- Laboratory studies are essential to gain process-level microphysics knowledge, but there is **uncertainty** in how to incorporate such data into schemes (limited sampling conditions, questions of how results scale to real clouds, etc).
- Wealth of **natural cloud and precipitation observations** but difficult to measure process rates directly, only net effects on hydrometeors —> an indirect constraint of bulk schemes

# Overview of the warm rain microphysics problem

**The BIG question:** How to use these various data sources — each with their own uncertainties — to constrain bulk schemes?

- As more complex bulk schemes are developed this makes indirect constraint (i.e., tuning) even more difficult...
- Simply stated: we want to incorporate uncertain “observations” (or process model data) in a parameterization with basic cloud physics knowledge in a rigorous way.
- This is a Bayesian problem, and we can therefore use Bayesian statistics to address it rigorously...



*Thomas Bayes (1701-1761)*

$$P(\mathbf{x}|\mathbf{y}) = \frac{P(\mathbf{y}|\mathbf{x})P(\mathbf{x})}{P(\mathbf{y})}$$

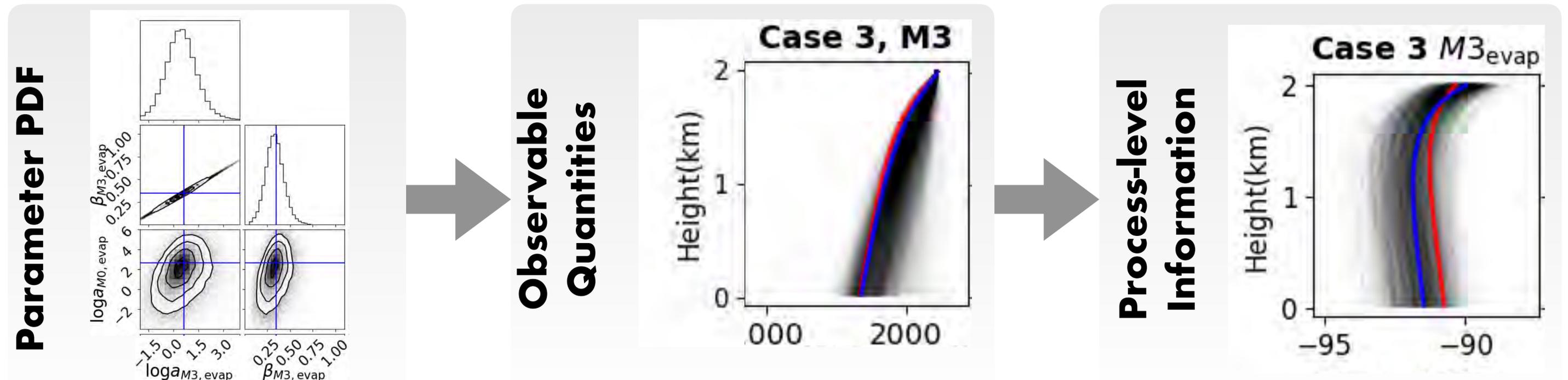
**BOSS**

# BOSS

- B**ayesian (we treat uncertainties robustly, uncertainties reside in parameters)
- O**bservationally-constrained (scheme is informed by comparison to observations)
- S**tatistical-physical (we don't just want a statistical scheme, but we will use statistics)
- S**cheme — bulk microphysics parameterization scheme (so far rain & cloud only)

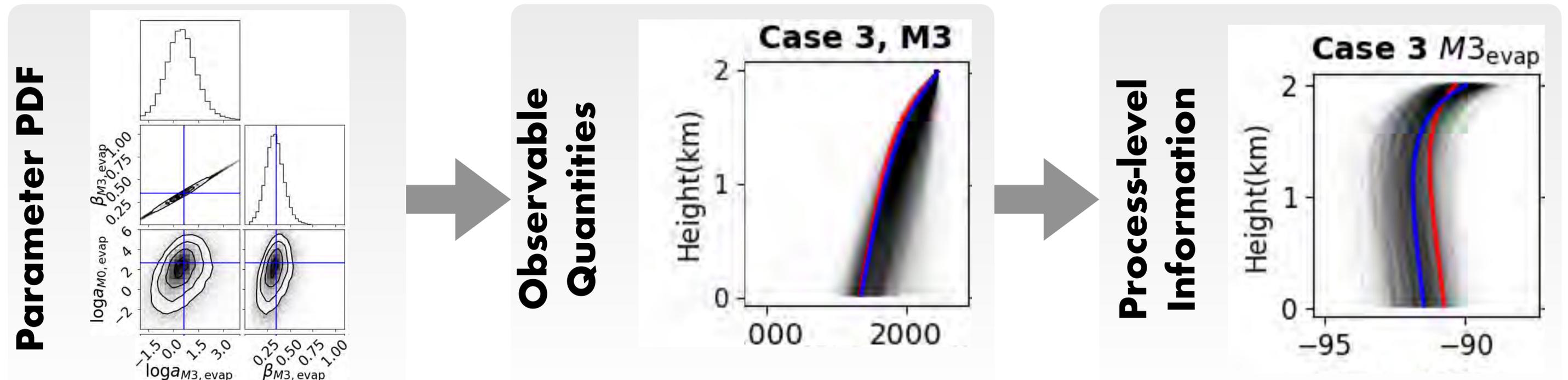
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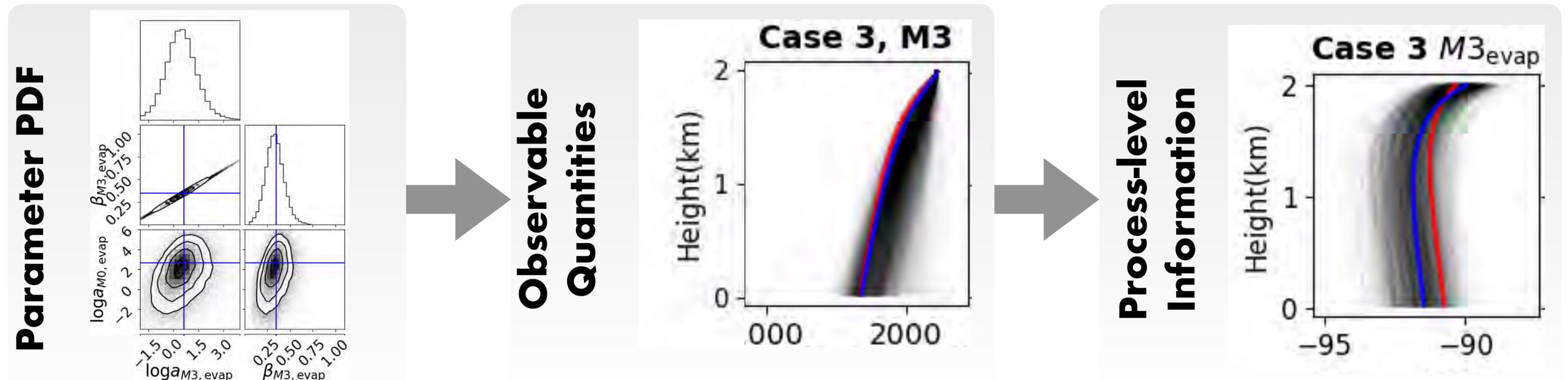
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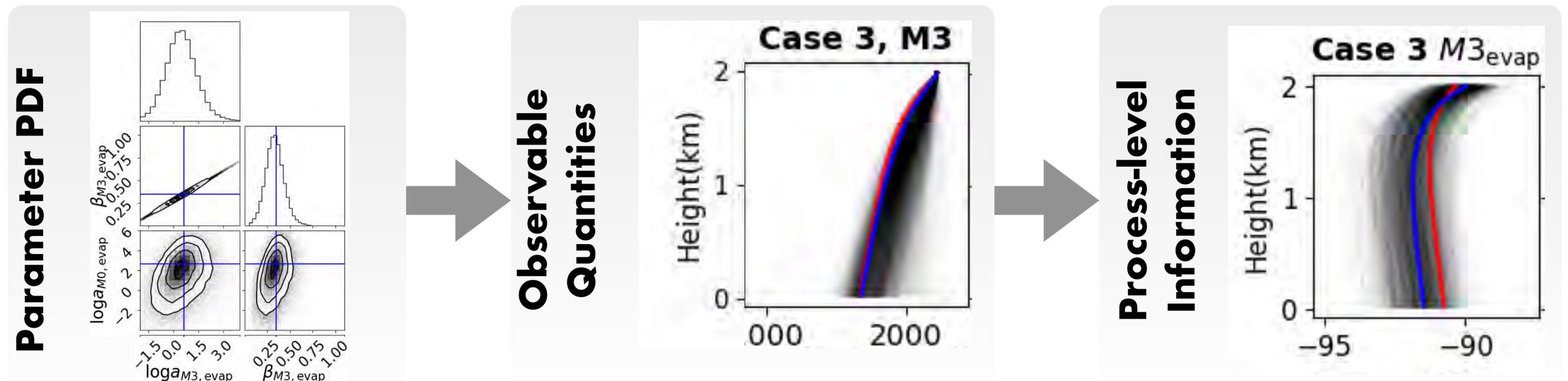


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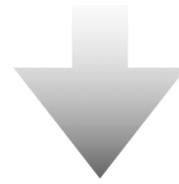
# The BOSS approach

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No assumed DSD functional form

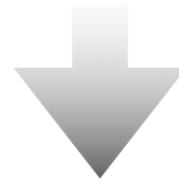
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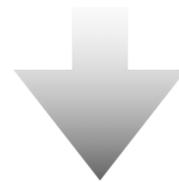
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Predict *moments* of the DSD  $M_k = \int_{D_{min}}^{D_{max}} D^k (\partial N / \partial D) dD$   
(M0=number, M3=mass, M6=reflectivity)

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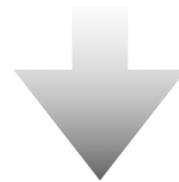


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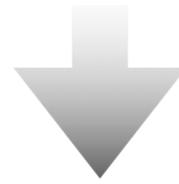
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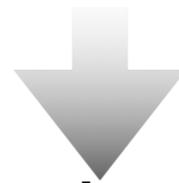
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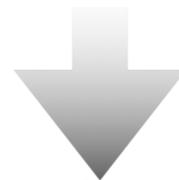


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Choose whatever moments are “best”

**Get rid of fixed process rate functions**

# Get rid of fixed process rate functions

Use a flexible (but sensible) functional basis set

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$$\frac{dM_k}{dt} \approx F(T, p, q) \sum_{l=1}^L a_{l,k} M_{p_1} \prod_{n=1}^{N-1} \left( \frac{M_{p_{n+1}}}{M_{p_n}} \right)^{\beta_{p_n, l, k}}$$

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Use Bayesian inference to estimate  $a, \beta, \delta$

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## Example of theoretical constraints on parsimony

A third moment (e.g. M6) can be used as a measure of DSD variance:

$$\sigma^2 = \frac{1}{M_{c0}} \int_0^\infty N(D)(D^3 - m_c)^2 dD = \frac{M_{c6}}{M_{c0}} - m_c^2$$

Constraint on the possible values of DSD variance enforces a structural form on the process rate for cloud self-collection (... some math...)

$$b_{6m,csc} = b_{0m,csc} + 2 \quad a_{6,csc} \geq a_{0,csc} \quad (1)$$

Similar arguments reduce the total number of BOSS parameters from 60+ to 37 for 3-moment cloud BOSS

# Directly fitting process rates to a Bin model

## Autoconversion rates: bin vs. BOSS fits

### Direct process fits with BOSS

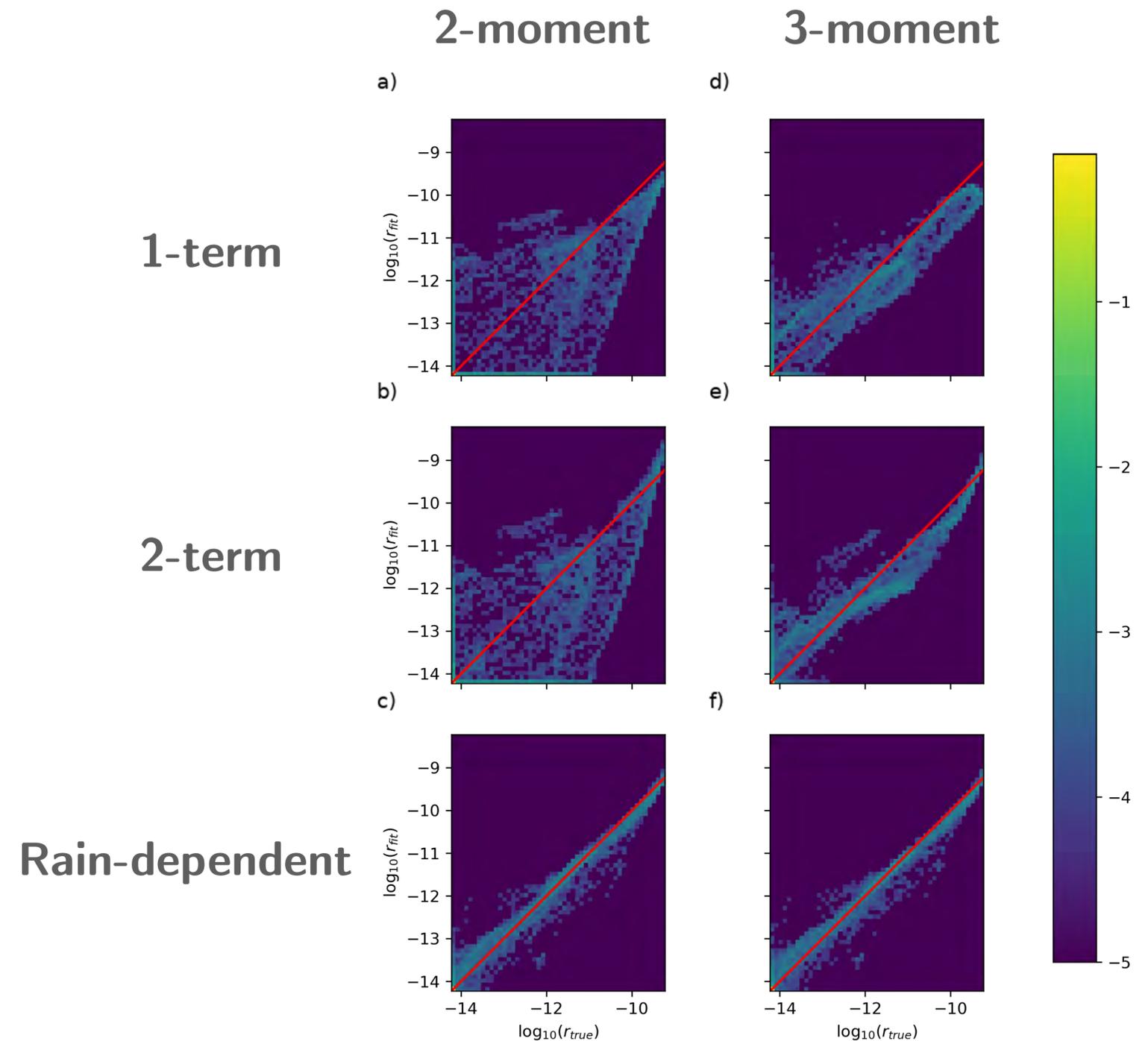
- Directly fit BOSS parameters to match existing TAU bin scheme autoconversion process rates
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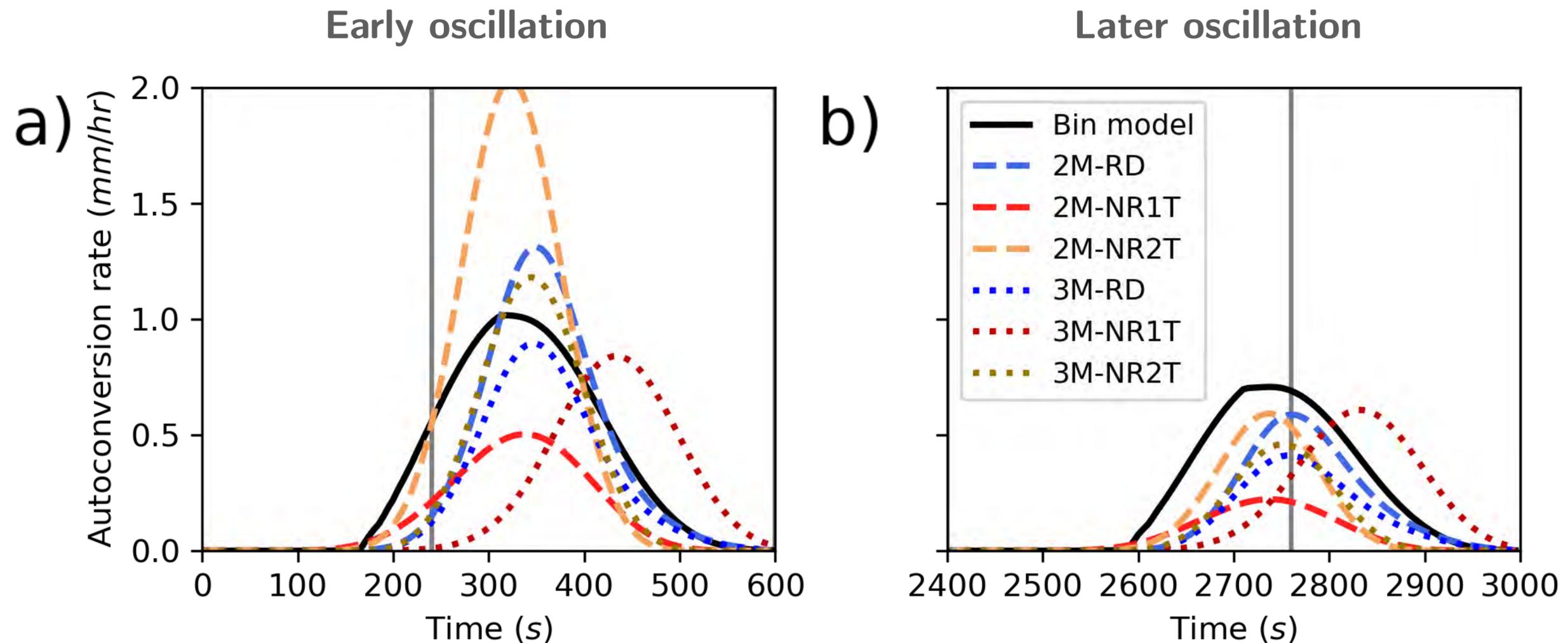
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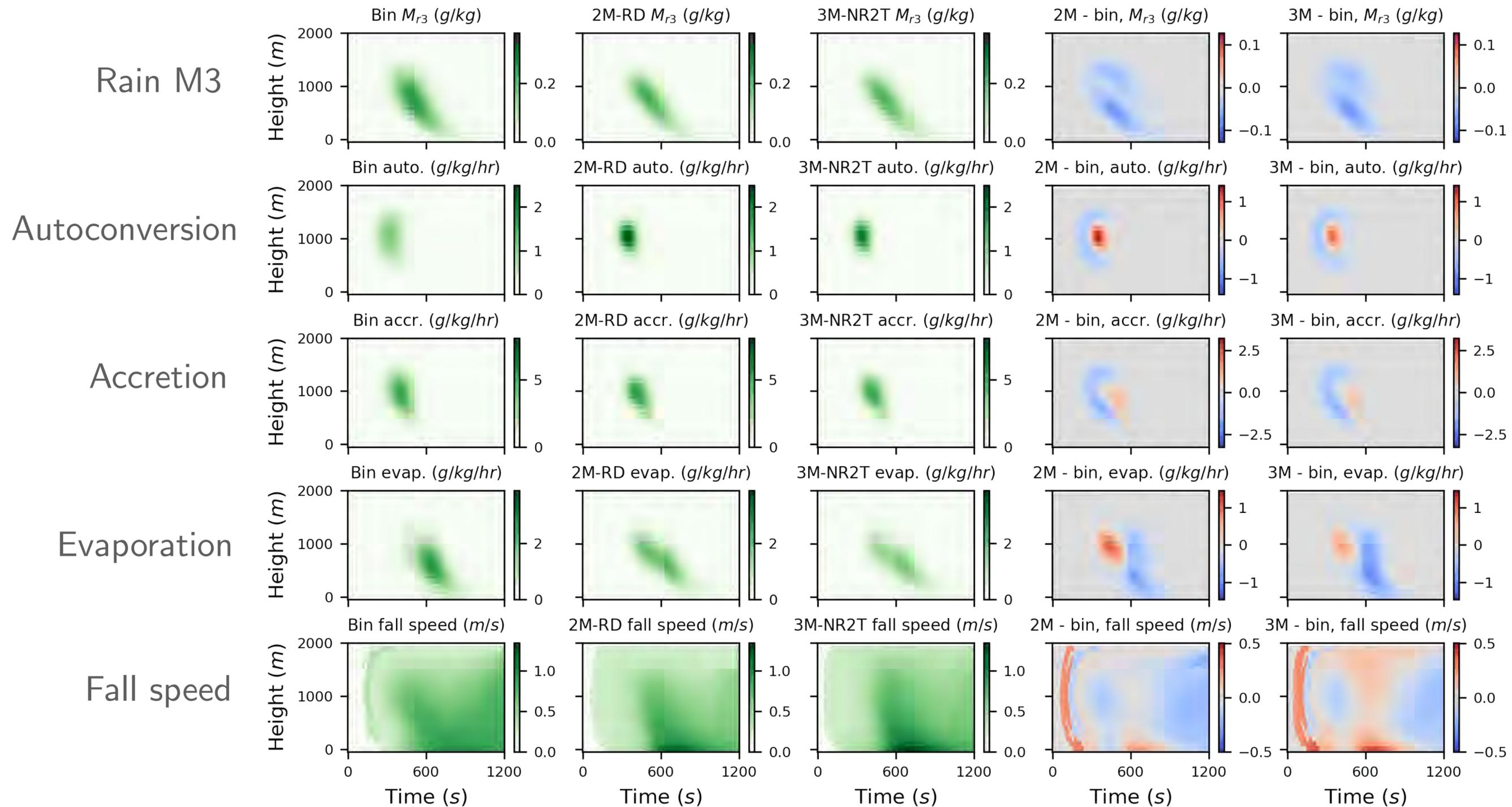


# Testing direct fits in time-evolving 1D model

Looking at autoconversion rates tuned via direct fitting in 1D model simulations



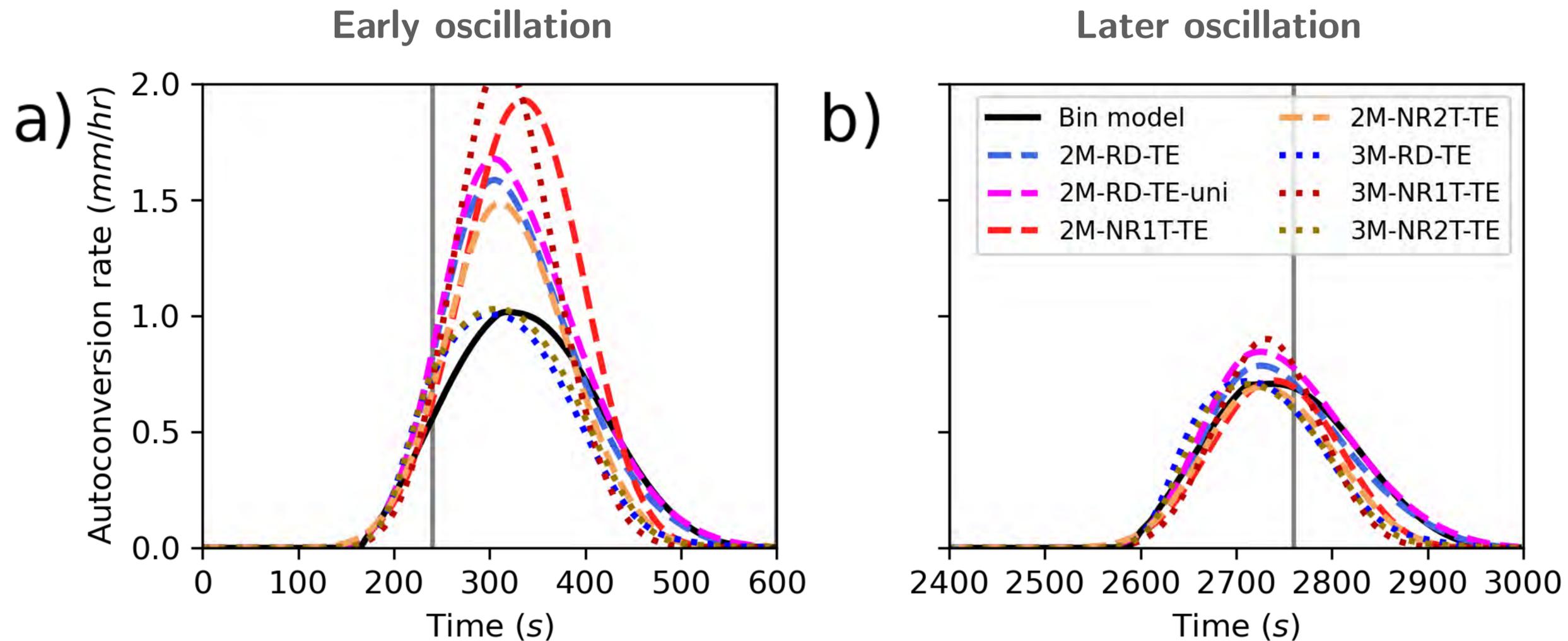
# Testing direct fits in 1D model (2M vs 3M)



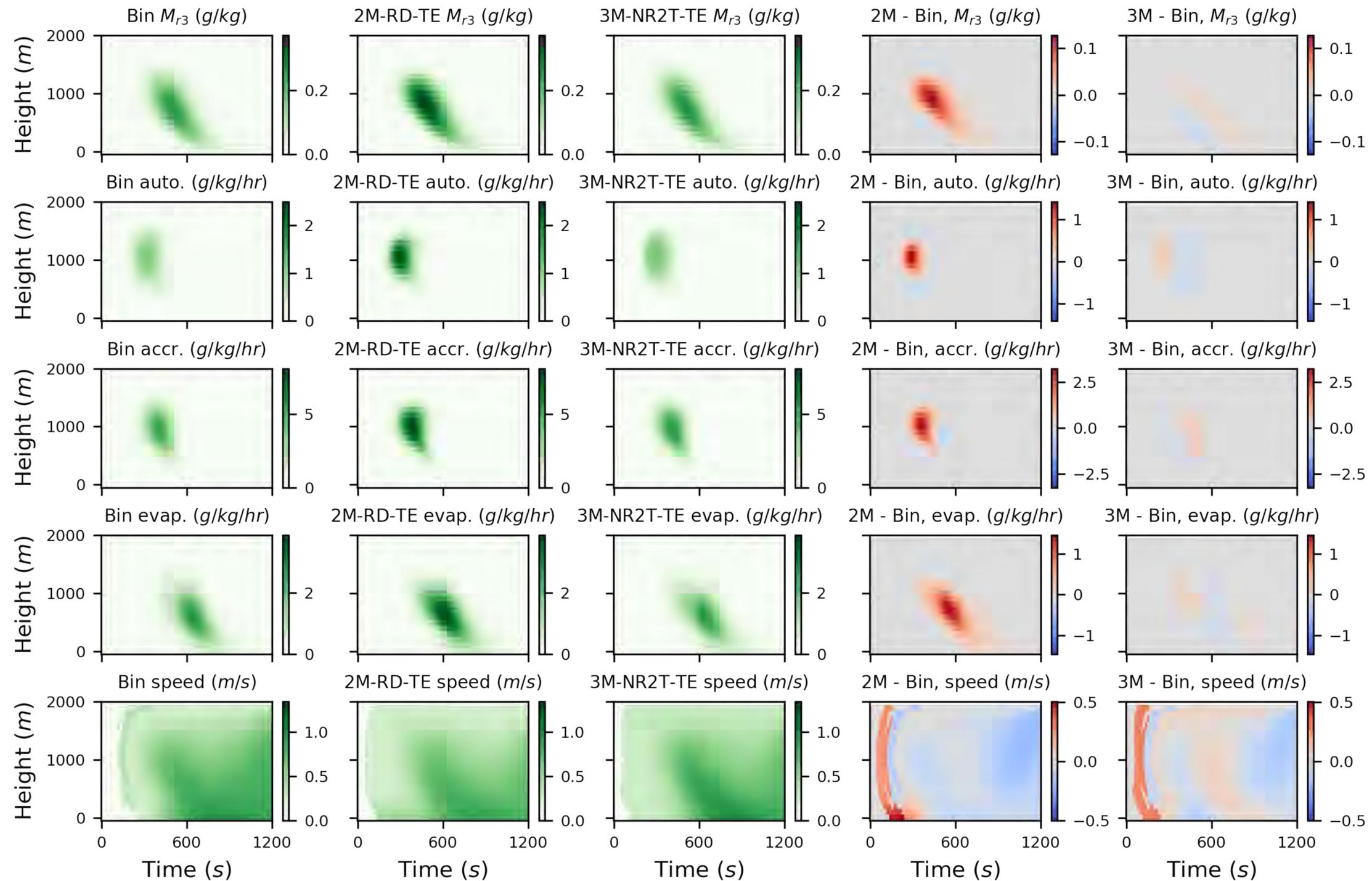
# Instead use direct fits as a (Bayesian) prior

\*Refine the prior with a likelihood using observations from *time-evolving sim'n*

## Autoconversion rates in 1D model



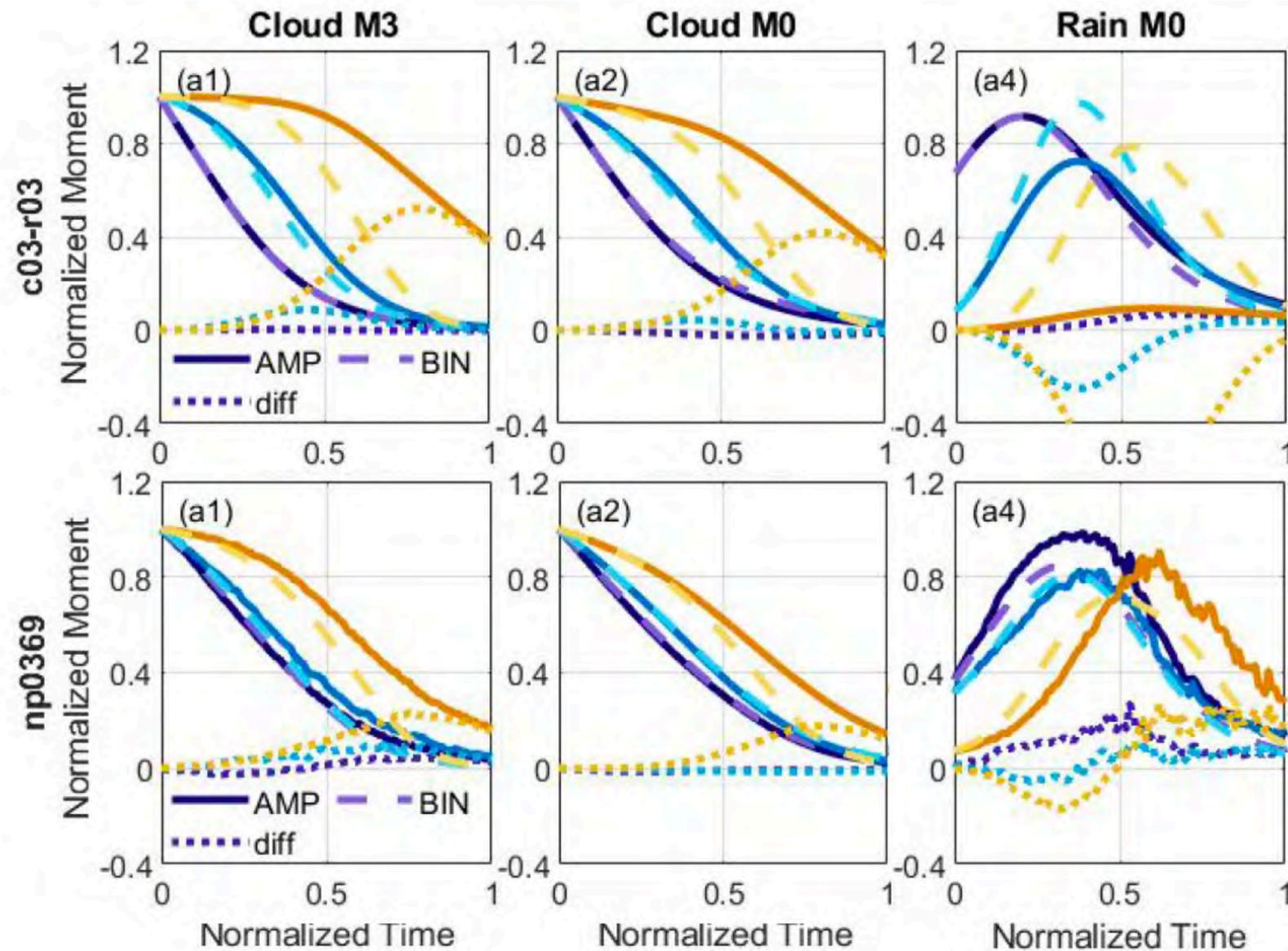
# Testing direct/1D fits in 1D model (2M vs 3M)



Structural choices must be evaluated in the context of adequate parameter constraint!

# A larger structural error?

Are separate cloud and rain categories the correct approach for bulk warm microphysics?

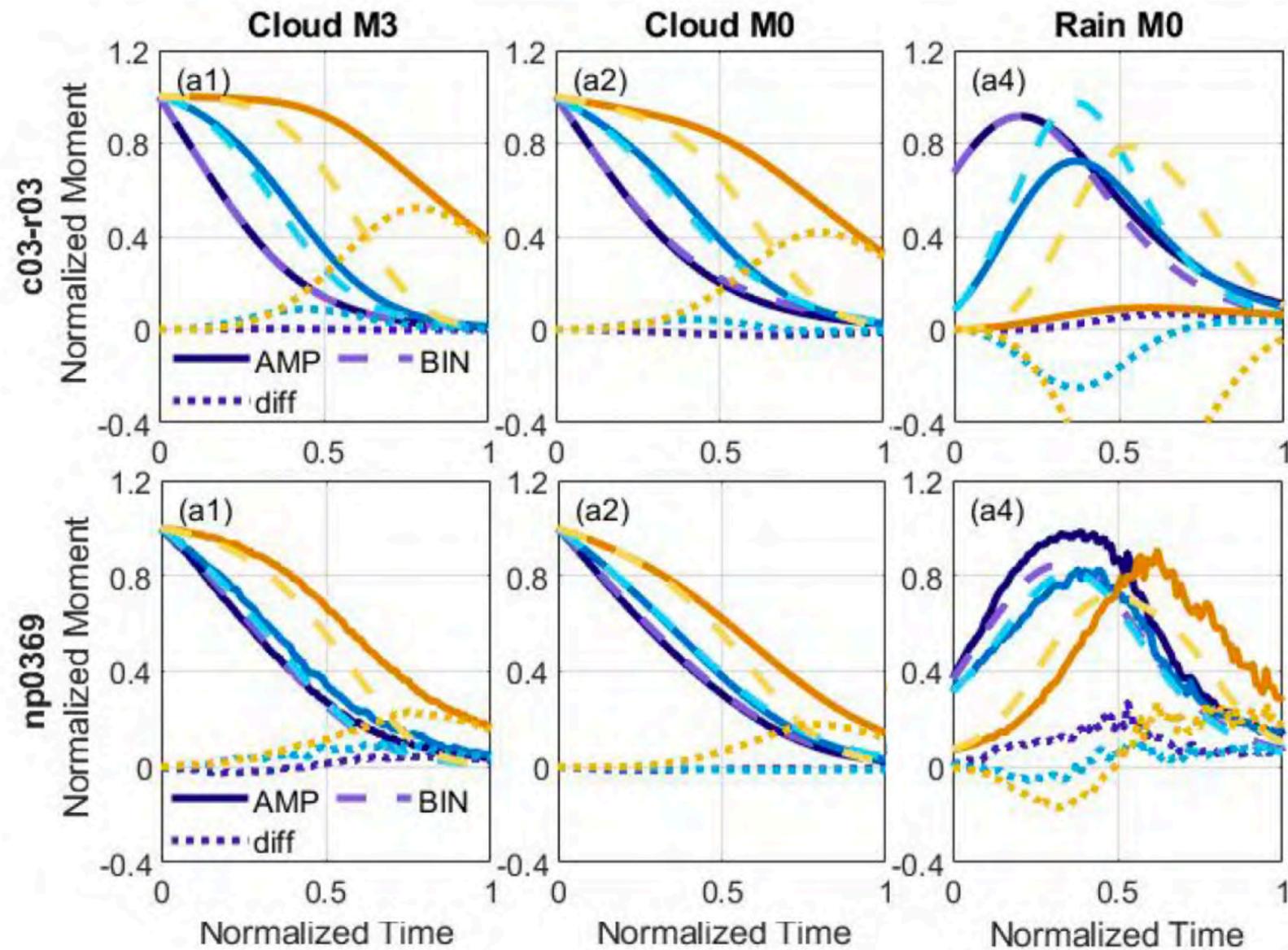


Adele L. Igel, H. Morrison, S. P. Santos, and M. van Lier-Walqui. *Limitations of separate cloud and rain categories in parameterizing collision-coalescence for bulk microphysics schemes.* JAMES, 2022.

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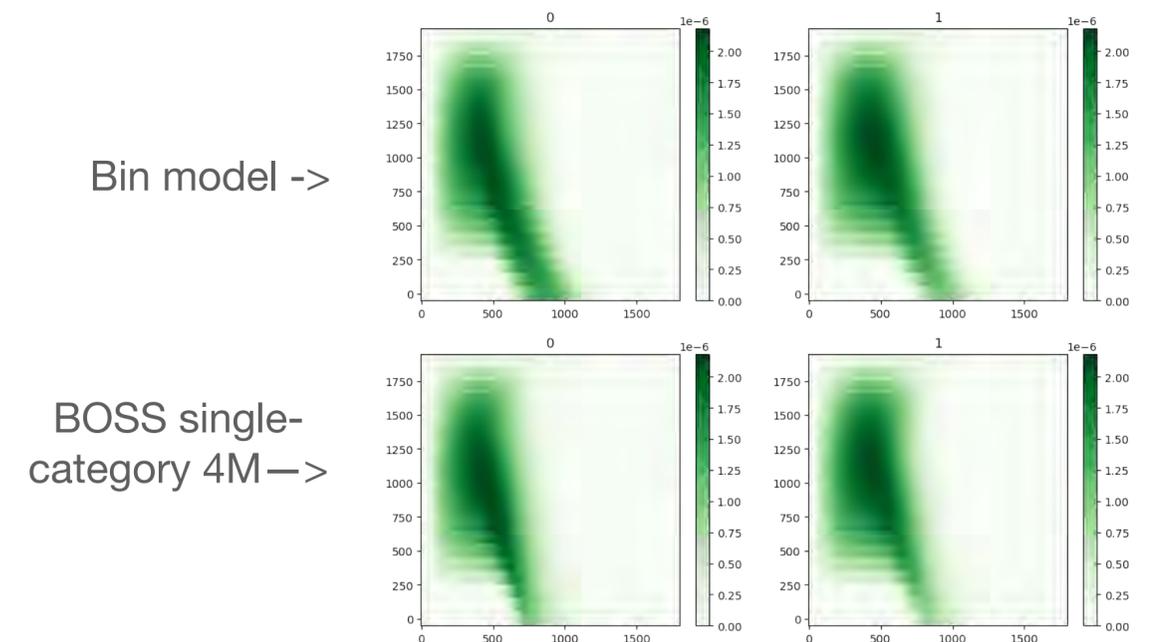
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*This is something we are currently testing with BOSS!*



# A spectrum of data and ways to constrain/inform BOSS

*Less expensive,  
less realistic*



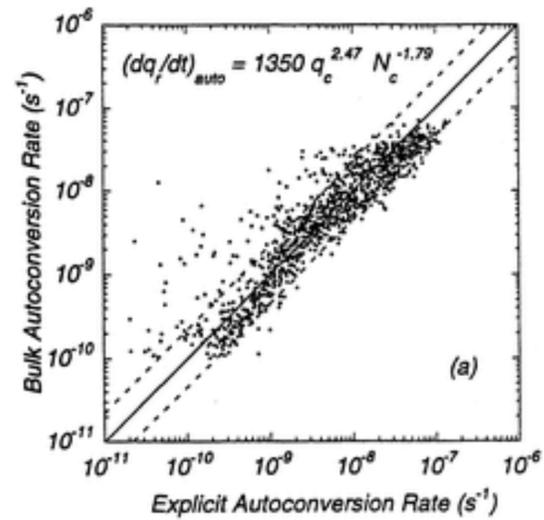
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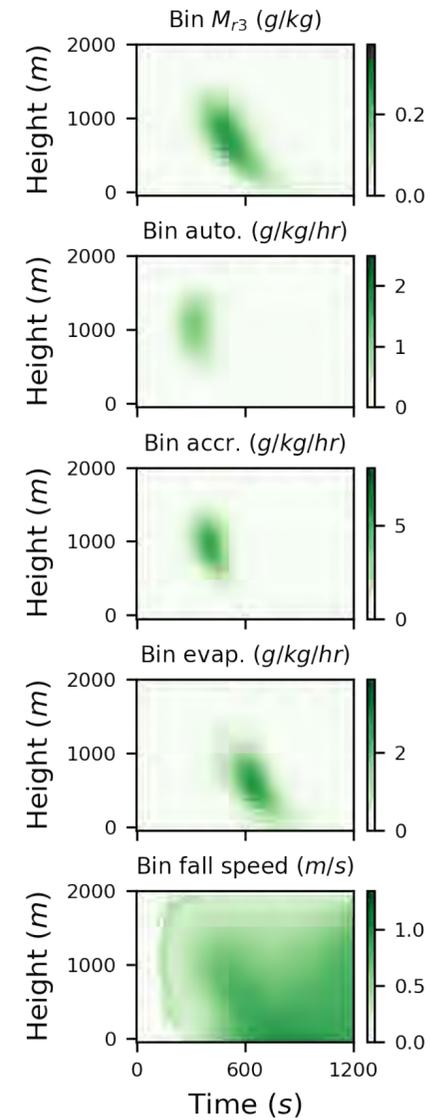
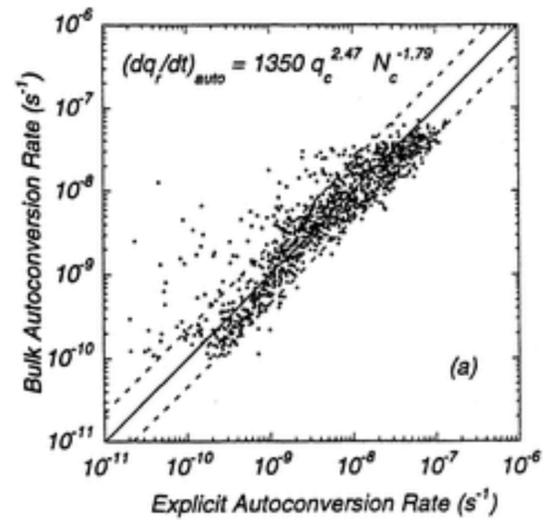
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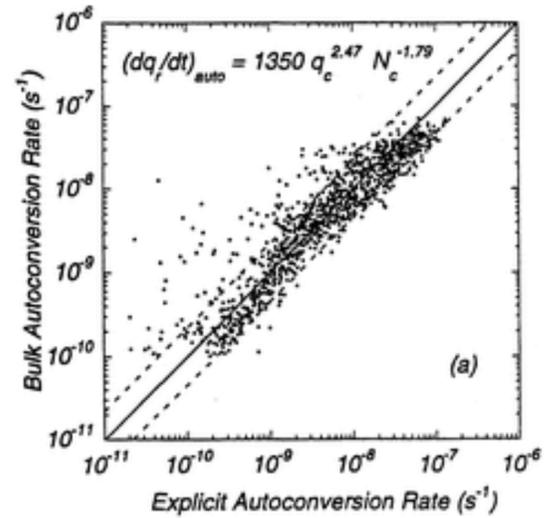
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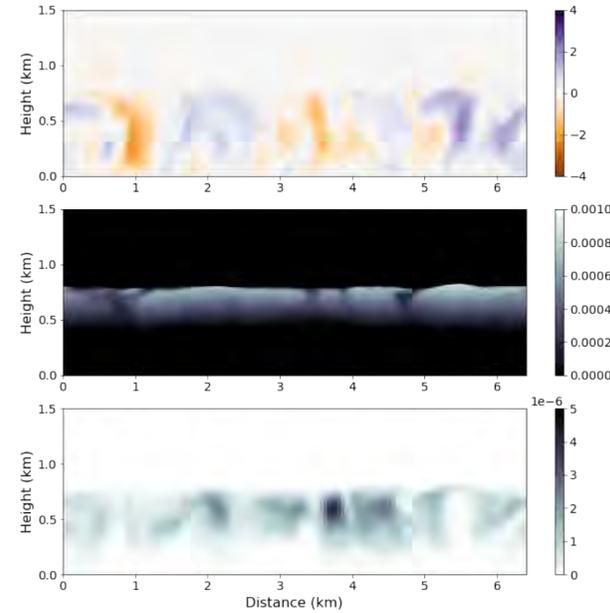
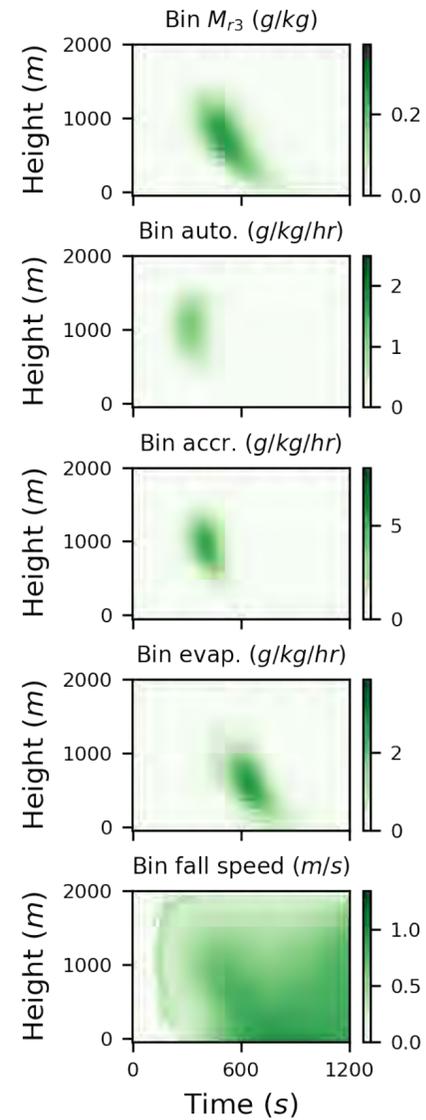
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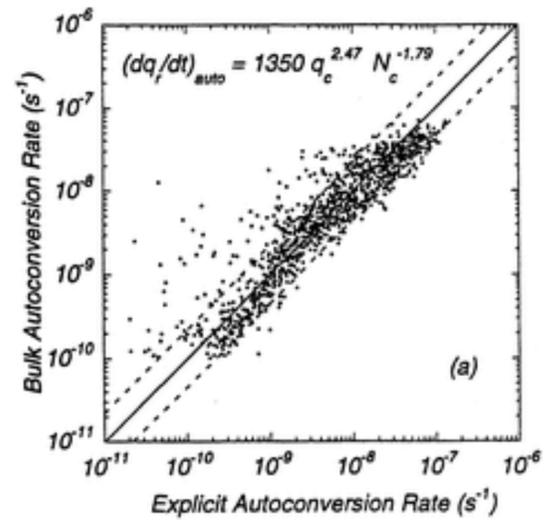
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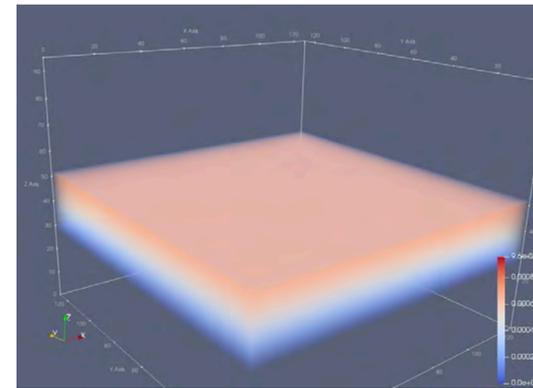
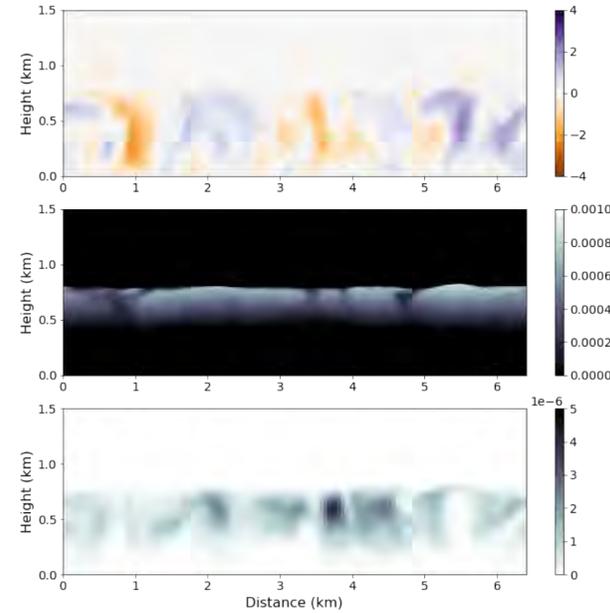
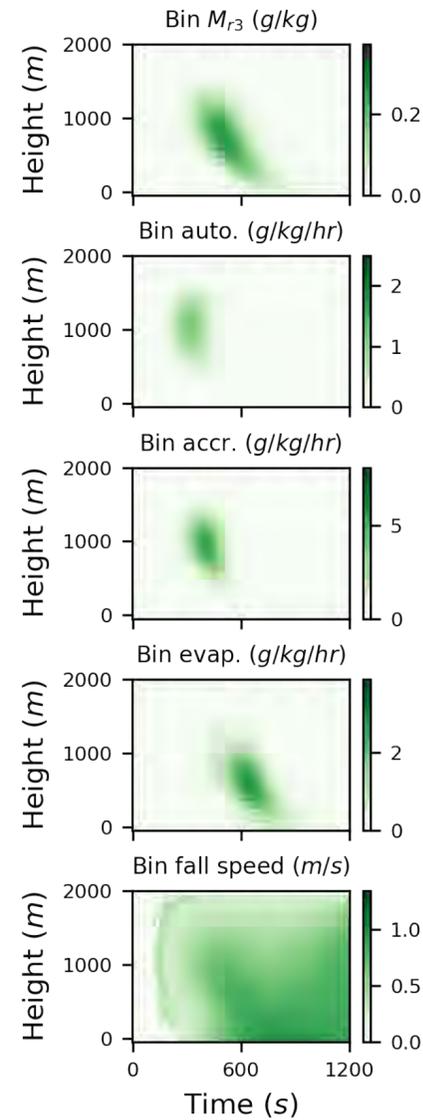
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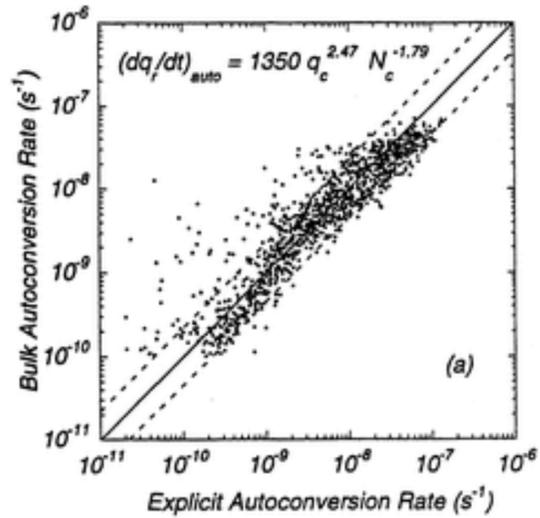
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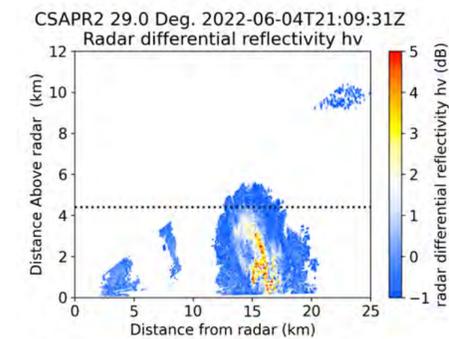
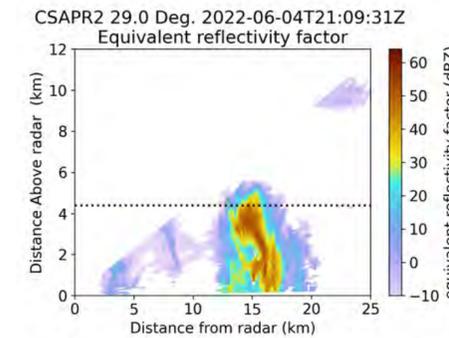
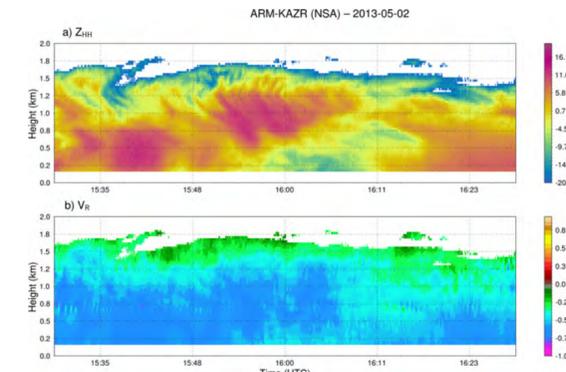
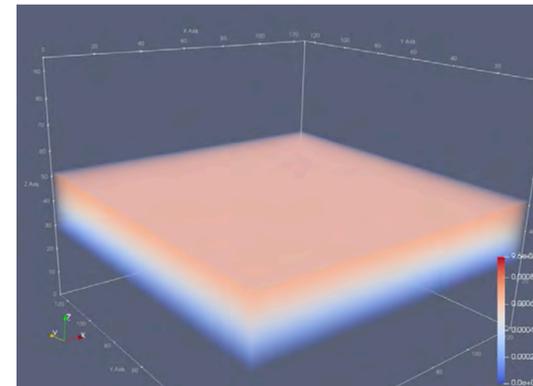
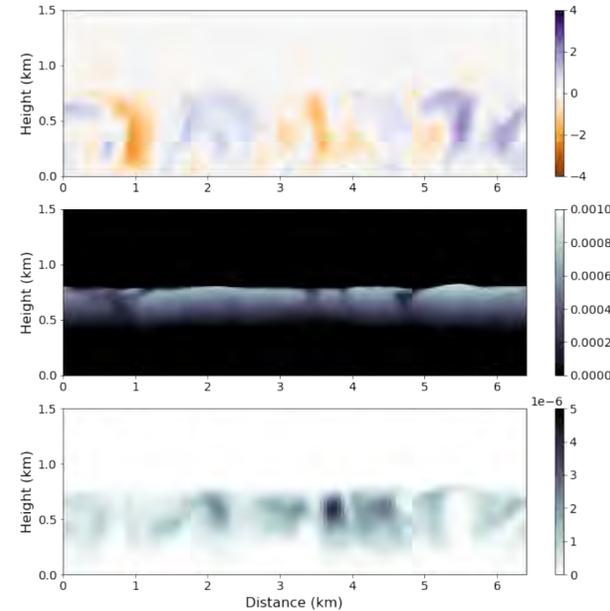
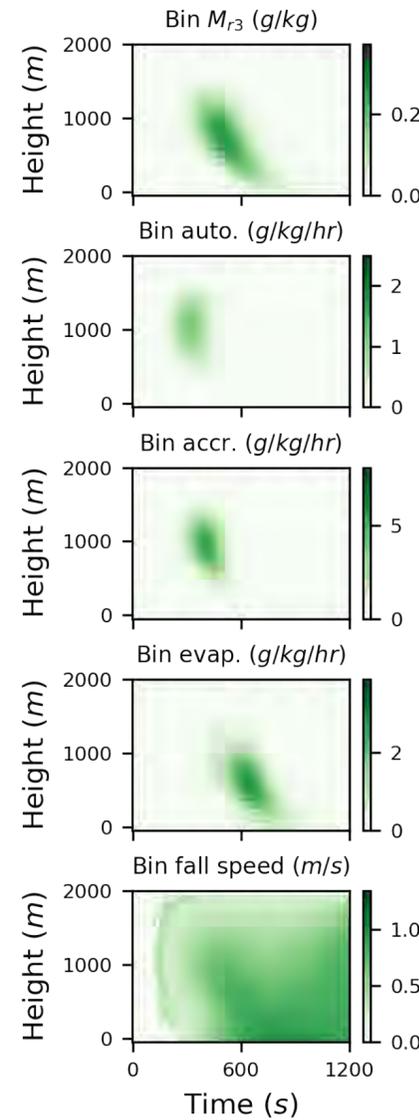


More expensive,  
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Real observations,  
real complications



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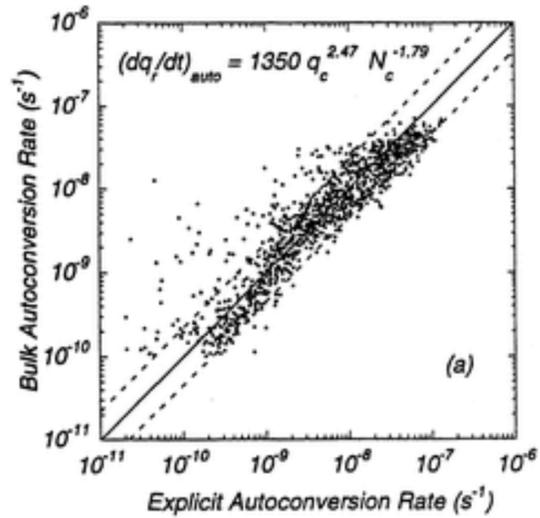
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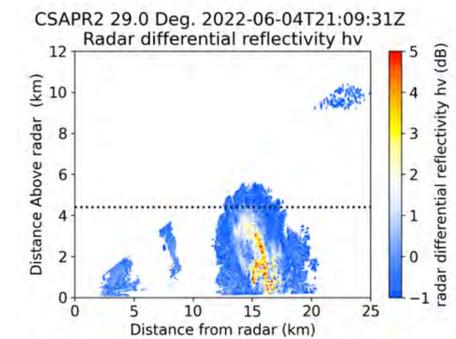
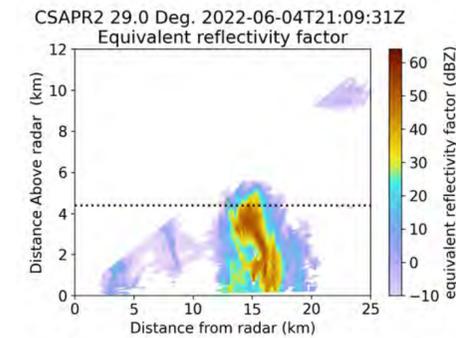
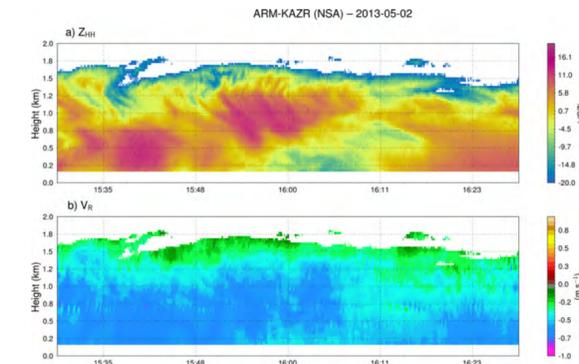
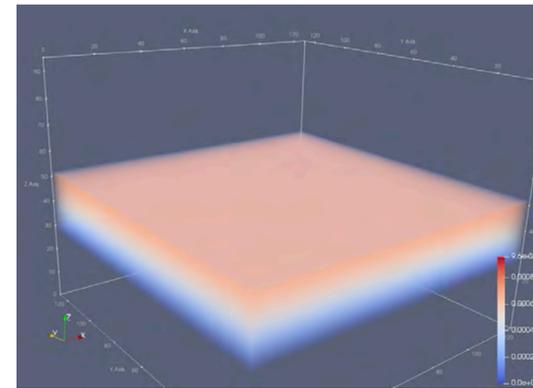
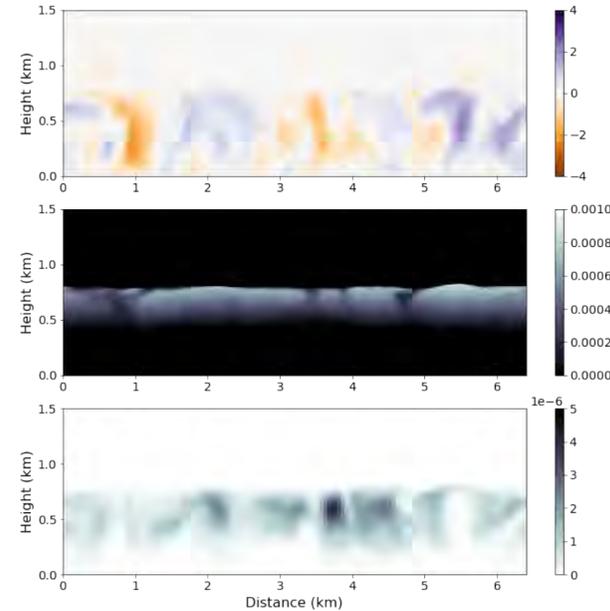
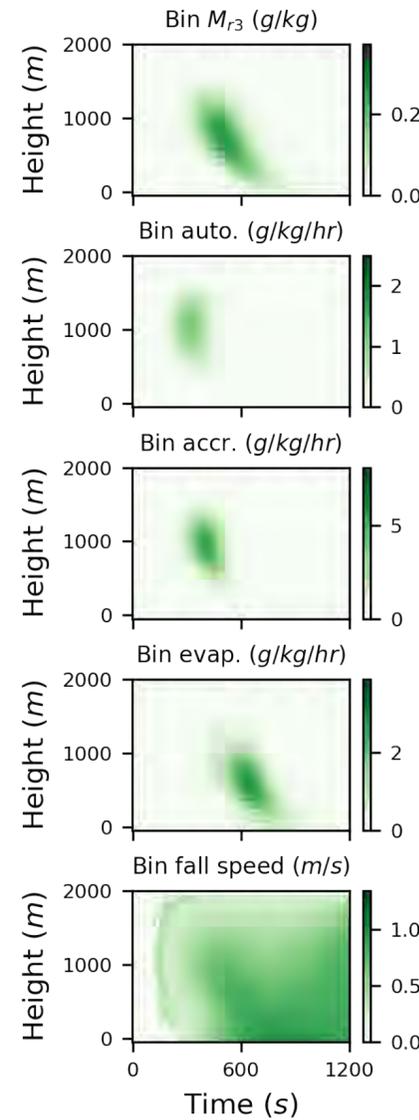


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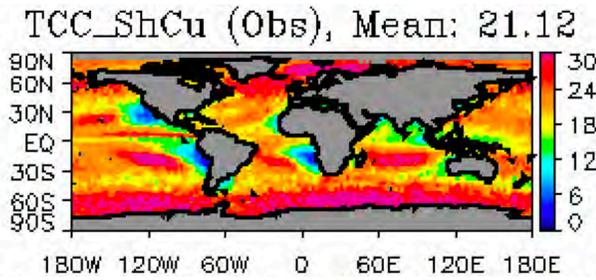
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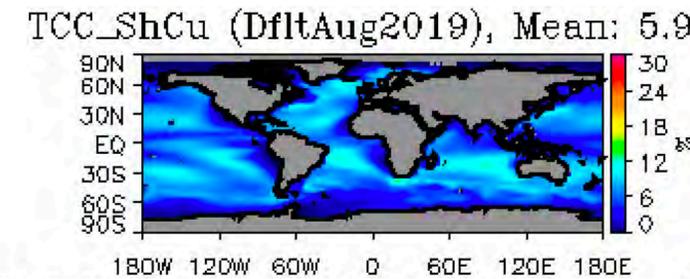
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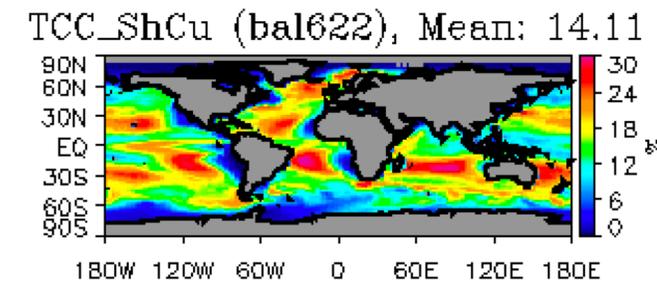
## Observed Shallow Cu



## Default Parameters



## Tuned Parameters



Directly fitting process rates to some "reference" scheme

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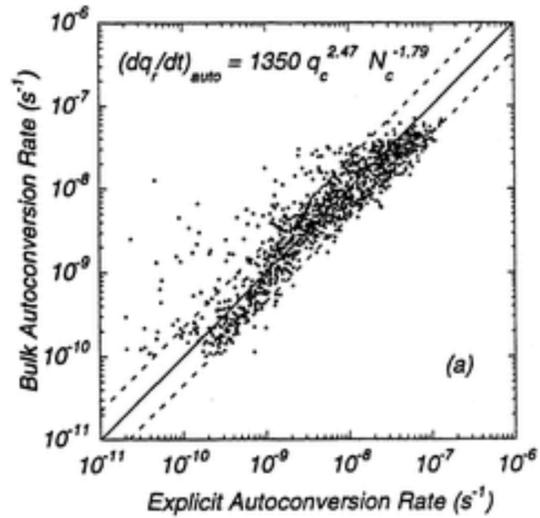
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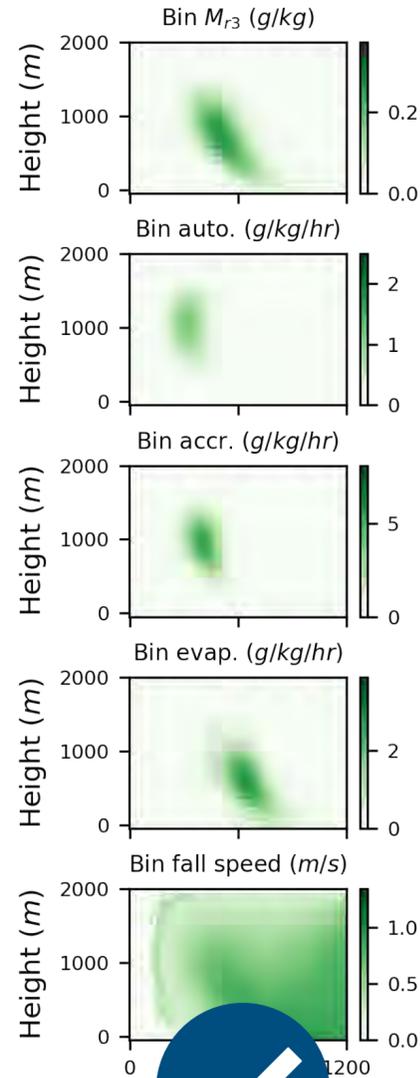
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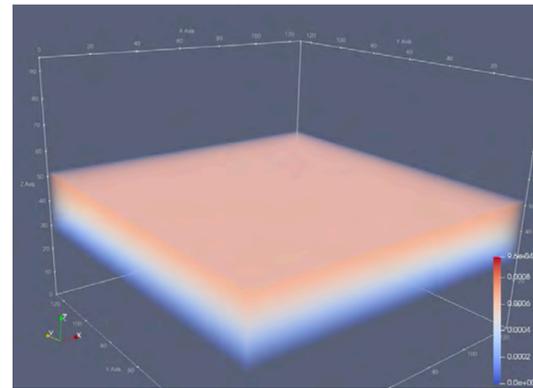
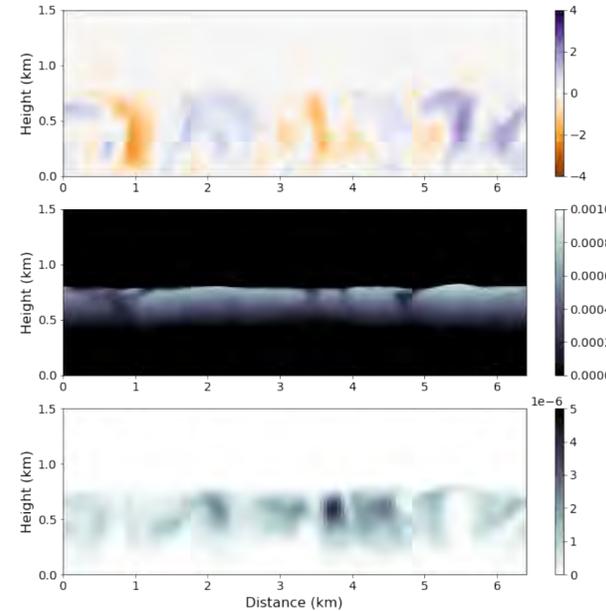
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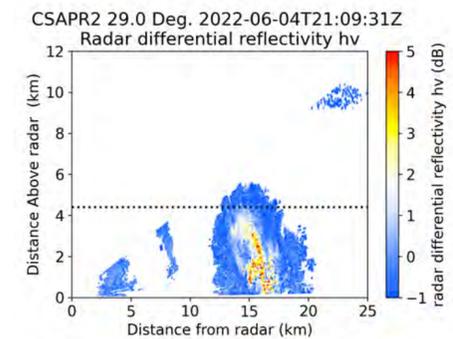
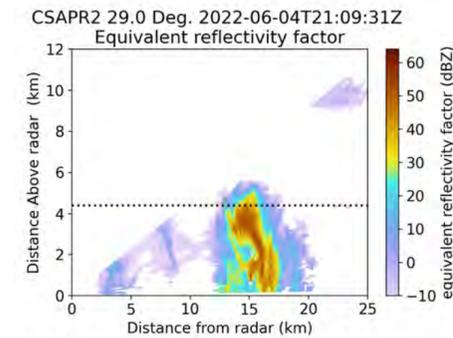
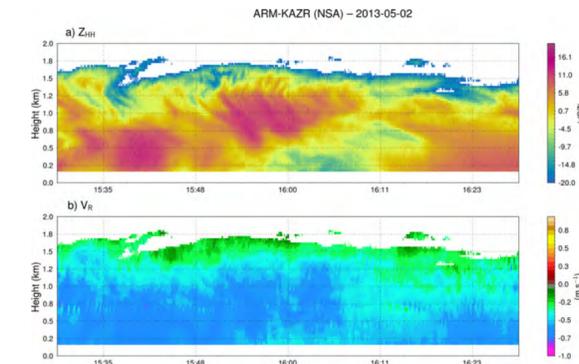
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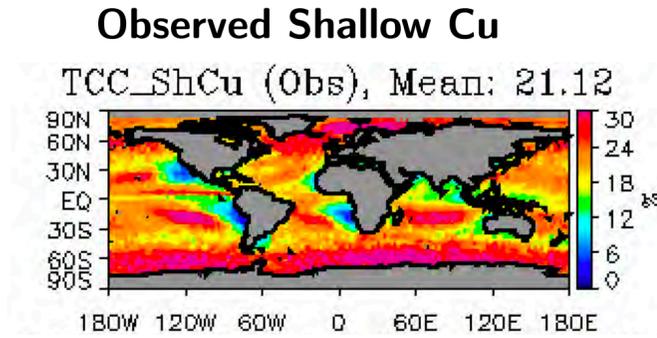
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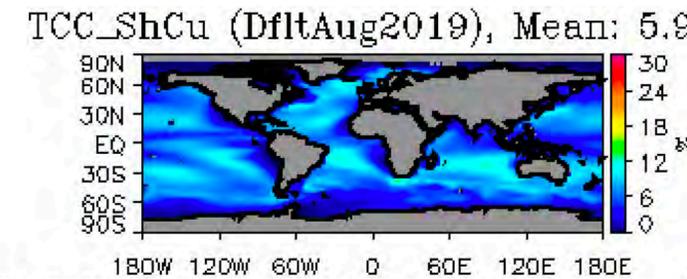
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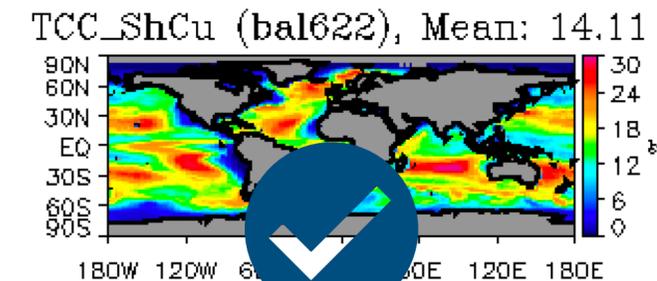
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# Conclusions & Acknowledgments



ASR Grant no. DE-SC0016579



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# Extra Slides

# JEFE (Sean P. Santos)

## JEFE: Measuring Predictability

### JEFE: Jacobian Evaluation of Functional Error

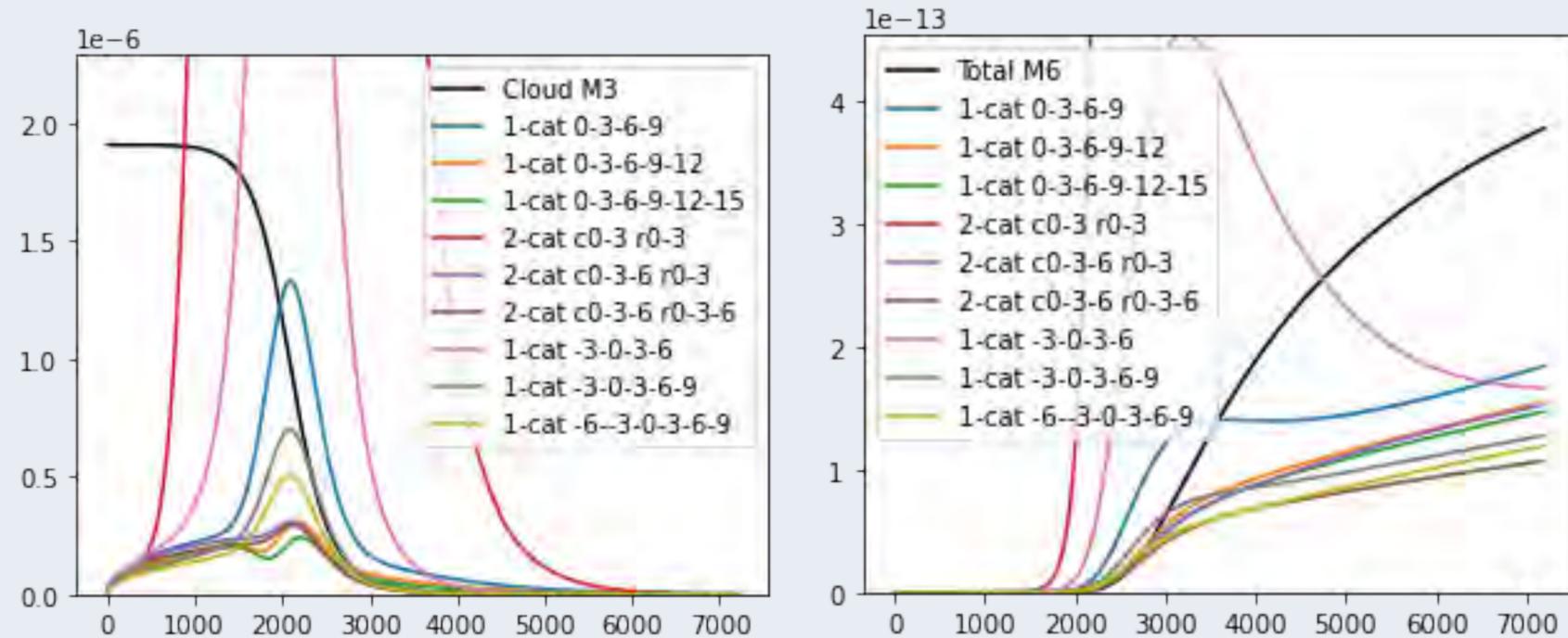
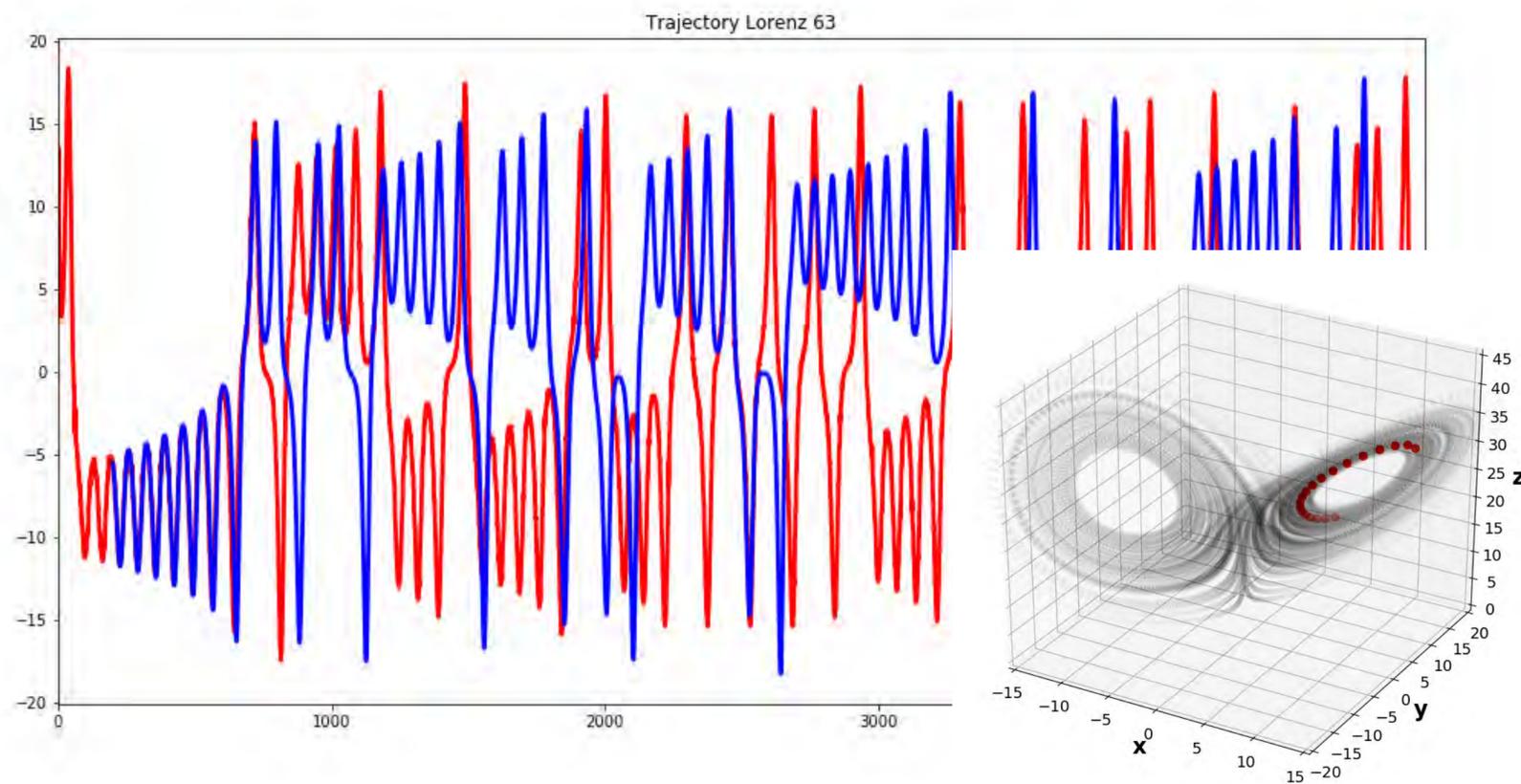


Figure 3: Adjoint-model-derived estimates of relative error of highly-accurate bulk schemes for cloud mass (left) and radar reflectivity (right).

A Challenge: inference complicated by state errors, initial & boundary condition uncertainty

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Some aspects of the atmosphere behave chaotically: errors grow nonlinearly from small perturbations, reducing predictability



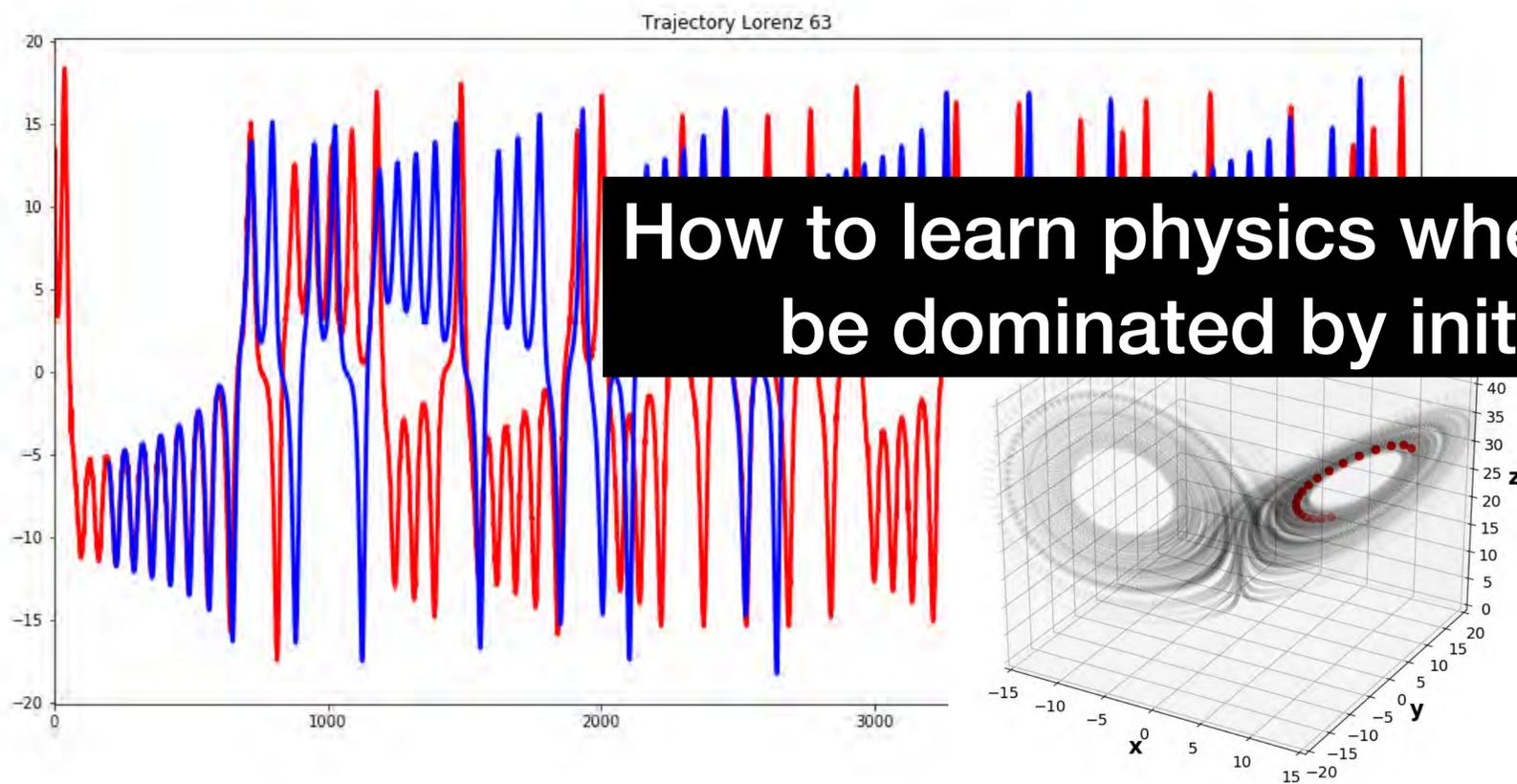
*Lorenz (1963)*



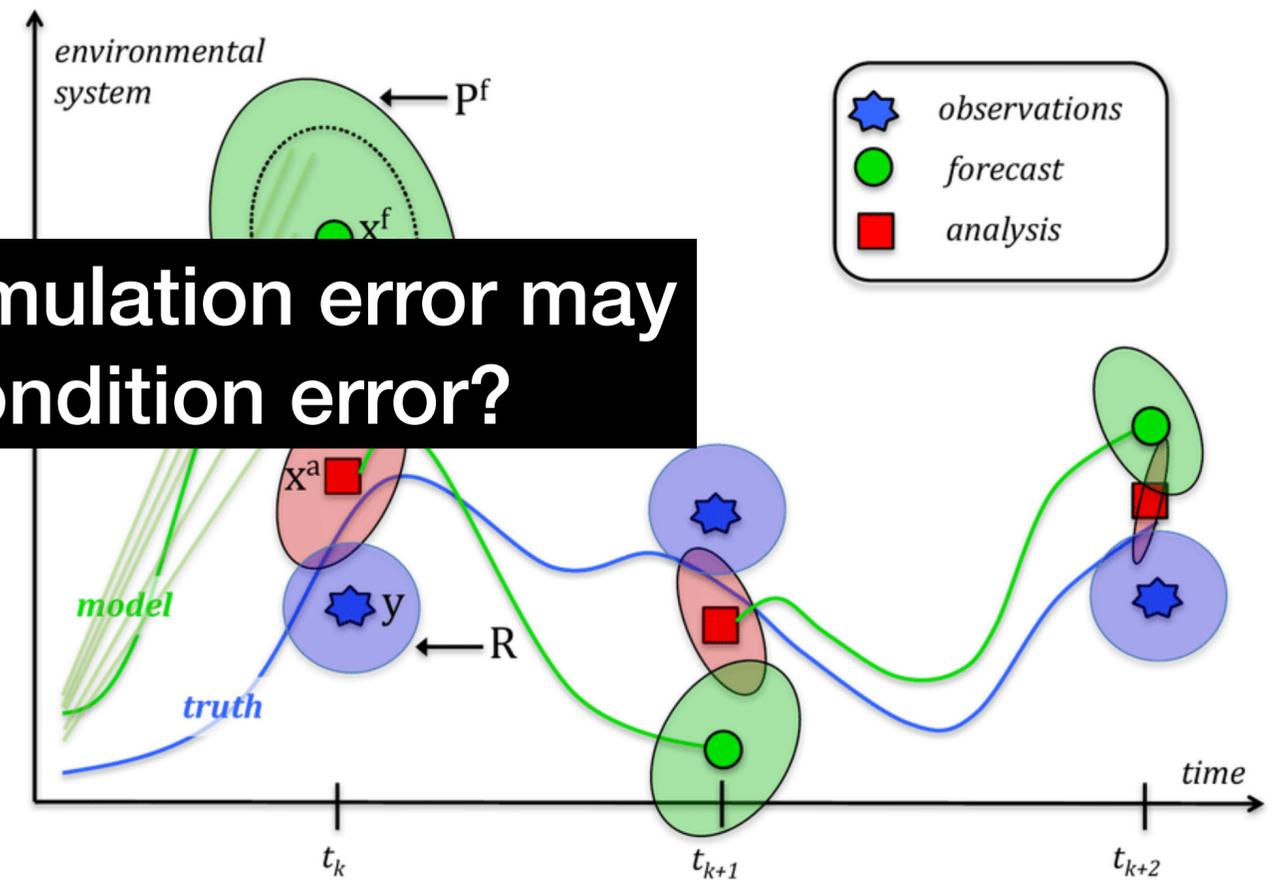
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“Data Assimilation” — correcting the state of a model forecast with observations



**How to learn physics when simulation error may be dominated by initial condition error?**

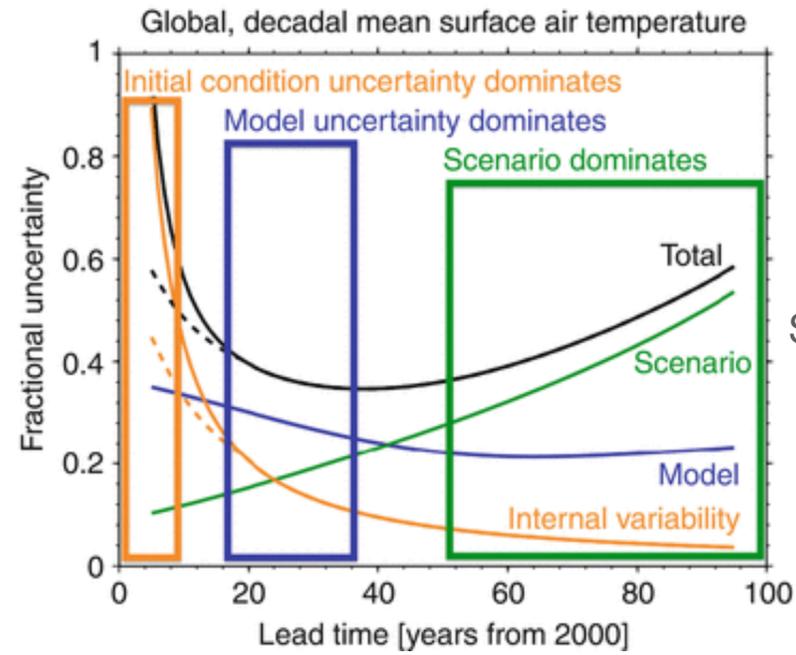


Lorenz (1963)

Tandeo et al. (2018)

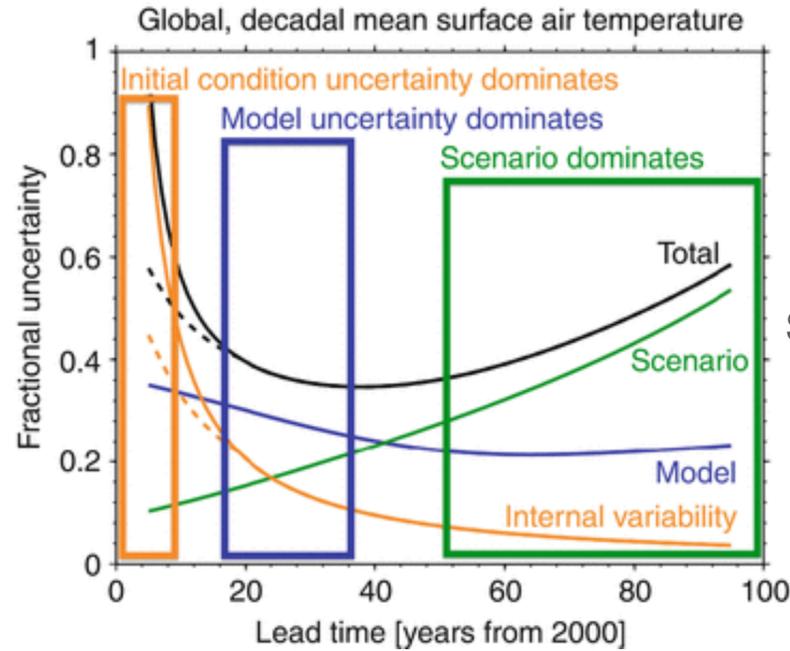
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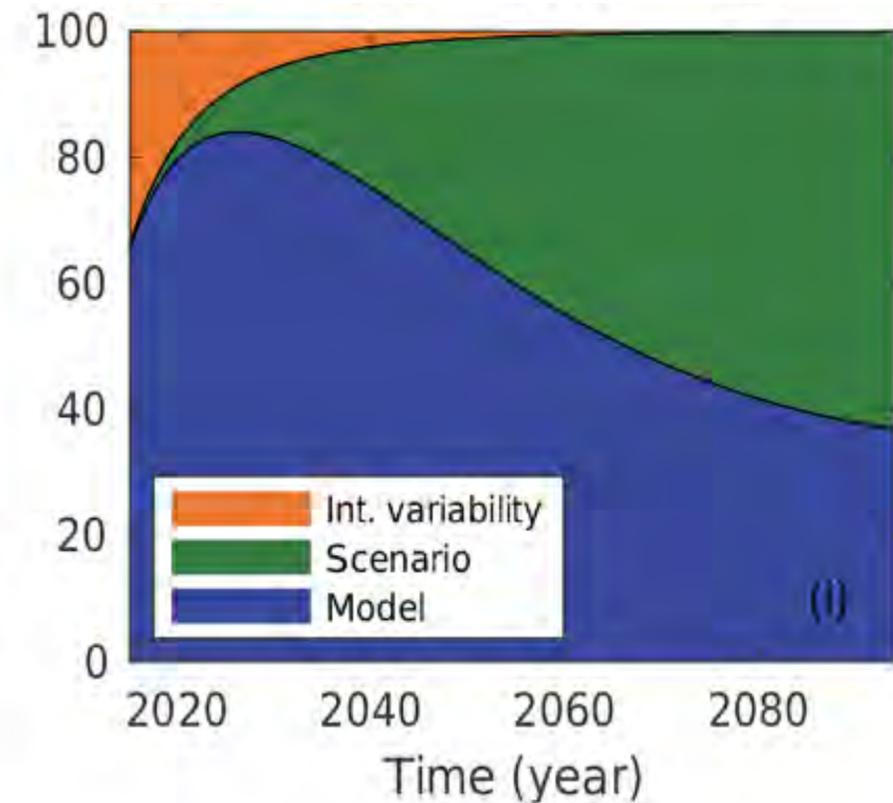
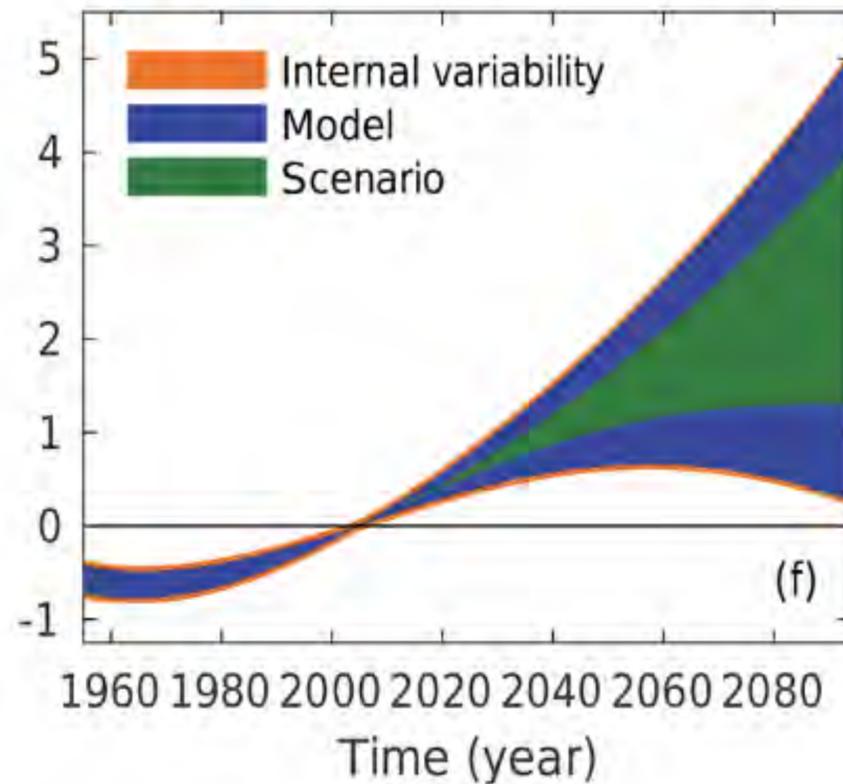
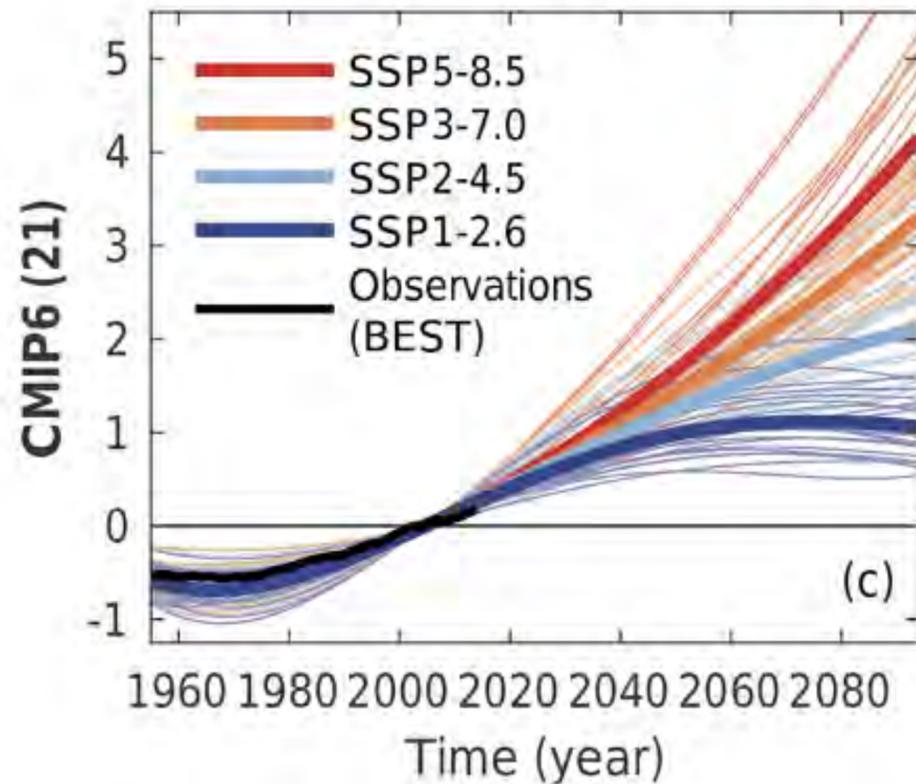


Sanderson & Knutti (2012)

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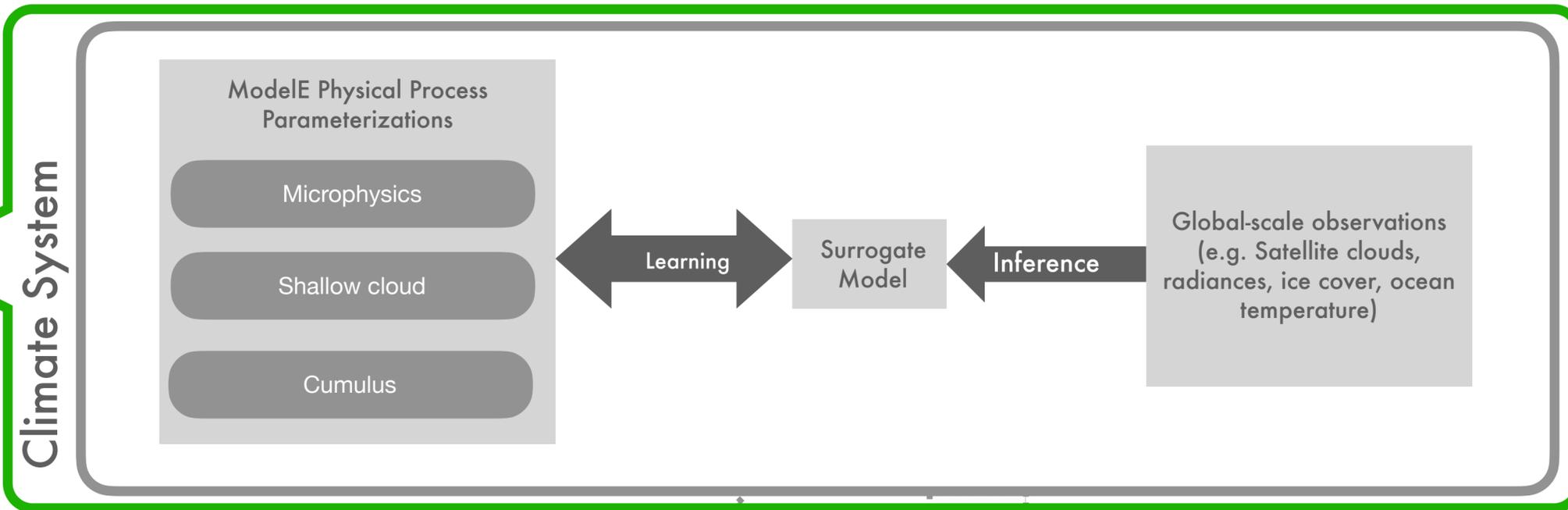


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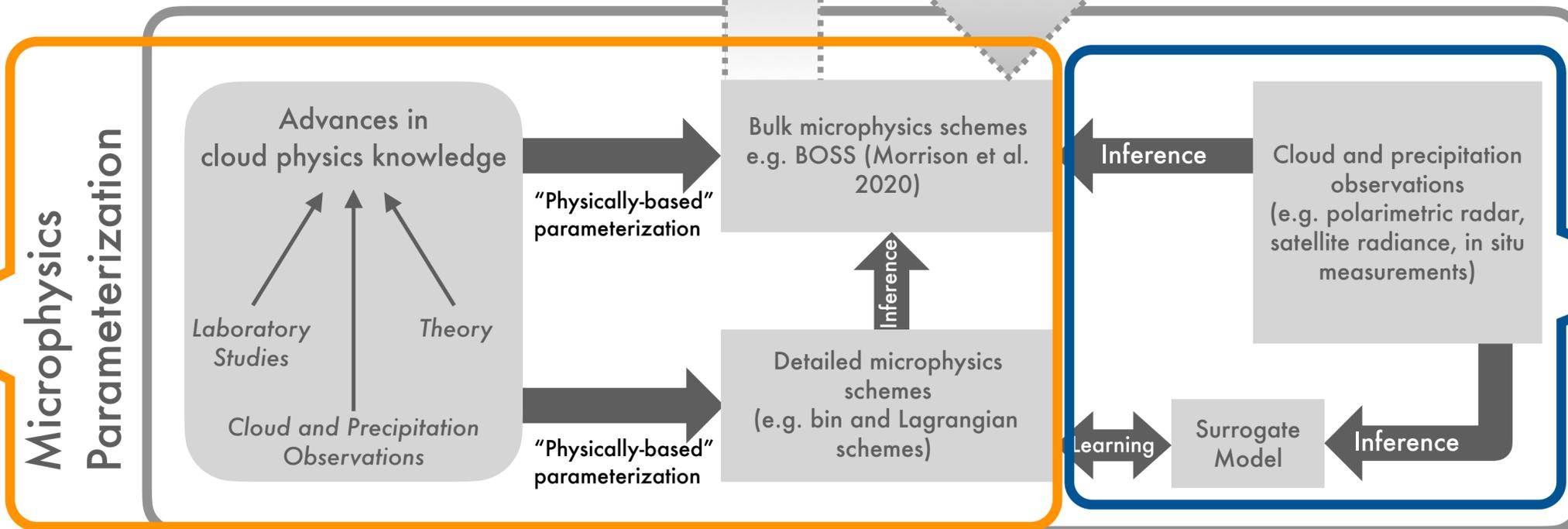


Lehner et al. (2020)

Top-down tuning of ModelE using MCMC and ML, informed by global satellite data



"Bottom-up" inference using MCMC, informed by detailed schemes and theory



Future work uniting bottom-up and top-down approaches

Future work using observations to improve process-level understanding

# Addressing structural errors in warm-rain microphysics with BOSS, a Bayesian data-driven physically-based bulk scheme

Marcus van Lier Walqui — CCSR Columbia University @ NASA/GISS

[mv2525@columbia.edu](mailto:mv2525@columbia.edu)

Sean Patrick Santos — Pacific Northwest National Laboratories

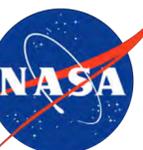
Hugh Morrison — National Center for Atmospheric Research

Karly Reimel — (prev.) Penn State University

Adele Igel — University of California Davis



ASR PI Meeting — Oct 27th 2022



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- Wealth of **natural cloud and precipitation observations** but difficult to measure process rates directly, only net effects on hydrometeors —> an indirect constraint of bulk schemes

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**The BIG question:** How to use these various data sources — each with their own uncertainties — to constrain bulk schemes?

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*Thomas Bayes (1701-1761)*

$$P(\mathbf{x}|\mathbf{y}) = \frac{P(\mathbf{y}|\mathbf{x})P(\mathbf{x})}{P(\mathbf{y})}$$

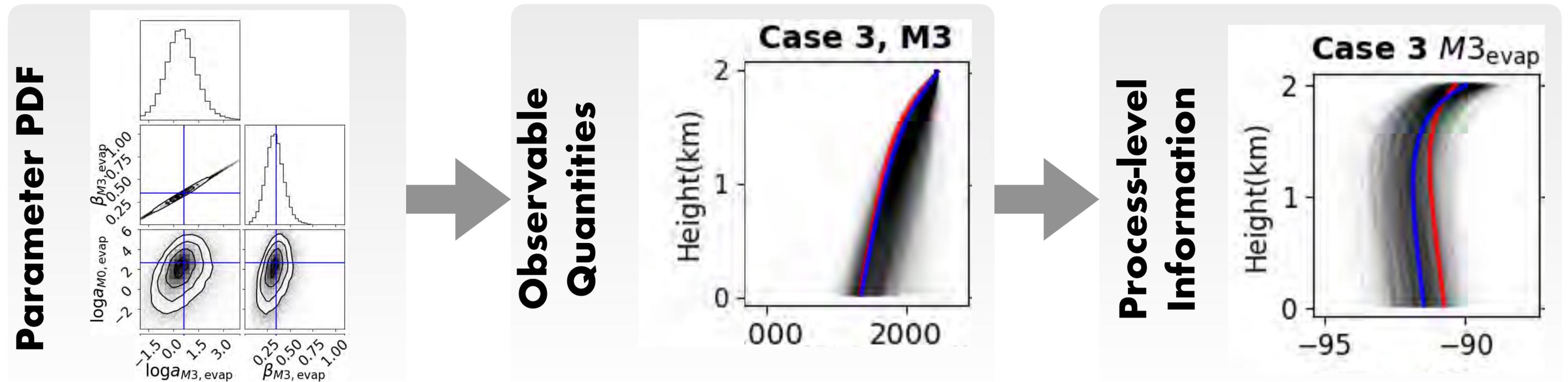
**BOSS**

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- B**ayesian (we treat uncertainties robustly, uncertainties reside in parameters)
- O**bservationally-constrained (scheme is informed by comparison to observations)
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- S**cheme — bulk microphysics parameterization scheme (so far rain & cloud only)

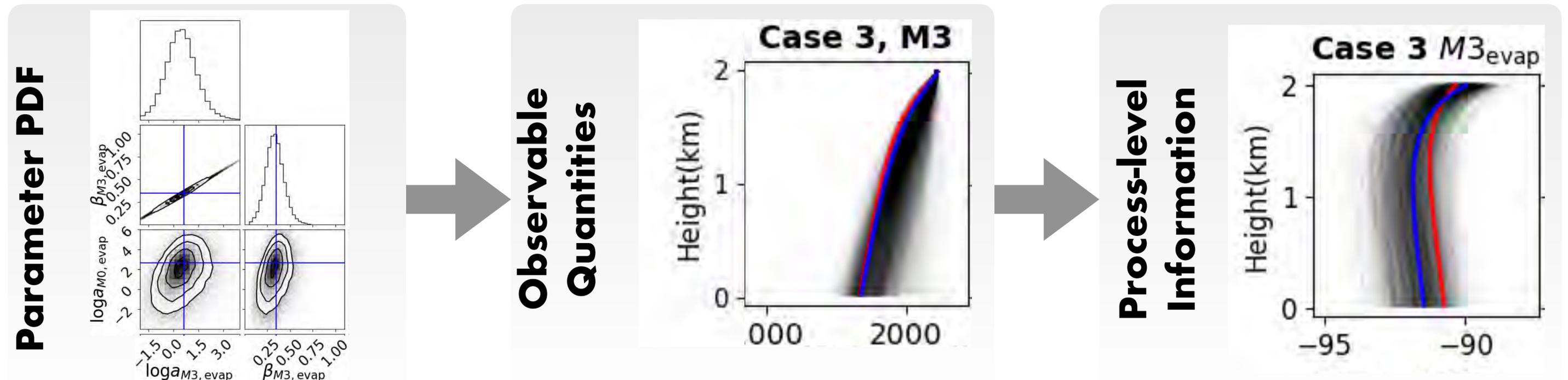
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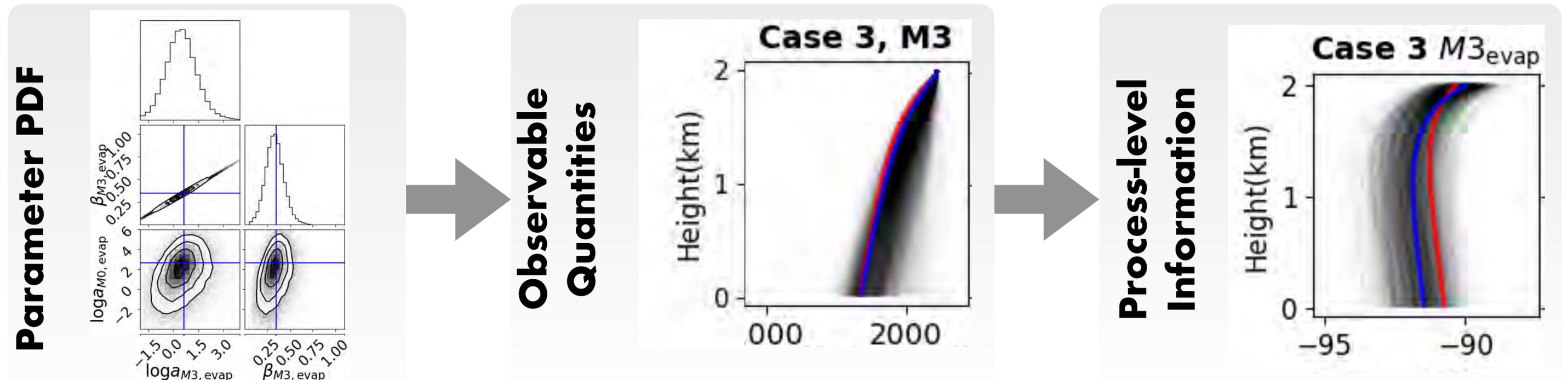
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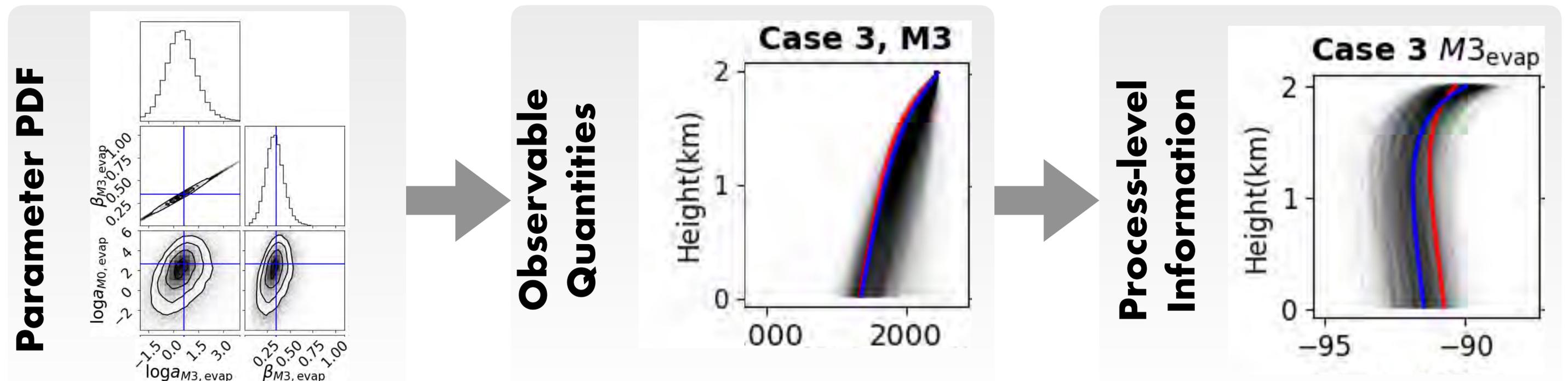


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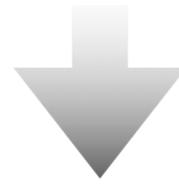
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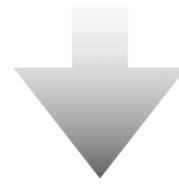
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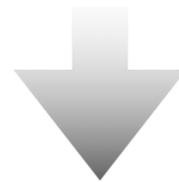
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Choose whatever moments are “best”

**Get rid of fixed process rate functions**

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Use Bayesian inference to estimate  $a, \beta, \delta$

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## Example of theoretical constraints on parsimony

A third moment (e.g. M6) can be used as a measure of DSD variance:

$$\sigma^2 = \frac{1}{M_{c0}} \int_0^\infty N(D)(D^3 - m_c)^2 dD = \frac{M_{c6}}{M_{c0}} - m_c^2$$

Constraint on the possible values of DSD variance enforces a structural form on the process rate for cloud self-collection (... some math...)

$$b_{6m,csc} = b_{0m,csc} + 2 \quad a_{6,csc} \geq a_{0,csc} \quad (1)$$

Similar arguments reduce the total number of BOSS parameters from 60+ to 37 for 3-moment cloud BOSS

# A spectrum of data and ways to constrain/inform BOSS

*Less expensive,  
less realistic*



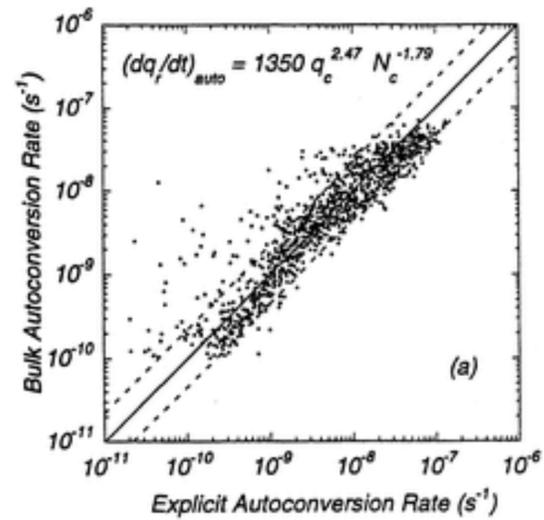
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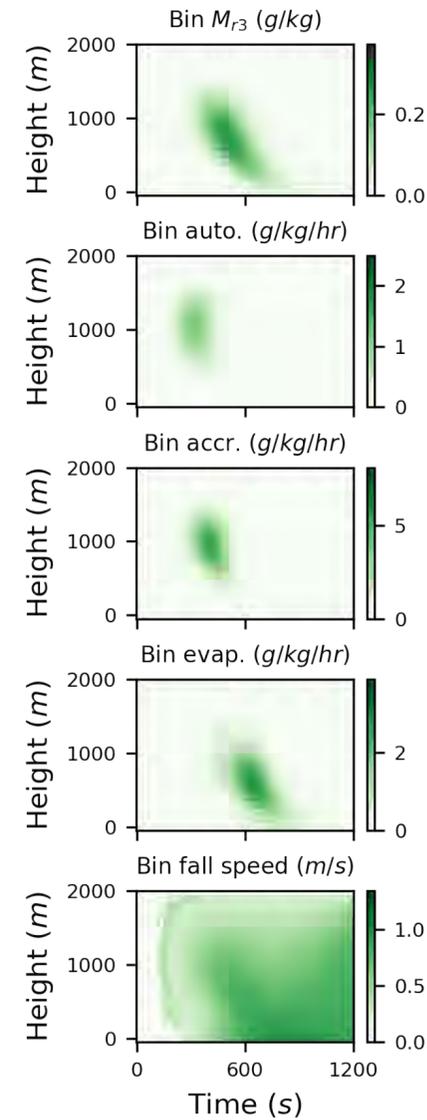
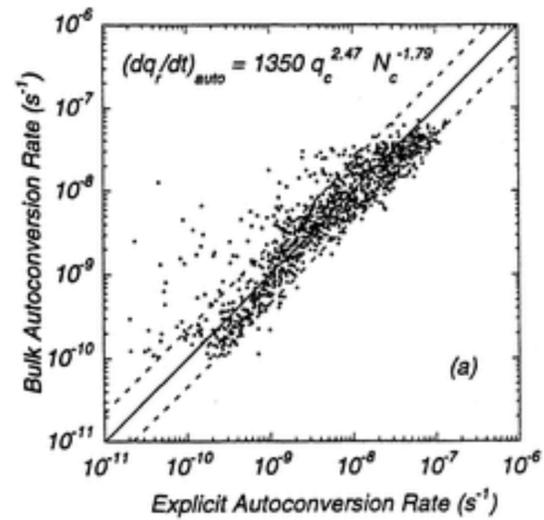
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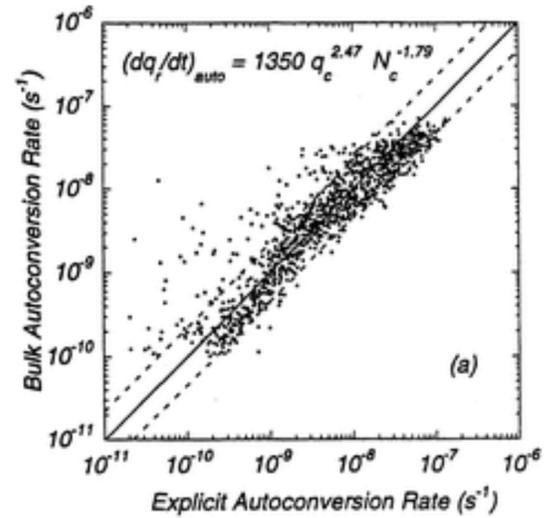
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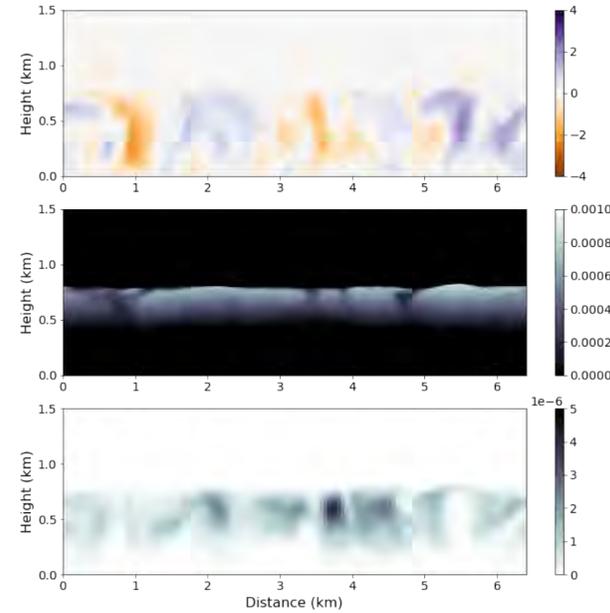
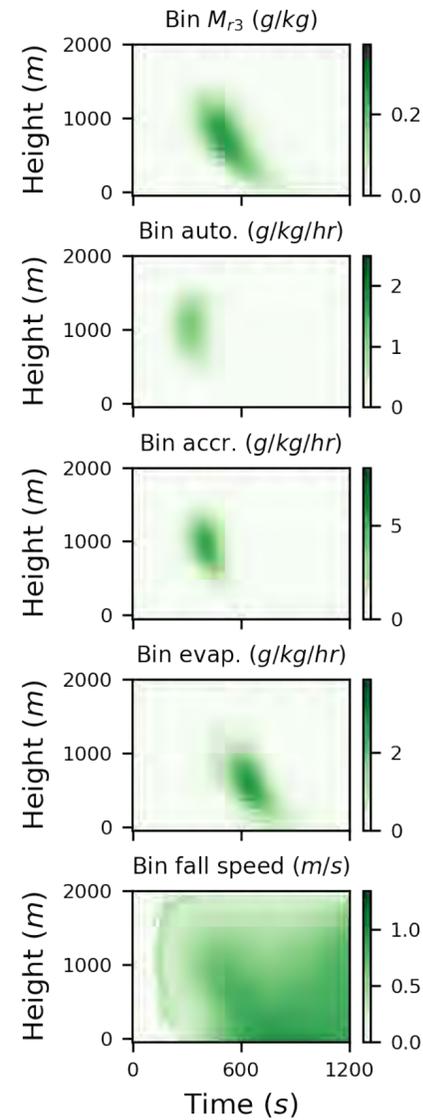
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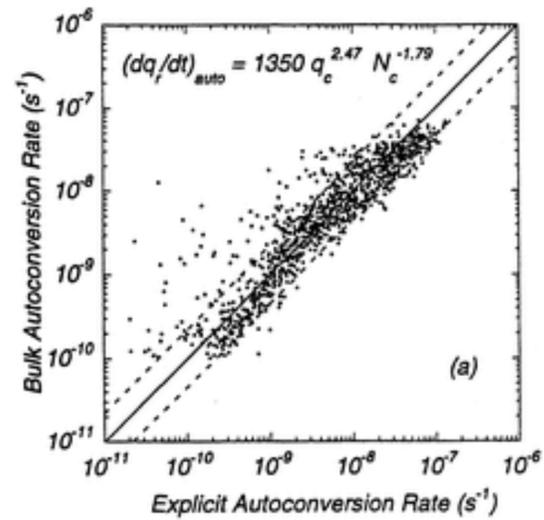
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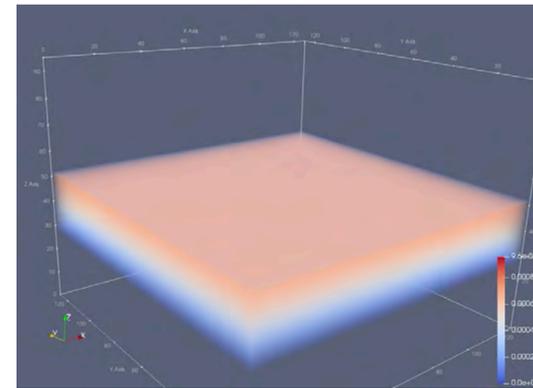
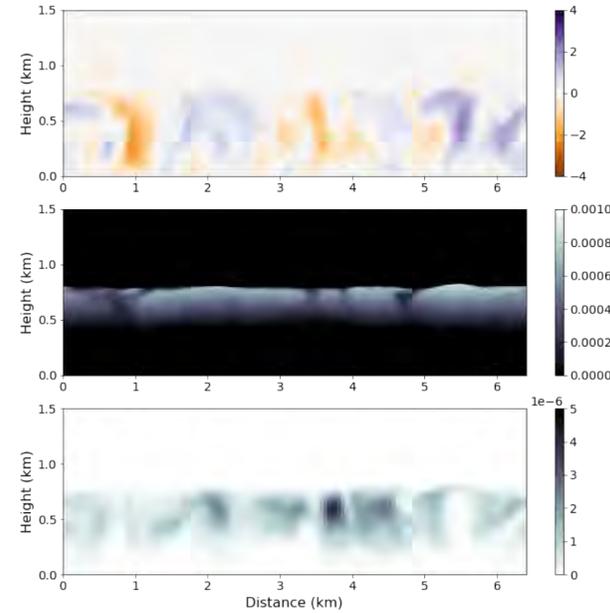
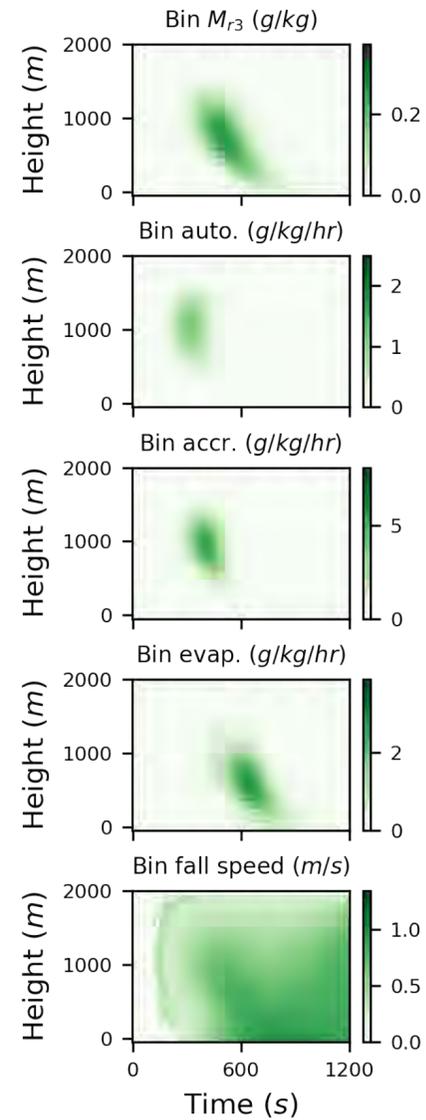
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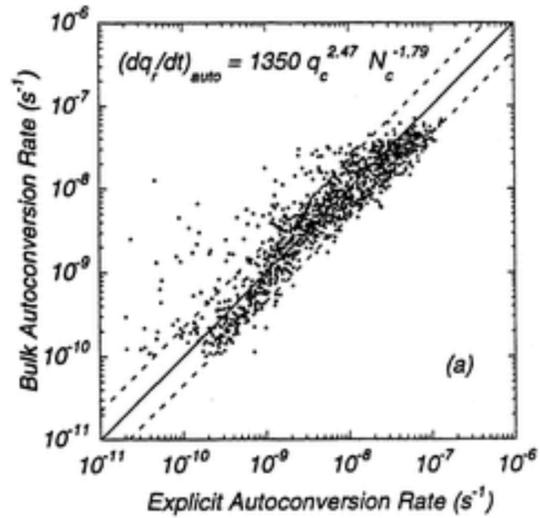
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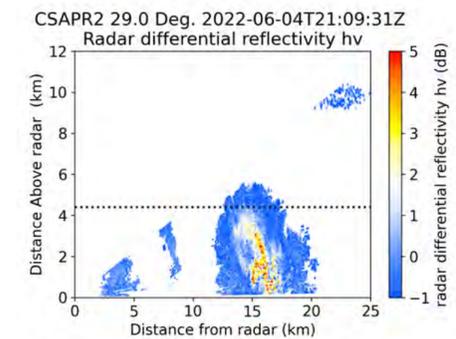
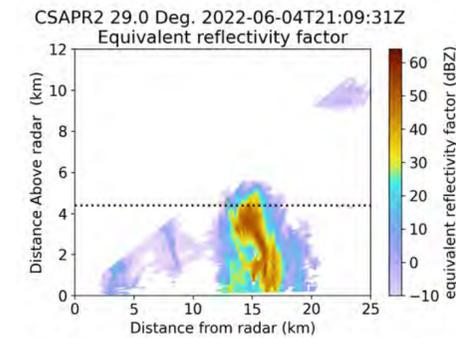
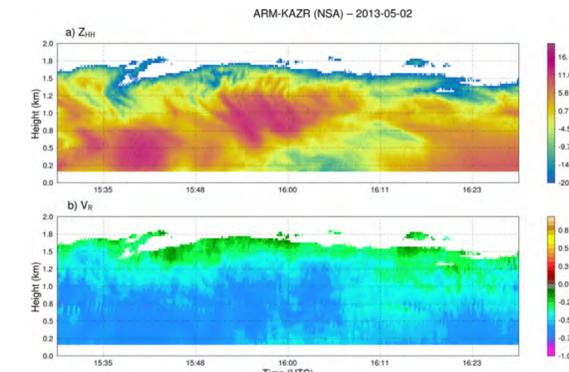
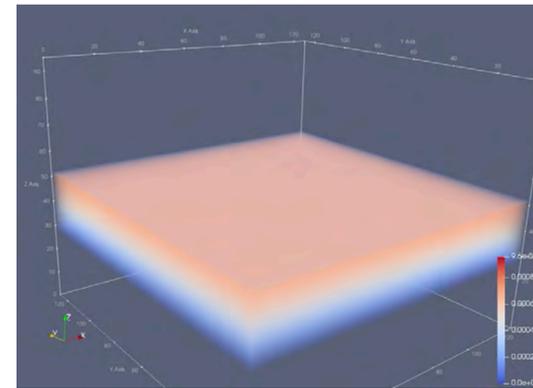
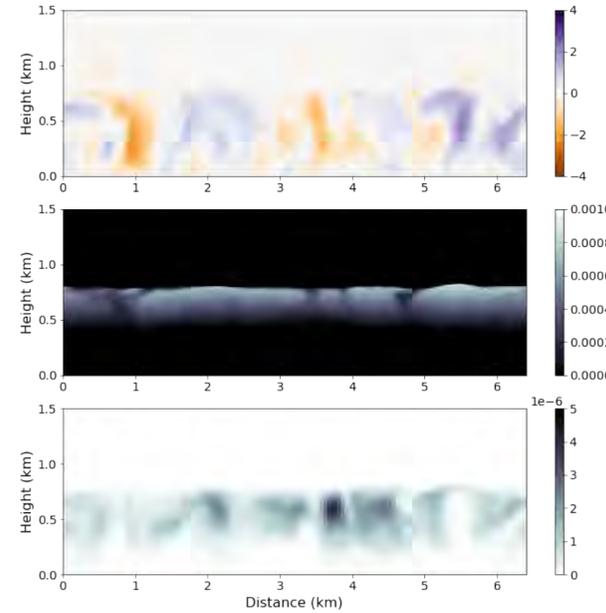
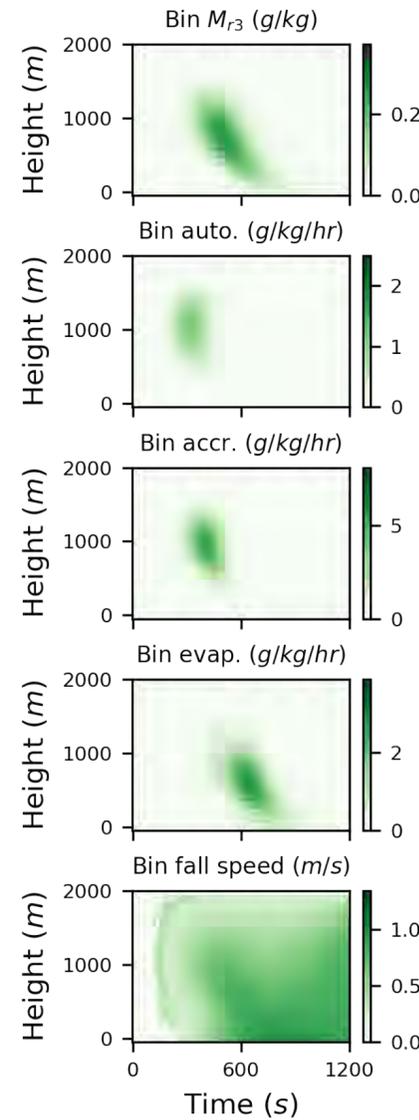


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Real observations,  
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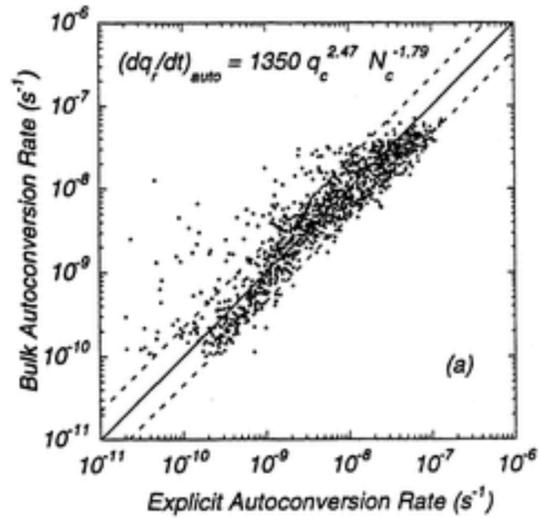
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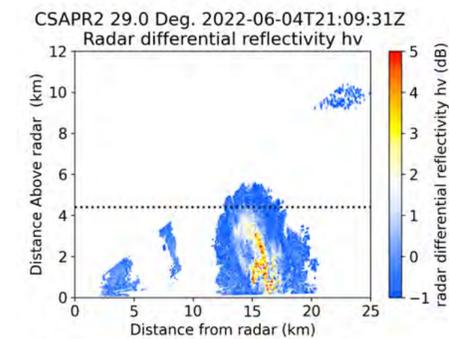
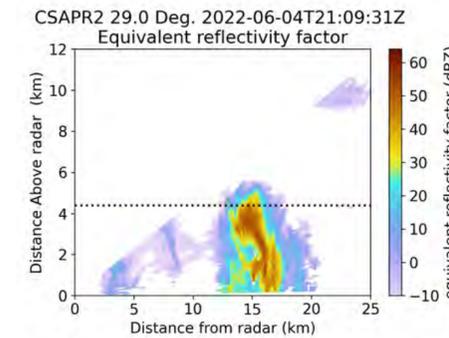
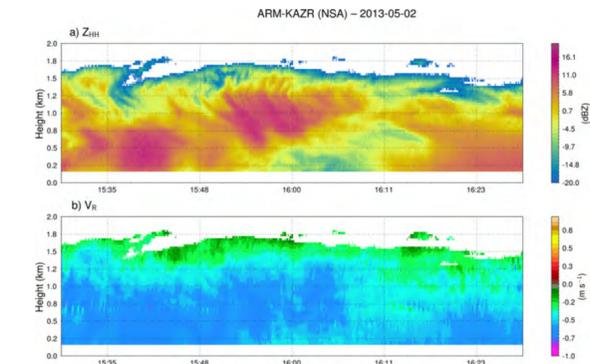
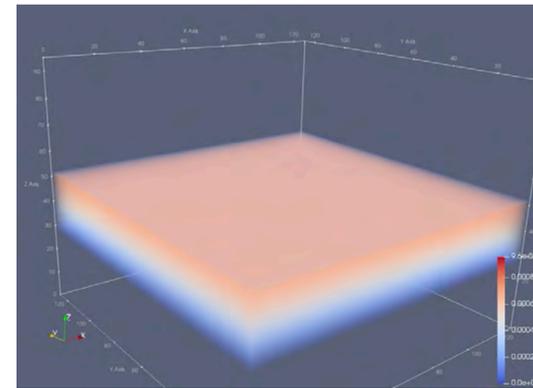
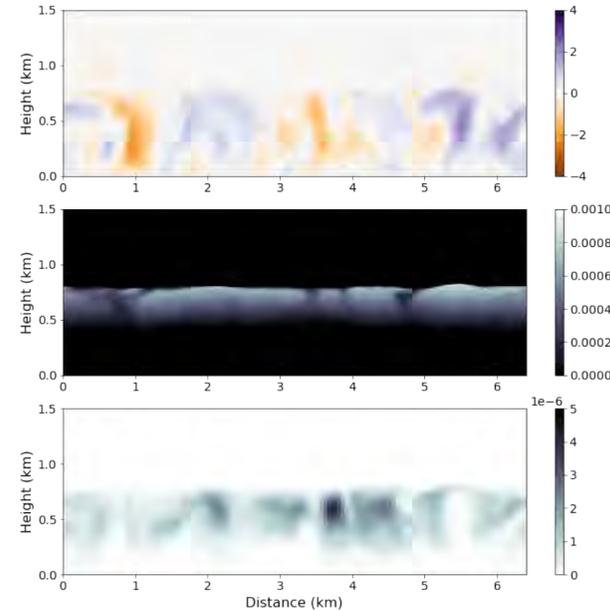
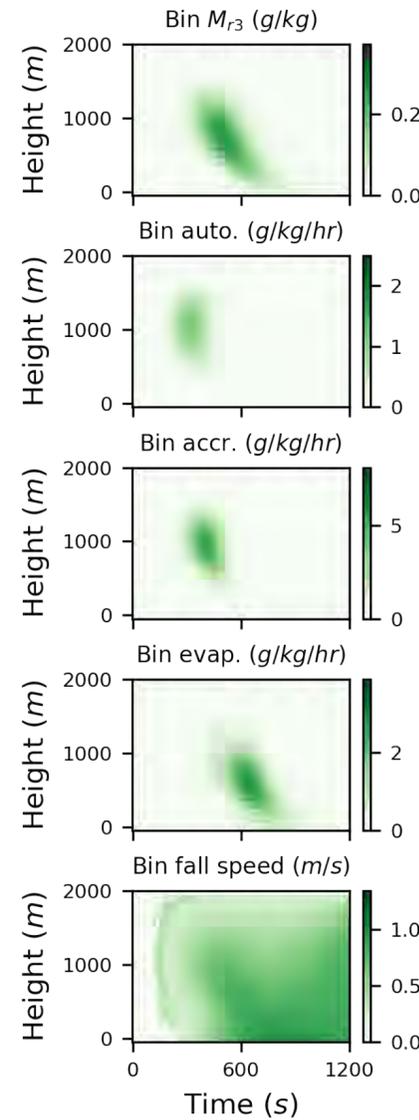


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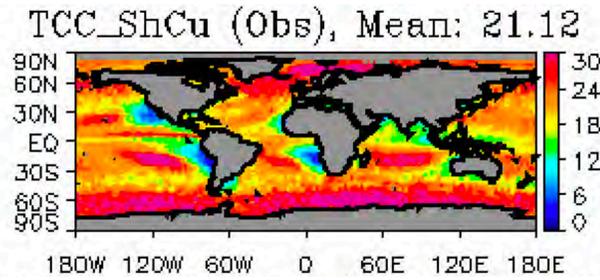
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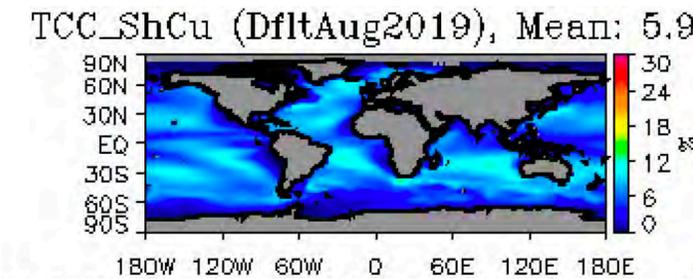
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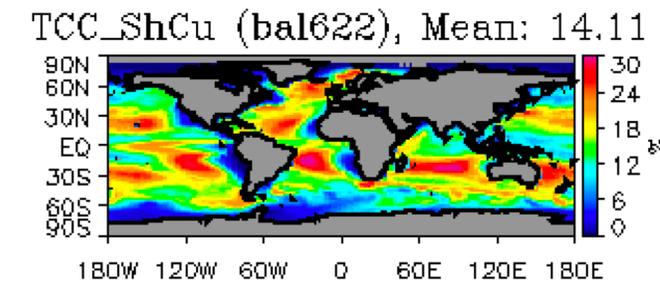
## Observed Shallow Cu



## Default Parameters



## Tuned Parameters



Directly fitting process rates to some "reference" scheme

Fit using a time-evolving kinematic 1D column model w/ reference scheme

Fit using "observations" from well-studied LES test cases (e.g. DYCOMS RF02) w reference scheme

Fit using observational "weather-scale" data, e.g. from DOE ARM cloud radars & LES

Fit within GCM global simulations, satellite data using ML and perturbed parameter ensembles

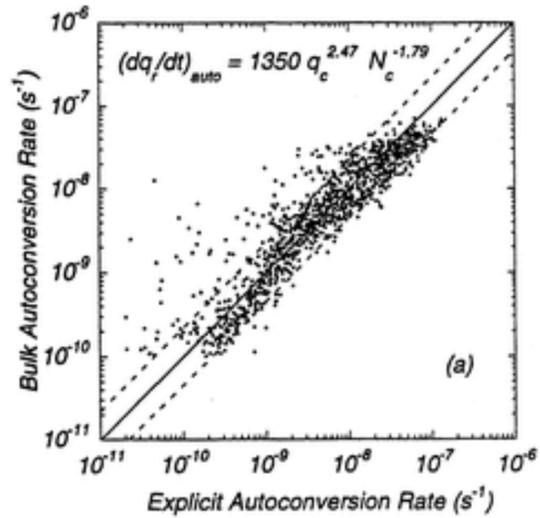
# A spectrum of data and ways to constrain/inform BOSS

Less expensive,  
less realistic



More expensive,  
more realistic

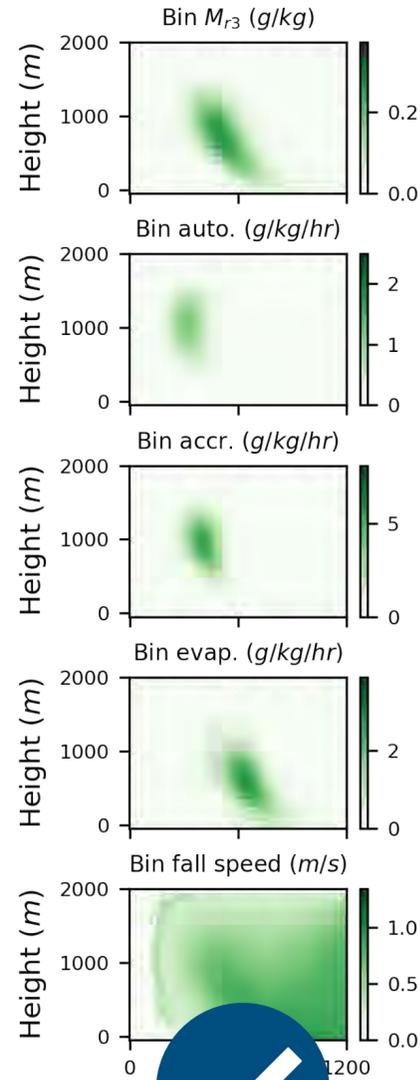
Real observations,  
real complications



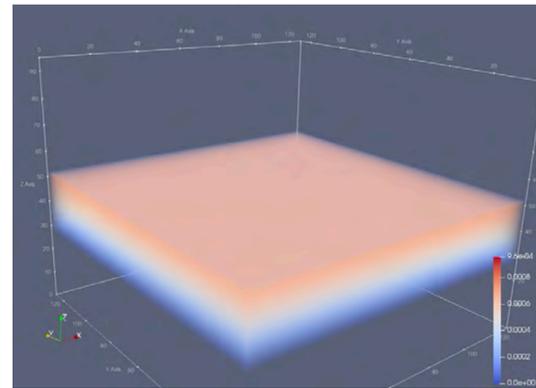
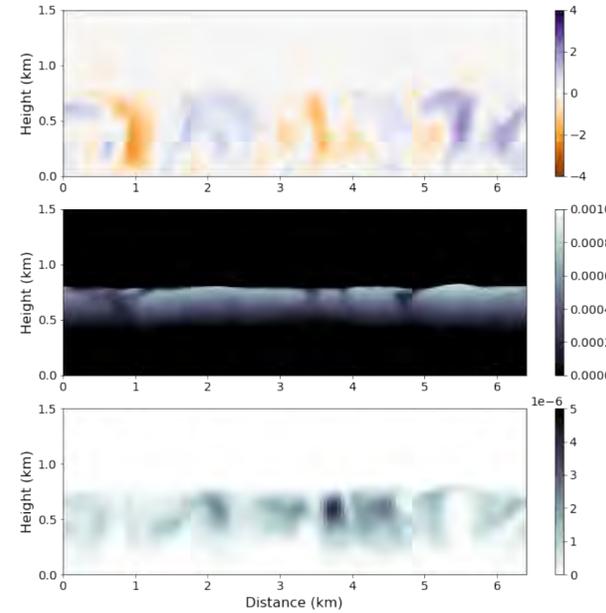
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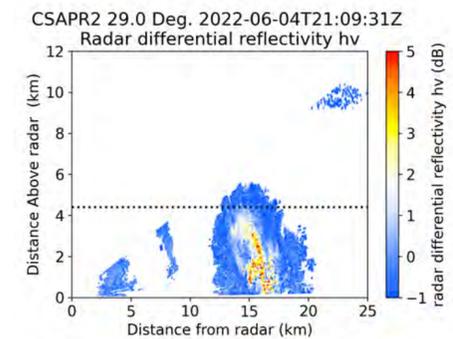
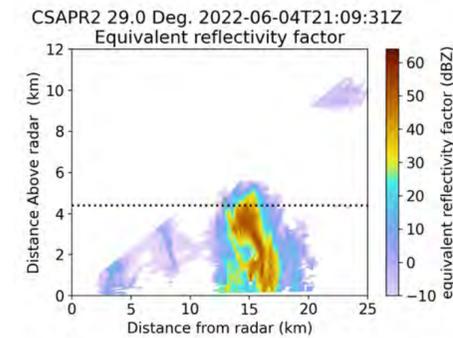
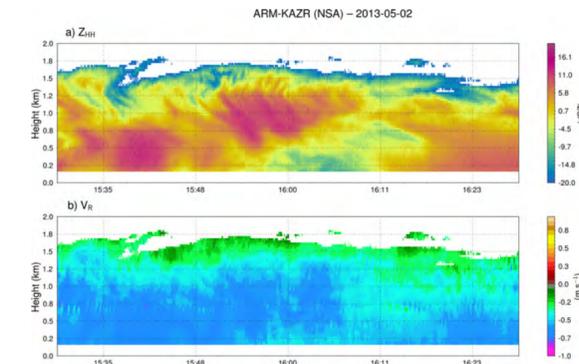
Directly fitting process rates to some “reference” scheme



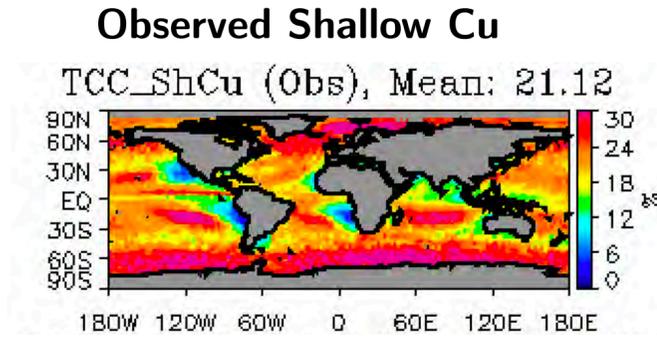
Fit using a time-evolving kinematic 1D column model w/ reference scheme



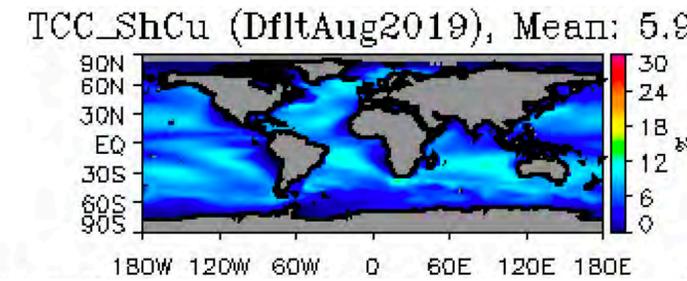
Fit using “observations” from well-studied LES test cases (e.g. DYCOMS RF02) w reference scheme



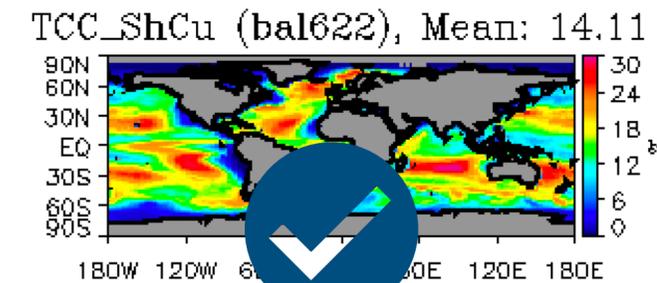
Fit using observational “weather-scale” data, e.g. from DOE ARM cloud radars & LES



Default Parameters



Tuned Parameters



Fit within GCM global simulations, satellite data using ML and perturbed parameter ensembles

# Directly fitting process rates to a Bin model

## Autoconversion rates: bin vs. BOSS fits

### Direct process fits with BOSS

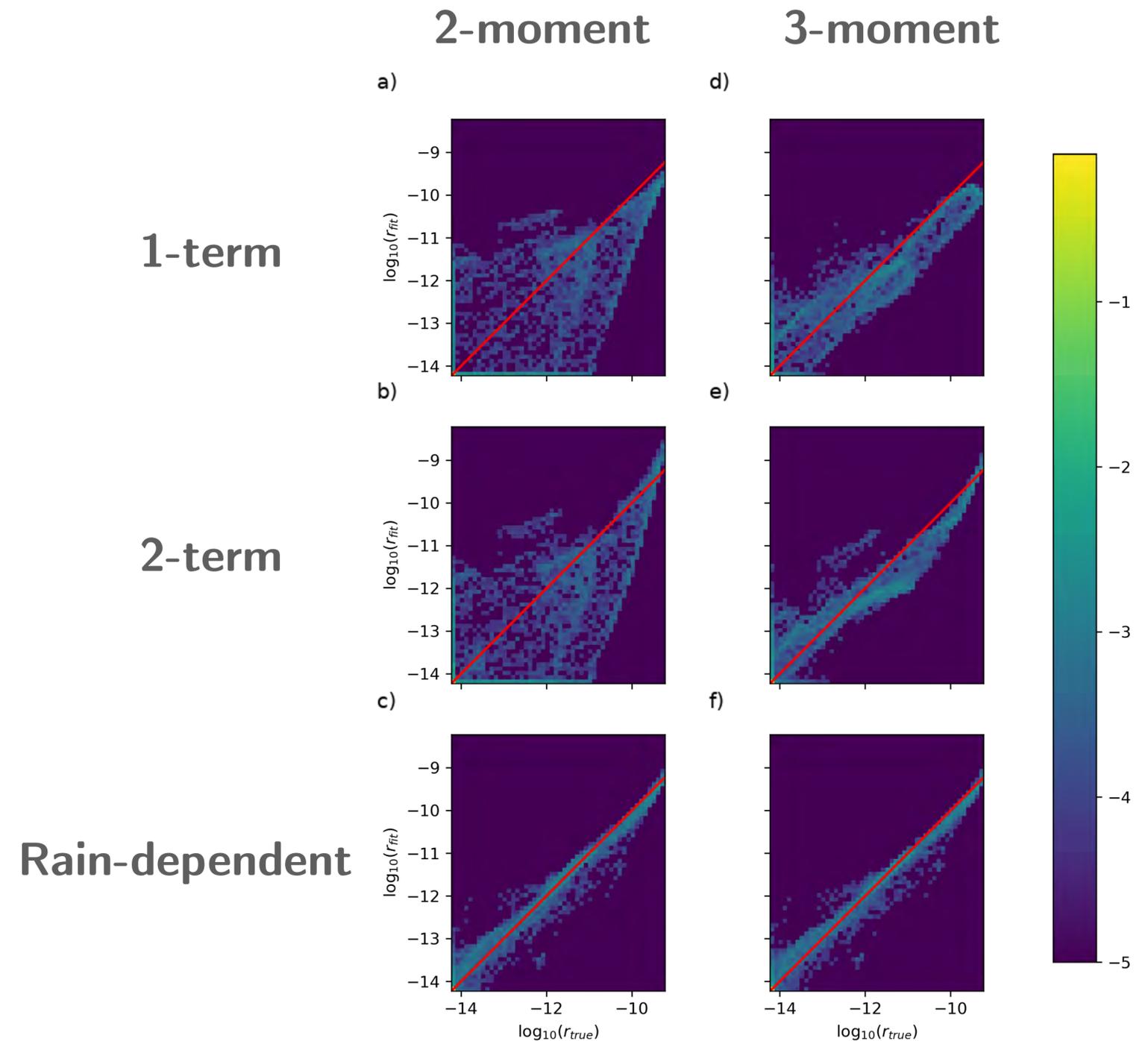
- Directly fit BOSS parameters to match existing TAU bin scheme autoconversion process rates
- Test 1-term process rate formulation vs. 2-term
- Test 2-moment cloud/rain vs. 3-moment cloud, 2-moment rain
- Test rain-dependent autoconversion term
- Observational uncertainty is treated as an unknown (using conjugate prior)

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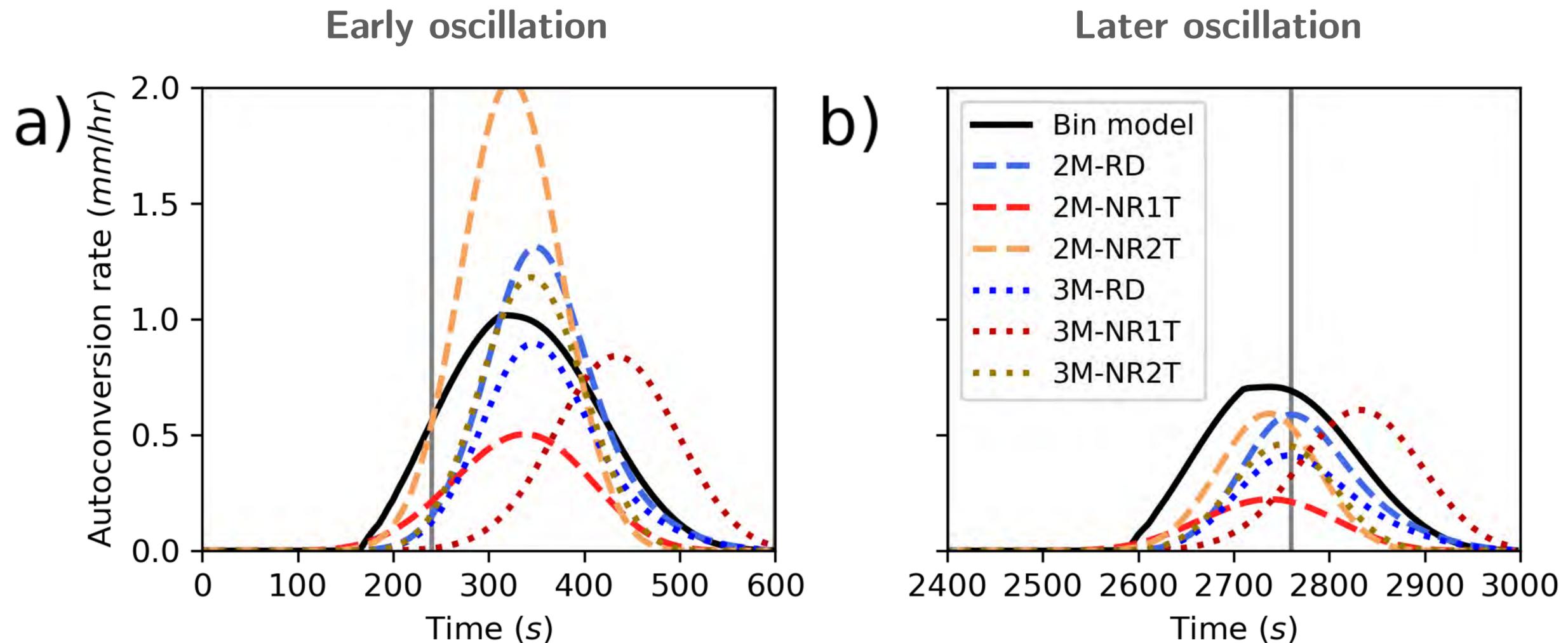
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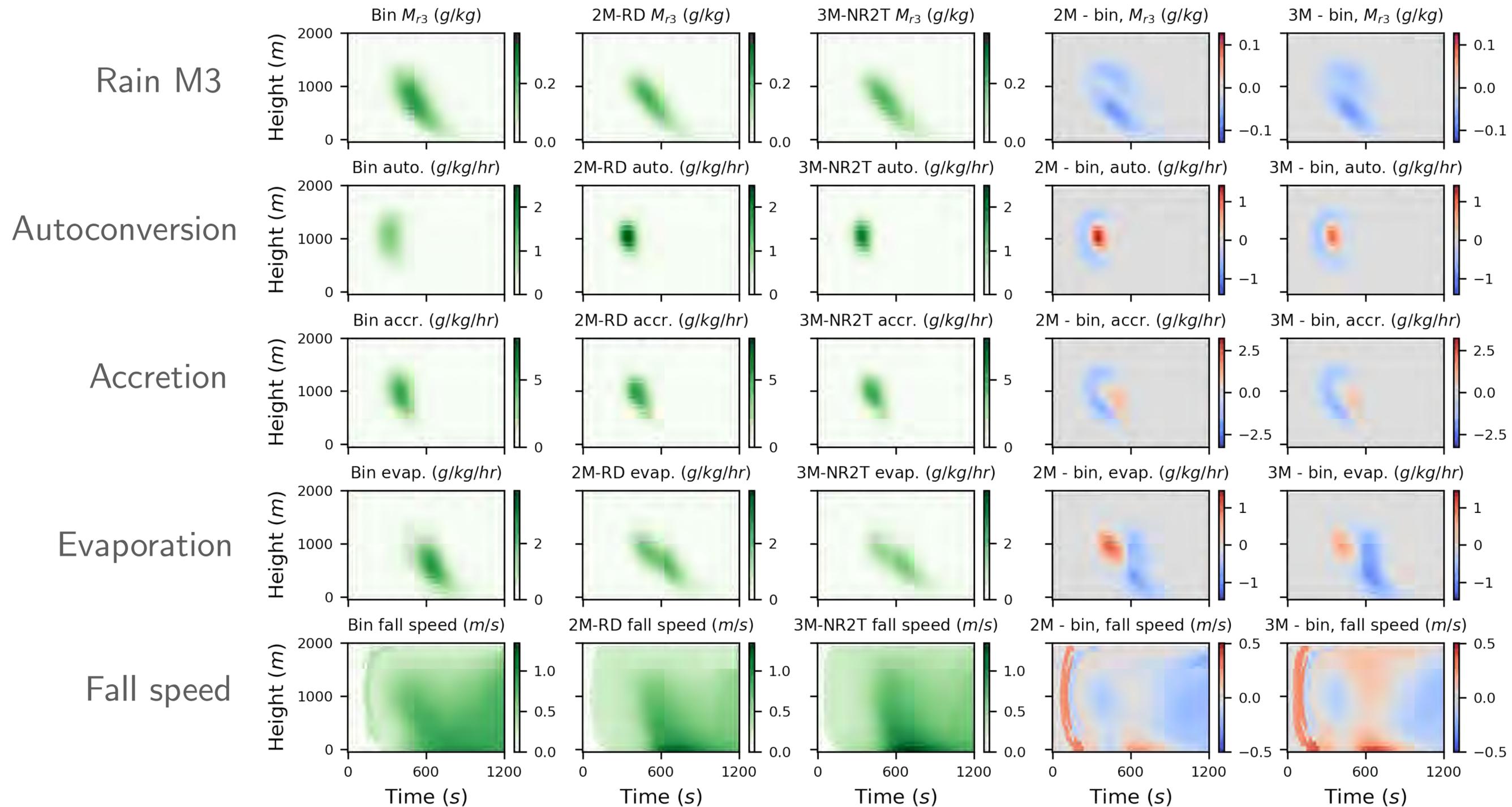


# Testing direct fits in time-evolving 1D model

Looking at autoconversion rates tuned via direct fitting in 1D model simulations



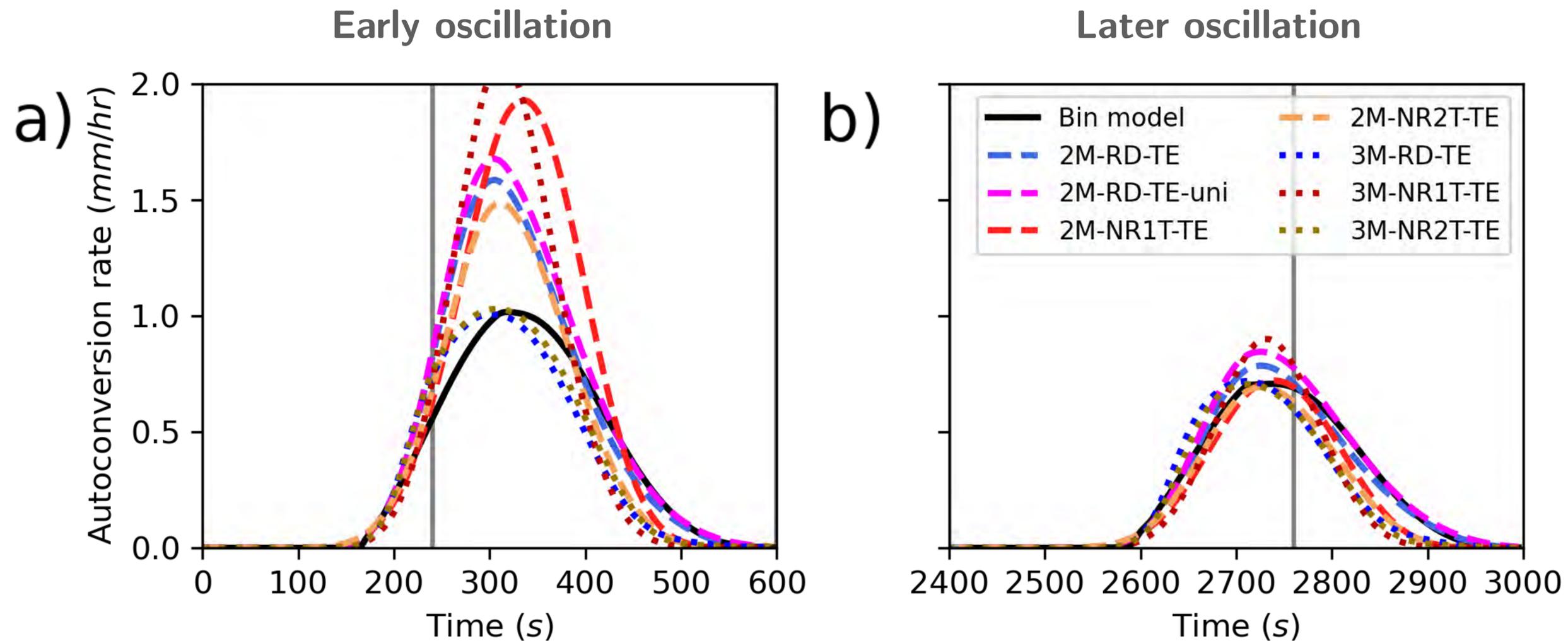
# Testing direct fits in 1D model (2M vs 3M)



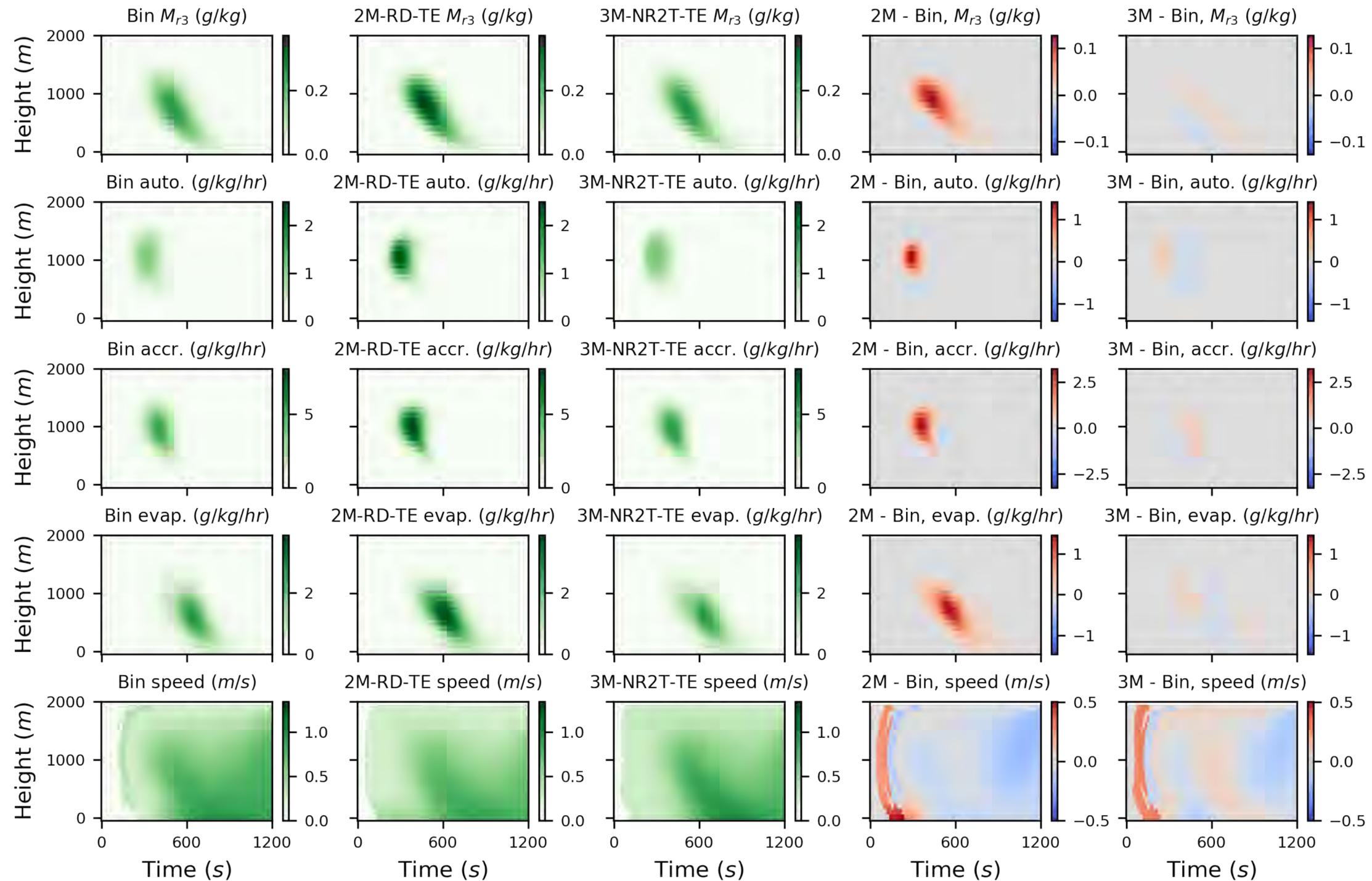
# Instead use direct fits as a (Bayesian) prior

\*Refine the prior with a likelihood using observations from *time-evolving sim'n*

## Autoconversion rates in 1D model



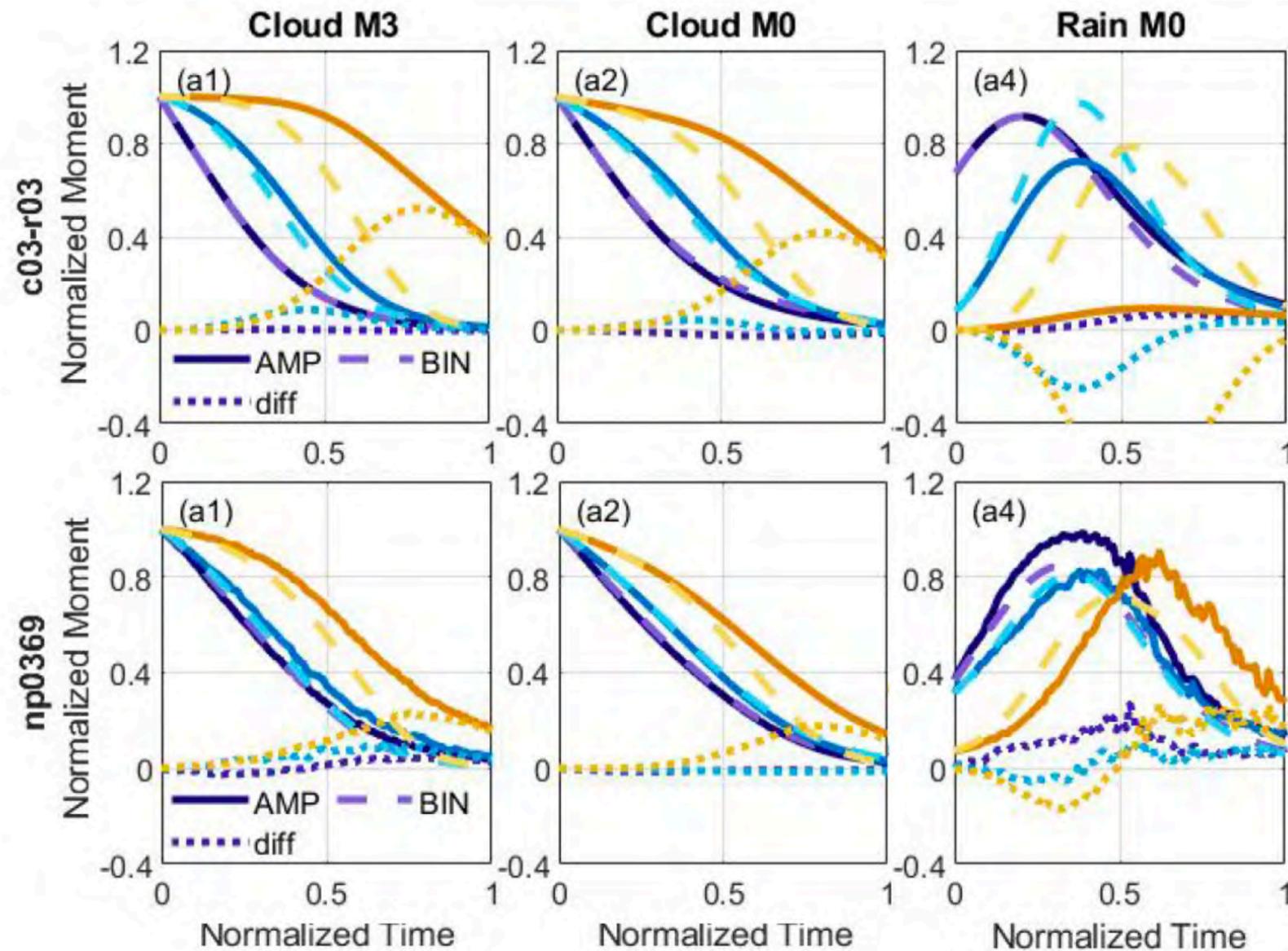
# Testing direct/1D fits in 1D model (2M vs 3M)



Structural choices must be evaluated in the context of adequate parameter constraint!

# A larger structural error?

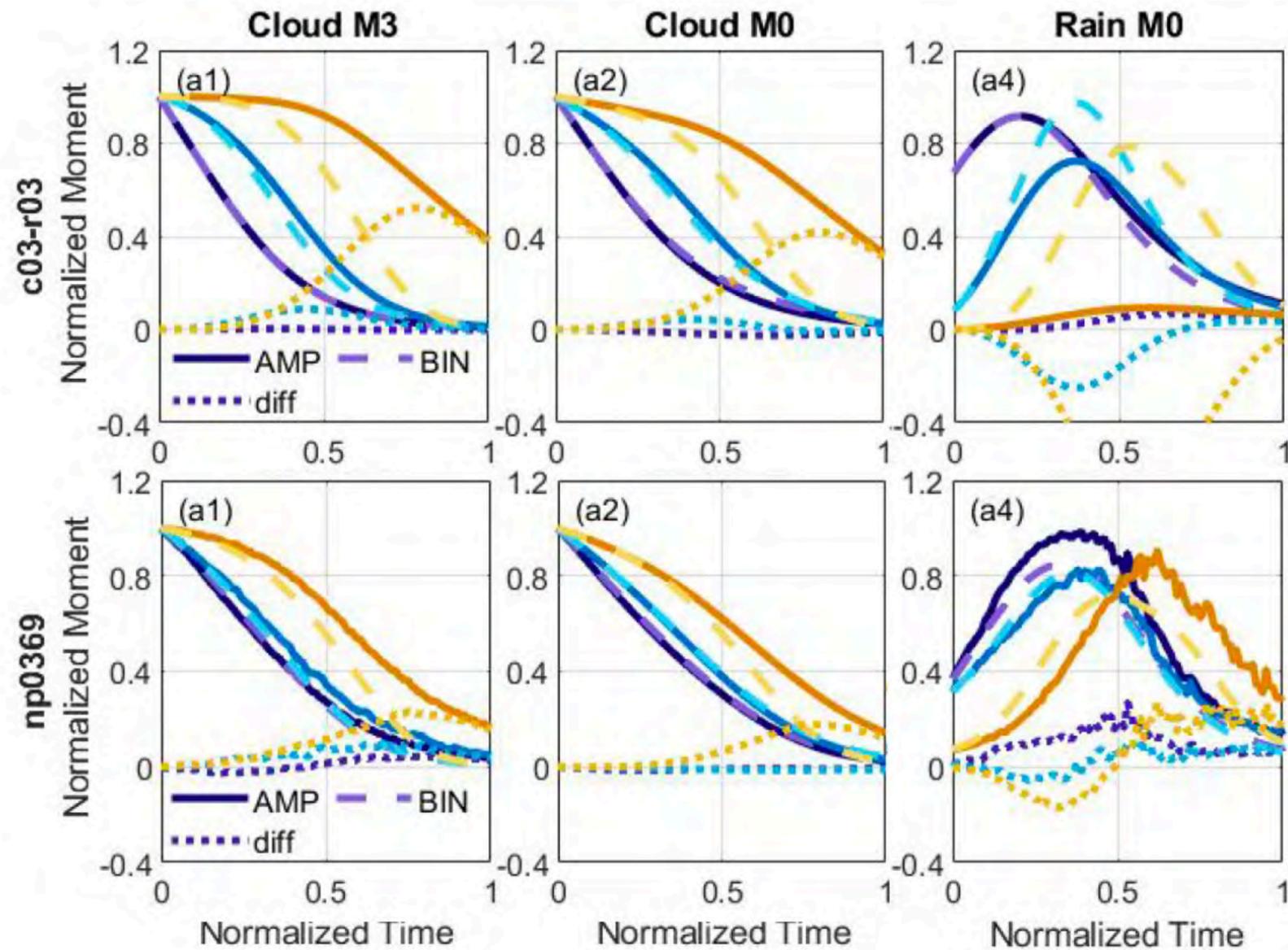
Are separate cloud and rain categories the correct approach for bulk warm microphysics?



Adele L. Igel, H. Morrison, S. P. Santos, and M. van Lier-Walqui. *Limitations of separate cloud and rain categories in parameterizing collision-coalescence for bulk microphysics schemes.* JAMES, 2022.

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*This is something we are currently testing with BOSS!*

