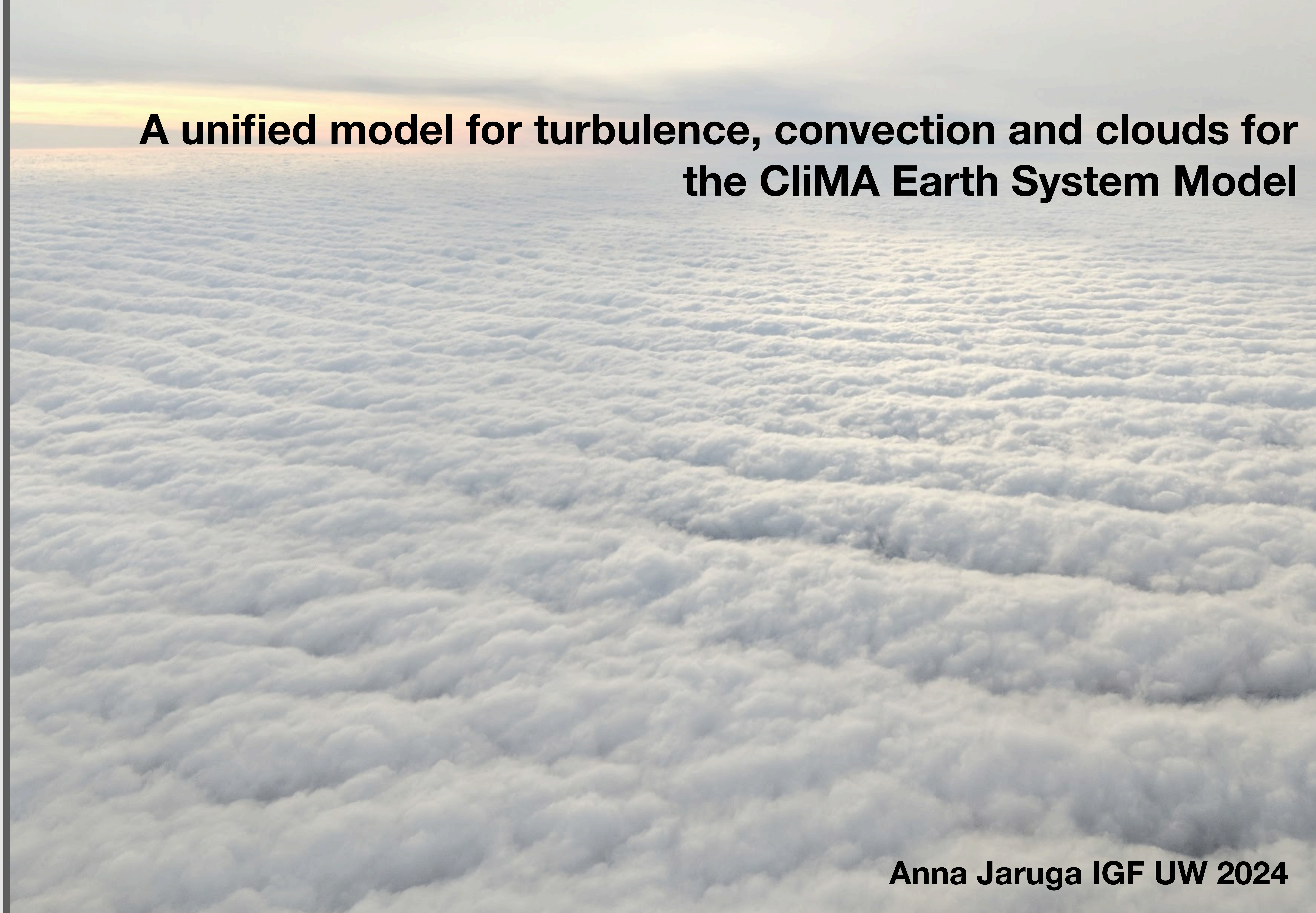


A unified model for turbulence, convection and clouds for the CliMA Earth System Model

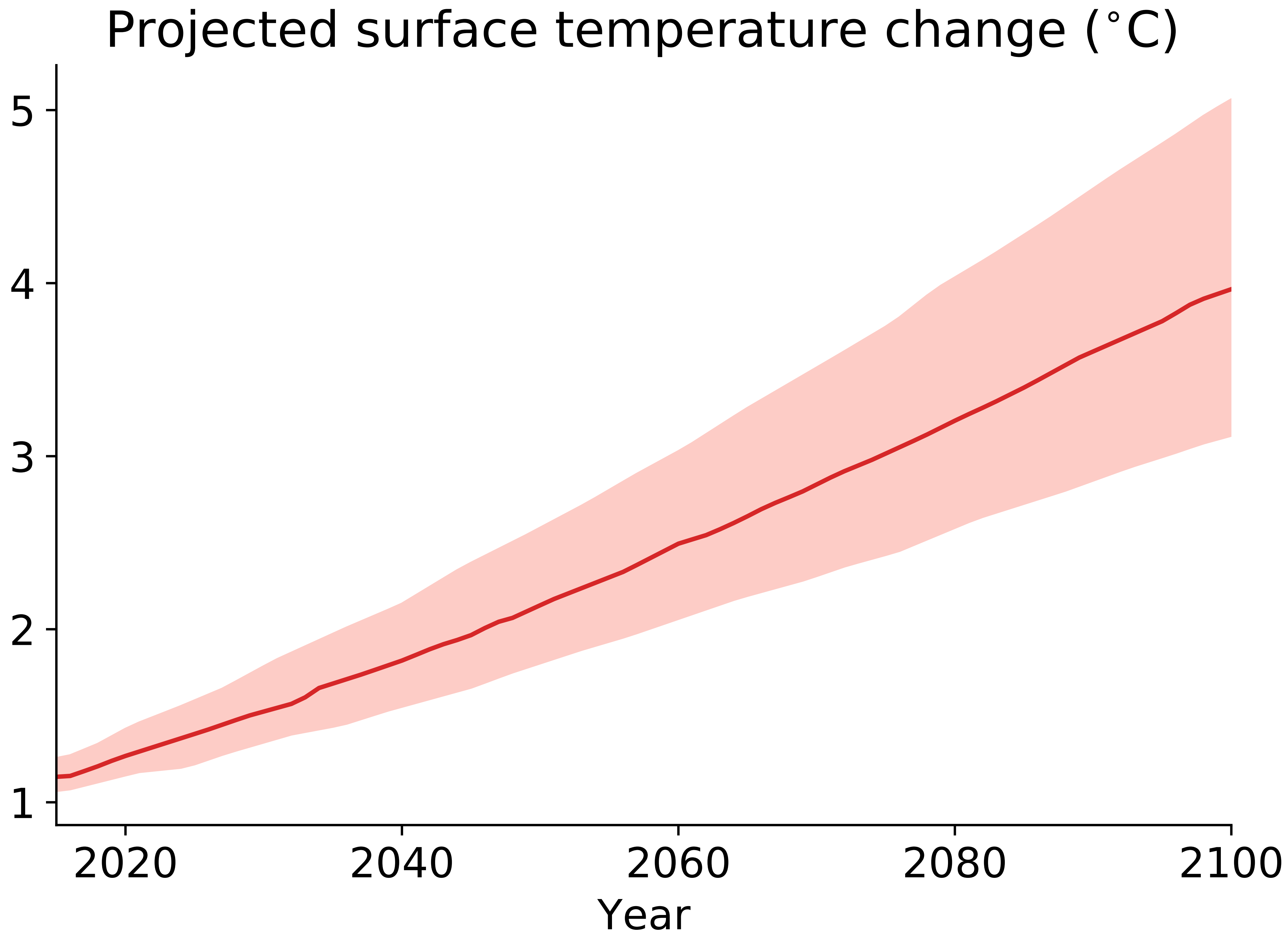
Anna Jaruga IGF UW 2024

Caltech

CliMA
CLIMATE MODELING ALLIANCE

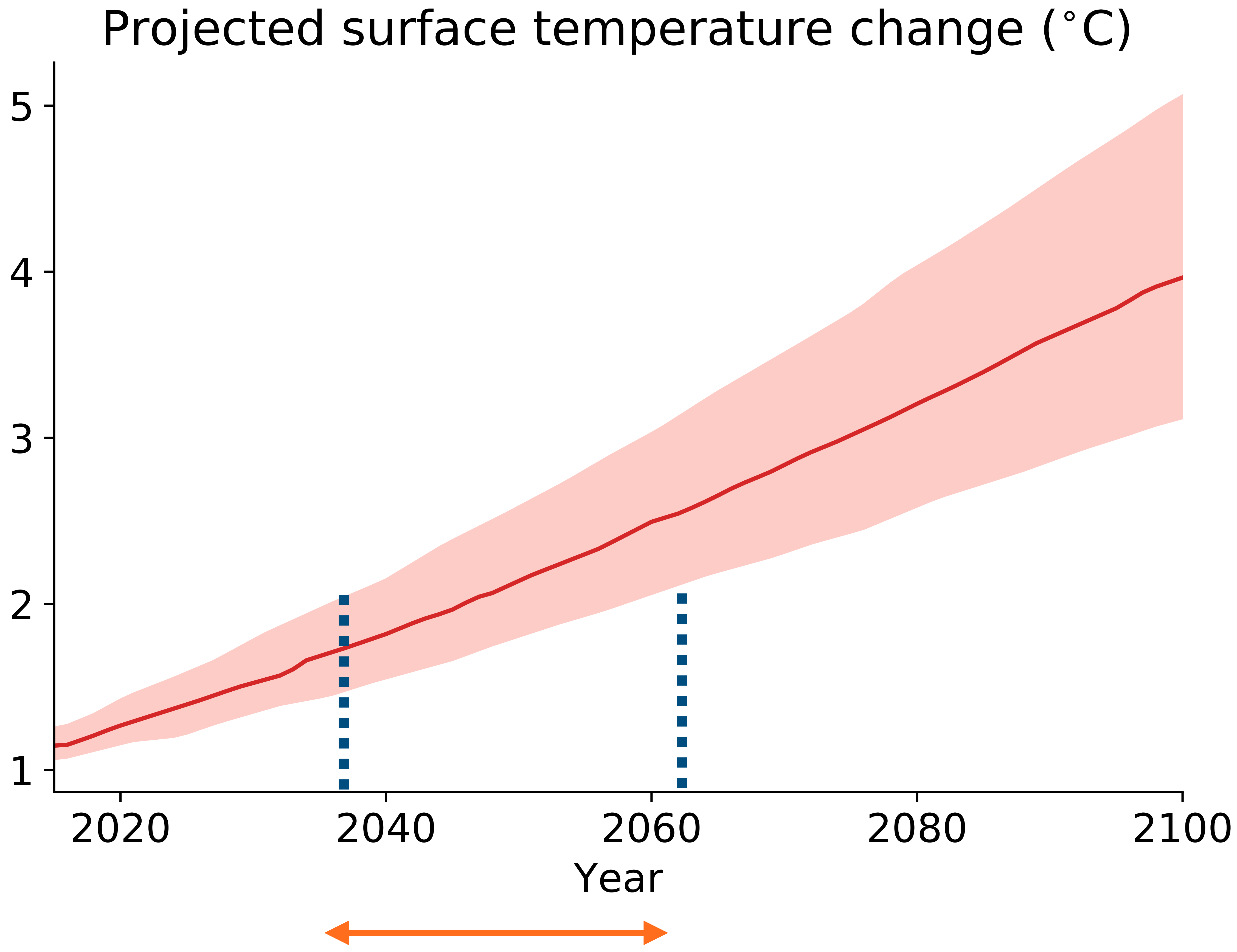
Clouds dominate uncertainties in climate projections

SSP3-7.0 scenario (IPCC, 2022)



Clouds dominate uncertainties in climate projections

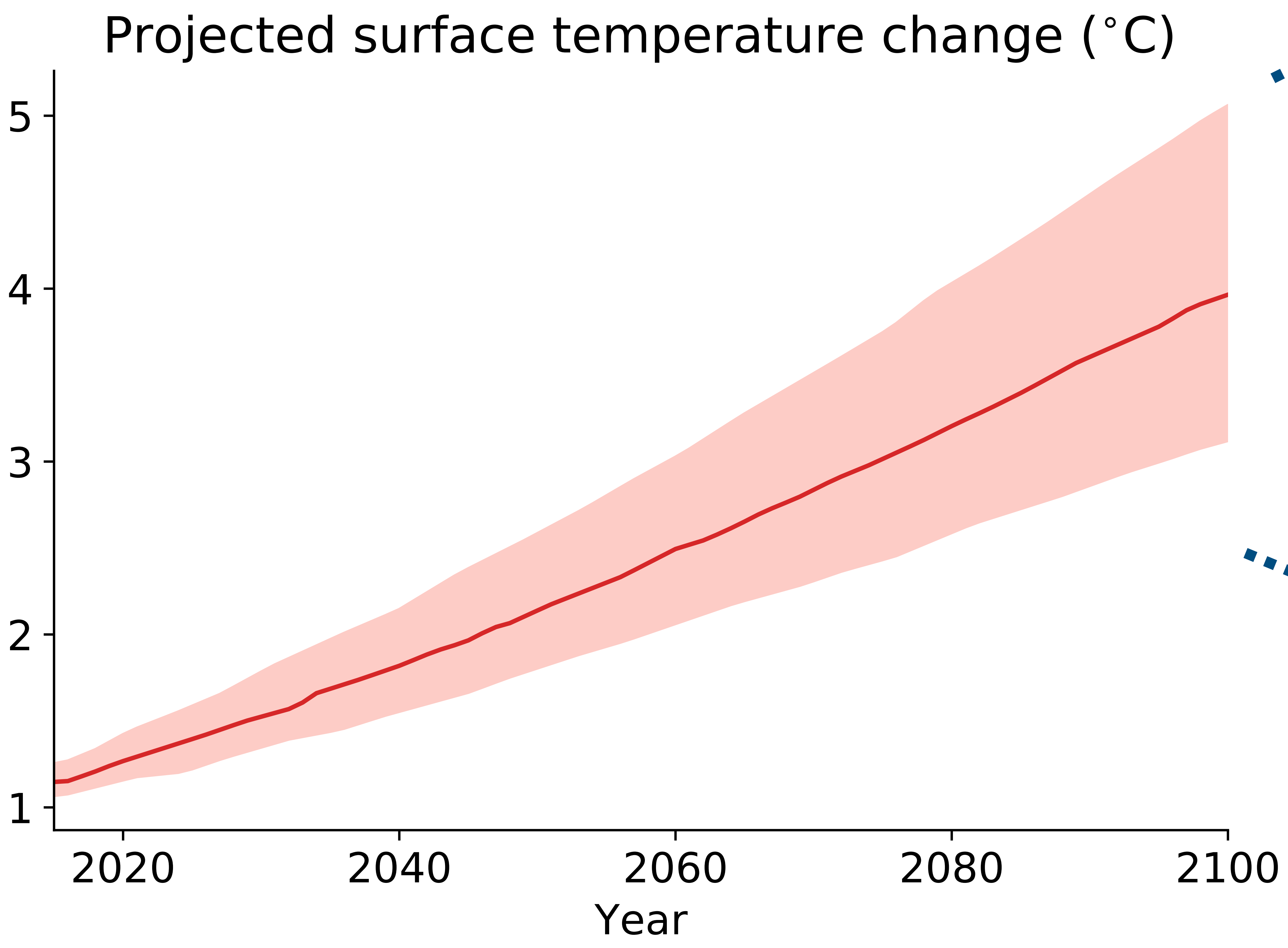
SSP3-7.0 scenario (IPCC, 2022)

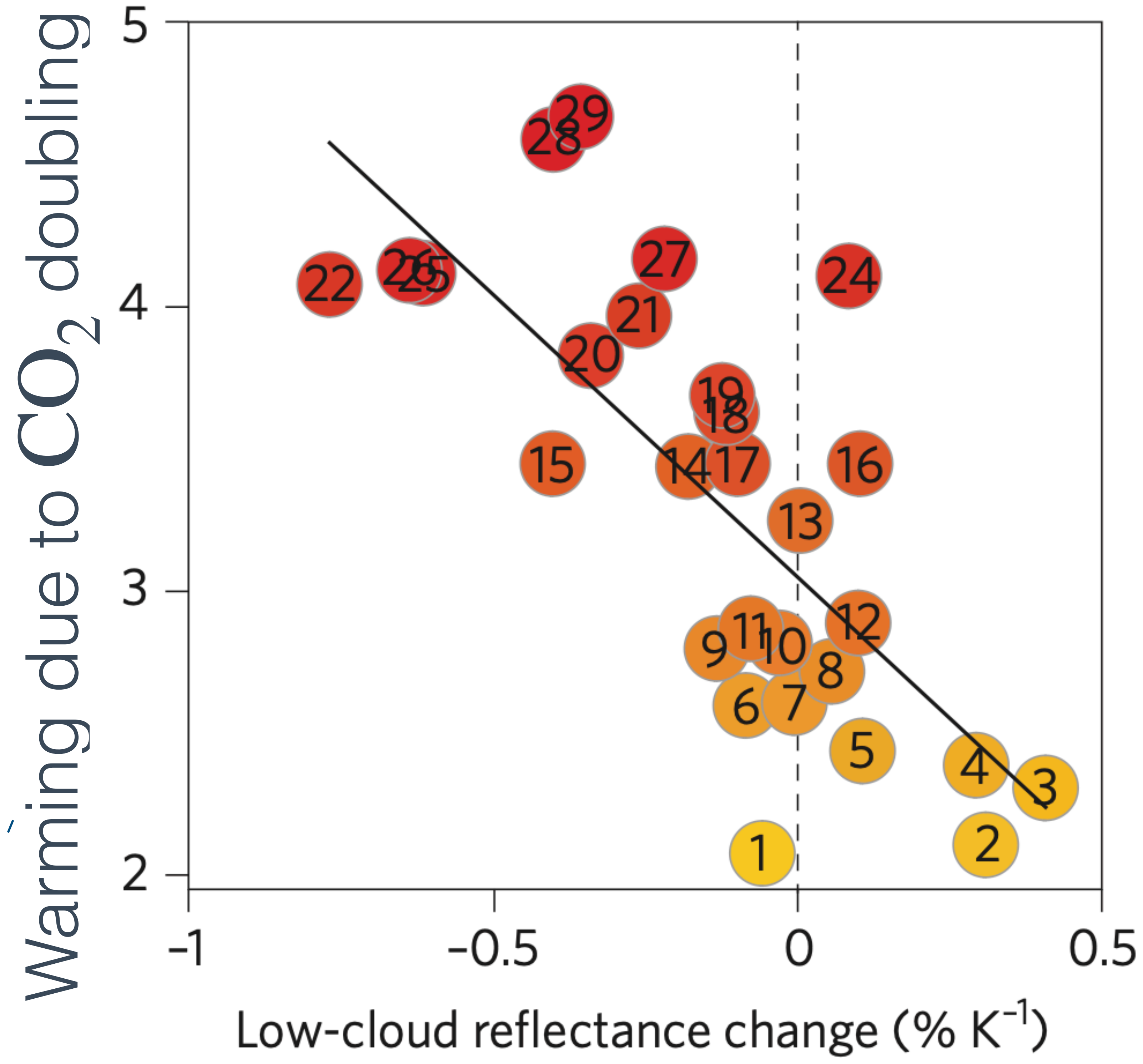


How much time do we have to act

Clouds dominate uncertainties in climate projections

SSP3-7.0 scenario (IPCC, 2022)





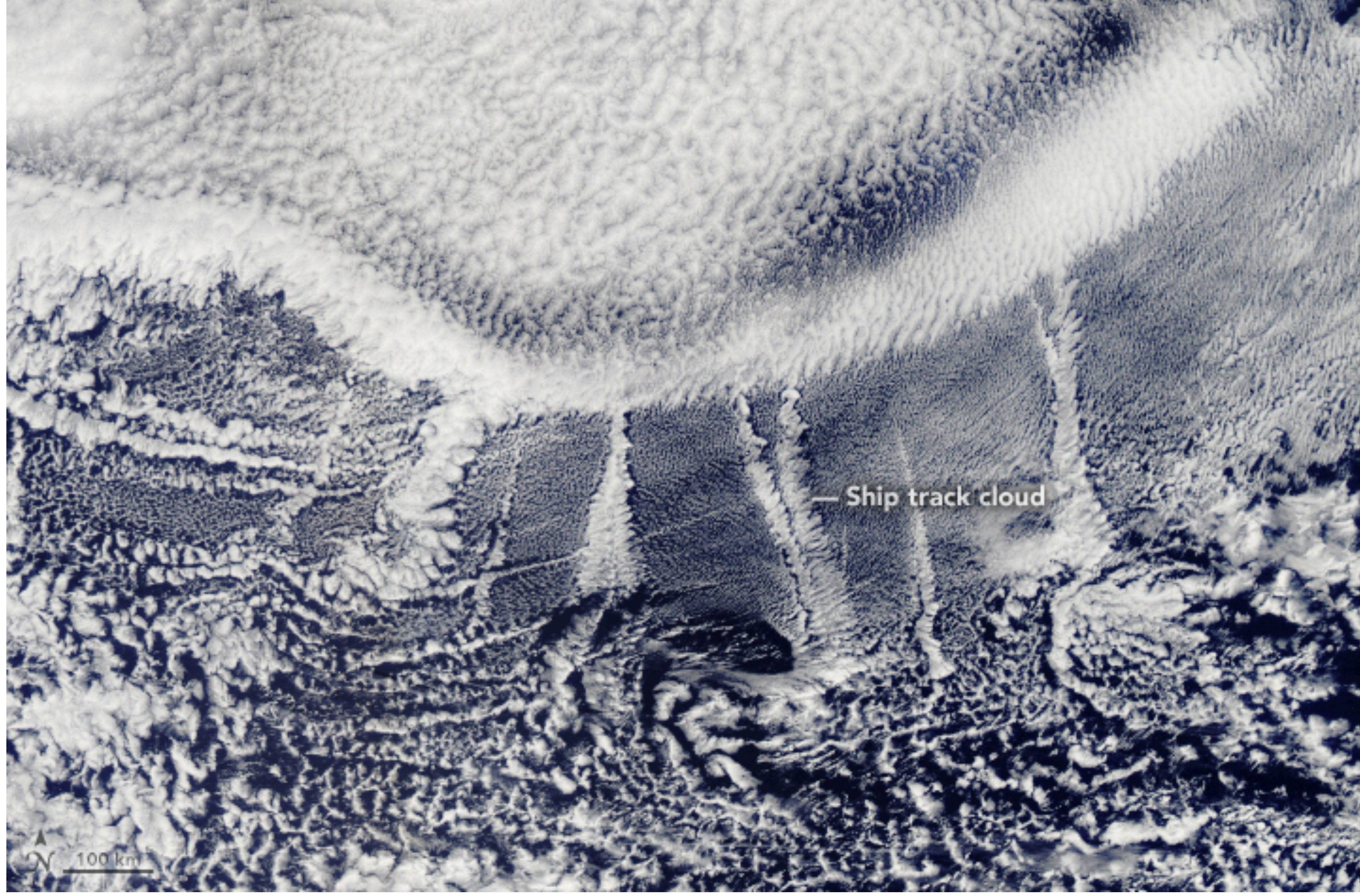
More clouds, less warming

Schneider et al., 2017:
Climate goals and computing the future of clouds

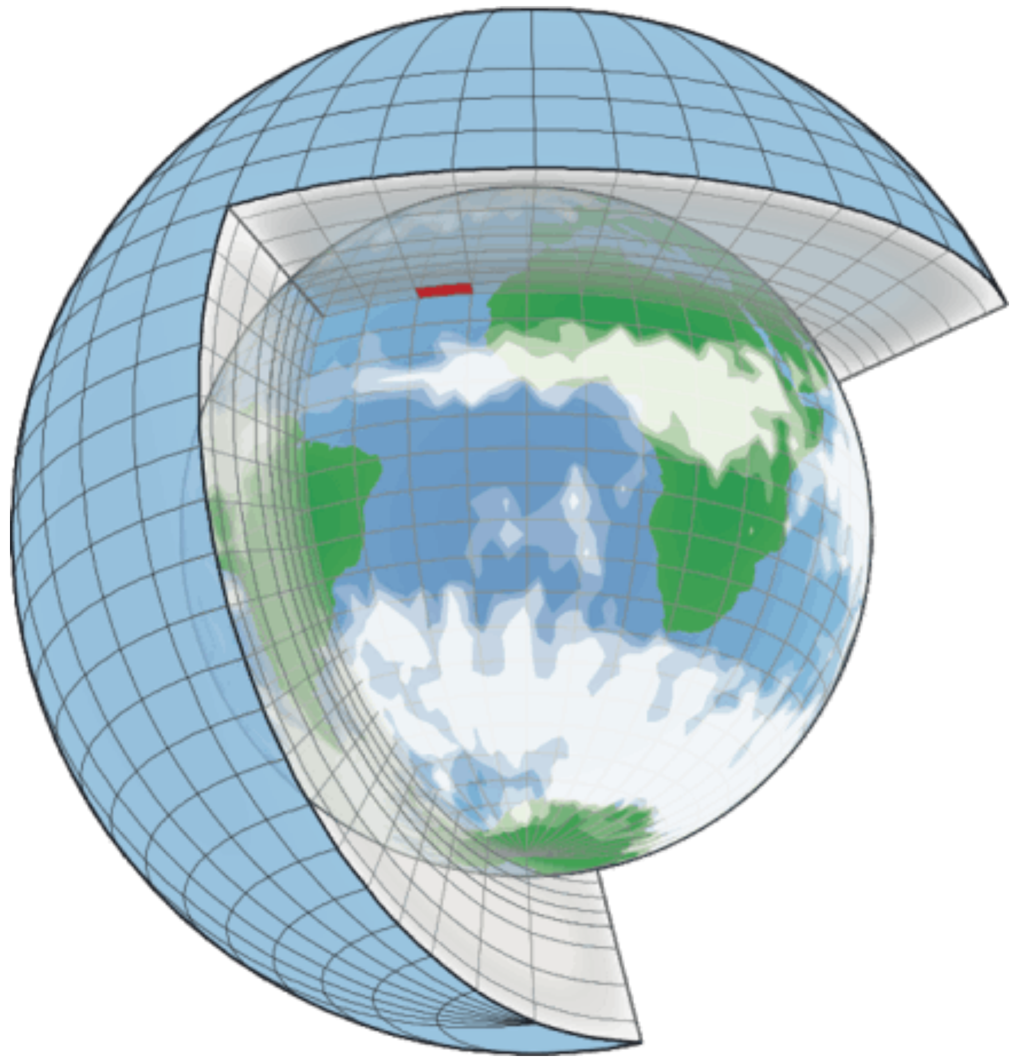
Clouds cannot be resolved in climate models

Need to represent subgrid-scale processes: turbulence, convection and cloud microphysics

~100 km 🟧



NASA MODIS: August 2018 clouds off the west coast of North America

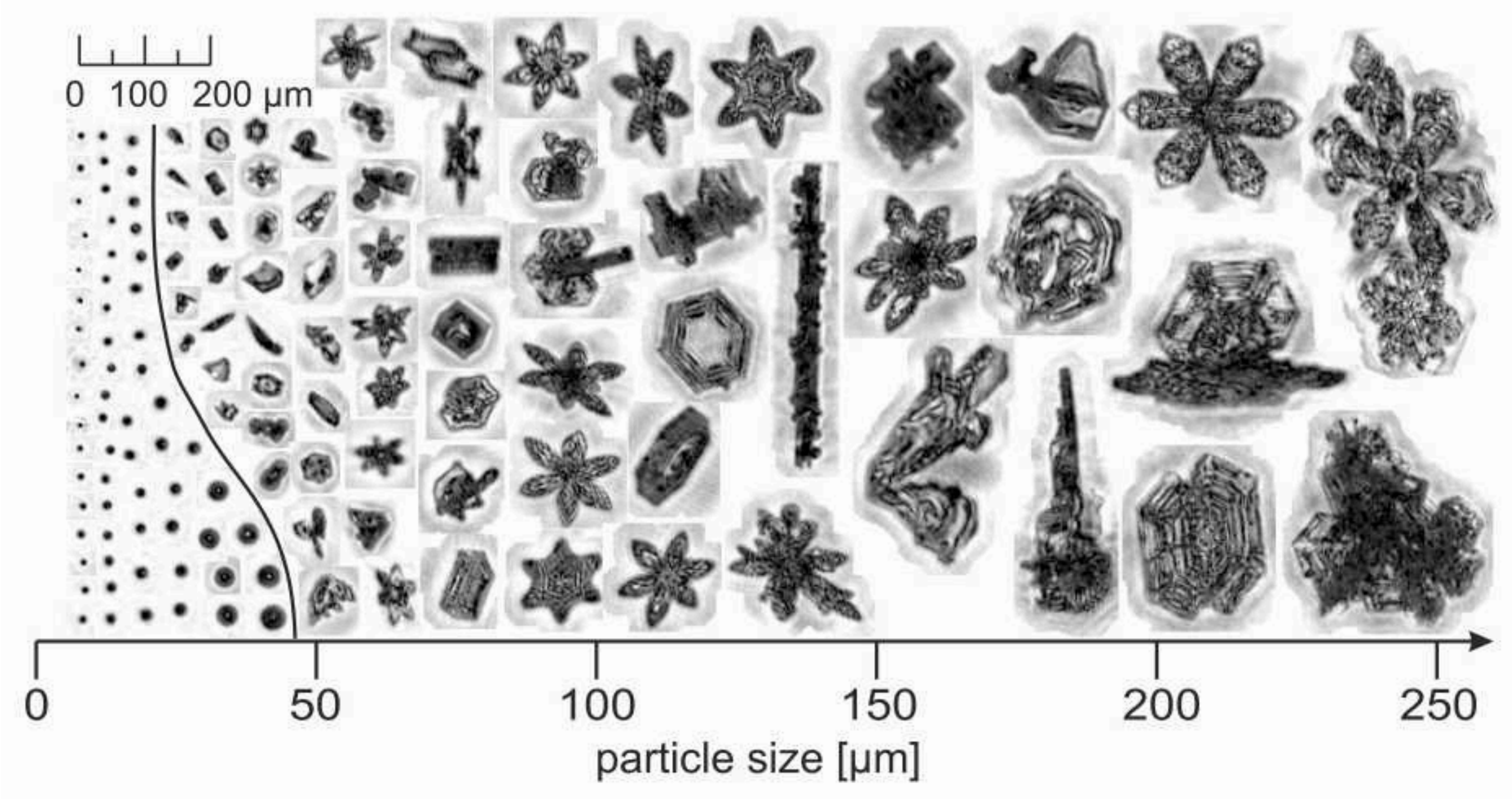


Global model:

~10-50 km resolution

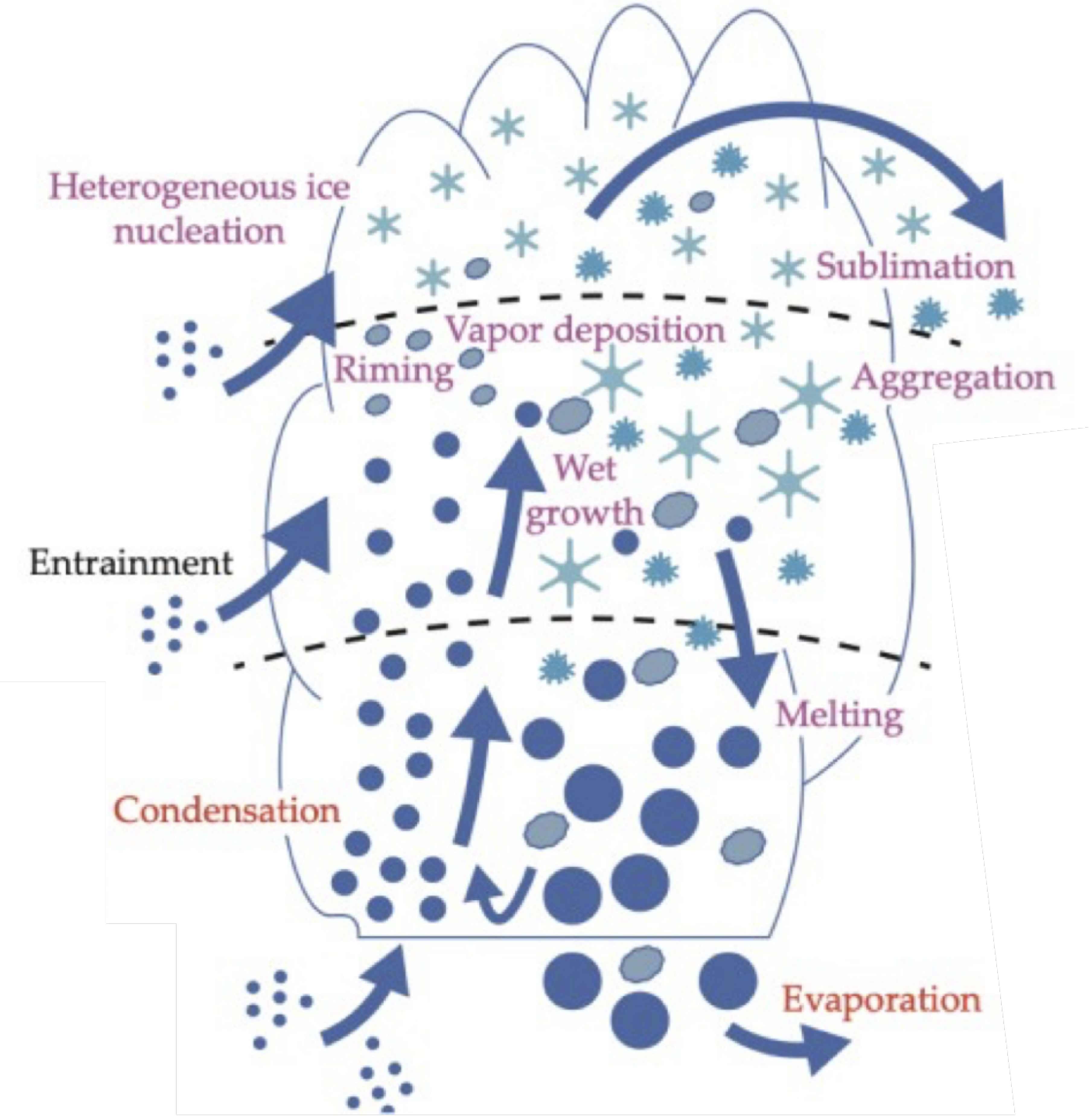
Cloud scales:
~10-100 m

Cloud microphysics scales: ~10^{-6} m



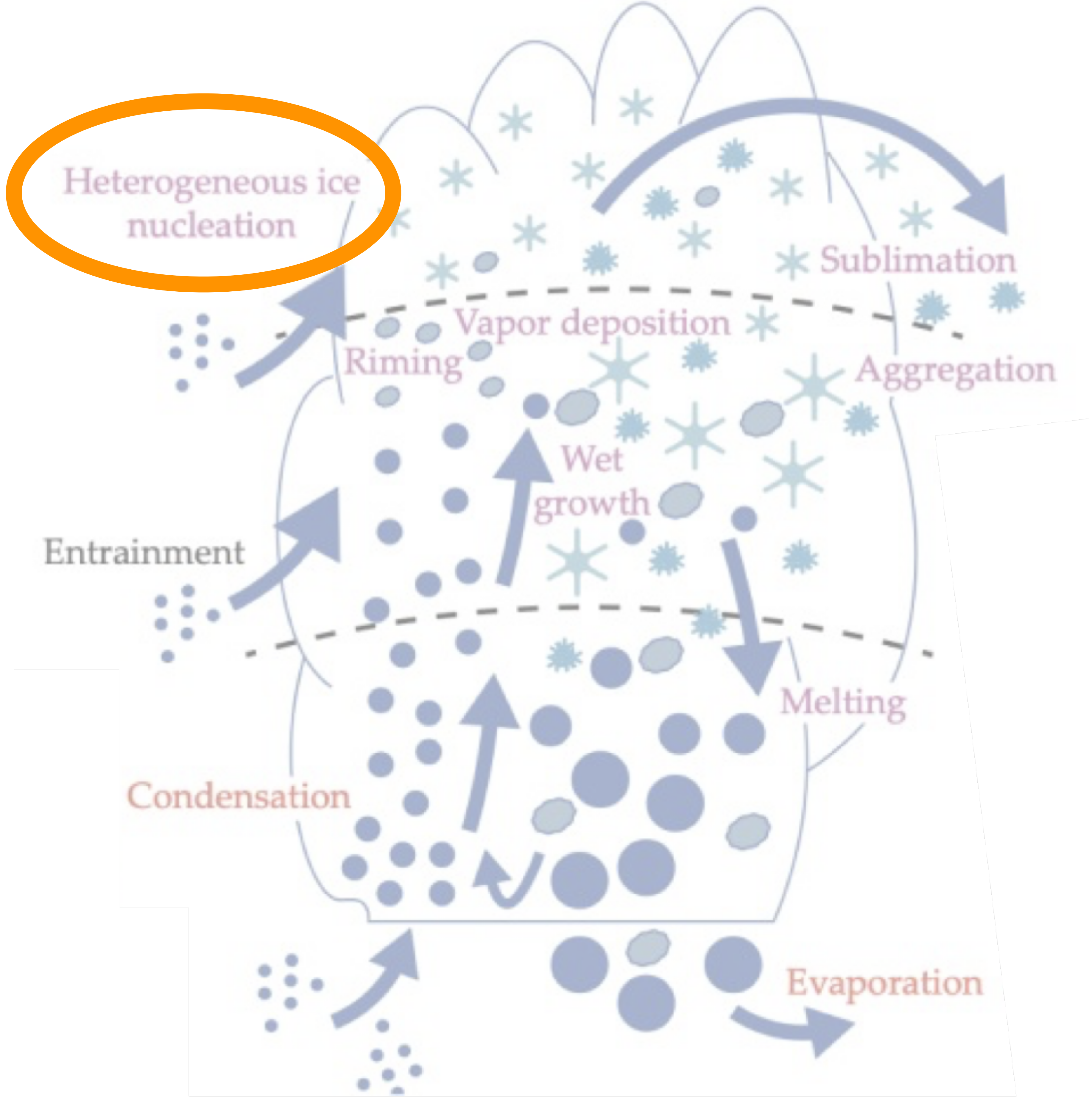
HOLIMO @ETH Zurich Field measurements with the holographic imager

Clouds cannot be resolved in climate models

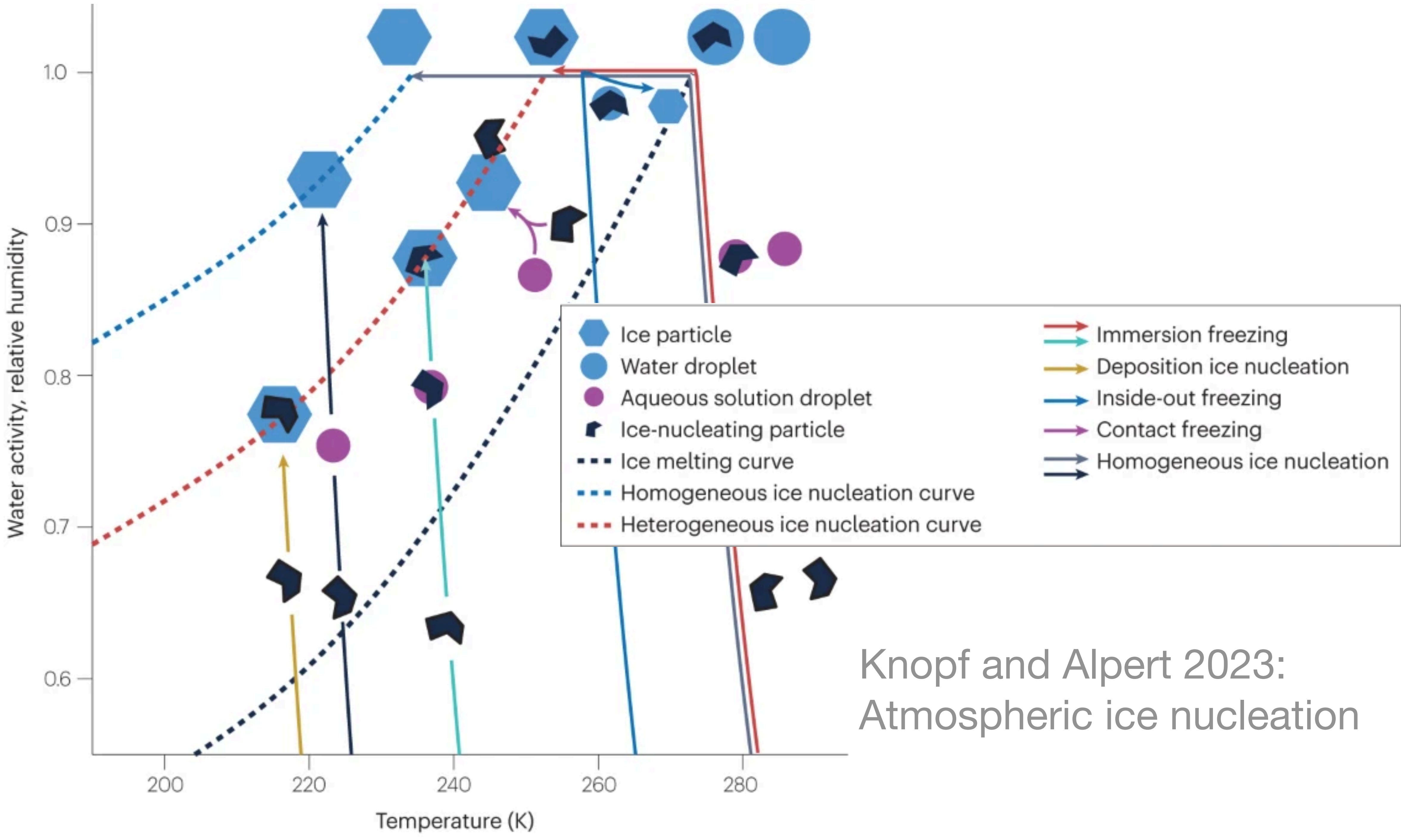


Morrison et al. 2020
Confronting the Challenge of Modeling Cloud and Precipitation Microphysics

Clouds cannot be resolved in climate models

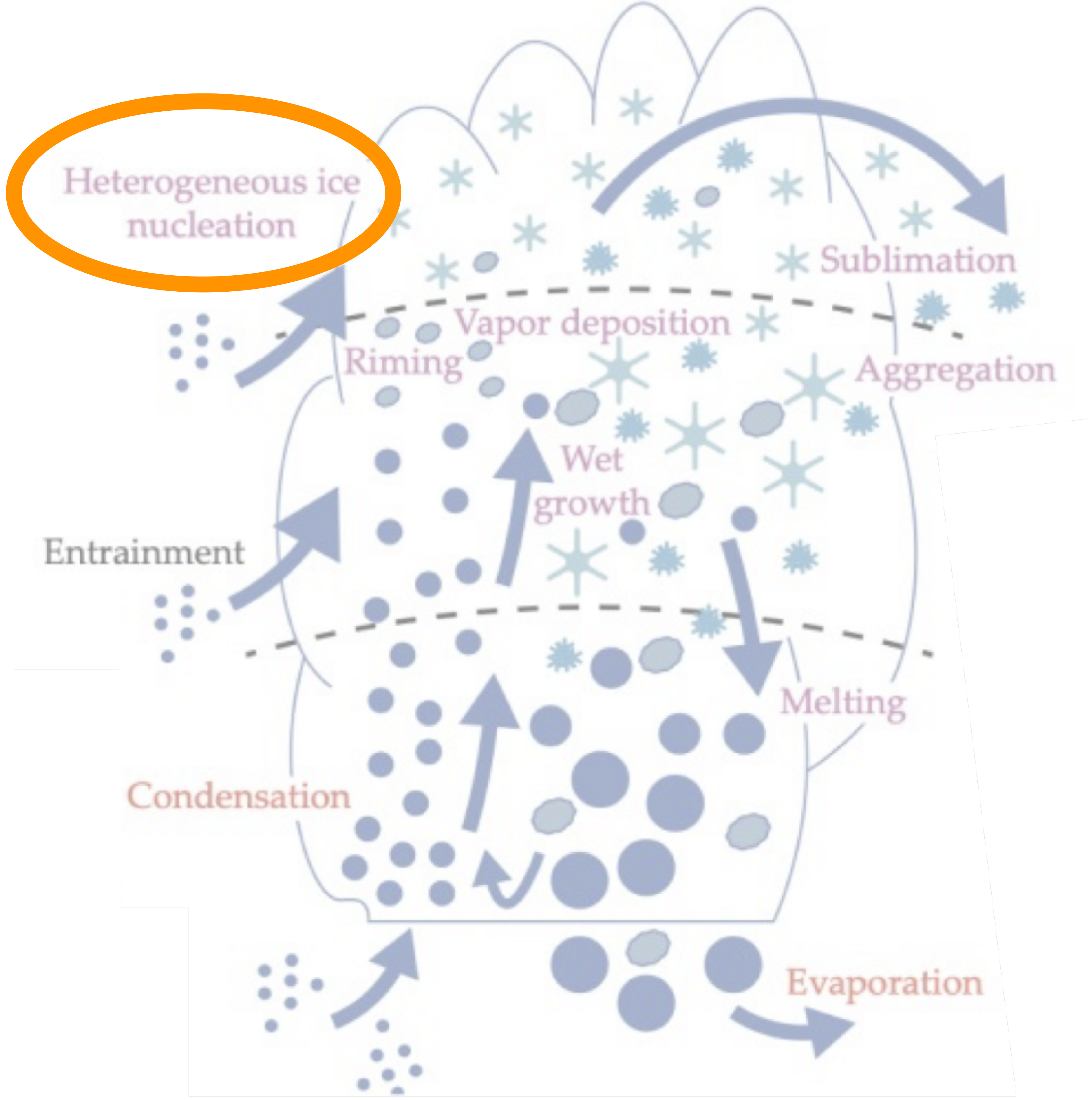


Morrison et al. 2020
Confronting the Challenge of Modeling Cloud and
Precipitation Microphysics

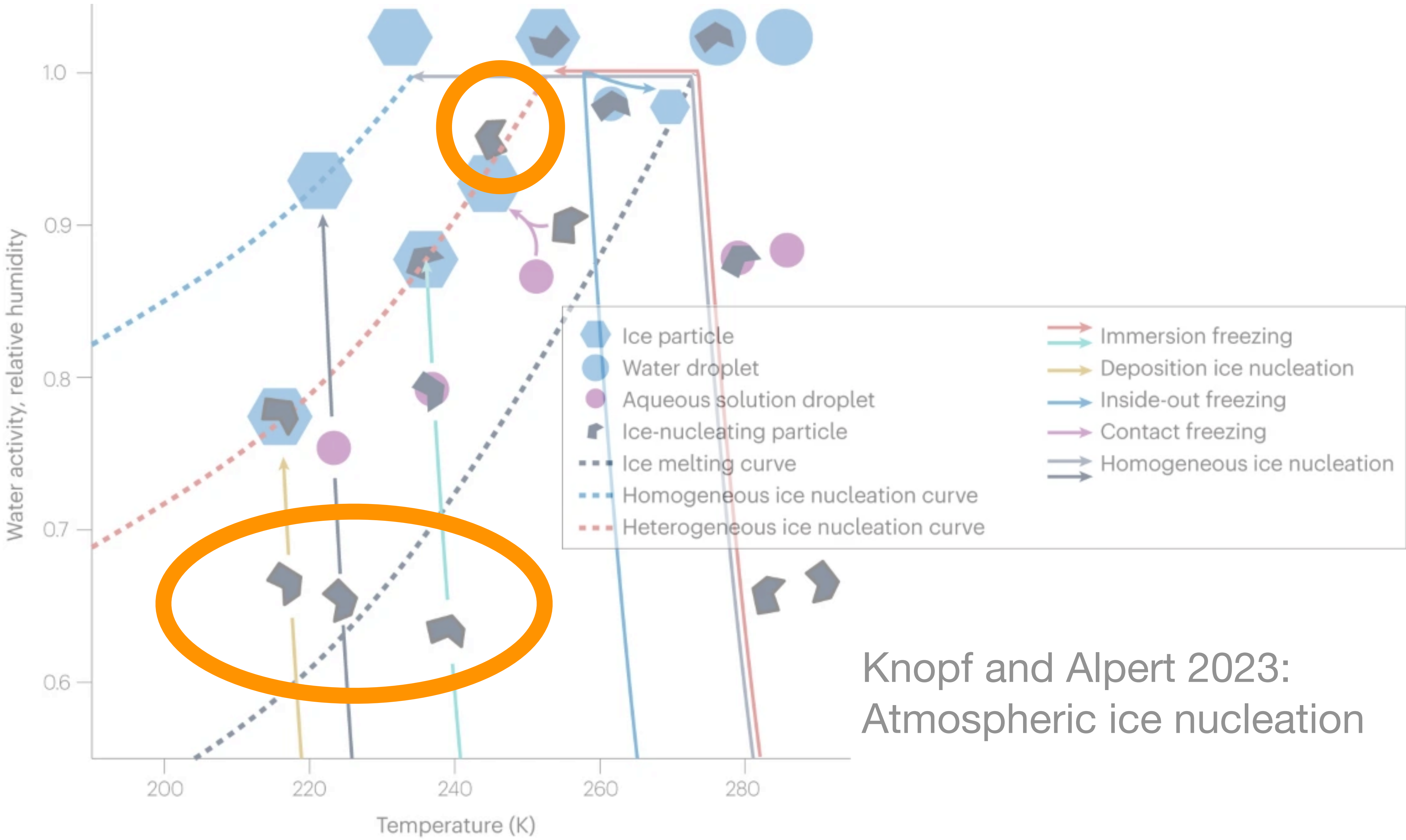


Knopf and Alpert 2023:
Atmospheric ice nucleation

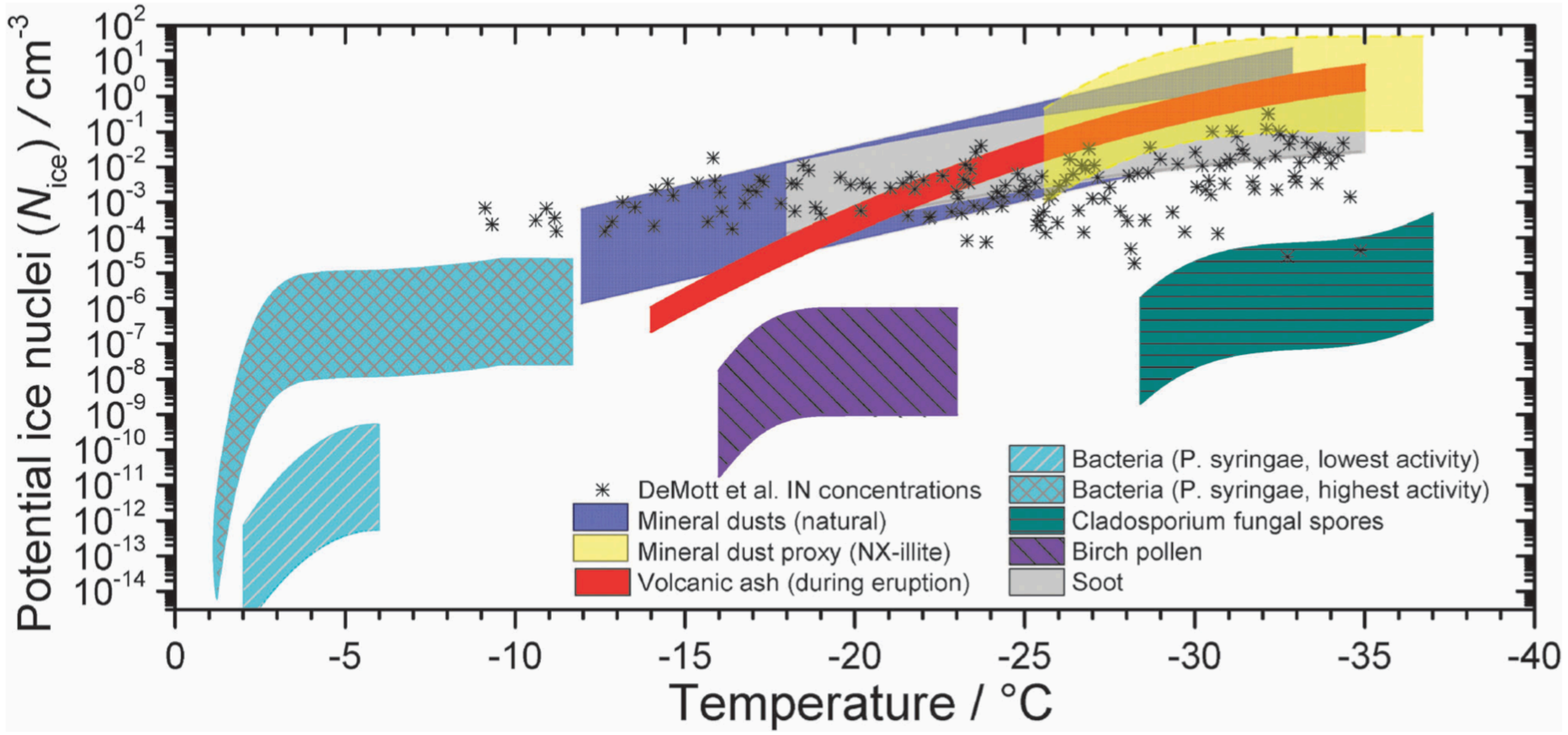
Clouds cannot be resolved in climate models



Morrison et al., 2020:
Confronting the Challenge of Modeling Cloud and Precipitation Microphysics

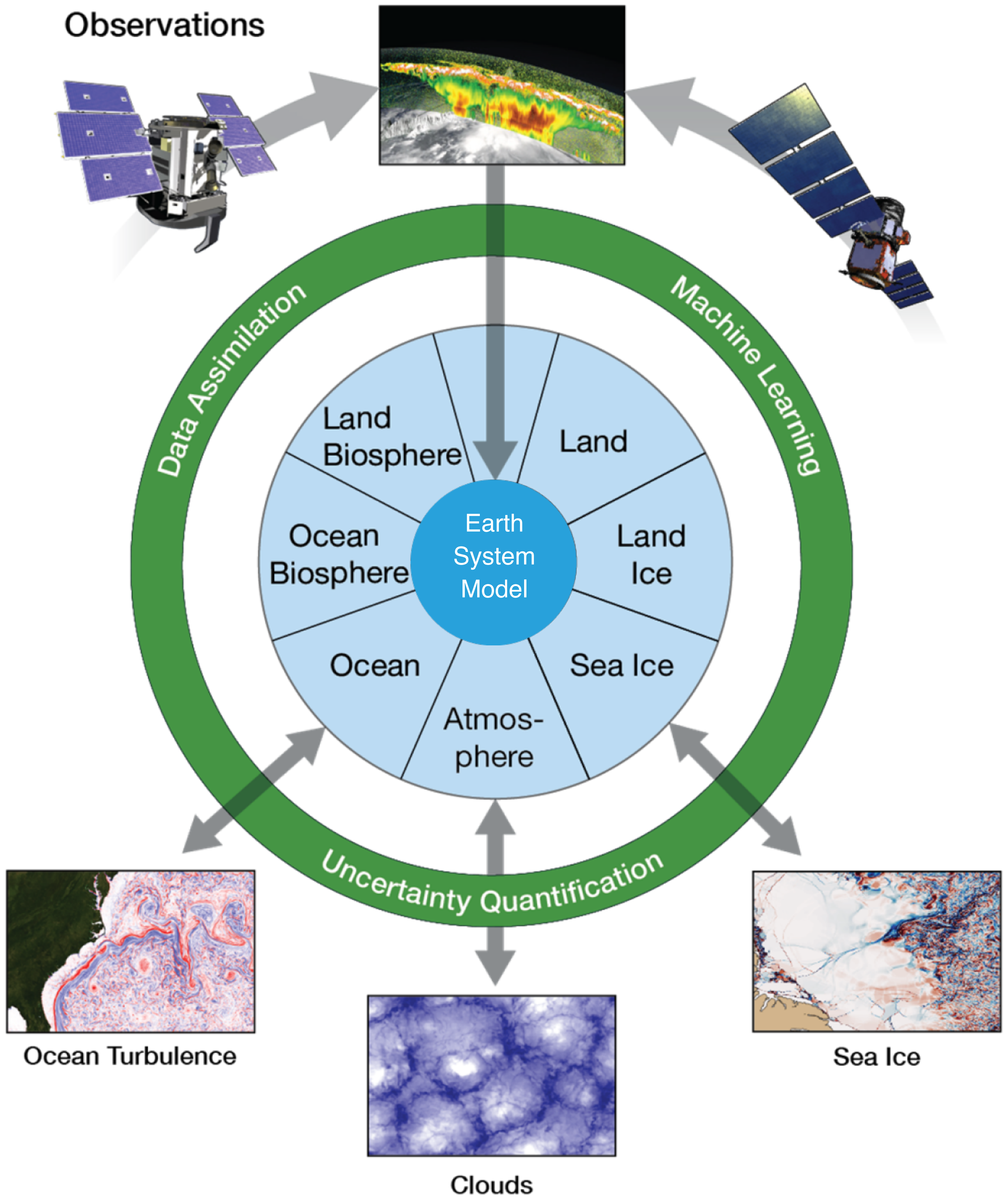


Knopf and Alpert 2023:
Atmospheric ice nucleation



Murray et. al., 2012:
Ice nucleation by particles immersed in supercooled cloud droplets

CliMA is building a **new Earth system model** whose components learn from observational and simulated data



Targeted High-Resolution Simulations

Atmosphere Model


Simon Byrne


Tapio Schneider


Sajjad Azimi


Valeria Barra


Jordan Benjamin


Tobias Bischoff


Costa Christopoulos


Yair Cohen


Oliver Dunbar


Emily de Jong


Nat Efrat-Henrici


Haakon Ervik


Jia He


Daniel Z. Huang


Anna Jaruga


Sriharsha Kandala


Charles Kawczynski


Oswald Knoth


Ignacio Lopez-Gomez


Amy Lu


Lenka Novak


Zhaoyi Shen


Clare Singer


Akshay Sridhar


Paul Ullrich


Dennis Yatunin

Outline

- **Physics based parameterizations**
- Data driven calibrations
- Software design

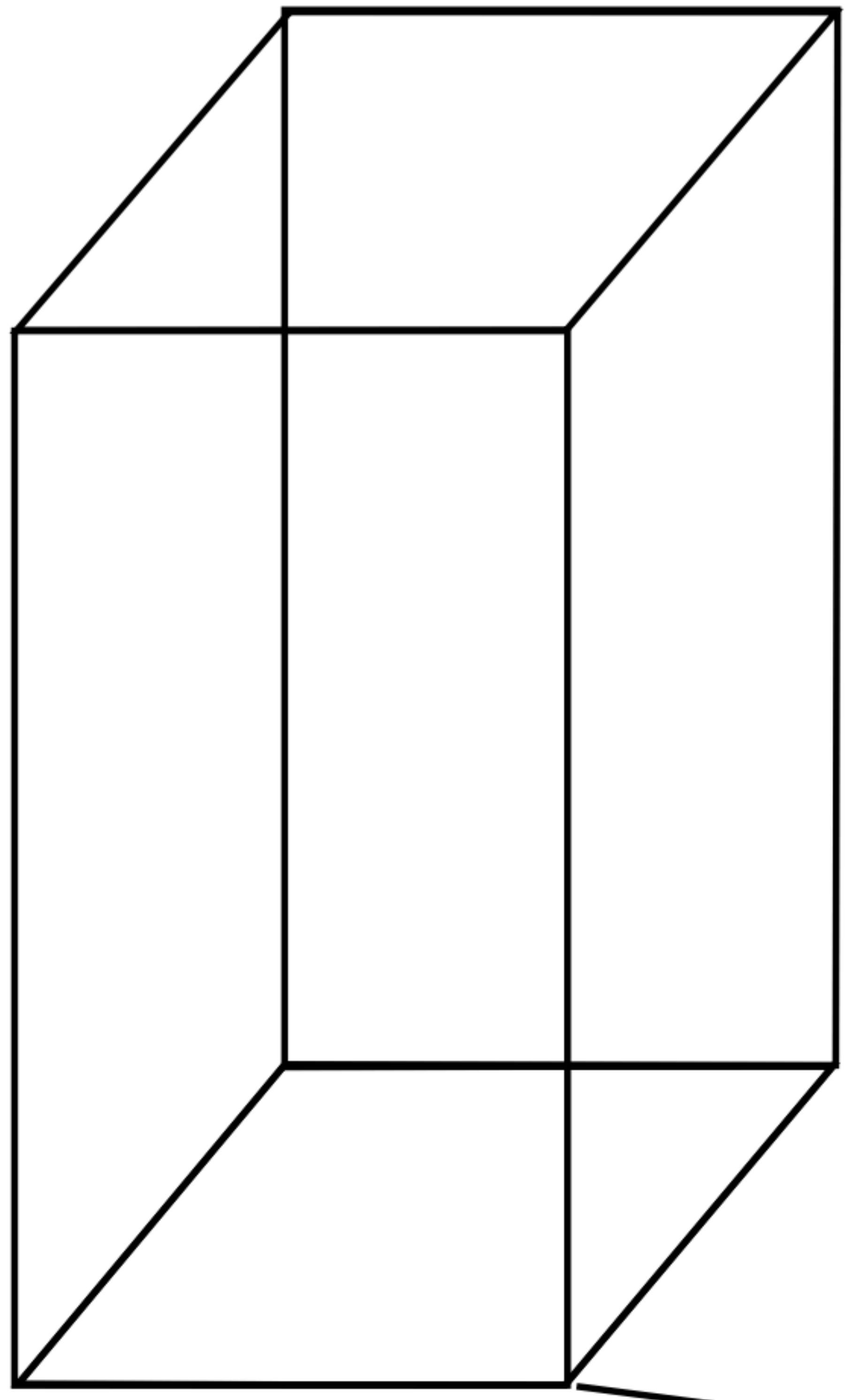
A unified physics-based model of turbulence, convection, …

GCM:

$$\frac{\partial\langle\phi\rangle}{\partial t}+\nabla_h\left(\langle\phi\rangle\langle\boldsymbol{u}\rangle\right)=-\frac{\partial}{\partial z}\left(\langle w\rangle\langle\phi\rangle\right)-\frac{\partial}{\partial z}\overset{?}{\boxed{\left\langle w^*\phi^*\right\rangle}}+\overset{?}{\boxed{\left\langle S_\phi\right\rangle}}$$

A **unified** physics-based model of turbulence, convection, ...

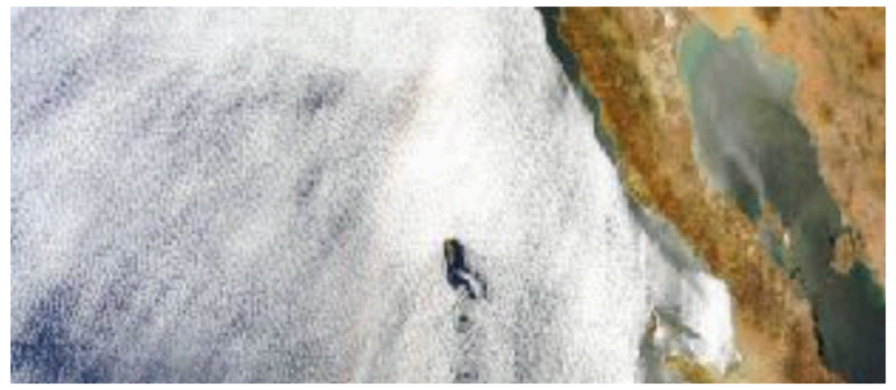
GCM column

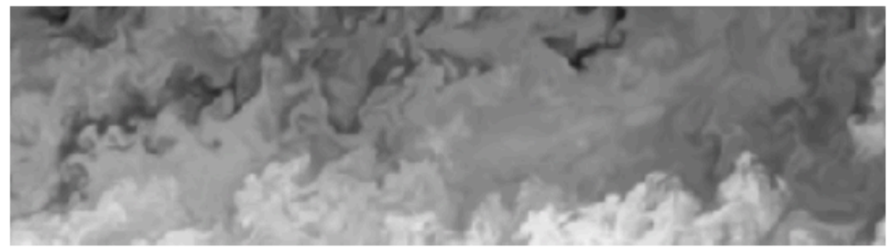


Deep convection

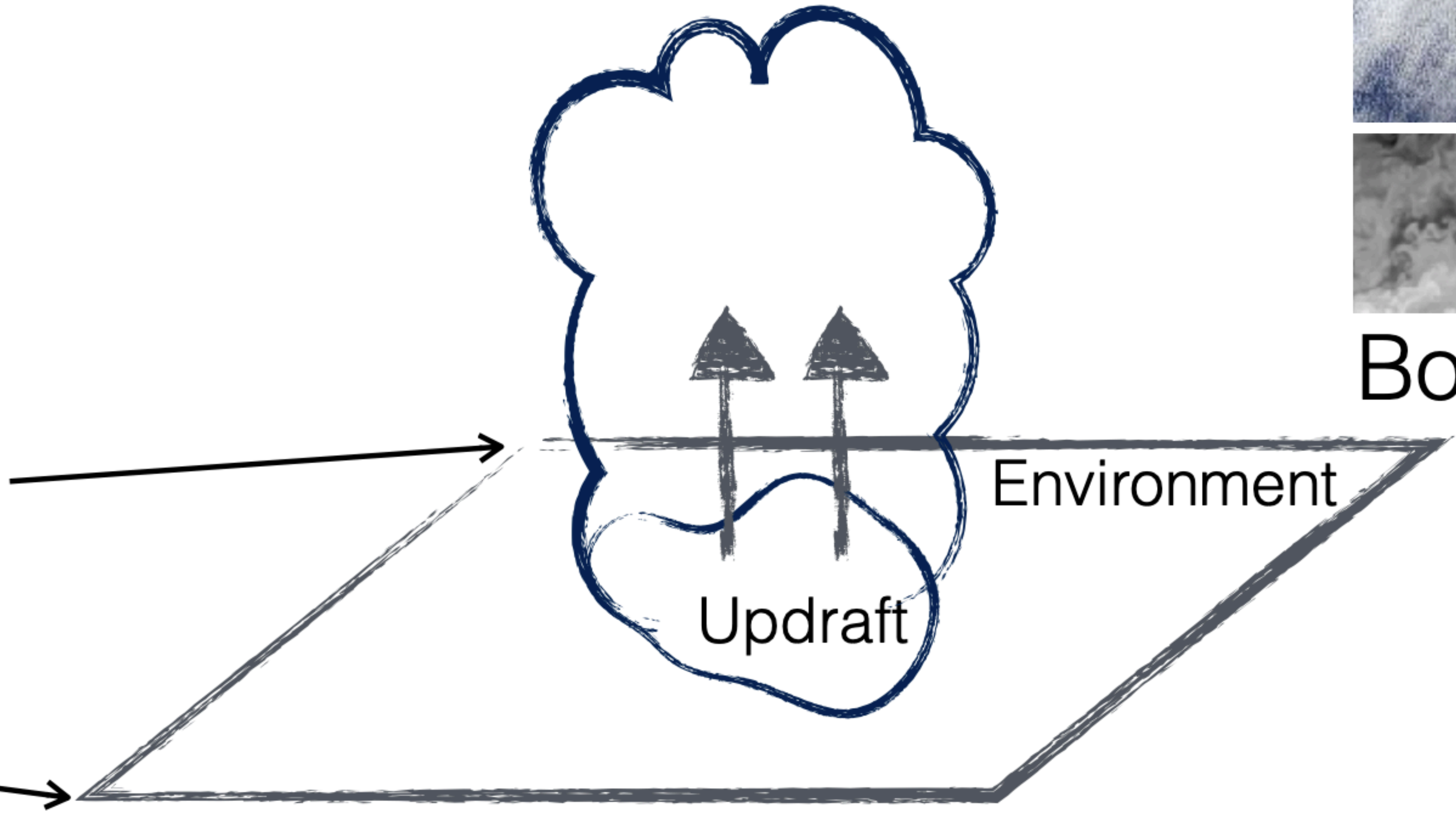
Shallow convection

Stratocumulus

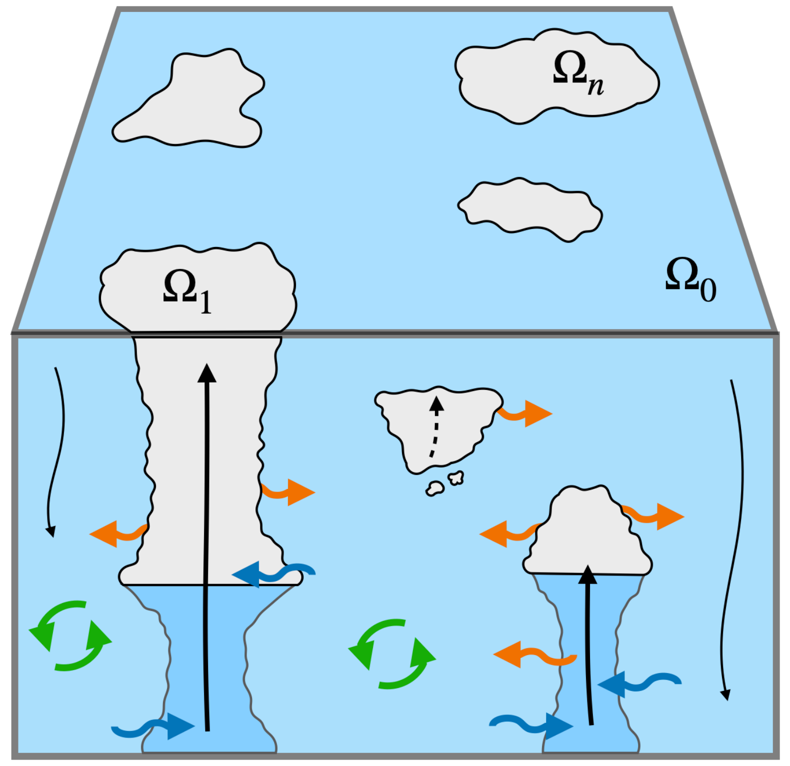


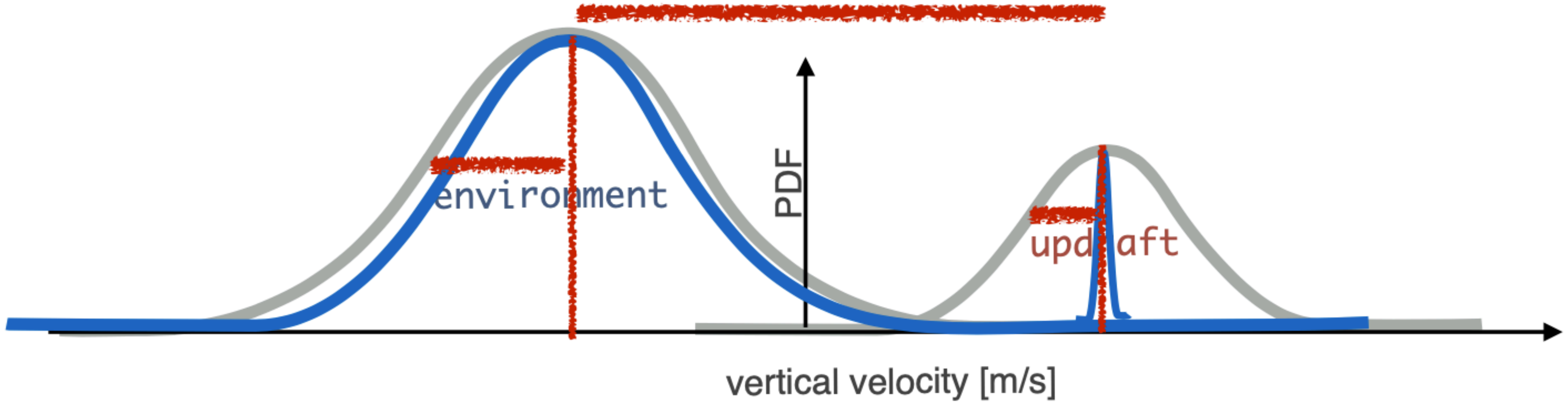


Boundary Layer



A unified physics-based model of turbulence, convection, …

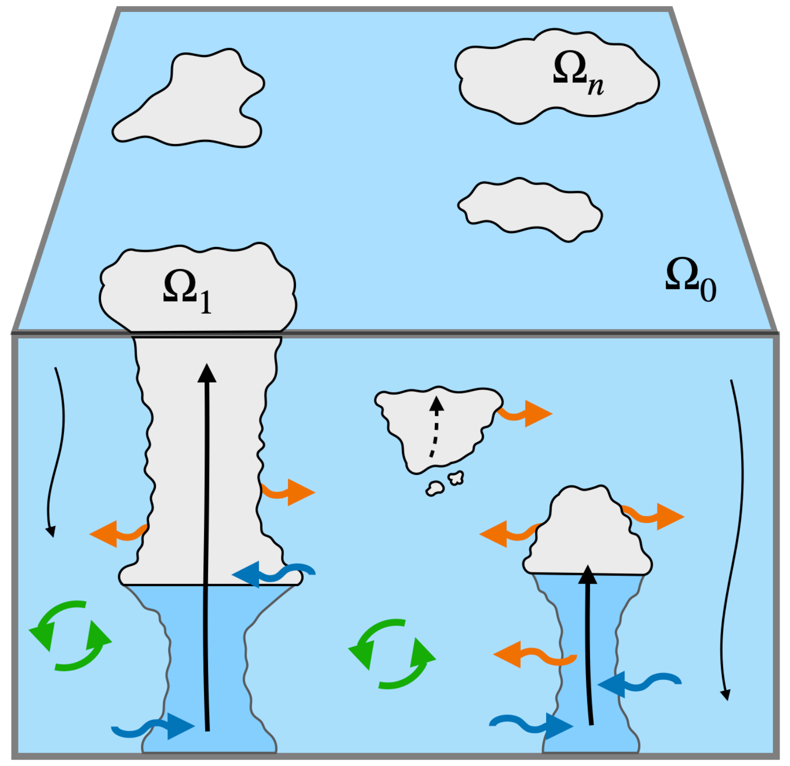


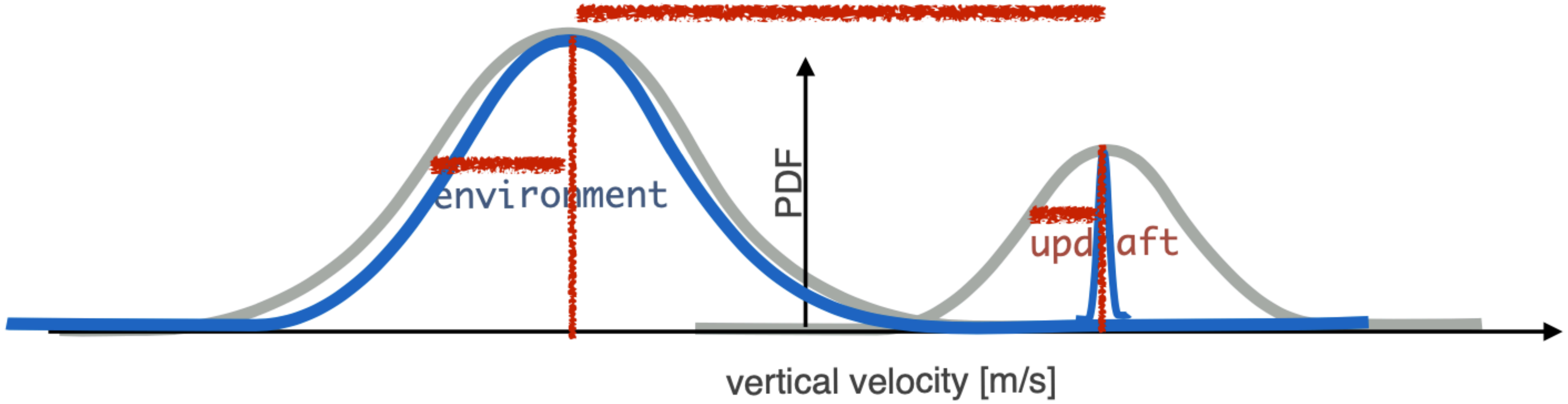


- Domain decomposed into sub-domains: coherent updrafts and isotropic environment

$$\langle\phi\rangle = a\boxed{\overline{\phi}_{up}} + (1-a)\boxed{\overline{\phi}_{env}}$$

A unified physics-based model of turbulence, convection, …





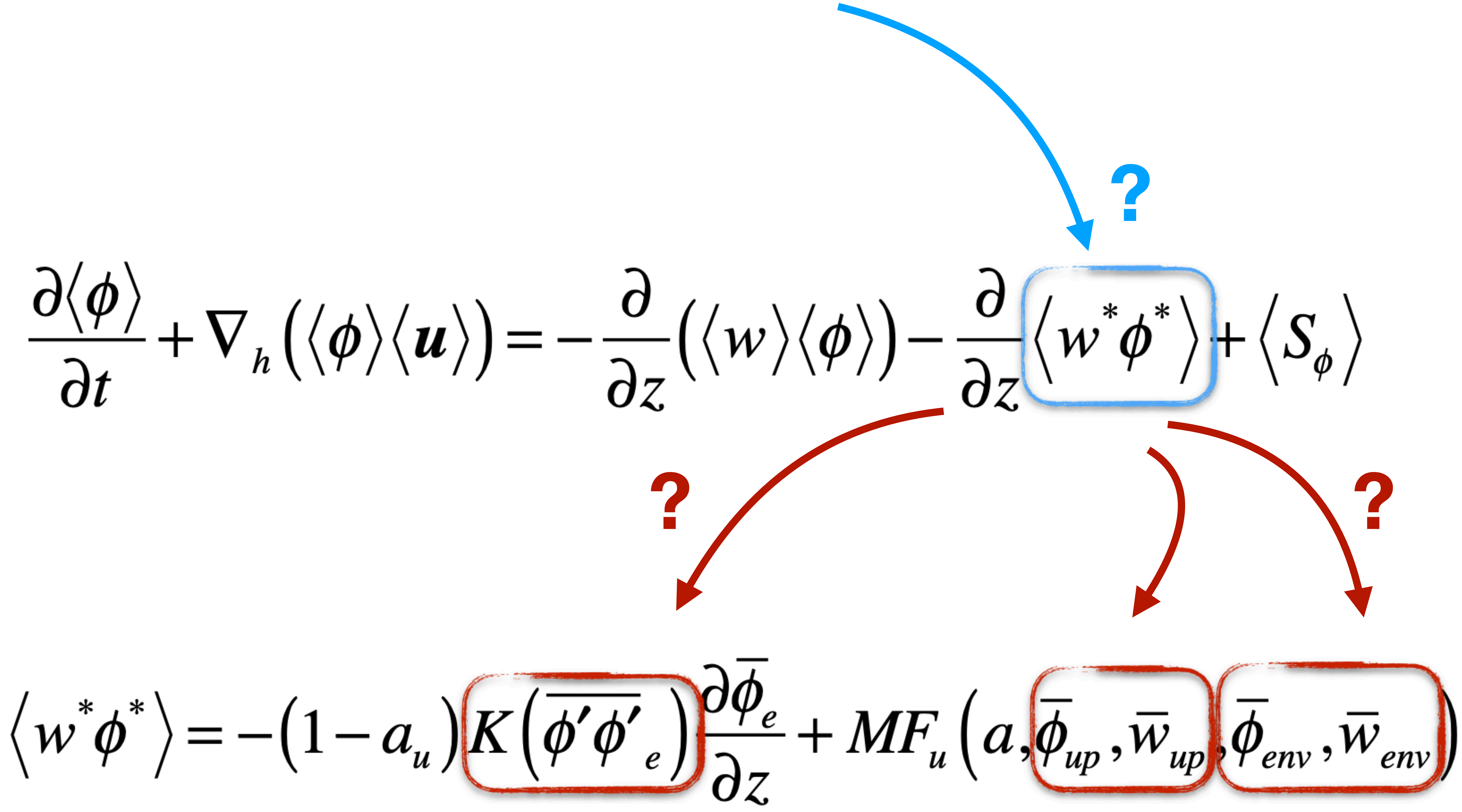
- Domain decomposed into sub-domains: coherent updrafts and isotropic environment

- Coarse-grain fluid equations by conditionally averaging over sub-domains,
  leading to exact conservation laws

$$\langle \phi \rangle = a\boxed{\bar{\phi}_{up}} + (1-a)\boxed{\bar{\phi}_{env}}$$

$$\langle w^{*}\phi^{*} \rangle = a\cancel{\boxed{\overline{w'\phi'}^{up}}} + (1-a)\boxed{\overline{w'\phi'}^{env}} + a(1-a)\boxed{\left(\bar{\phi}_u - \bar{\phi}_e\right)\left(\bar{w}_u - \bar{w}_e\right)}$$

A unified physics-based model of turbulence, convection, …



GCM:

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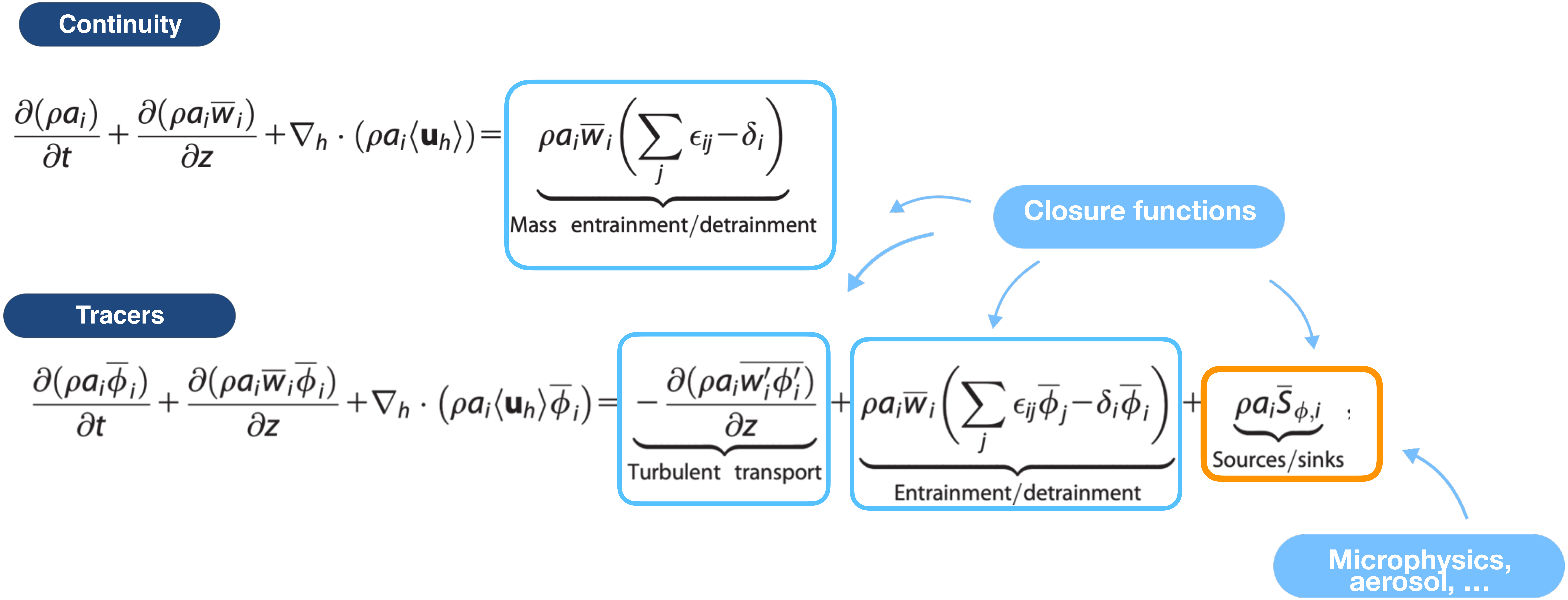
SGS model:

$$\langle w^*\phi^*\rangle=-(1-a_u)\boxed{K\left(\overline{\phi'\phi'}_e\right)}\frac{\partial\bar{\phi}_e}{\partial z}+MF_u\left(a,\boxed{\bar{\phi}_{up},\bar{w}_{up}},\boxed{\bar{\phi}_{env},\bar{w}_{env}}\right)$$

A unified physics-based model of turbulence, convection, …



Continuity

$$\frac{\partial(\rho a_i)}{\partial t}+\frac{\partial(\rho a_i\overline{w}_i)}{\partial z}+\nabla_h\cdot(\rho a_i\langle\mathbf{u}_h\rangle)=\boxed{\underbrace{\rho a_i\overline{w}_i\left(\sum_j\epsilon_{ij}-\delta_i\right)}_{\text{Mass entrainment/detrainment}}}$$

Tracers

$$\frac{\partial(\rho a_i\overline{\phi}_i)}{\partial t}+\frac{\partial(\rho a_i\overline{w}_i\overline{\phi}_i)}{\partial z}+\nabla_h\cdot(\rho a_i\langle\mathbf{u}_h\rangle\overline{\phi}_i)=\boxed{\underbrace{-\frac{\partial(\rho a_i\overline{w_i'\phi_i'})}{\partial z}}_{\text{Turbulent transport}}}+\boxed{\underbrace{\rho a_i\overline{w}_i\left(\sum_j\epsilon_{ij}\overline{\phi}_j-\delta_i\overline{\phi}_i\right)}_{\text{Entrainment/detrainment}}}+\boxed{\underbrace{\rho a_i\overline{S}_{\phi,i}}_{\text{Sources/sinks}}}$$

Closure functions

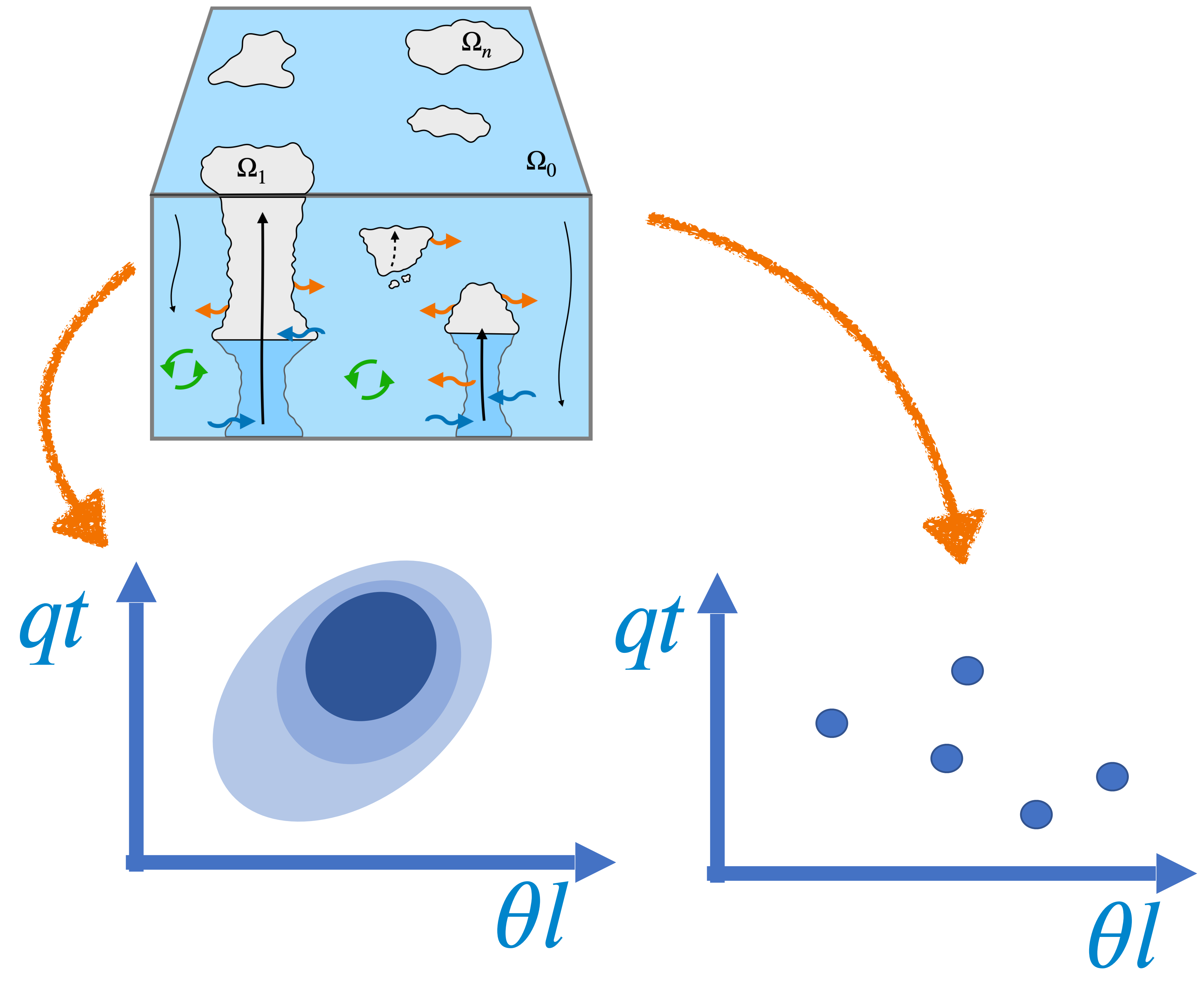
Microphysics, aerosol, …

Tan et al., 2018: An Extended Eddy-Diffusivity Mass-Flux Scheme for Unified Representation of Subgrid-Scale Turbulence and Convection
Cohen et al. 2020: Unified Entrainment and Detrainment Closures for Extended Eddy-Diffusivity Mass-Flux Schemes
Lopez-Gomez et al., 2020: A Generalized Mixing Length Closure for Eddy-Diffusivity Mass-Flux Schemes of Turbulence and Convection

A unified physics-based model of turbulence, convection and clouds

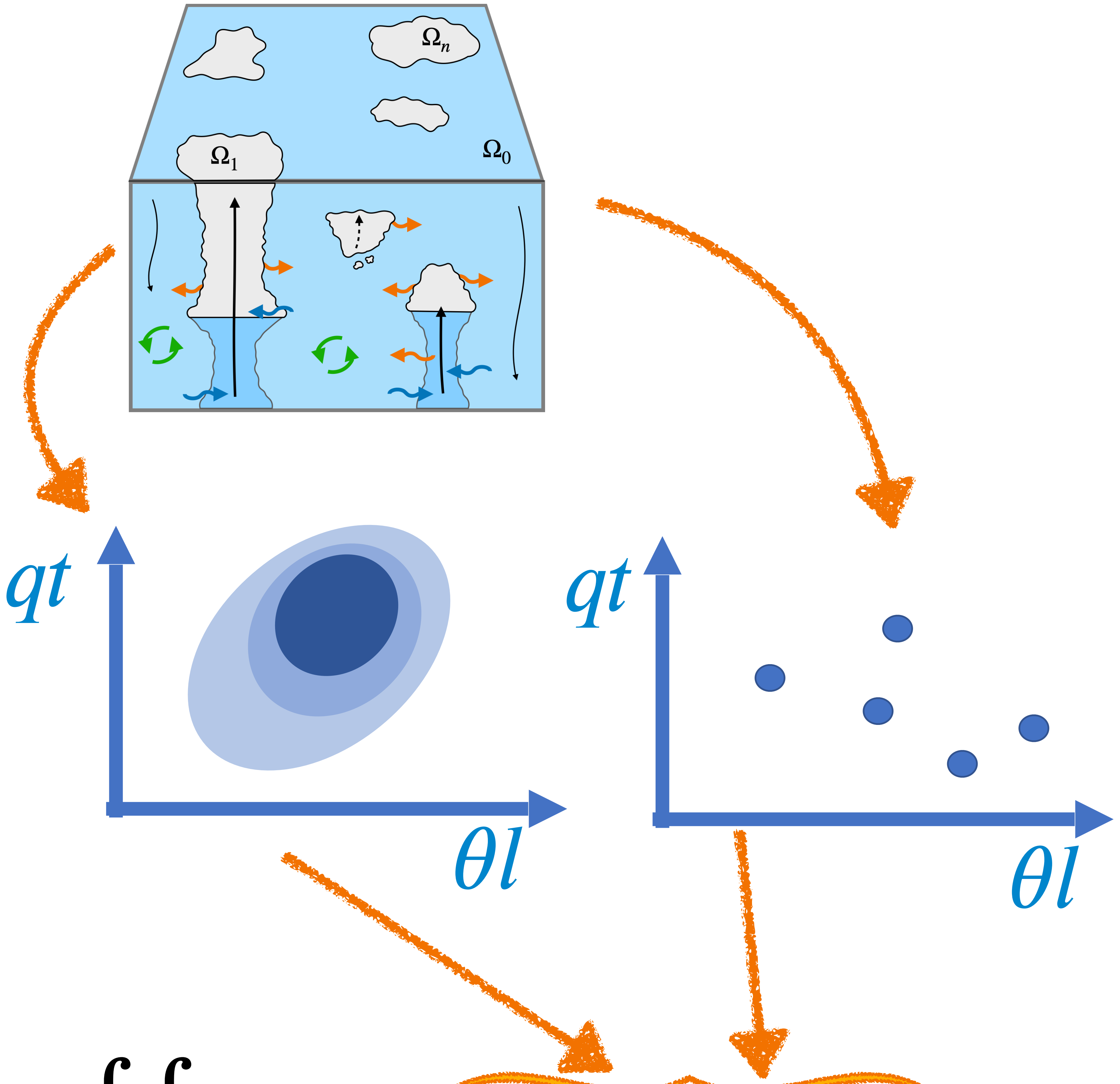
- SGS scheme provides information on the sub-grid scale environment (co)variances of (q_t, θ) and mean updraft values

- When coupling with cloud microphysics scheme we assume a distribution shape:
  Log-normal or Gaussian



A unified physics-based model of turbulence, convection and clouds

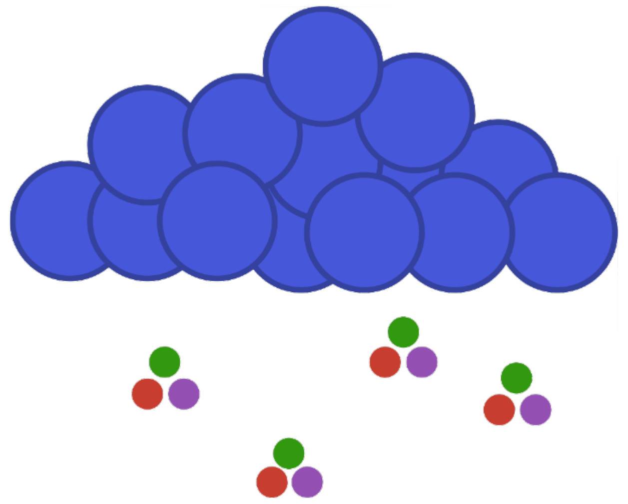
- SGS scheme provides information on the sub-grid scale environment (co)variances of (q_t, θ) and mean updraft values
- When coupling with cloud microphysics scheme we assume a distribution shape:
  Log-normal or Gaussian
- Microphysics autoconversion and accretion sources are computed by integrating over $P(\theta, q_t)$
    - Environment: Numerical quadratures
    - Updrafts: Sum of δ functions



$$S = \int\int \underbrace{f(\theta, q_t)}_{} \overbrace{P(\theta, q_t) d\theta dq_t}^{}$$

Microphysics, aerosol, …

A library of bulk microphysics and aerosol schemes



CloudMicrophysics.jl

Currently available:

- **1-moment microphysics** (cloud water and ice, rain, snow)
- **2-moment microphysics** (Seifert and Beheng 2006, + 4 autoconversion and accretion options)

A library of bulk microphysics and aerosol schemes

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- **Aerosol activation** (Abdul-Razzak and Ghan 2000 + ML calibrated options)
- **Ice nucleation** (Mohler et al 2006, water activity based: Knopf and Alpert 2013, Koop et al 2000)
- **Aerosol nucleation** (CLOUD experiments at CERN, Duane et. al. 2016, Kirkby et al 2016, Riccobono et al 2014)

A library of bulk microphysics and aerosol schemes

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- **Precipitation susceptibility tests** (Glassmeier and Lohmann 2016)
- **Terminal velocity** (Chen et. al. 2022)

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- **Terminal velocity** (Chen et. al. 2022)

Next development steps:

- More ice nucleation paths (?)
- Aerosol model (?)
- P3 snow/ice microphysics scheme (Morrison and Milbrandt 2015)
- Replace unknown parametric functions with NNs
- Calibrate with observations (e.g., CloudSat, MODIS)

Summary

GCM:

$$\frac{\partial\langle\phi\rangle}{\partial t}+\nabla_h\left(\langle\phi\rangle\langle\boldsymbol{u}\rangle\right)=-\frac{\partial}{\partial z}\left(\langle w\rangle\langle\phi\rangle\right)-\frac{\partial}{\partial z}\boxed{\langle w^*\phi^*\rangle}+\boxed{\langle S_\phi\rangle}$$

“dynamical core”

$$\frac{\partial(\rho a_i\overline{\phi}_i)}{\partial t}+\frac{\partial(\rho a_i\overline{w}_i\overline{\phi}_i)}{\partial z}+\nabla_h\cdot\left(\rho a_i\langle\mathbf{u}_h\rangle\overline{\phi}_i\right)=\boxed{\underbrace{-\frac{\partial(\rho a_i\overline{w'_i\phi'_i})}{\partial z}}_{\text{Turbulent transport}}}+\boxed{\underbrace{\rho a_i\overline{w}_i\left(\sum_j\epsilon_{ij}\overline{\phi}_j-\delta_i\overline{\phi}_i\right)}_{\text{Entrainment/detrainment}}}+\boxed{\underbrace{\rho a_i\overline{S}_{\phi,i}}_{\text{Sources/sinks}}}$$

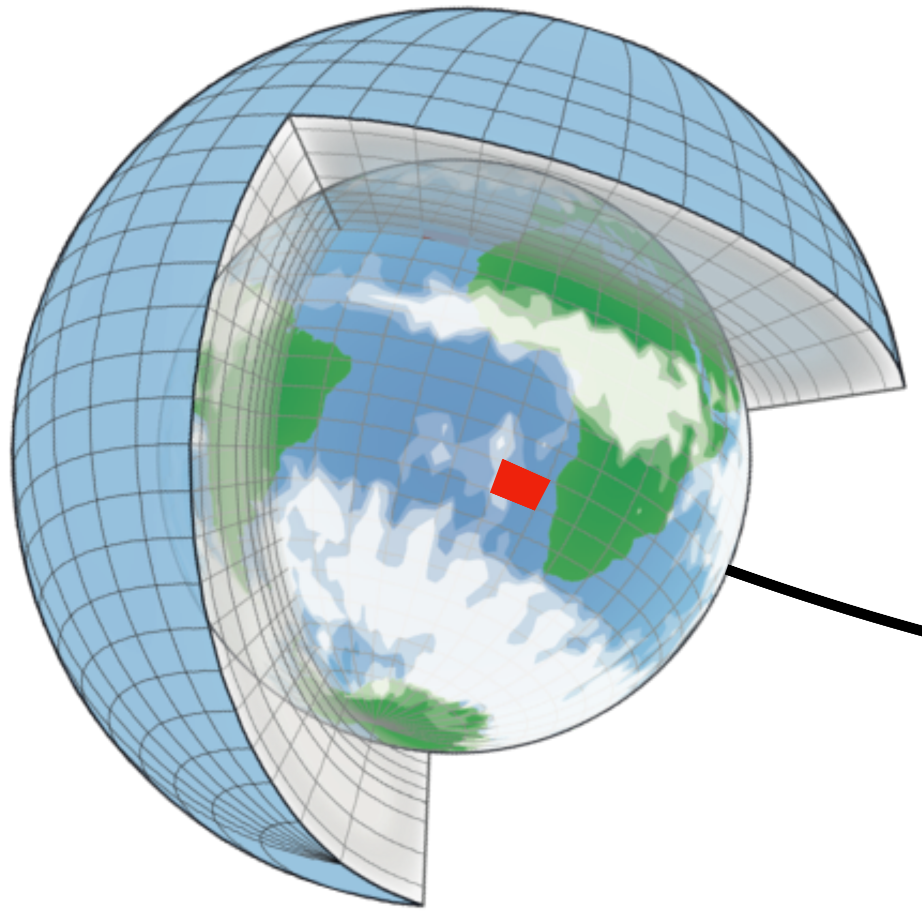
“physics” parameterizations

Outline

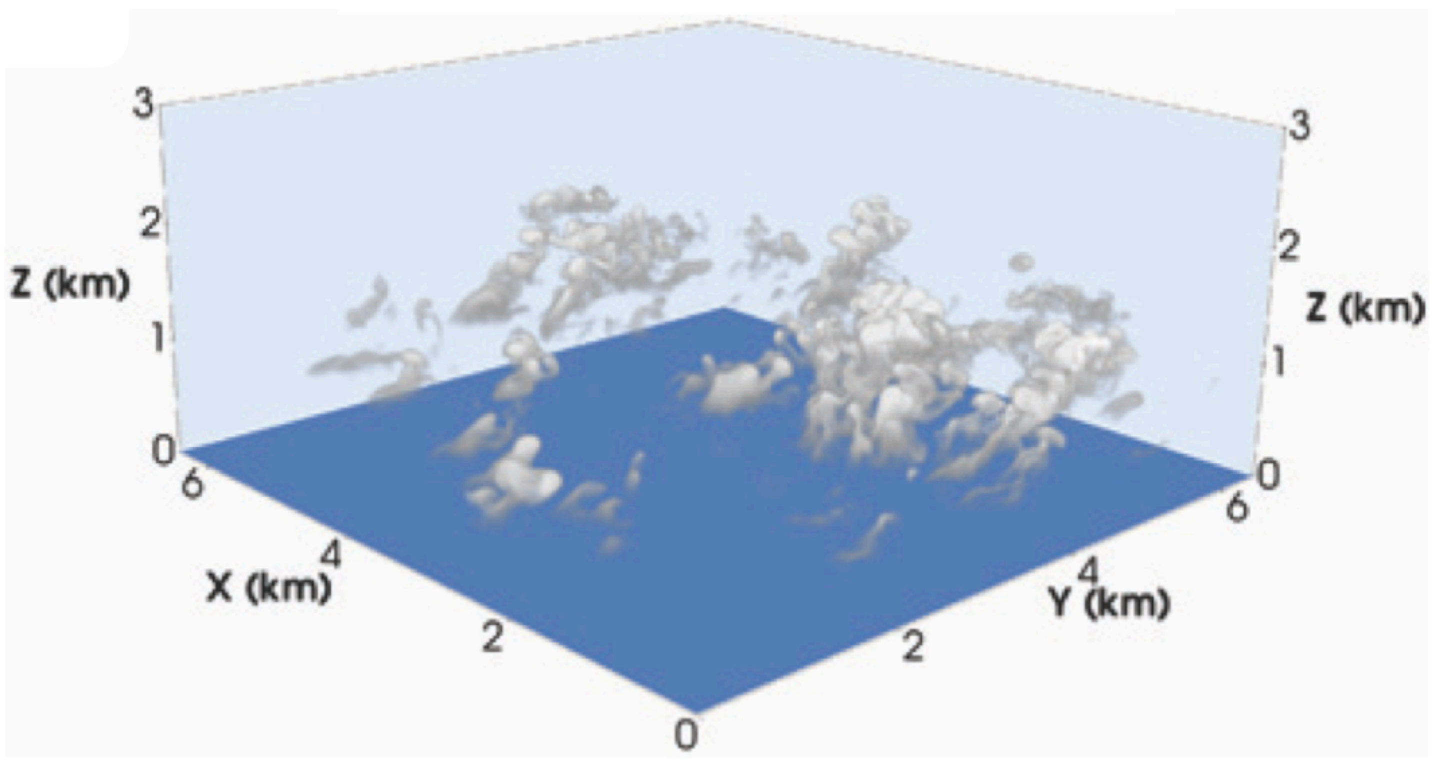
- Physics based parameterizations
- **Data driven calibrations**
- Software design

Learning from data

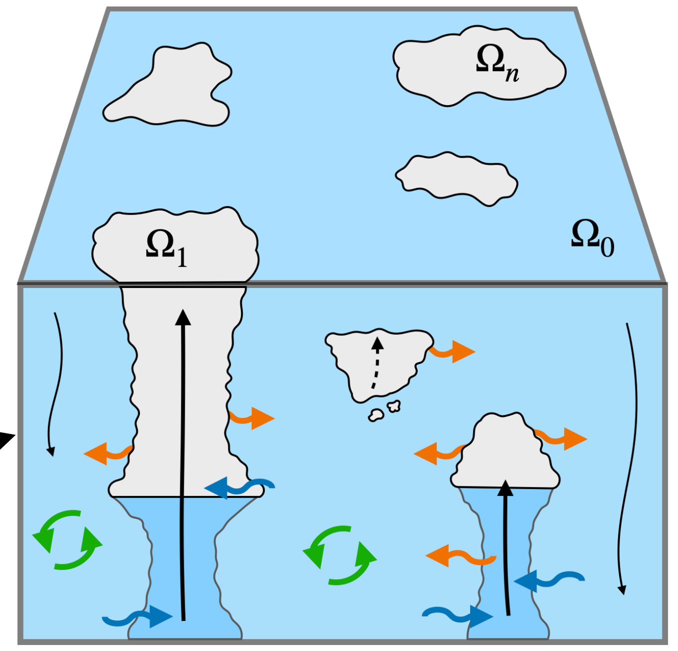
for turbulence and convection model



Targeted data acquisition



3D LES high resolution simulations of turbulence and convection



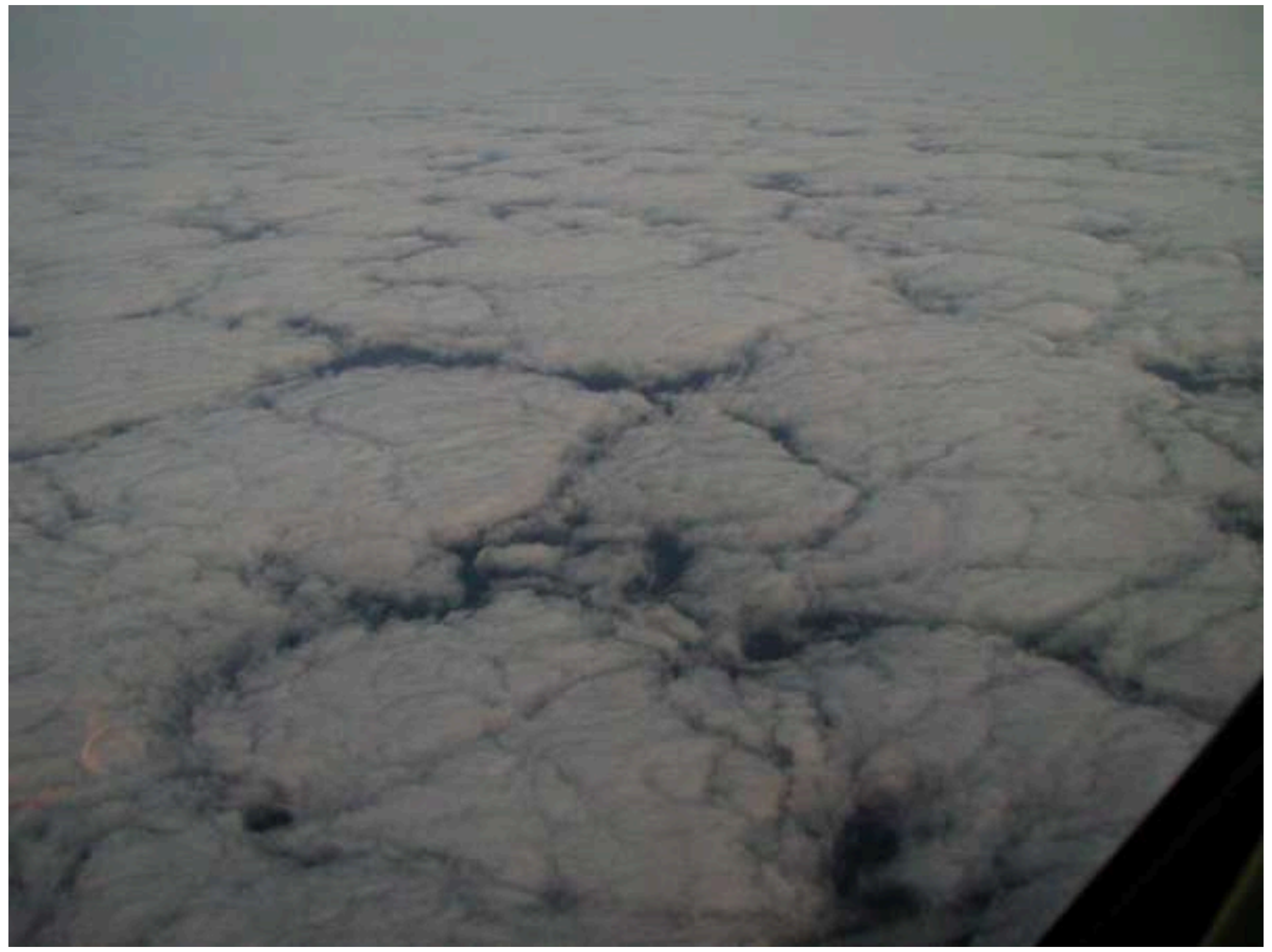
Process-level learning
Uncertainty quantification

Lopez-Gomez et al. 2022: Training Physics-Based Machine-Learning Parameterizations With Gradient-Free Ensemble Kalman Methods
Dunbar et al. 2022: Ensemble-based experimental design for targeted high-resolution simulations to inform climate models

Individual test cases

Dycoms RF02
Drizzling Sc trapped under inversion

Ackerman et al., 2009: Large-Eddy Simulations of a Drizzling, Stratocumulus-Topped Marine Boundary Layer



Rico
Precipitating shallow trade wind convection

Van Zanten et.al., 2011: Controls on precipitation and cloudiness in simulations of trade-wind cumulus as observed during RICO

TRMM LBA
Development of deep convection over Amazon

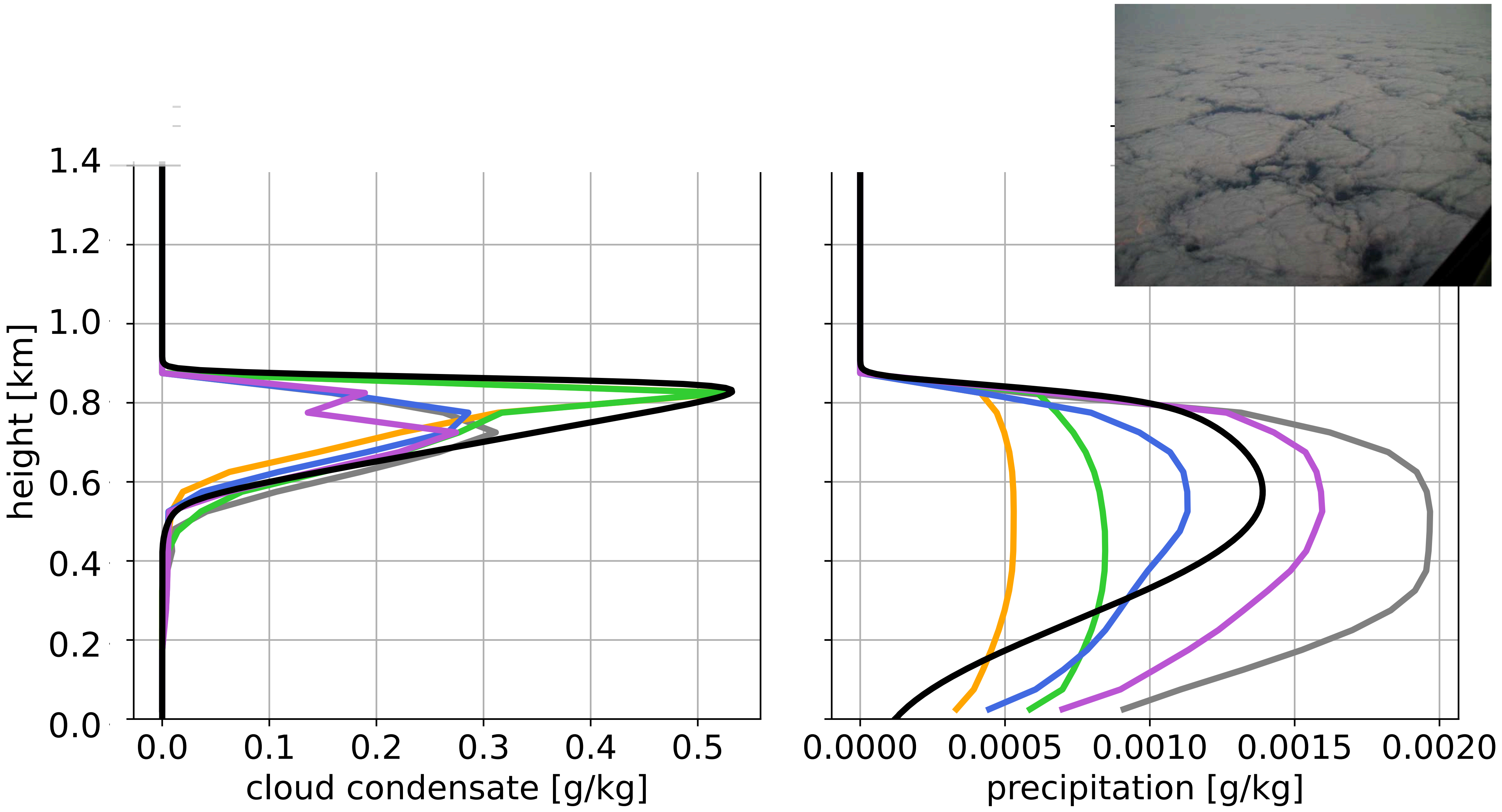
Grabowski et. al., 2006: Daytime convective development over land: A model intercomparison based on LBA observations

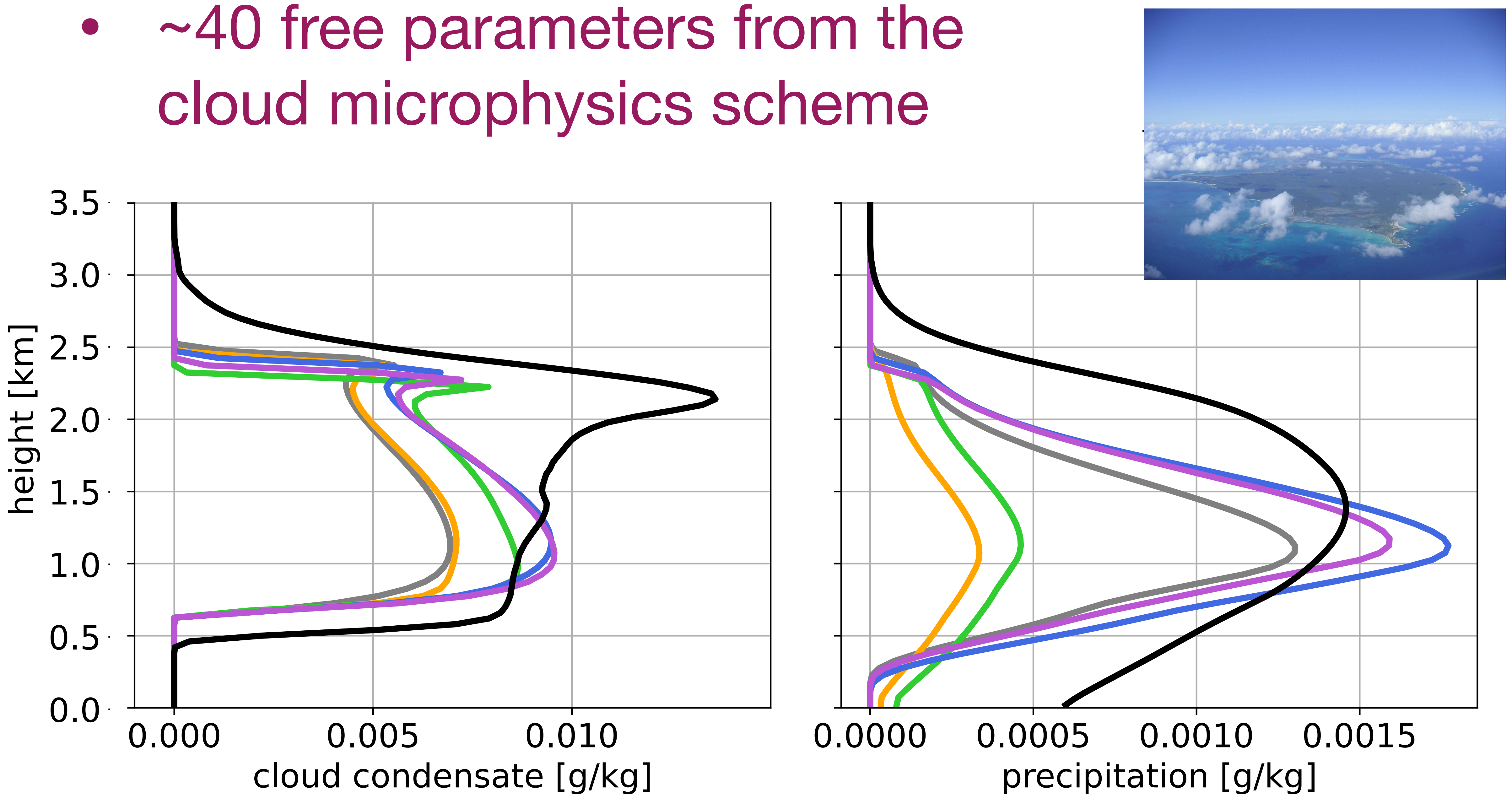
Individual test cases

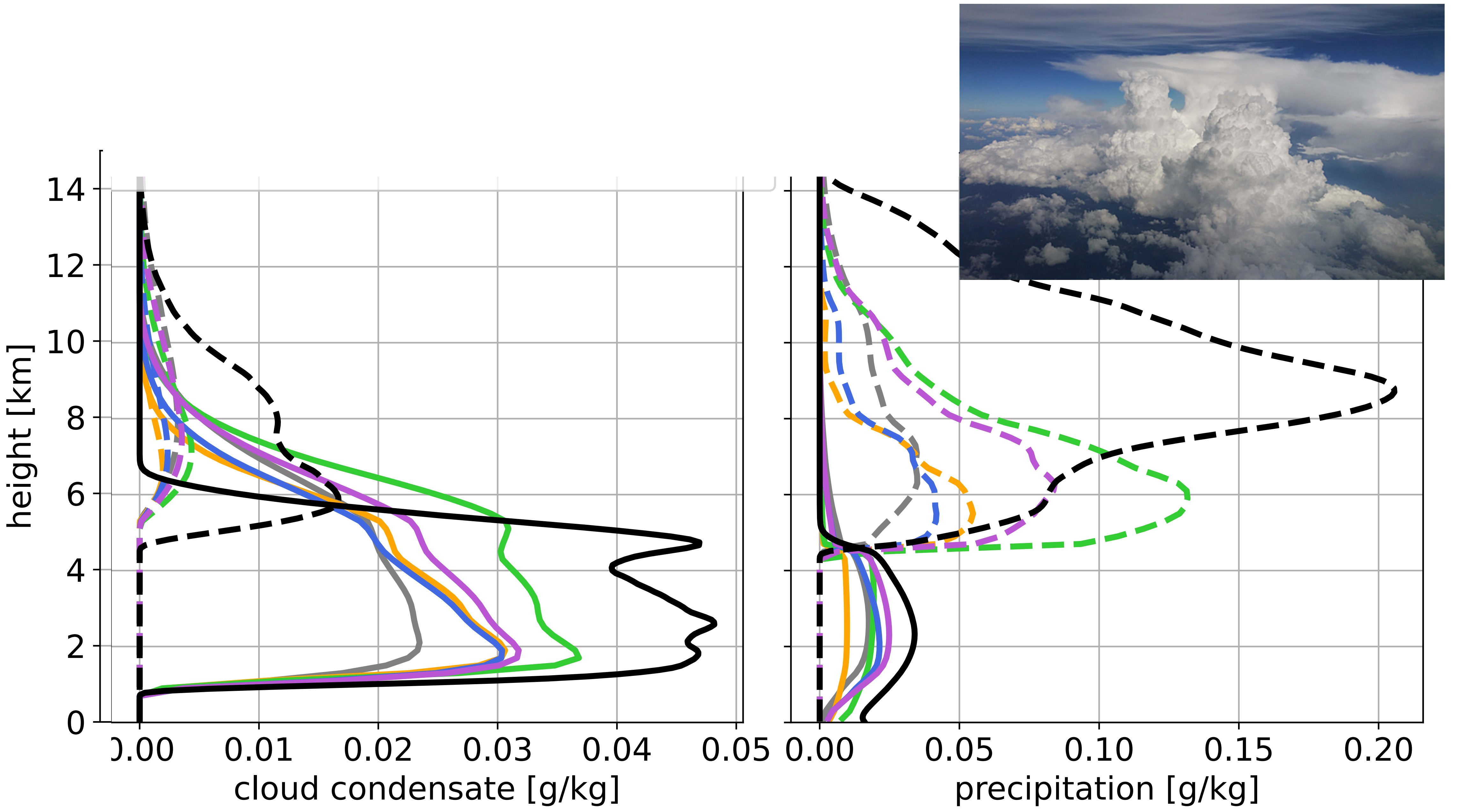
3D LES data (observations)

Calibrated SGS model

- ~20 free parameters from SGS scheme
- ~40 free parameters from the cloud microphysics scheme



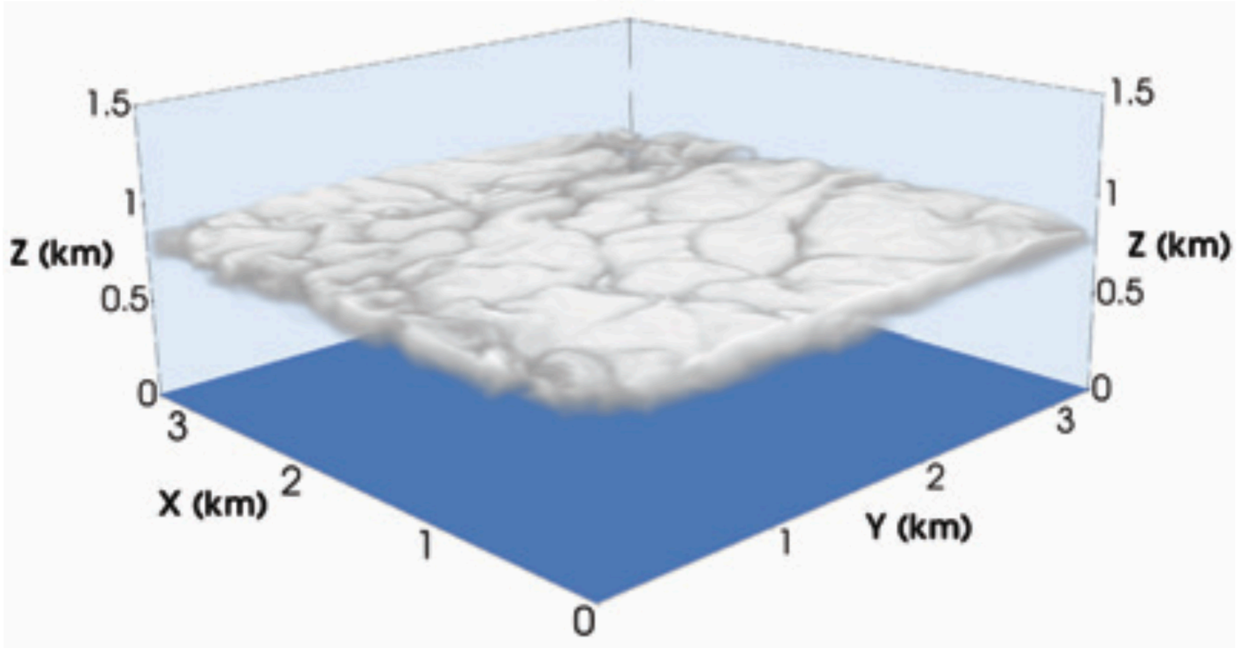




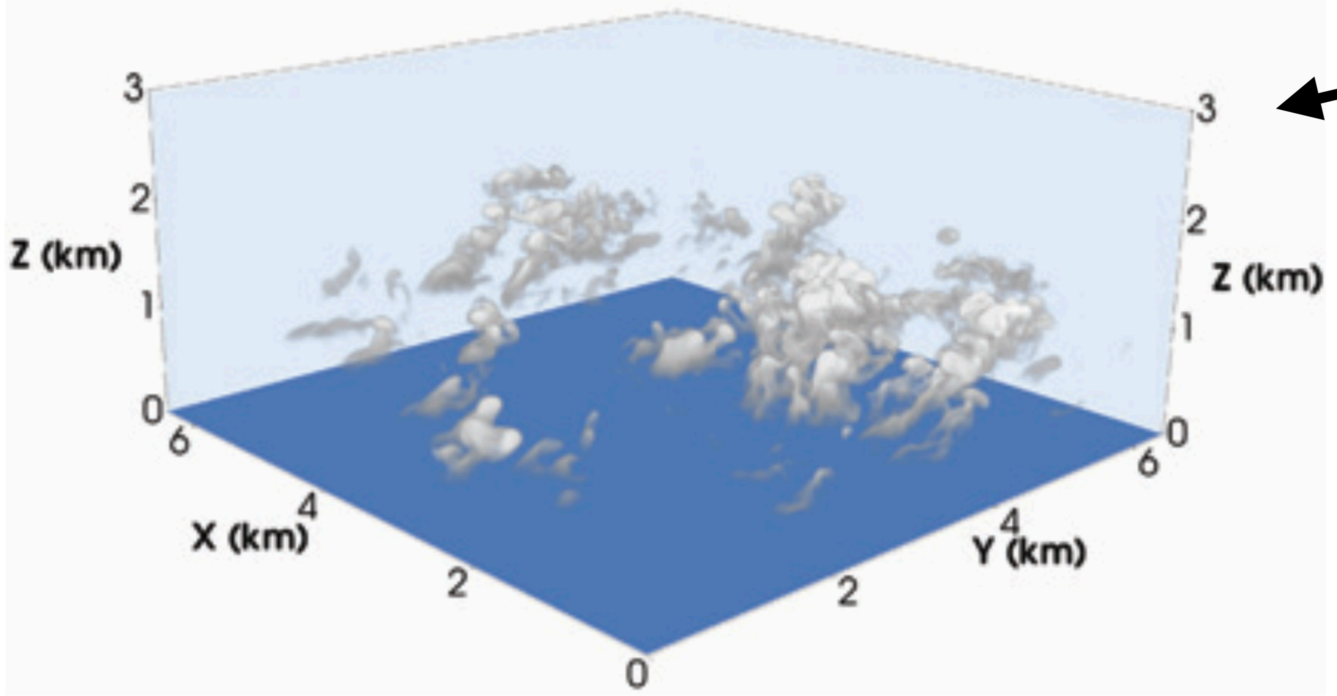
Jaruga et al. in prep.

Libraries of cases

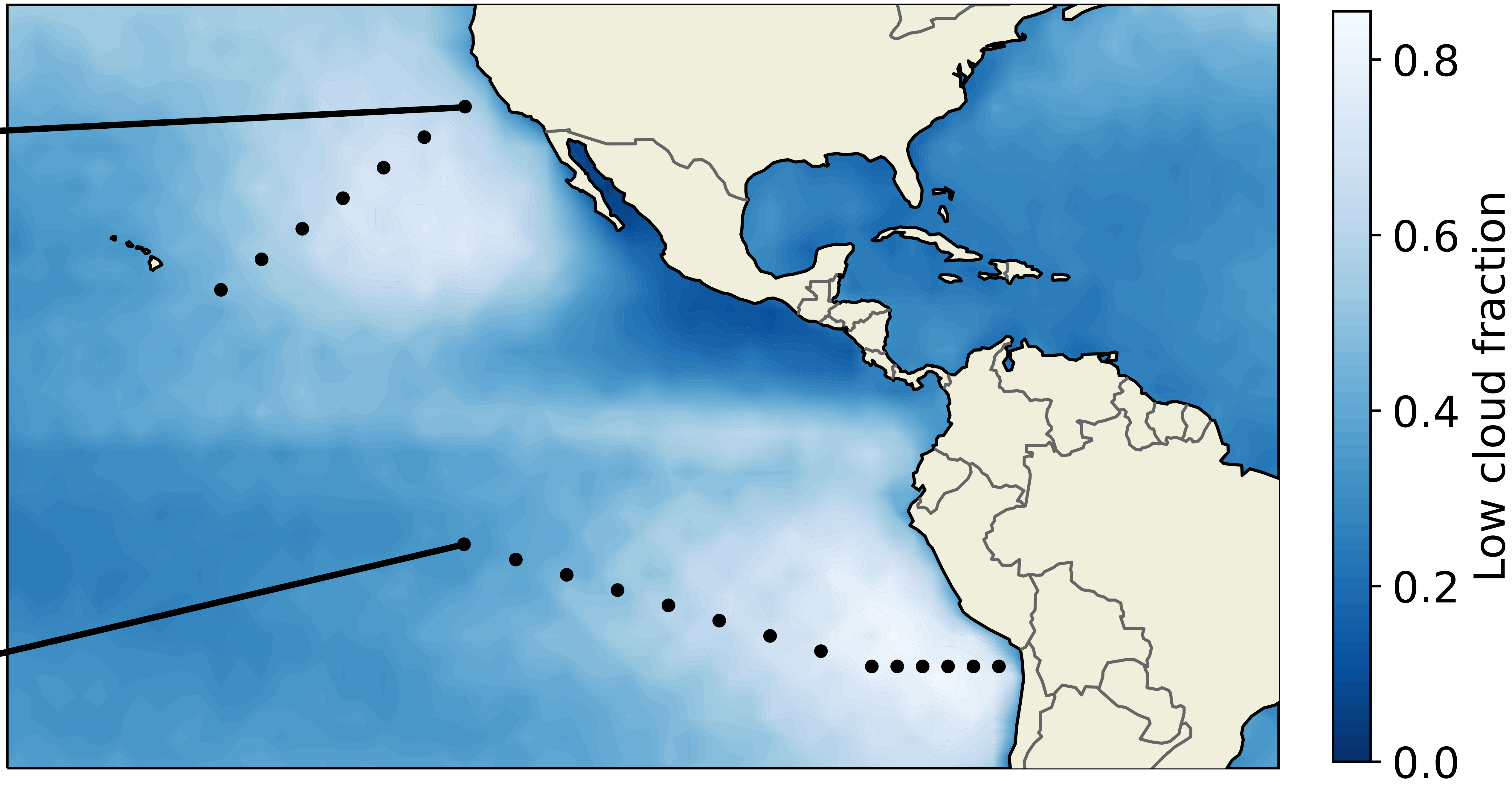
Stratocumulus



Shallow cumulus



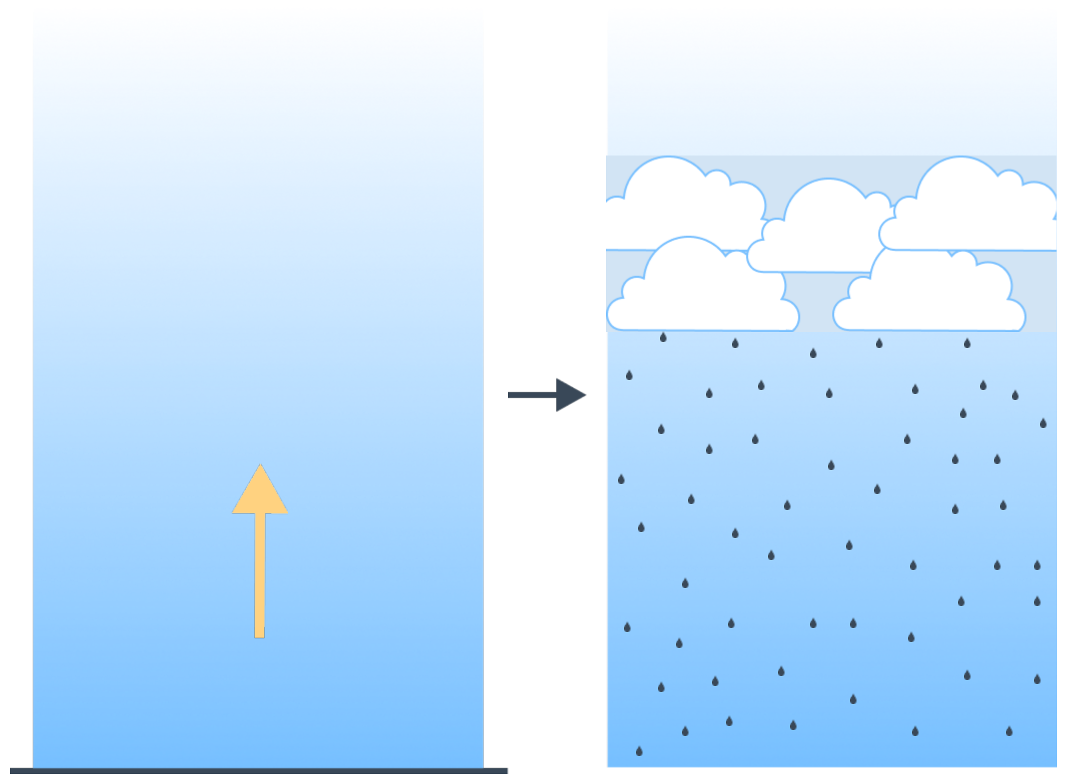
Synthetic data generation in different seasons and climates



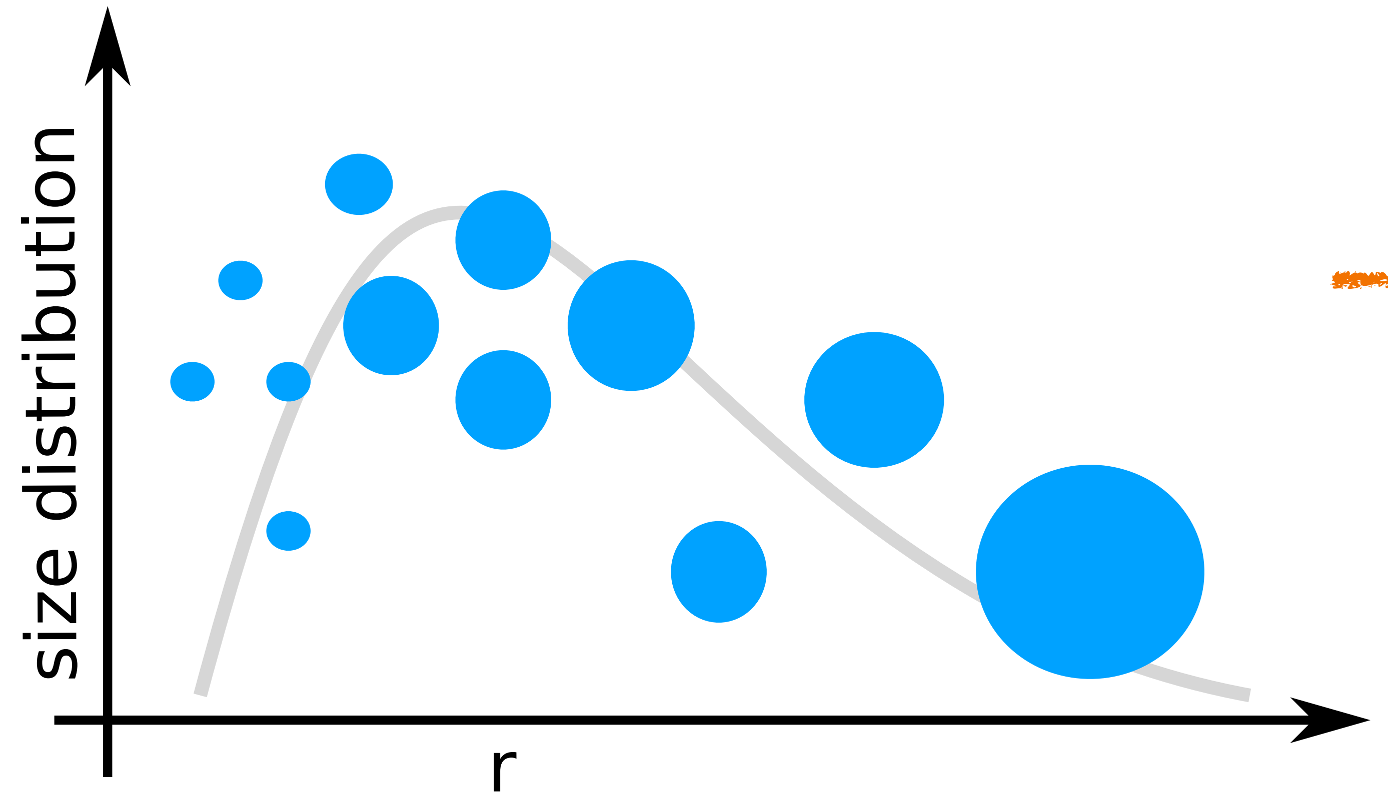
Shen et al. 2022: A Library of Large-Eddy Simulations Forced by Global Climate Models

Learning from data

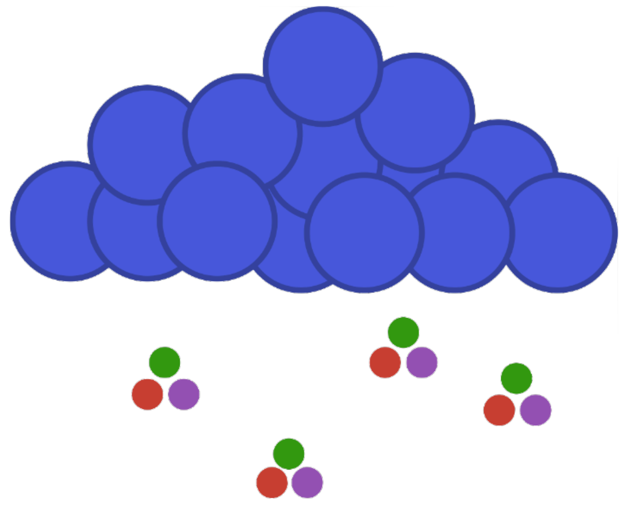
for cloud microphysics and aerosol models



Simple driver models (prescribed flow, single column)



High resolution simulations of particles dynamics (focus on PySDM and cloud microphysics)



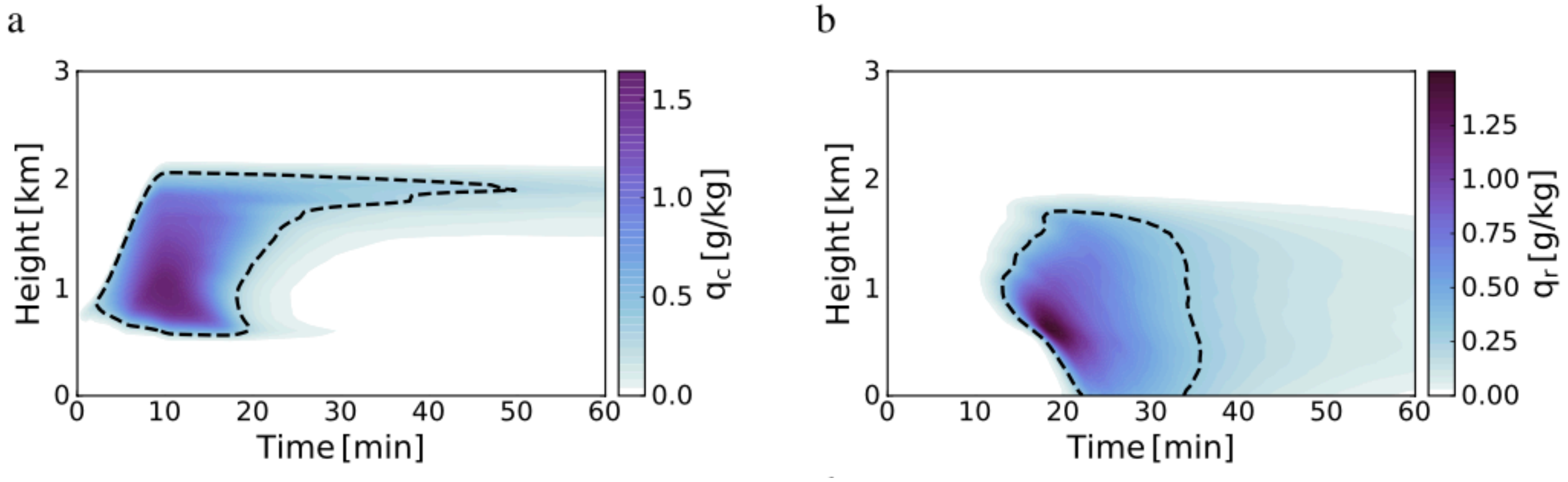
CloudMicrophysics.jl

Process-level learning
Uncertainty quantification

Bartman et al JOSS 2021: PySDM v1 particle-based cloud modeling package for warm-rain microphysics and aqueous chemistry
Shipway and Hill QJRMS 2012: Diagnosis of systematic differences between multiple parametrizations of warm rain microphysics using a kinematic framework

Learning from data

for cloud microphysics and aerosol models



A library of rainshaft superdroplet simulations with varying updraft speed, surface pressure and droplet concentration. (49 cases in total)

Calibration pipeline for bulk microphysics schemes against superdroplet simulations.

Azimi et al. 2023 (submitted):
Training warm-rain bulk microphysics schemes using super-droplet simulations

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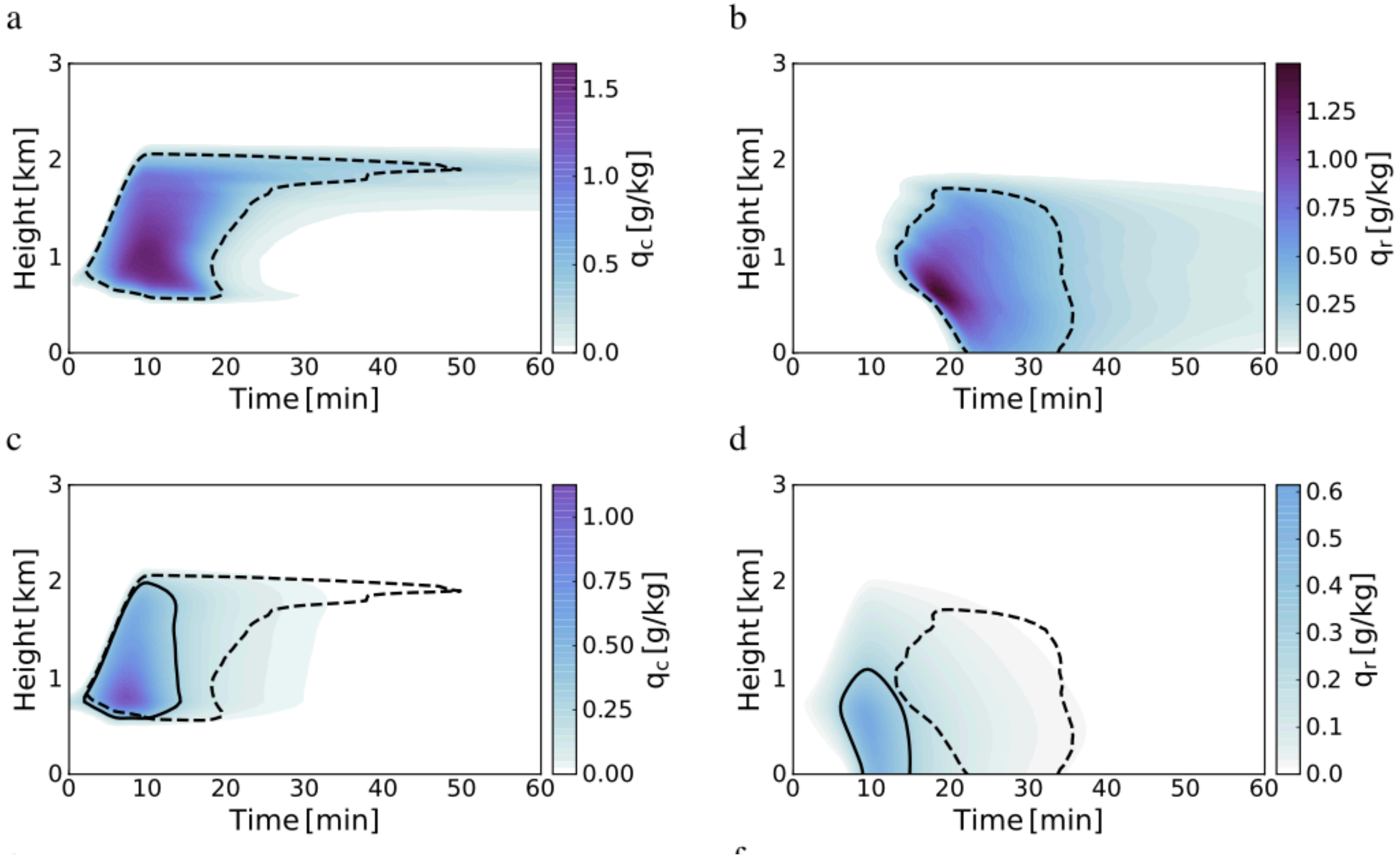
for cloud microphysics and aerosol models

A library of rainshaft superdroplet simulations with varying updraft speed, surface pressure and droplet concentration. (49 cases in total)

Calibration pipeline for bulk microphysics schemes against superdroplet simulations.



Azimi et al. 2023 (submitted):
Training warm-rain bulk microphysics schemes using super-droplet simulations

Learning from data

for cloud microphysics and aerosol models

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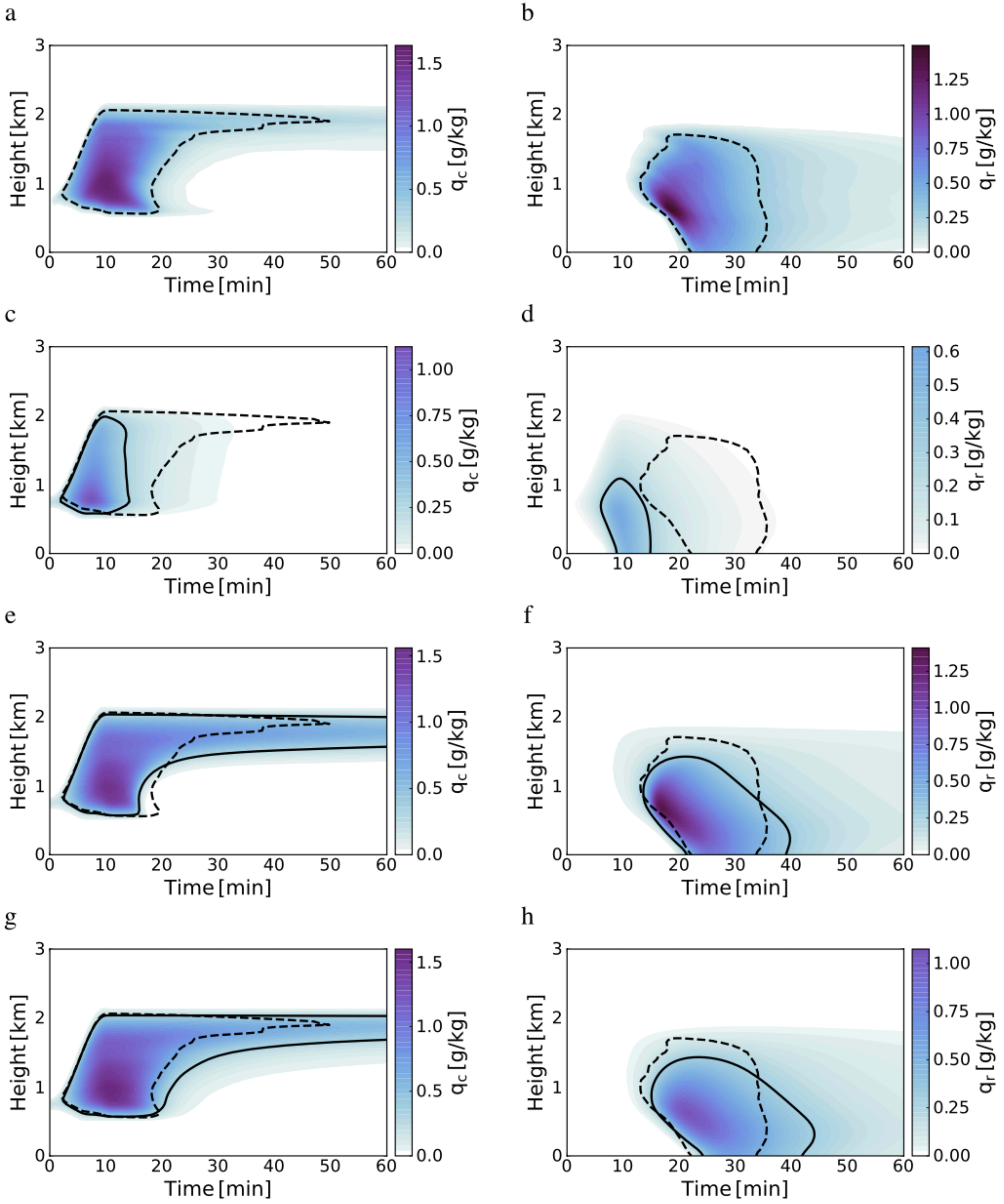

EKI

UKI

Azimi et al. 2023 (submitted):
Training warm-rain bulk microphysics schemes using super-droplet simulations

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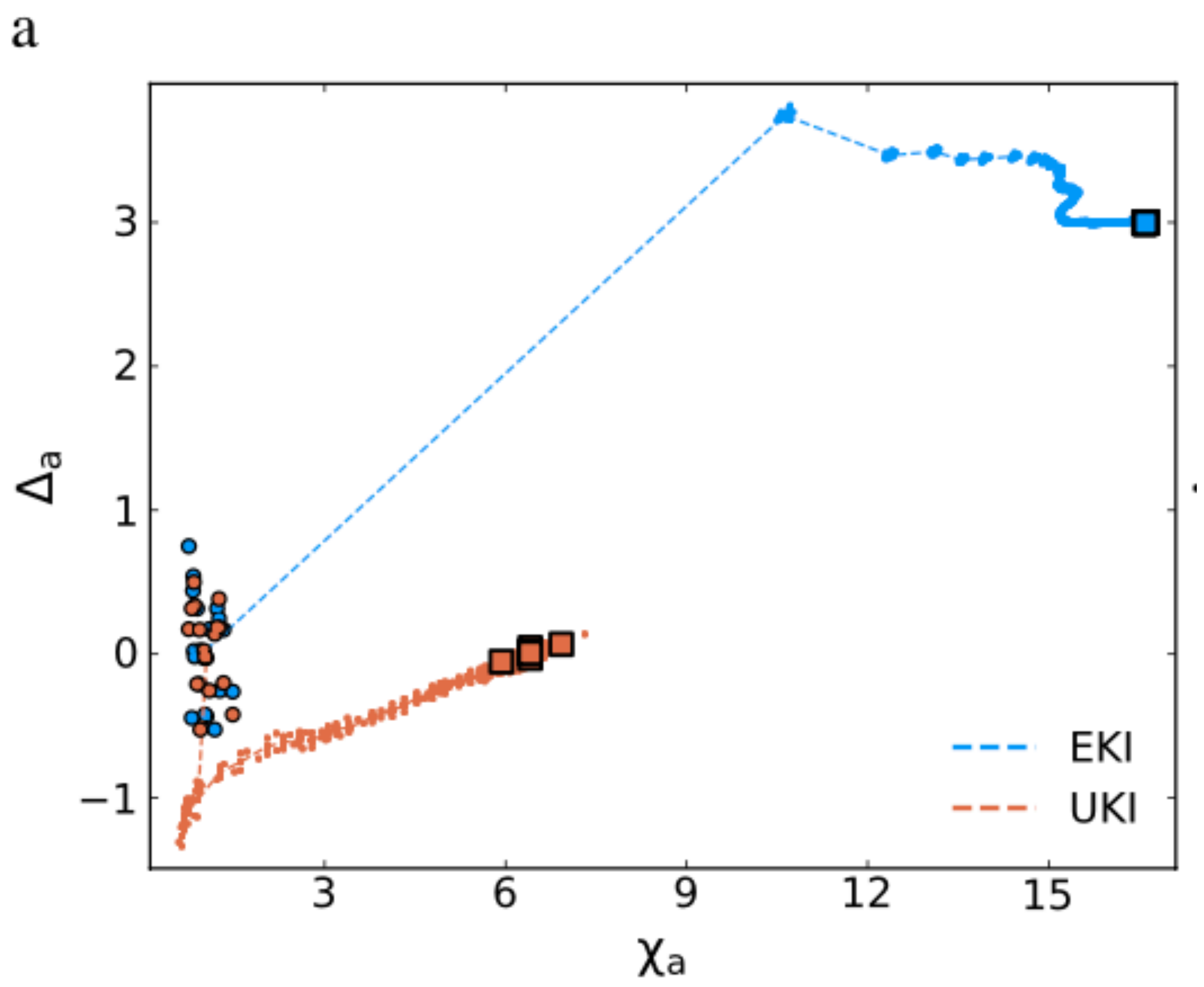
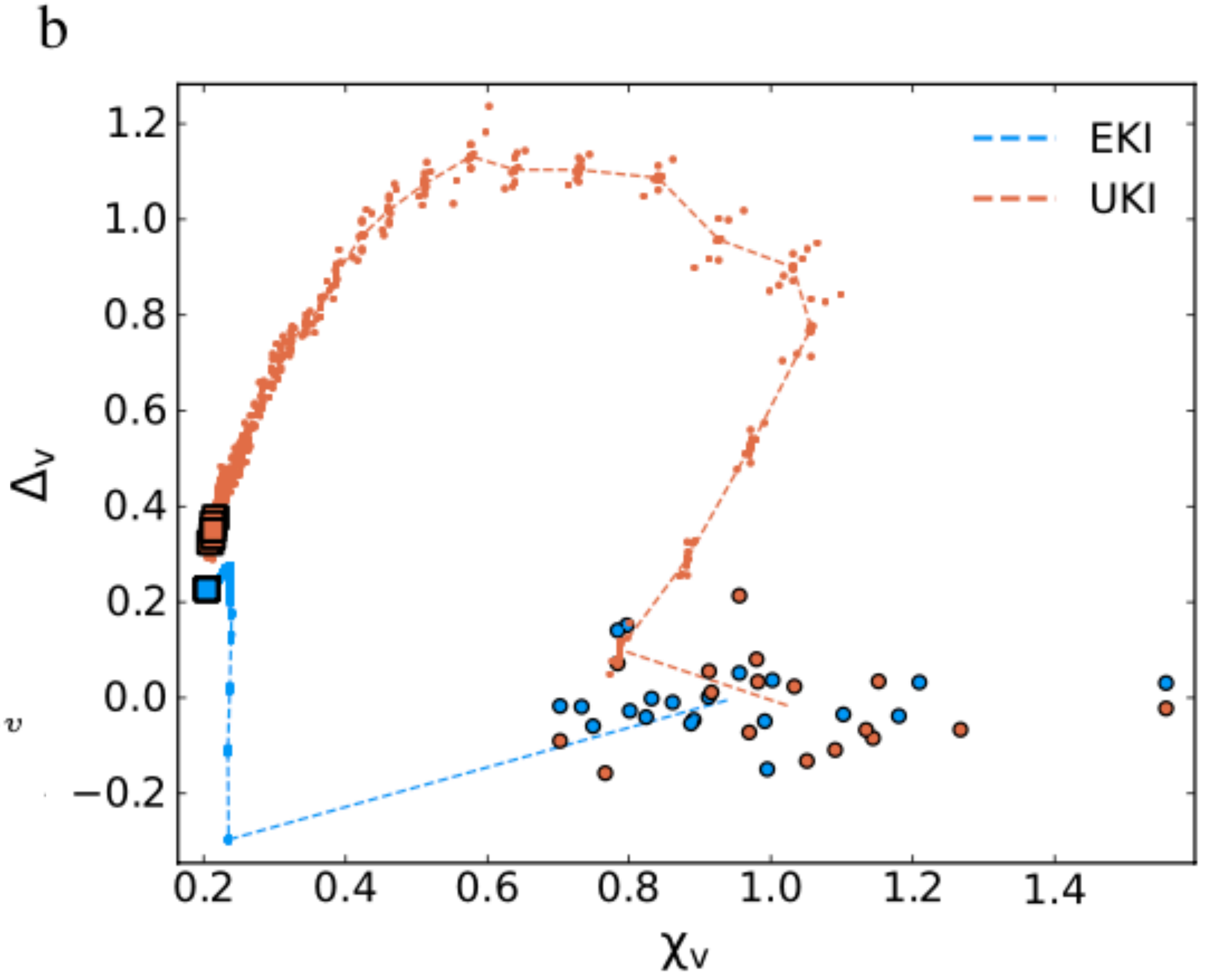
Parameter name	Description
τ_{cond}	Condensation time scale
$\tau_{acnv,0}$	Auto-conversion time scale
α_{acnv}	Auto-conversion coefficient
χ_v	Terminal velocity coefficient
Δ_v	Terminal velocity coefficient
χ_a	Accretion coefficient
Δ_a	Accretion coefficient
a_{vent}	Evaporation coefficient
b_{vent}	Evaporation coefficient
r_0	Reference raindrop radius
n_0	Size distribution parameter
C_d	Raindrop drag coefficient
E_{cr}	Collision efficiency

$$a(r) = \chi_a a_0 \left(\frac{r}{r_0}\right)^{2+\Delta_a}$$





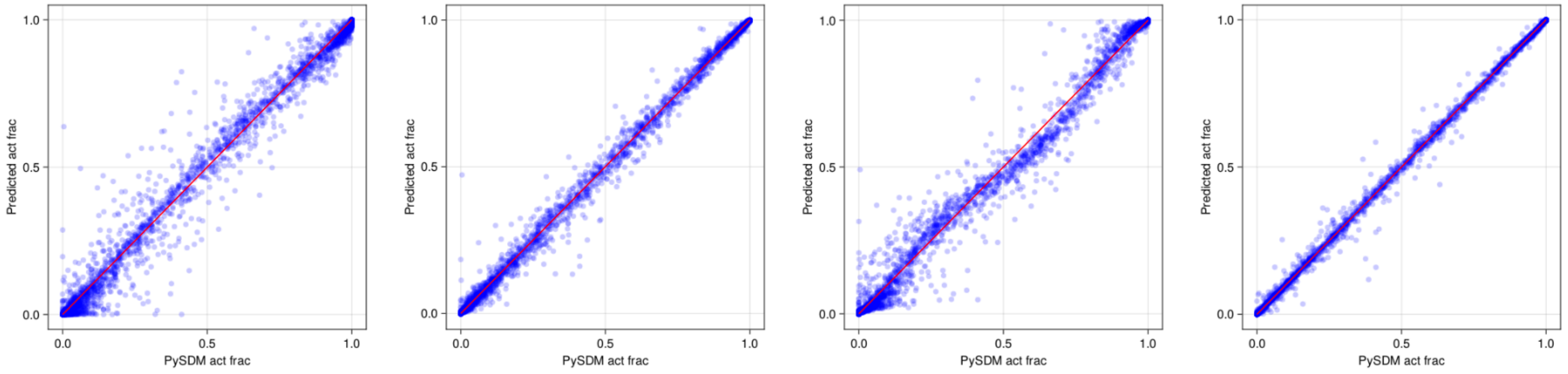
$$v(r) = \chi_v v_0 \left(\frac{r}{r_0}\right)^{1/2+\Delta_v}$$

Azimi et al. 2023 (submitted):
Training warm-rain bulk microphysics schemes using super-droplet simulations

Learning from data

for cloud microphysics and aerosol models
-> Example summer internship project

Training in 0-dimensional parcel model, 1-mode aerosol distribution



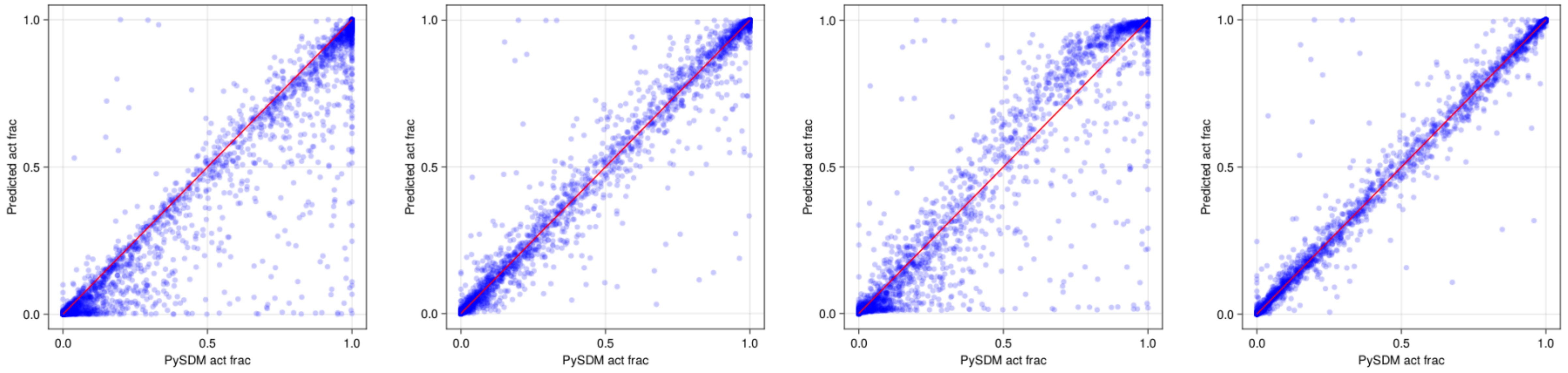
(a) Re-calibrated ARG scheme

(b) ARG-informed EvoTree model

(c) ARG-informed GP model

(d) Naive DNN model

Training in 0-dimensional parcel model, 2-mode aerosol distribution



(a) Re-calibrated ARG scheme

(b) ARG-informed EvoTree model

(c) ARG-informed GP model

(d) Naive DNN model

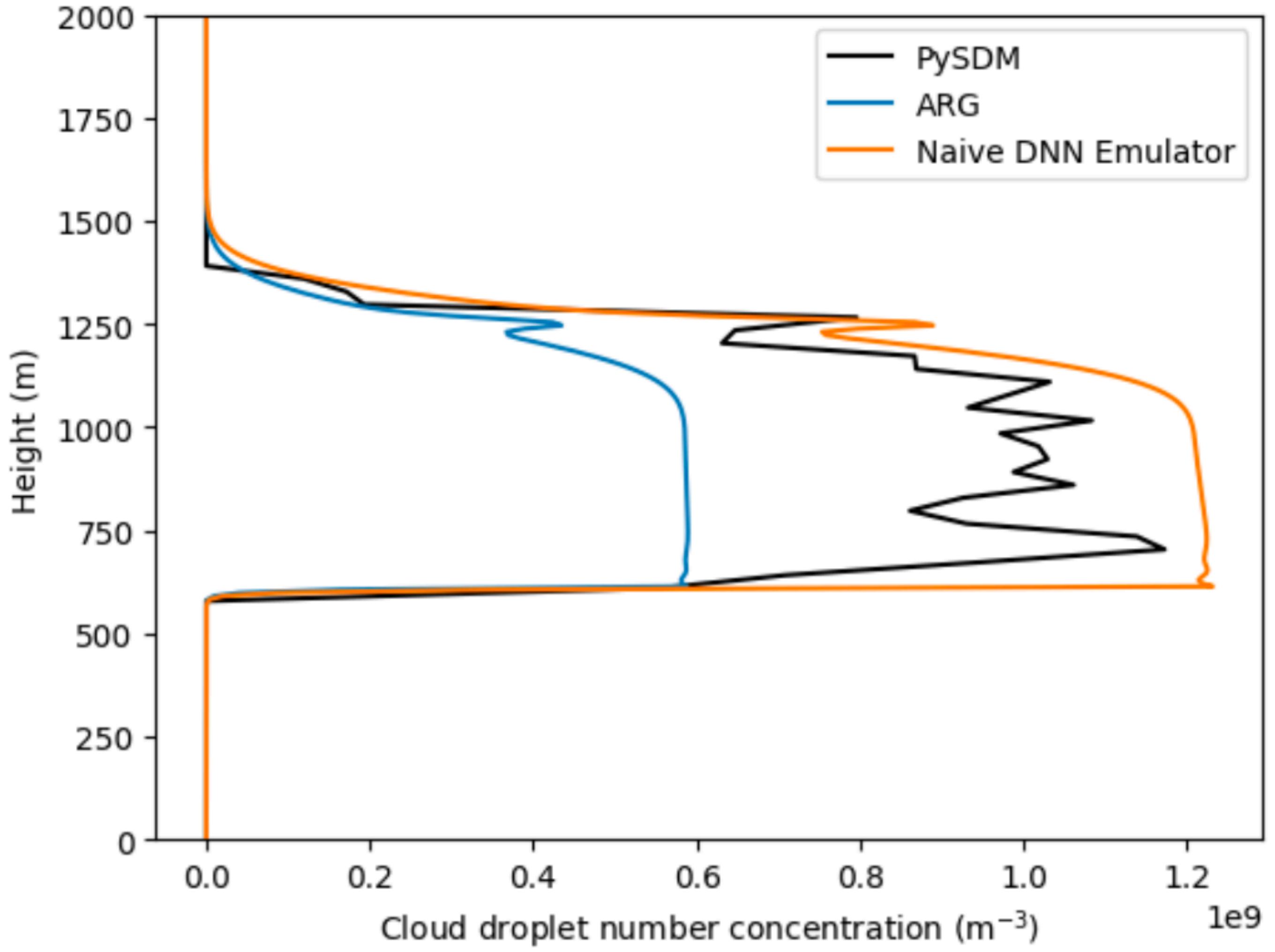
Abdul-Razzak and Ghan 2000 aerosol activation

$$S_{max} = \left\{ \sum_{i=1}^{I} \left[f_i \left(\frac{\zeta}{\eta_i} \right)^{3/2} + g_i \left(\frac{S_{mi}^2}{\eta_i + 3\zeta} \right)^{3/4} \right] \right\}^{-1/2}$$

$$f_i = 0.5 \exp(2.5 \ln^2 \sigma_i)$$

$$g_i = 1 + 0.25 \ln \sigma_i$$

Testing in 1-dimensional rain shaft model



Mikhail Mints 2023

Summary

GCM: $$\frac{\partial\langle\phi\rangle}{\partial t}+\nabla_h\left(\langle\phi\rangle\langle\boldsymbol{u}\rangle\right)=-\frac{\partial}{\partial z}\left(\langle w\rangle\langle\phi\rangle\right)-\frac{\partial}{\partial z}\boxed{\langle w^{*}\phi^{*}\rangle}+\boxed{\langle S_{\phi}\rangle}$$

“dynamical core”

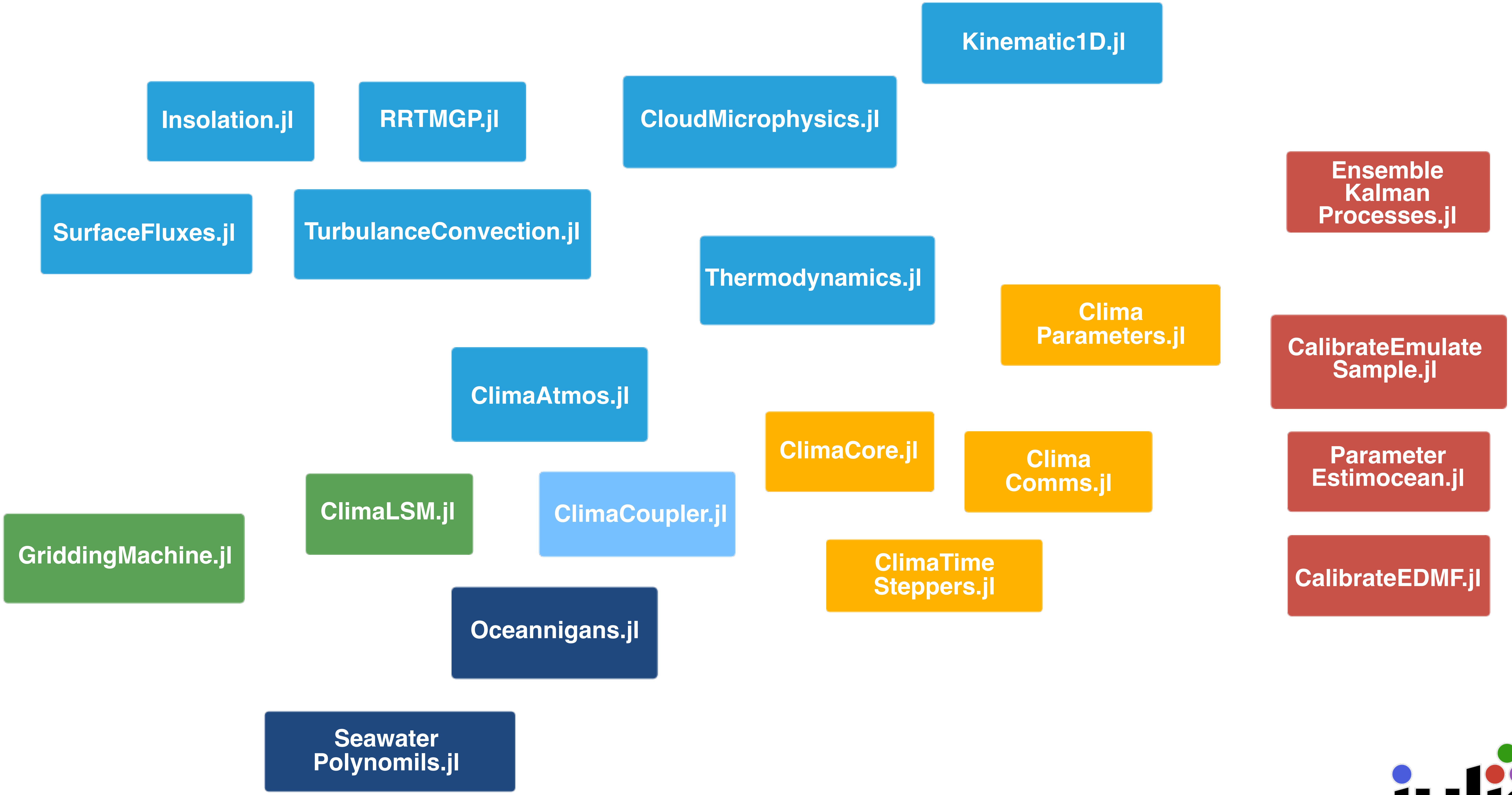
$$\frac{\partial(\rho a_i\overline{\phi}_i)}{\partial t}+\frac{\partial(\rho a_i\overline{w}_i\overline{\phi}_i)}{\partial z}+\nabla_h\cdot\left(\rho a_i\langle\mathbf{u}_h\rangle\overline{\phi}_i\right)=\boxed{\underbrace{-\frac{\partial(\rho a_i\overline{w_i'\phi_i'})}{\partial z}}_{\text{Turbulent transport}}}+\boxed{\underbrace{\rho a_i\overline{w}_i\left(\sum_j\epsilon_{ij}\overline{\phi}_j-\delta_i\overline{\phi}_i\right)}_{\text{Entrainment/detrainment}}}+\boxed{\underbrace{\rho a_i\overline{S}_{\phi,i}}_{\text{Sources/sinks}}}$$

“physics” parameterizations, data driven calibrations

Outline

- Physics based parameterizations
- Data driven calibrations
- **Software design**

Building blocks of CliMA ESM



Kinematic1D.jl

Insolation.jl

RRTMGP.jl

CloudMicrophysics.jl

Ensemble Kalman Processes.jl

SurfaceFluxes.jl

TurbulanceConvection.jl

Thermodynamics.jl

Clima Parameters.jl

CalibrateEmulate Sample.jl

ClimaAtmos.jl

ClimaCore.jl

Clima Comms.jl

Parameter Estimocean.jl

ClimaLSM.jl

ClimaCoupler.jl

GriddingMachine.jl

ClimaTime Steppers.jl

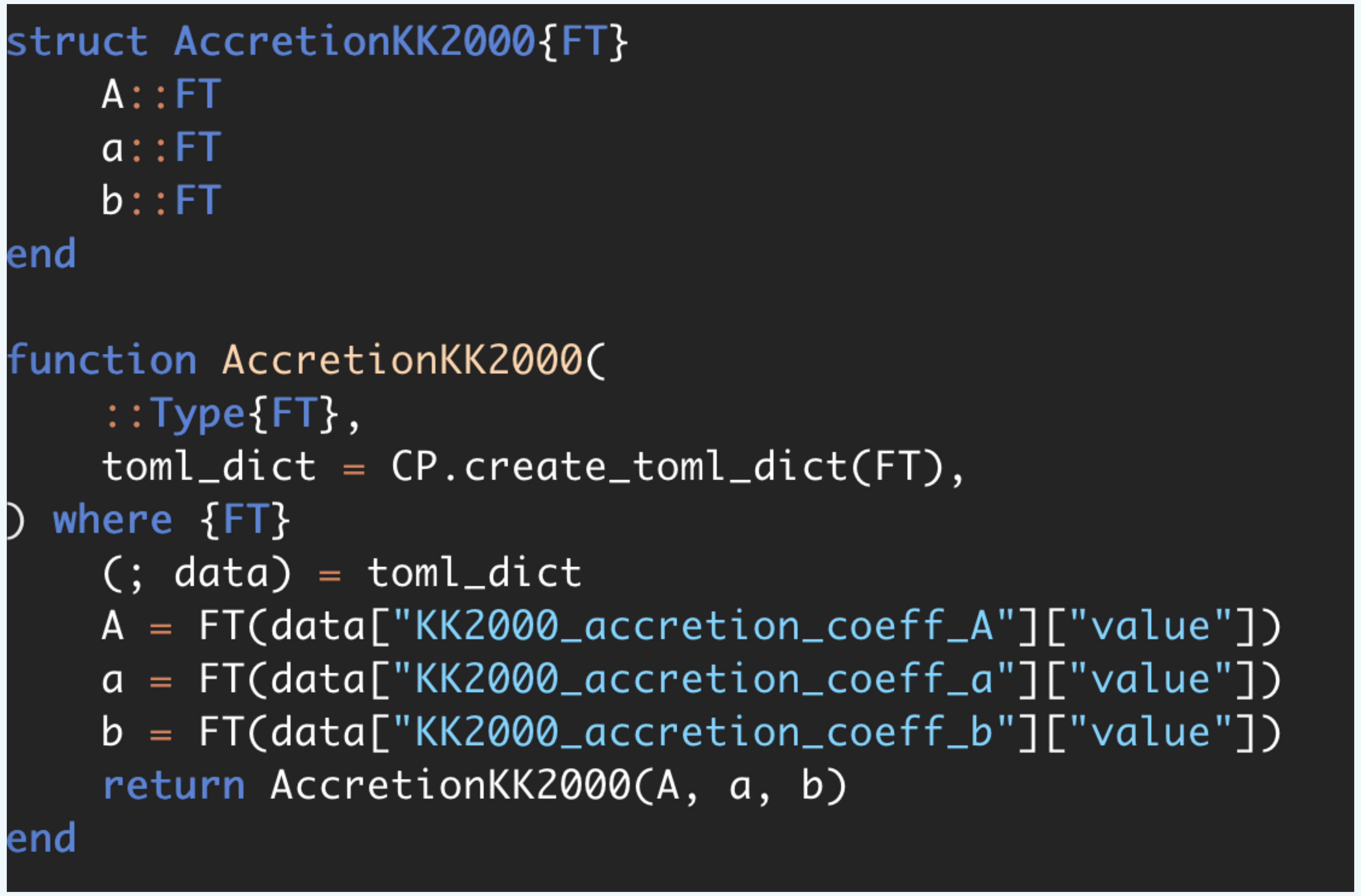
CalibrateEDMF.jl

Oceannigans.jl

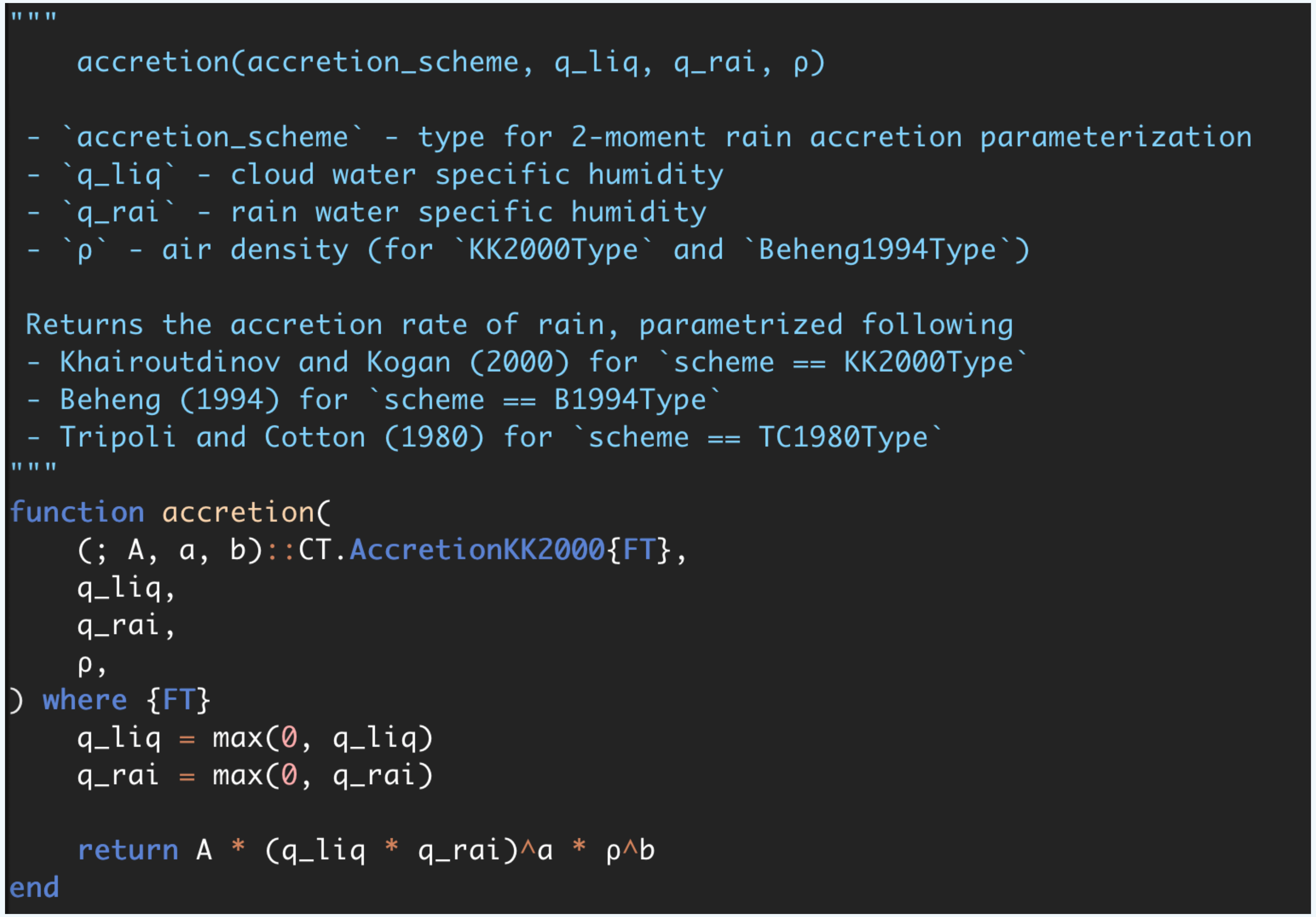
Seawater Polynomils.jl

github.com/CliMA

Workflow highlights: design for ML applications



```
struct AccretionKK2000{FT}
    A::FT
    a::FT
    b::FT
end

function AccretionKK2000(
    ::Type{FT},
    toml_dict = CP.create_toml_dict(FT),
) where {FT}
    (; data) = toml_dict
    A = FT(data["KK2000_accretion_coeff_A"]["value"])
    a = FT(data["KK2000_accretion_coeff_a"]["value"])
    b = FT(data["KK2000_accretion_coeff_b"]["value"])
    return AccretionKK2000(A, a, b)
end
```

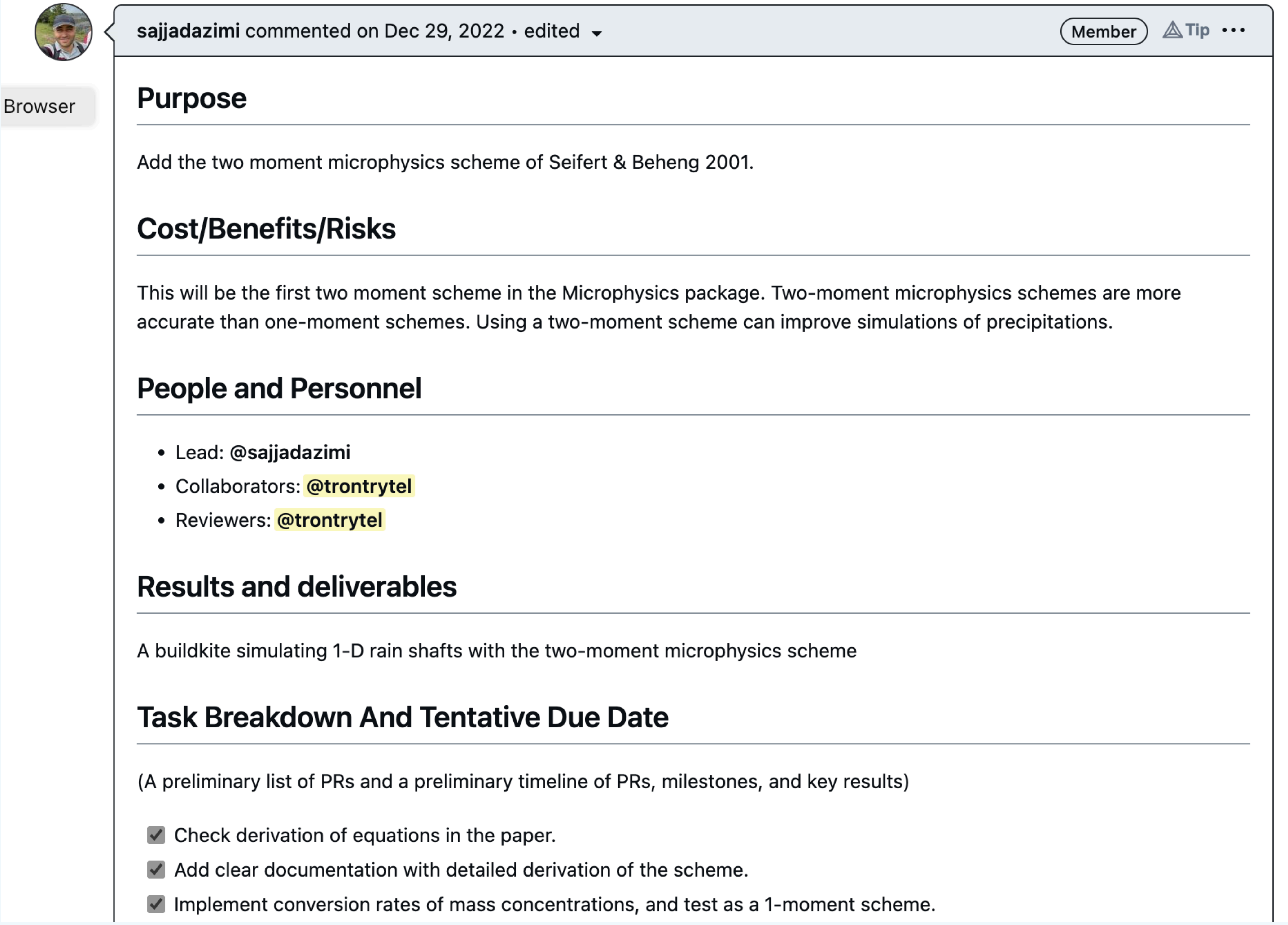


```
"""
    accretion(accretion_scheme, q_liq, q_rai, ρ)

 - `accretion_scheme` - type for 2-moment rain accretion parameterization
 - `q_liq` - cloud water specific humidity
 - `q_rai` - rain water specific humidity
 - `ρ` - air density (for `KK2000Type` and `Beheng1994Type`)

 Returns the accretion rate of rain, parametrized following
 - Khairoutdinov and Kogan (2000) for `scheme == KK2000Type`
 - Beheng (1994) for `scheme == B1994Type`
 - Tripoli and Cotton (1980) for `scheme == TC1980Type`
"""
function accretion(
    (; A, a, b)::CT.AccretionKK2000{FT},
    q_liq,
    q_rai,
    ρ,
) where {FT}
    q_liq = max(0, q_liq)
    q_rai = max(0, q_rai)

    return A * (q_liq * q_rai)^a * ρ^b
end
```

Free parameters are stored separately in text files (interface with ML calibration pipelines)

They are passed in as arguments to all functions

Workflow highlights: design planning



sajjadazimi commented on Dec 29, 2022 • edited

Purpose

Add the two moment microphysics scheme of Seifert & Beheng 2001.

Cost/Benefits/Risks

This will be the first two moment scheme in the Microphysics package. Two-moment microphysics schemes are more accurate than one-moment schemes. Using a two-moment scheme can improve simulations of precipitations.

People and Personnel

- Lead: **@sajjadazimi**
- Collaborators: **@trontrytel**
- Reviewers: **@trontrytel**

Results and deliverables

A buildkite simulating 1-D rain shafts with the two-moment microphysics scheme

Task Breakdown And Tentative Due Date

(A preliminary list of PRs and a preliminary timeline of PRs, milestones, and key results)

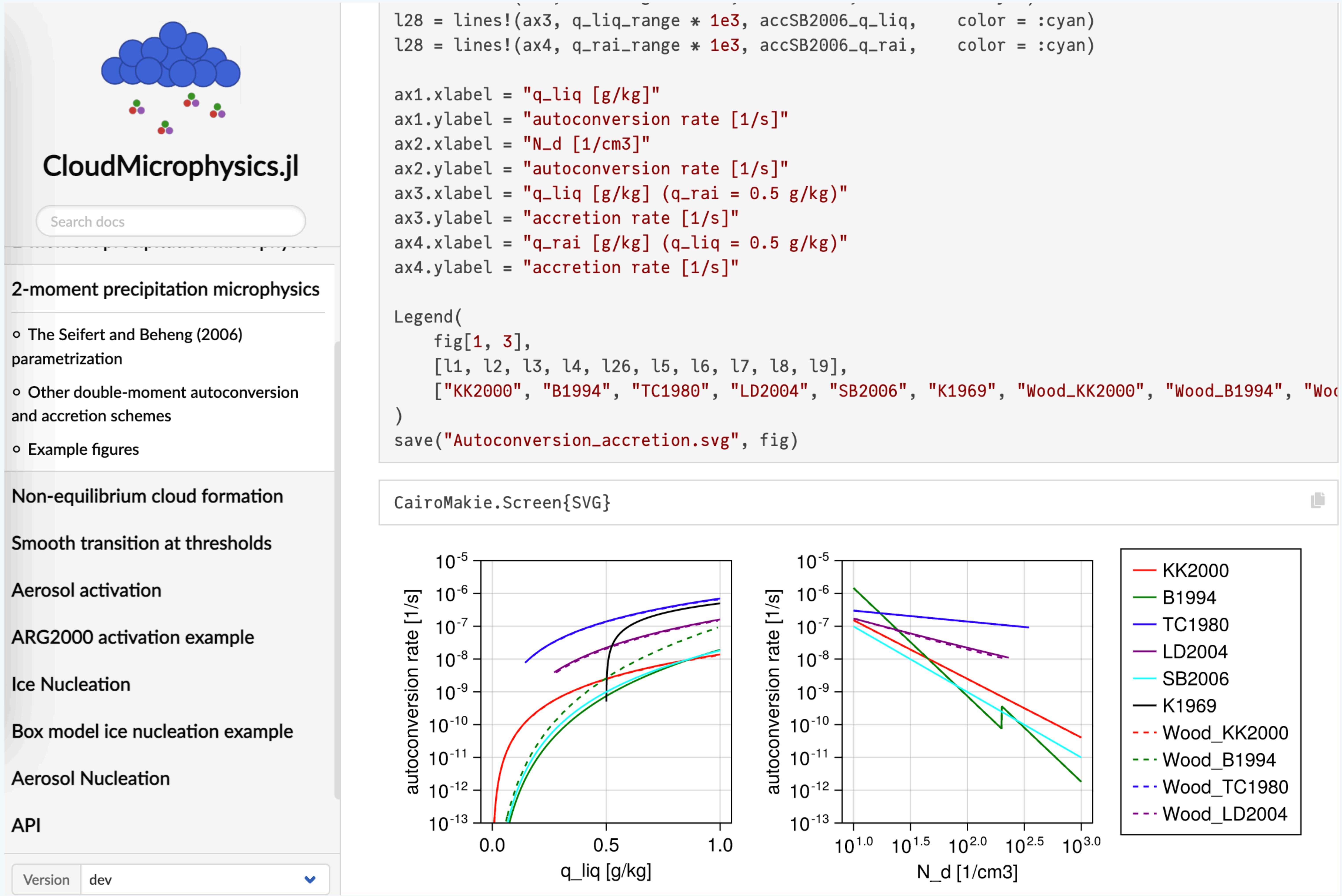
- ☑ Check derivation of equations in the paper.
- ☑ Add clear documentation with detailed derivation of the scheme.
- ☑ Implement conversion rates of mass concentrations, and test as a 1-moment scheme.

Discuss the design and objectives before starting

Get feedback from software engineers and scientists

Define intermediate steps

Workflow highlights: documentation



CloudMicrophysics.jl

Search docs

2-moment precipitation microphysics

- The Seifert and Beheng (2006) parametrization
- Other double-moment autoconversion and accretion schemes
- Example figures

Non-equilibrium cloud formation

Smooth transition at thresholds

Aerosol activation

ARG2000 activation example

Ice Nucleation

Box model ice nucleation example

Aerosol Nucleation

API

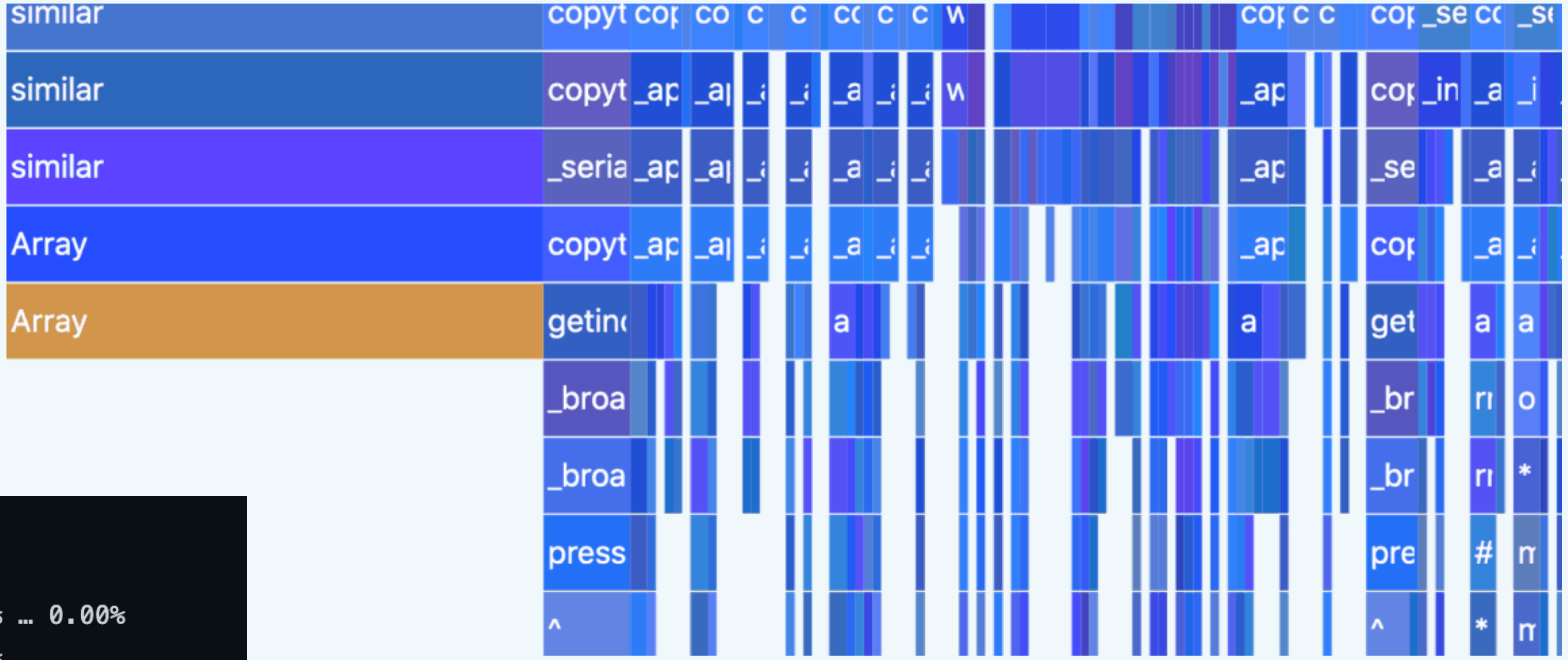
Version dev

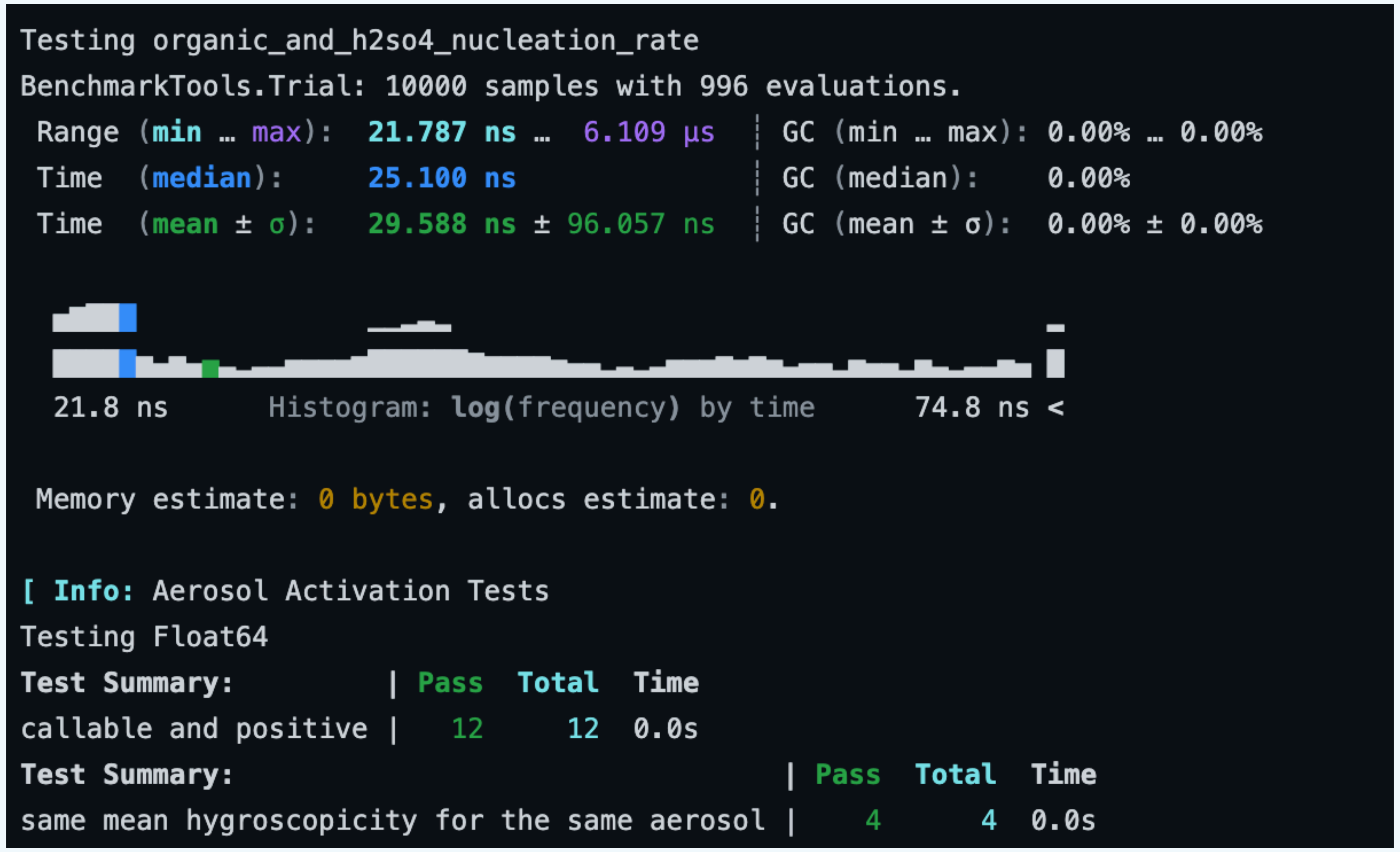
```
l28 = lines!(ax3, q_liq_range * 1e3, accSB2006_q_liq,    color = :cyan)
l28 = lines!(ax4, q_rai_range * 1e3, accSB2006_q_rai,    color = :cyan)

ax1.xlabel = "q_liq [g/kg]"
ax1.ylabel = "autoconversion rate [1/s]"
ax2.xlabel = "N_d [1/cm3]"
ax2.ylabel = "autoconversion rate [1/s]"
ax3.xlabel = "q_liq [g/kg] (q_rai = 0.5 g/kg)"
ax3.ylabel = "accretion rate [1/s]"
ax4.xlabel = "q_rai [g/kg] (q_liq = 0.5 g/kg)"
ax4.ylabel = "accretion rate [1/s]"

Legend(
    fig[1, 3],
    [l1, l2, l3, l4, l26, l5, l6, l7, l8, l9],
    ["KK2000", "B1994", "TC1980", "LD2004", "SB2006", "K1969", "Wood_KK2000", "Wood_B1994", "Woo
)
save("Autoconversion_accretion.svg", fig)
```

```
CairoMakie.Screen{SVG}
```

Workflow highlights: testing, performance monitoring

ClimaCore performance CI





```
Testing organic_and_h2so4_nucleation_rate
BenchmarkTools.Trial: 10000 samples with 996 evaluations.
 Range (min … max):  21.787 ns …  6.109 μs  ┊ GC (min … max): 0.00% … 0.00%
 Time  (median):     25.100 ns              ┊ GC (median):    0.00%
 Time  (mean ± σ):   29.588 ns ± 96.057 ns  ┊ GC (mean ± σ):  0.00% ± 0.00%

  21.8 ns       Histogram: log(frequency) by time       74.8 ns <

 Memory estimate: 0 bytes, allocs estimate: 0.

[ Info: Aerosol Activation Tests
Testing Float64
Test Summary:          | Pass  Total  Time
callable and positive |   12     12  0.0s
Test Summary:                             | Pass  Total  Time
same mean hygroscopicity for the same aerosol |    4      4  0.0s
```

CloudMicrophysics performance CI

Instead of a summary:

- Climate modelling has followed ***mirror view*** approach:
    - Deducing representation from detailed first-principles
    - Adding more detail leads to representing system better
    - Complexity and uncertainty of the system can be tackled with physics
- Other approaches could be:
    - ***heuristic*** (prioritise generating understanding)
    - ***predictive*** (prioritise predictive capabilities).
- Complexity needs to be tailored to model's purpose.

Ulrike Proske et. al. 2023: https://doi. org/10.1029/2022MS003571
Addressing complexity in global aerosol climate model cloud microphysics.

Instead of a summary:

- Hindered understanding - model as a book-keeper of added processes
- Generative entrenchment
- Parameters
- Over-interpretation vs negligence
- No reduction in uncertainty
- Opacity, authority
- Transparency about other factors influencing model choices

Ulrike Proske et. al. 2023: https://doi. org/10.1029/2022MS003571
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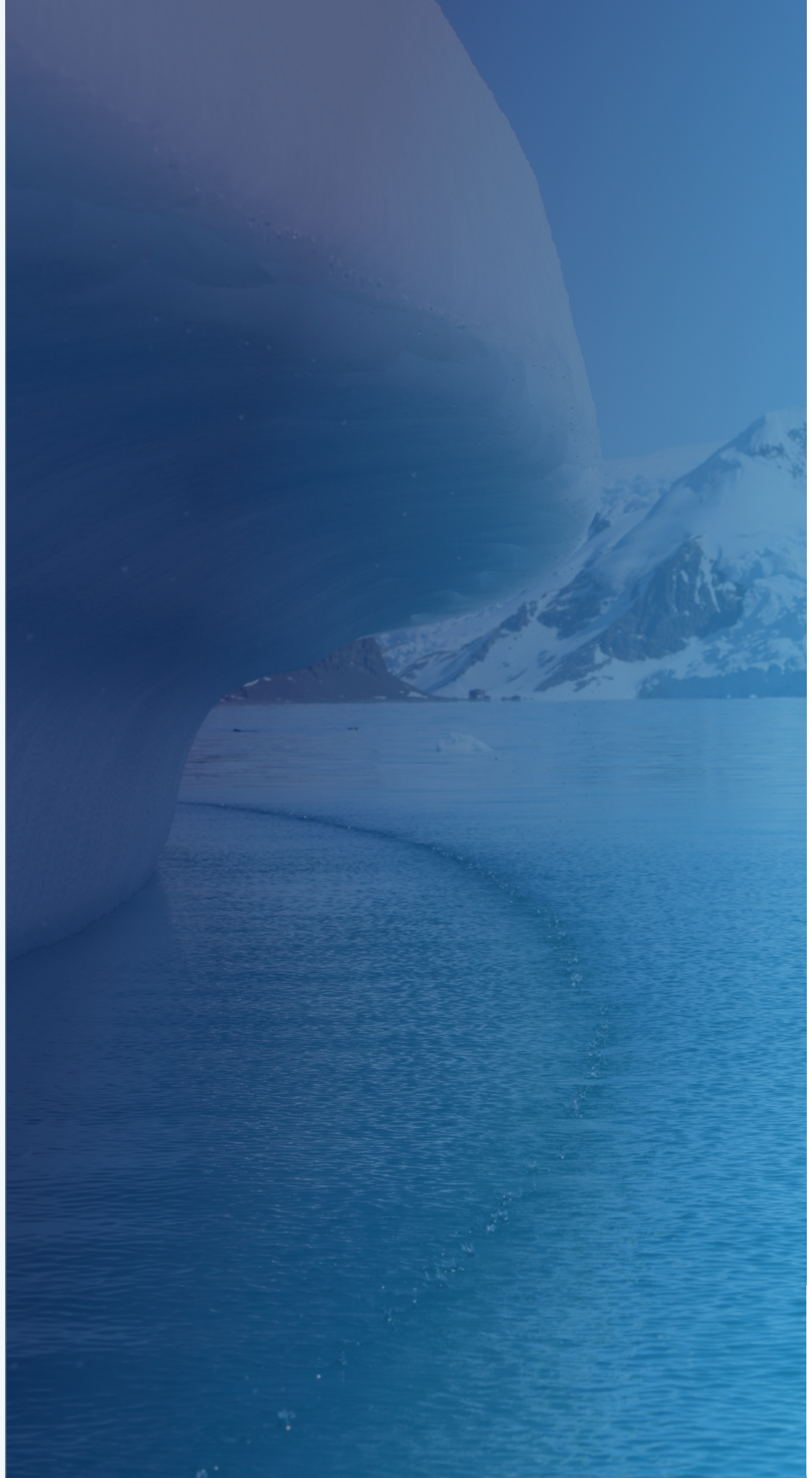

Thank you for your attention!

ajaruga@caltech.edu

github.com/CliMA

clima.caltech.edu

We are funded by a consortium of private foundations and federal agencies, led by the generosity of Eric and Wendy Schmidt by recommendation of the Schmidt Futures program, and the National Science Foundation.