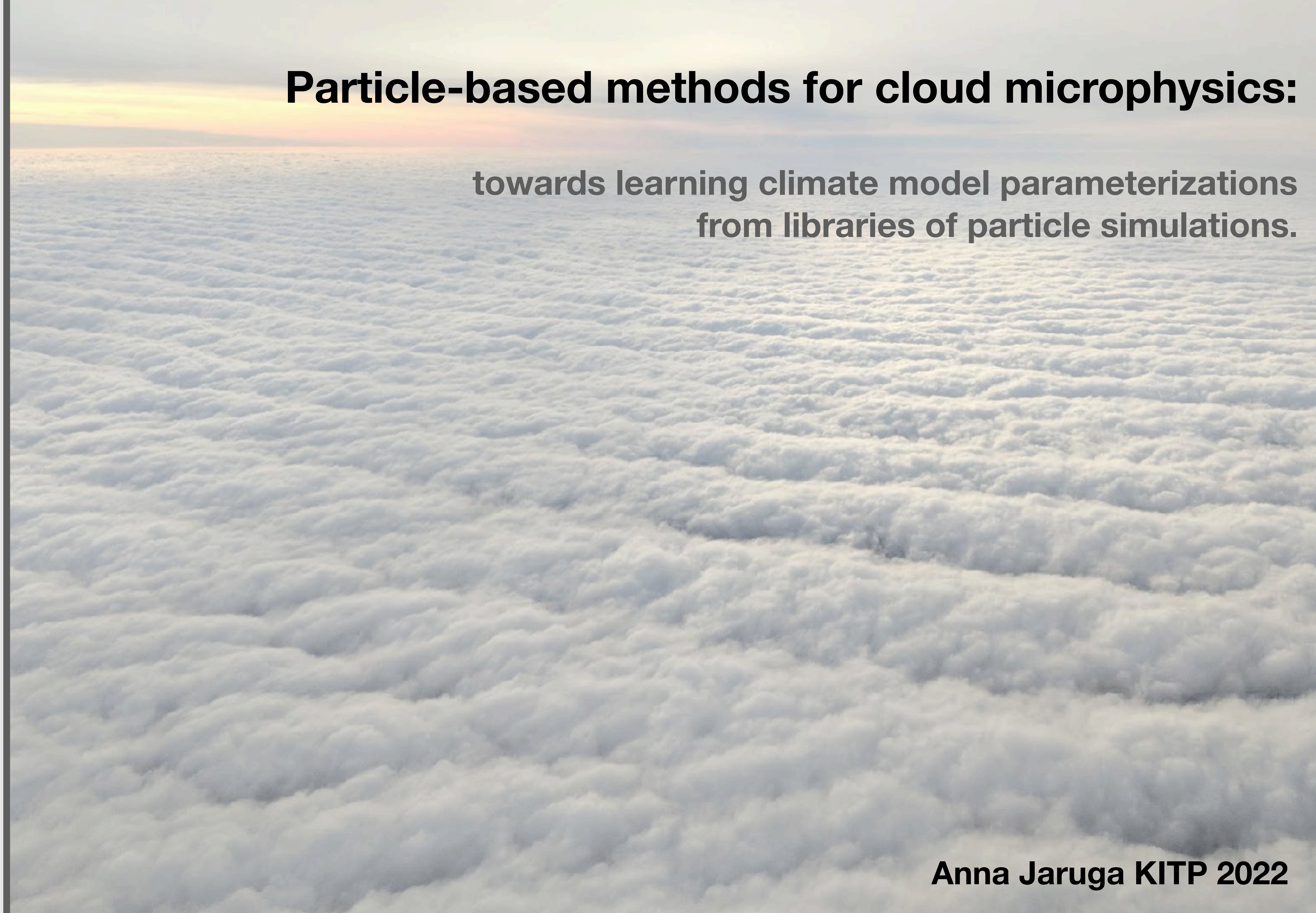


Particle-based methods for cloud microphysics:

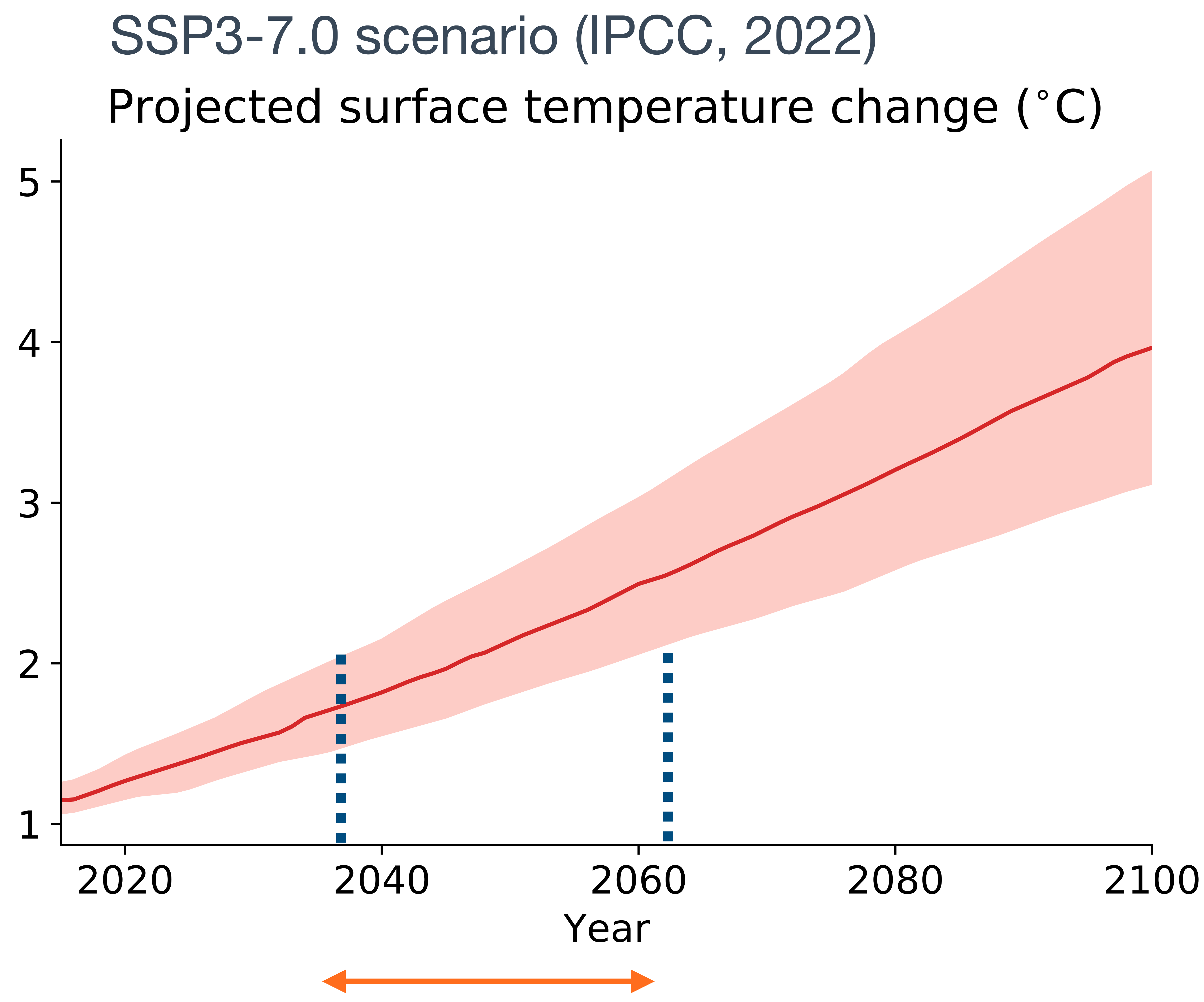
towards learning climate model parameterizations from libraries of particle simulations.

Anna Jaruga KITP 2022

Caltech

CliMA
CLIMATE MODELING ALLIANCE

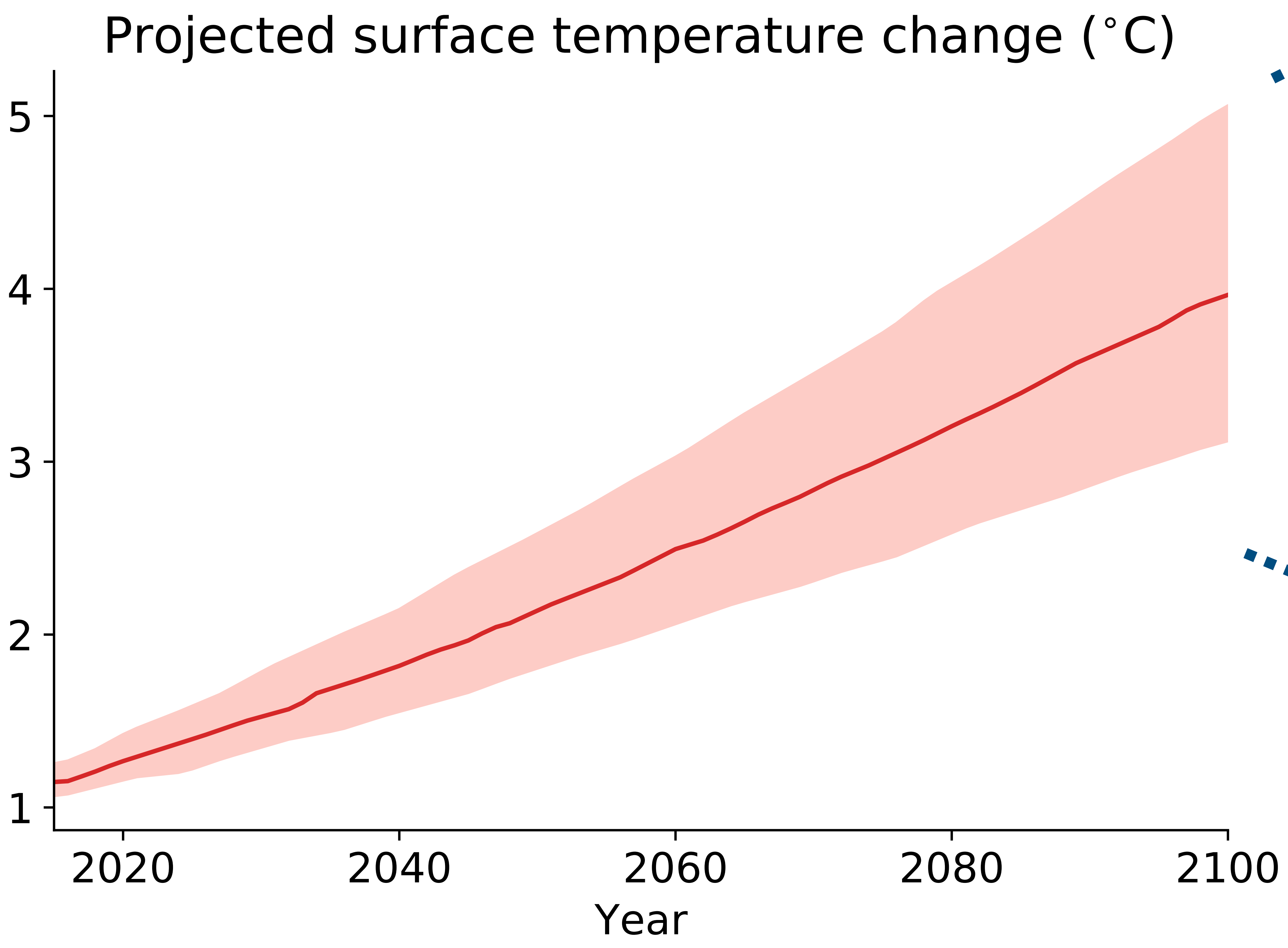
Clouds dominate uncertainties in climate projections

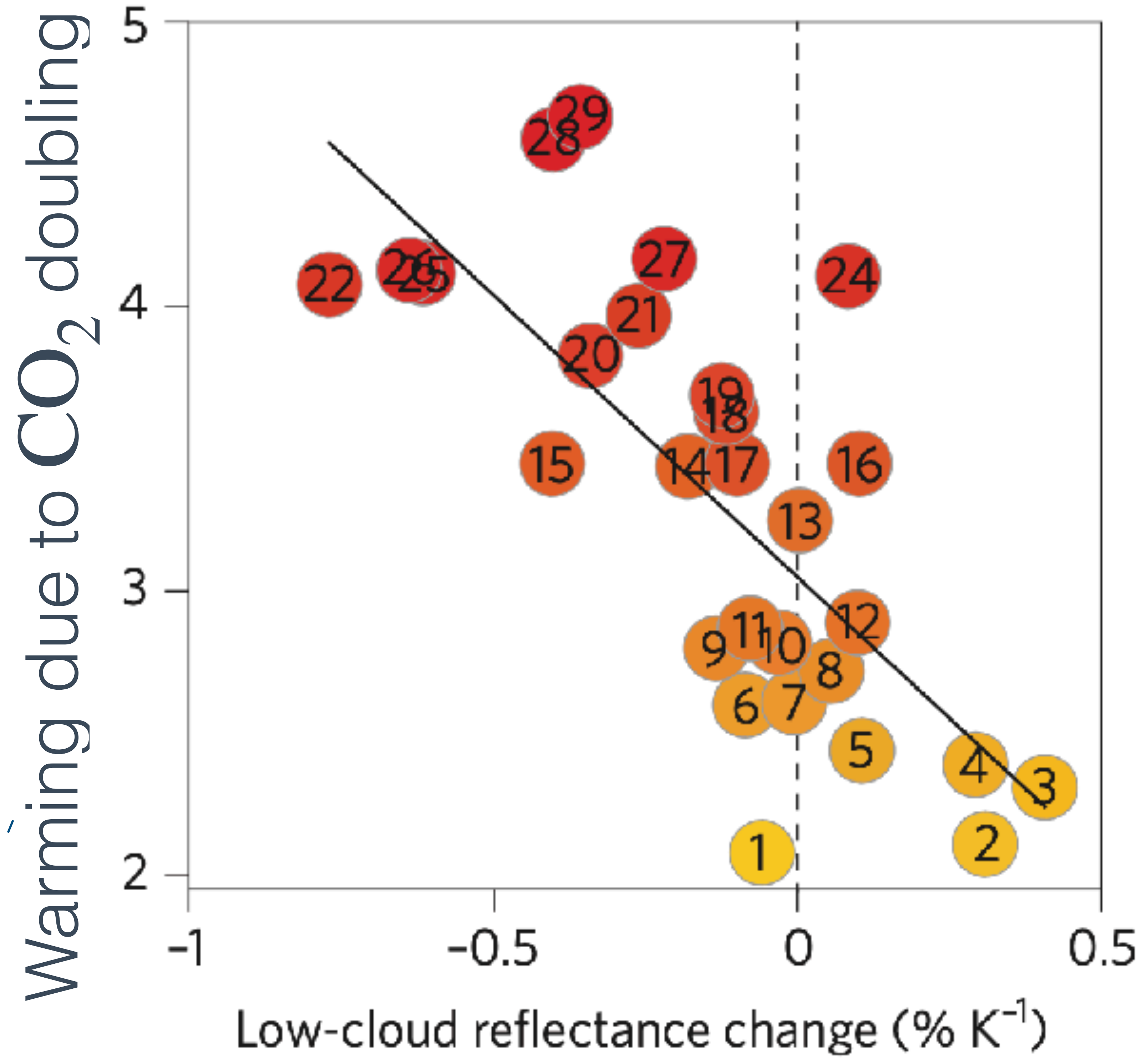


How much time do we have to act

Clouds dominate uncertainties in climate projections

SSP3-7.0 scenario (IPCC, 2022)





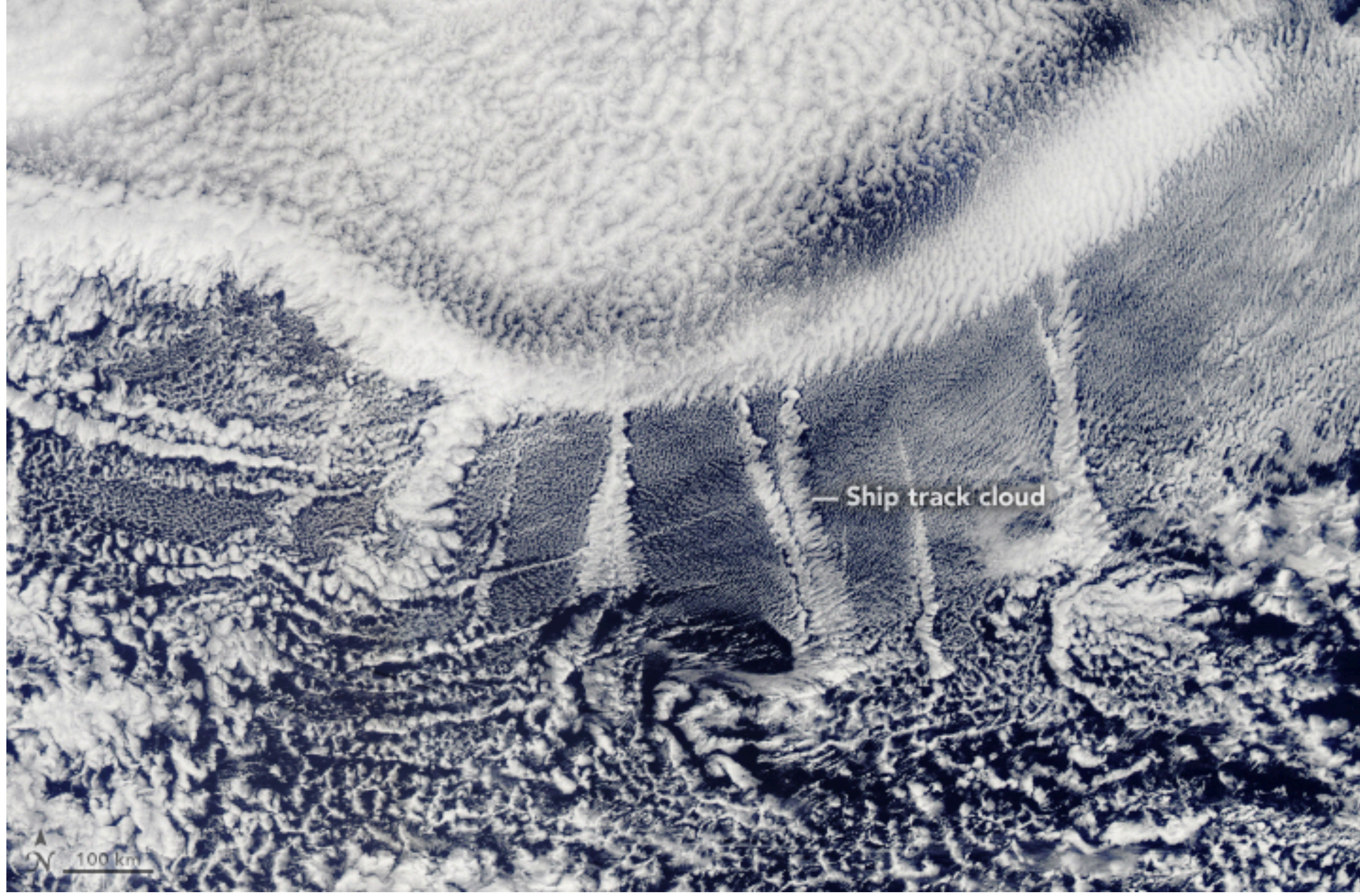
More clouds, less warming

Schneider et al., *Nat. Clim. Change* 2017:
Climate goals and computing the future of clouds

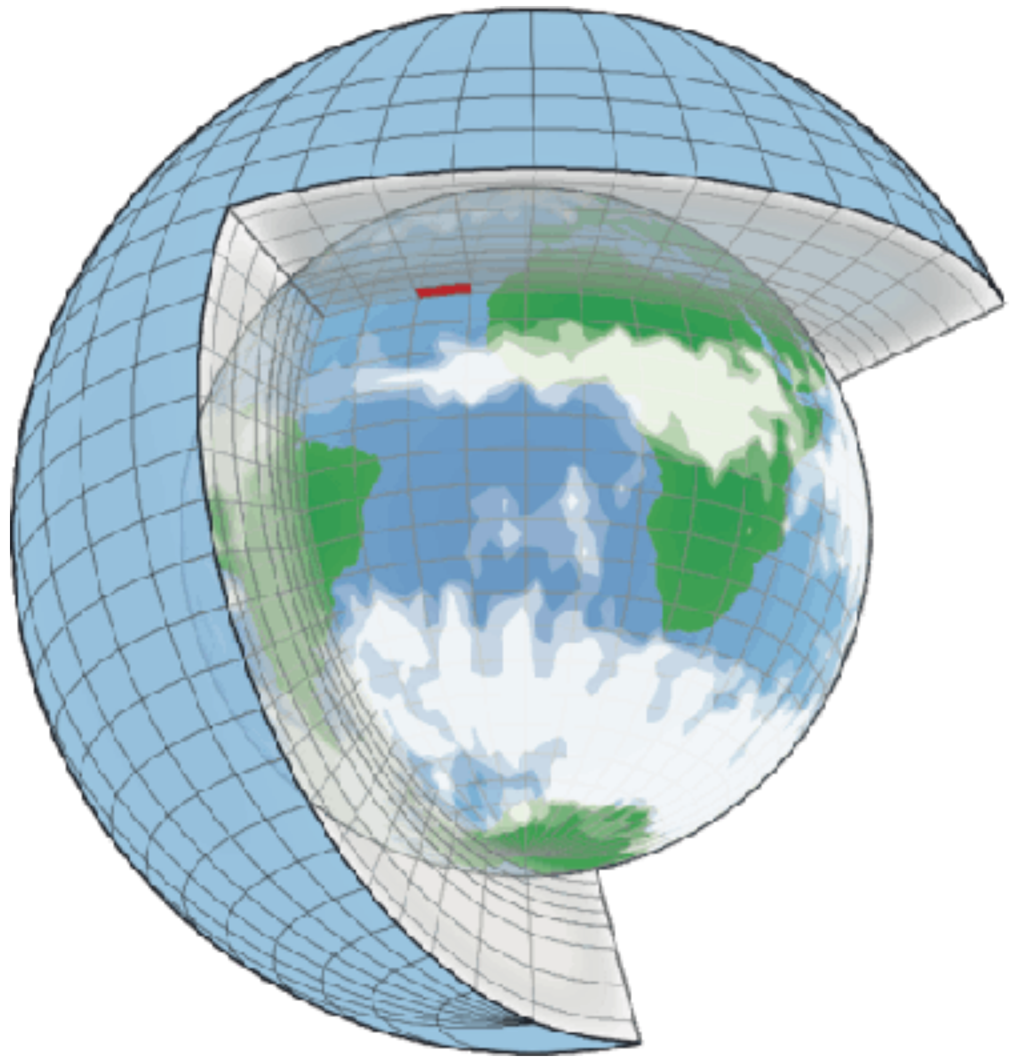
Clouds cannot be resolved in climate models

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

~100 km



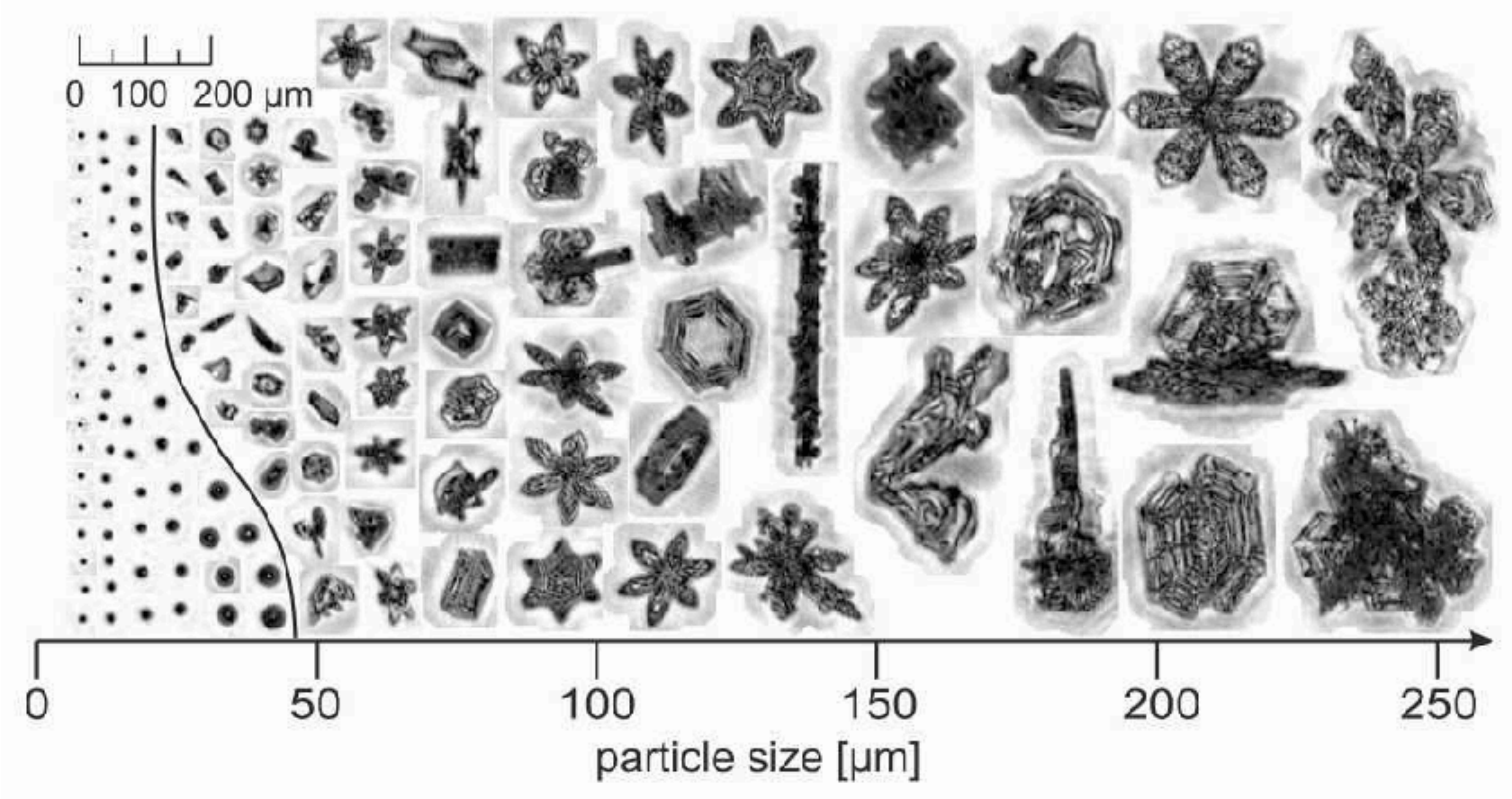
NASA MODIS: August 2018 clouds off the west coast of North America



Global model:
~10-50 km resolution

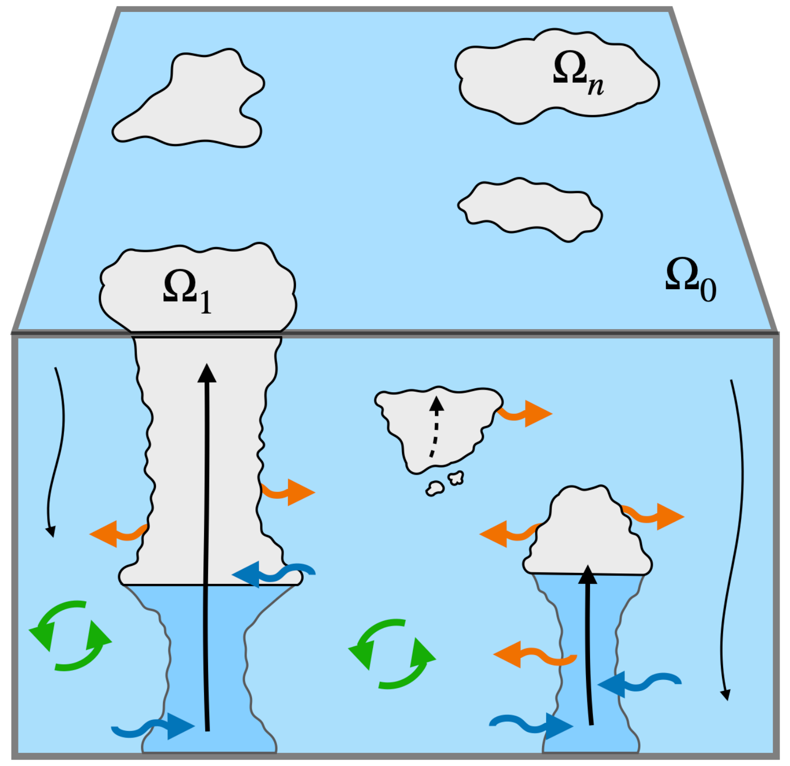
Cloud scales:
~10-100 m

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



HOLIMO @ETH Zurich Field measurements with the holographic imager

TurbulenceConvection.jl



- 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

- Closures:
  - entrainment/detrainment
  - mixing length
  - pressure drag,
  - microphysics,
  - …

Continuity

$$\frac{\partial(\rho a_i)}{\partial t} + \frac{\partial(\rho a_i \overline{w}_i)}{\partial z} + \nabla_h \cdot (\rho a_i \langle \mathbf{u}_h \rangle) = \rho a_i \overline{w}_i \left(\sum_j \epsilon_{ij} - \delta_i \right)$$

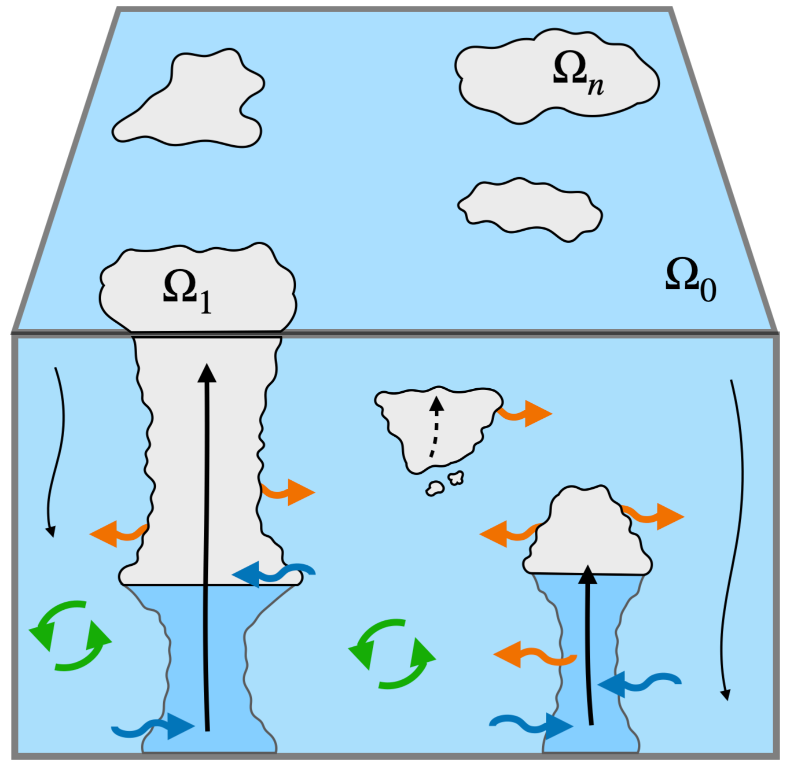
Scalar mean

$$\frac{\partial(\rho a_i \bar{\phi}_i)}{\partial t} + \nabla_h \cdot (\rho a_i \langle \mathbf{u}_h \rangle \bar{\phi}_i) + \frac{\partial(\rho a_i \bar{w}_i \bar{\phi}_i)}{\partial z} =$$

$$\rho a_i \bar{w}_i \sum_{j \neq i} \left((\epsilon_{ij} + \hat{\epsilon}_{ij}) \bar{\phi}_j - (\delta_{ij} + \hat{\epsilon}_{ij}) \bar{\phi}_i \right) - \frac{\partial(\rho a_i \overline{w_i' \phi_i'})}{\partial z} + \boxed{\rho a_i \overline{S_{\phi,i}},}$$

Tan et al., JAMES 2018,
Cohen et al. JAMES 2020,
Lopez-Gomez et al. JAMES 2020

TurbulenceConvection.jl



- 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

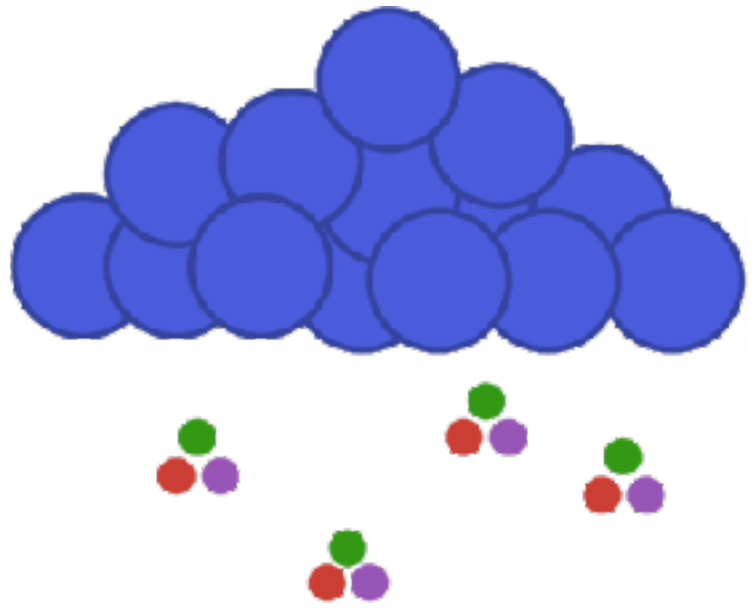
Scalar covariance

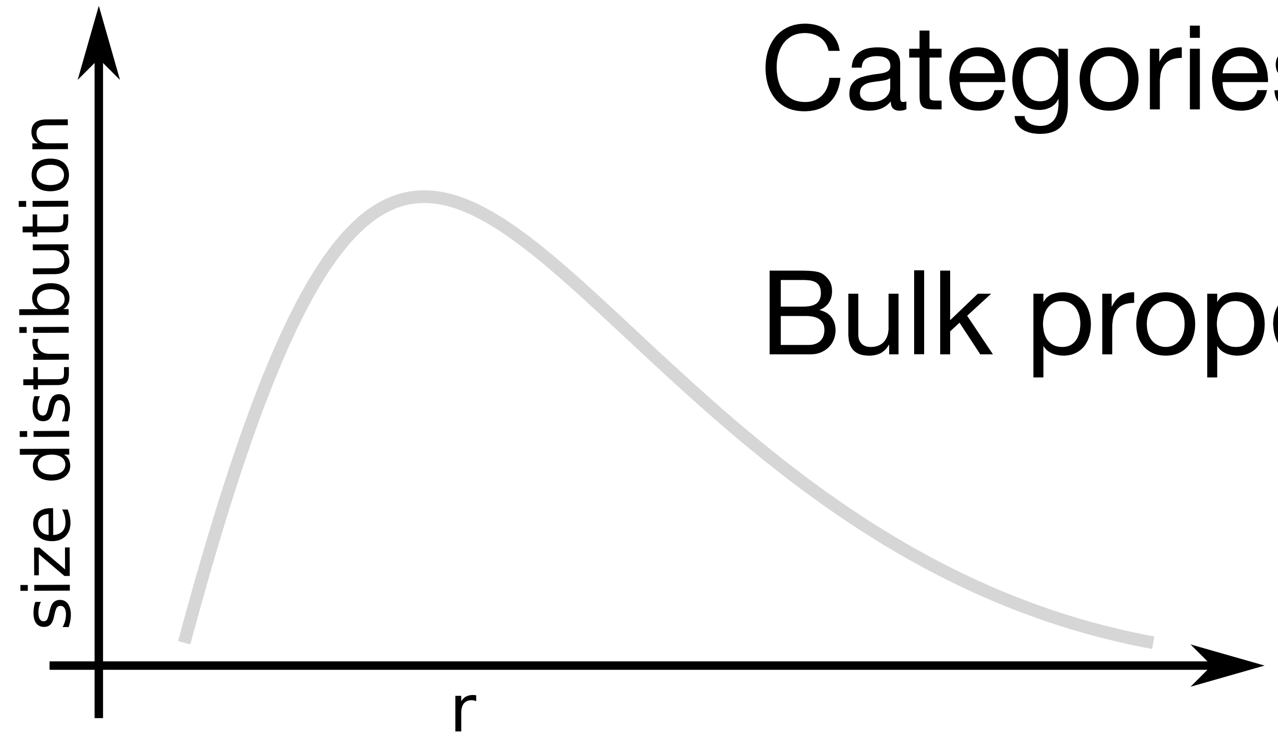
- Closures:
  - entrainment/detrainment
  - mixing length
  - pressure drag,
  - microphysics,
  - …

$$\frac{\partial(\rho a_i \overline{\phi_i'\psi_i'})}{\partial t} + \nabla_h \cdot (\rho a_i \langle \mathbf{u}_h \rangle \overline{\phi_i'\psi_i'}) + \frac{\partial(\rho a_i \bar{w}_i \overline{\phi_i'\psi_i'})}{\partial z} =$$
$$\rho a_i \bar{w}_i \sum_{j\neq i} \left(\epsilon_{ij} (\bar{\psi}_i - \bar{\psi}_j)(\bar{\phi}_i - \bar{\phi}_j) - \delta_{ij} \overline{\phi_i'\psi_i'} \right) +$$
$$\rho a_i \bar{w}_i \sum_{j\neq i} \left(\hat{\epsilon}_{ij} (\bar{\phi}_i^* (\bar{\psi}_i - \bar{\psi}_j) + \bar{\psi}_i^* (\bar{\phi}_i - \bar{\phi}_j)) - \hat{\epsilon}_{ij} \overline{\phi_i'\psi_i'} \right) -$$
$$\frac{\partial(\rho a_i \overline{w_i'\phi_i'\psi_i'})}{\partial z} - \rho a_i (\overline{w_i'\phi_i'} \frac{\partial \bar{\psi}_i}{\partial z} + \overline{w_i'\psi_i'} \frac{\partial \bar{\phi}_i}{\partial z}) + \boxed{\rho a_i (\overline{\mathcal{S}_{\phi,i}'\psi_i'} + \overline{\mathcal{S}_{\psi,i}'\phi_i'})} - \rho a_i \overline{D_{\phi_i'\psi_i'}},$$

Tan et al., JAMES 2018,
Cohen et al. JAMES 2020,
Lopez-Gomez et al. JAMES 2020

CloudMicrophysics.jl





Categories: cloud water and ice, rain and snow, …

Bulk properties: total mass of water in each category

- assumed particle size distributions

$$n(r) = n_0 exp\,(-\lambda\, r)$$

- mass(size), area(size) and terminal velocity(size)

$$m(r) = \chi_m\, m_0 \left(\frac{r}{r_0}\right)^{m_e + \Delta_m}$$

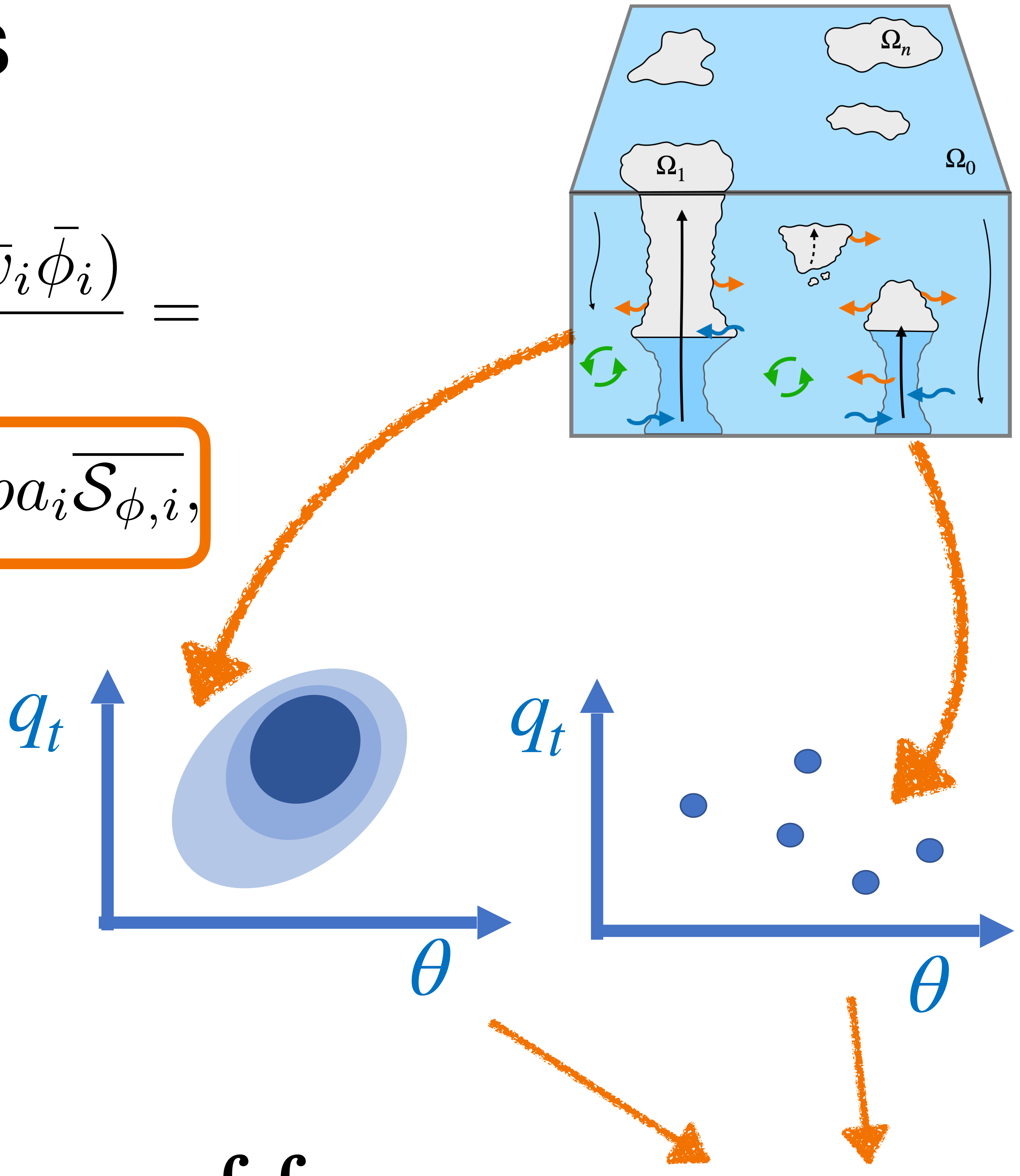
- physics closures

$$\left.\frac{d\,q_c}{dt}\right|_{accr} = - \int_0^\infty n_p(r)\, a^p(r)\, v_{term}(r)\, E_{cp}\, q_c\, dr$$

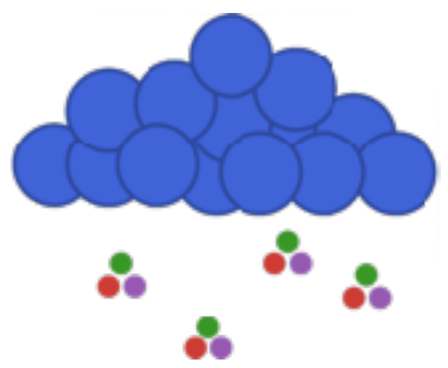
Representing clouds in climate models

$$\frac{\partial(\rho a_i \bar{\phi}_i)}{\partial t} + \nabla_h \cdot (\rho a_i \langle \mathbf{u}_h \rangle \bar{\phi}_i) + \frac{\partial(\rho a_i \bar{w}_i \bar{\phi}_i)}{\partial z} =$$

$$\rho a_i \bar{w}_i \sum_{j\neq i}\left((\epsilon_{ij}+\hat{\epsilon}_{ij})\bar{\phi}_j - (\delta_{ij}+\hat{\epsilon}_{ij})\bar{\phi}_i\right) - \frac{\partial(\rho a_i \overline{w_i'\phi_i'})}{\partial z} + \boxed{\rho a_i \overline{\mathcal{S}_{\phi,i}},}$$



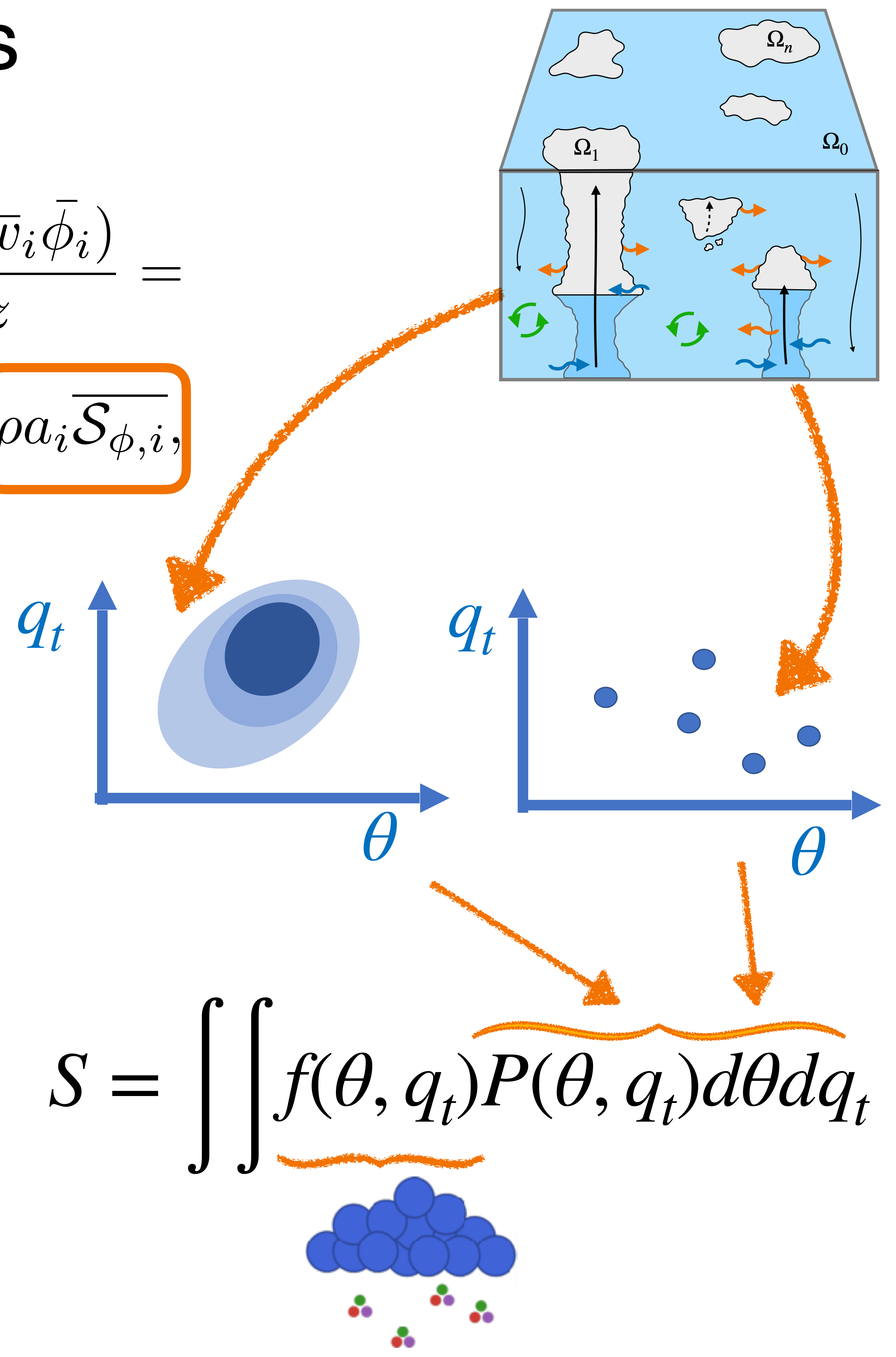
$$S = \iint f(\theta, q_t) P(\theta, q_t)\, d\theta\, dq_t$$



Representing clouds in climate models

$$\frac{\partial(\rho a_i \bar{\phi}_i)}{\partial t} + \nabla_h \cdot (\rho a_i \langle \mathbf{u}_h \rangle \bar{\phi}_i) + \frac{\partial(\rho a_i \bar{w}_i \bar{\phi}_i)}{\partial z} =$$

$$\rho a_i \bar{w}_i \sum_{j \neq i} \Big((\epsilon_{ij} + \hat{\epsilon}_{ij}) \bar{\phi}_j - (\delta_{ij} + \hat{\epsilon}_{ij}) \bar{\phi}_i \Big) - \frac{\partial(\rho a_i \overline{w_i' \phi_i'})}{\partial z} + \boxed{\rho a_i \overline{\mathcal{S}_{\phi,i}},}$$



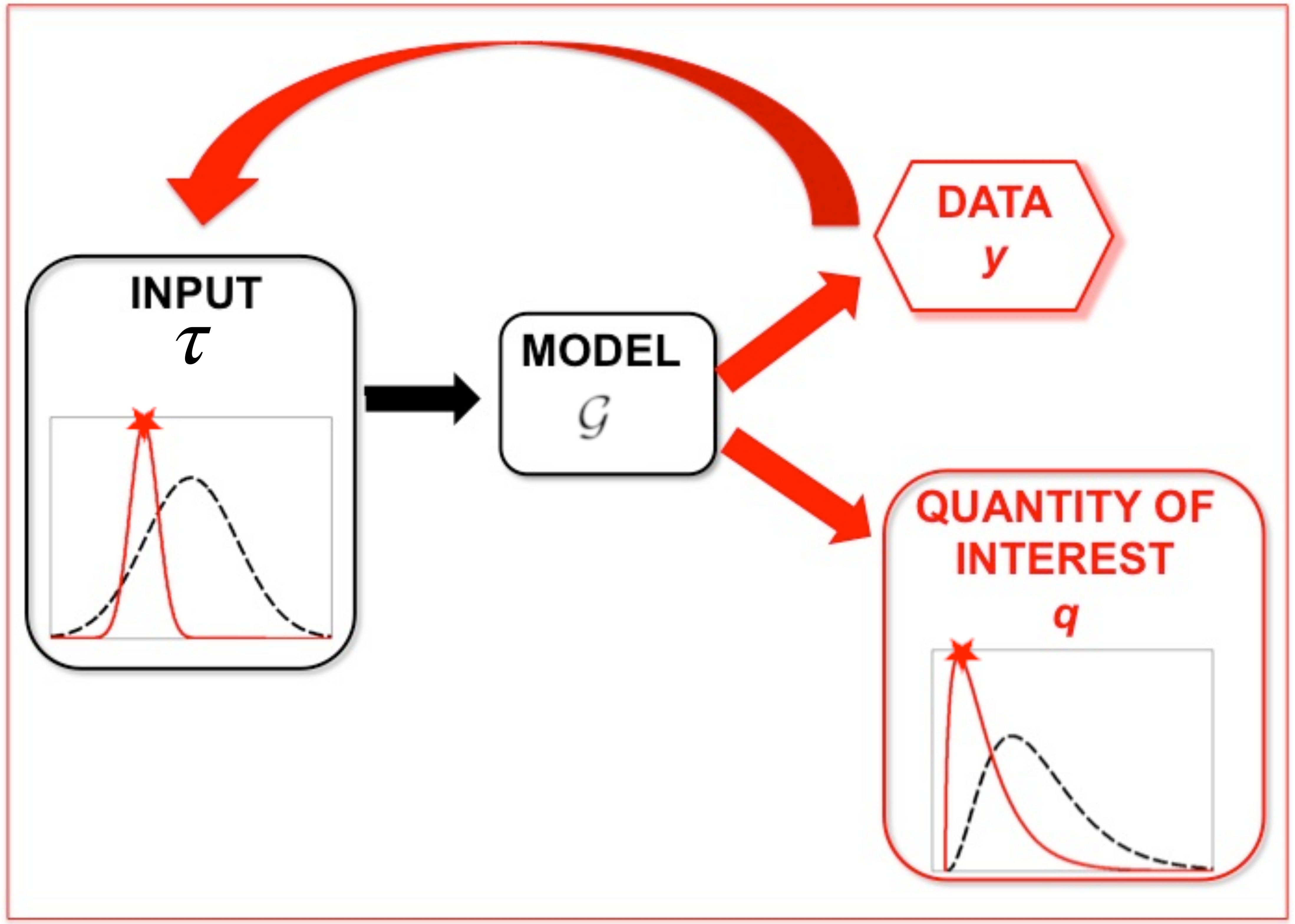
- ~20 free parameters from SGS scheme

- ~40 free parameters from the cloud microphysics scheme

Learn the free parameters from data as Bayesian inverse problem

Our sub-grid scale + cloud microphysics model is a map from space of parameters to climate statistics.

We want to learn the distribution of free parameters and update prior on τ (- -) with observation *y* (—).

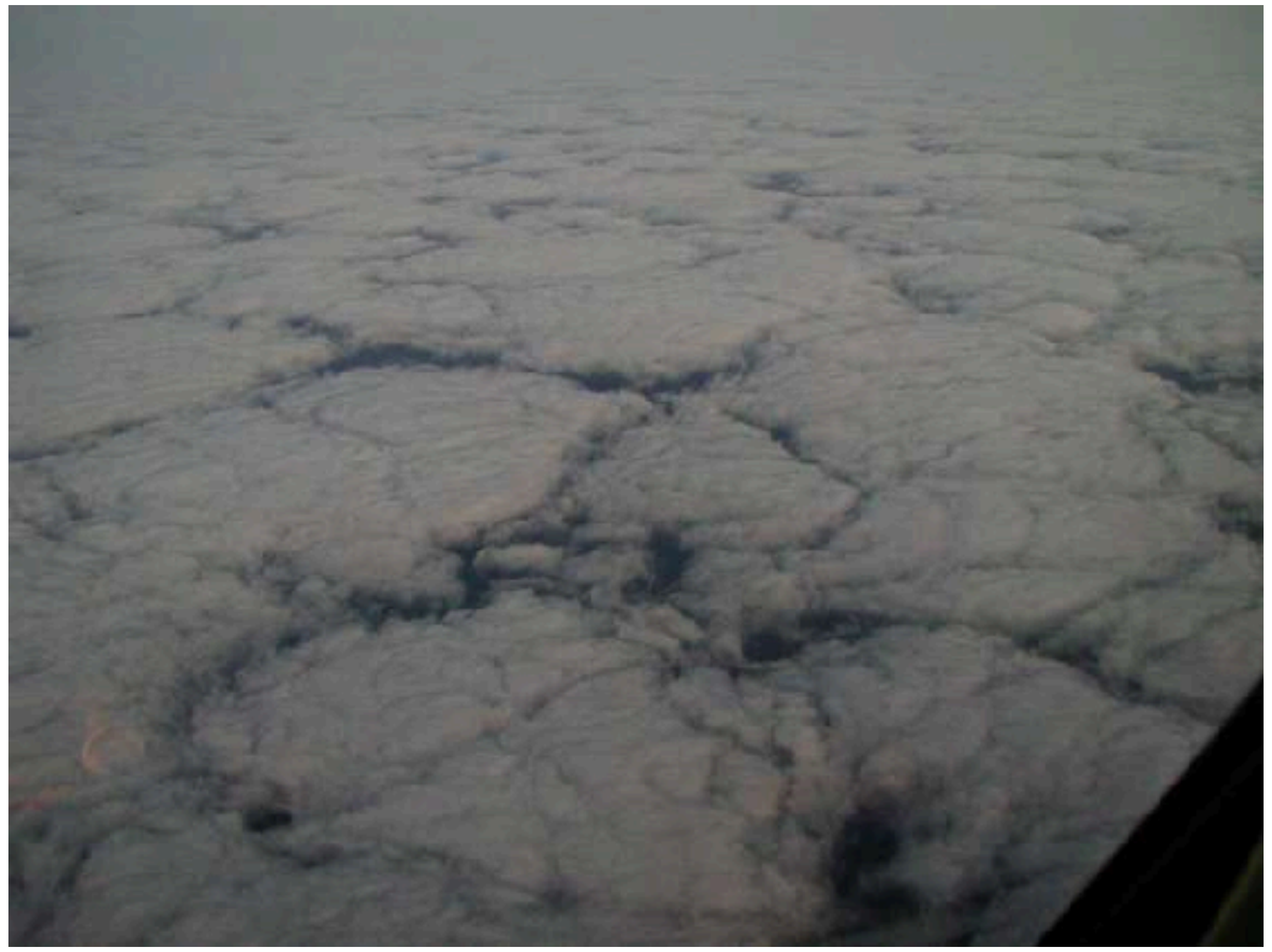


Cleary et al. 2021; Dunbar, Garbuno-Inigo, et al. 2021.

Individual test cases

Dycoms RF02
Drizzling Sc trapped under inversion

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



CliMA CLIMATE MODELING ALLIANCE

Rico
Precipitating shallow trade wind convection

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

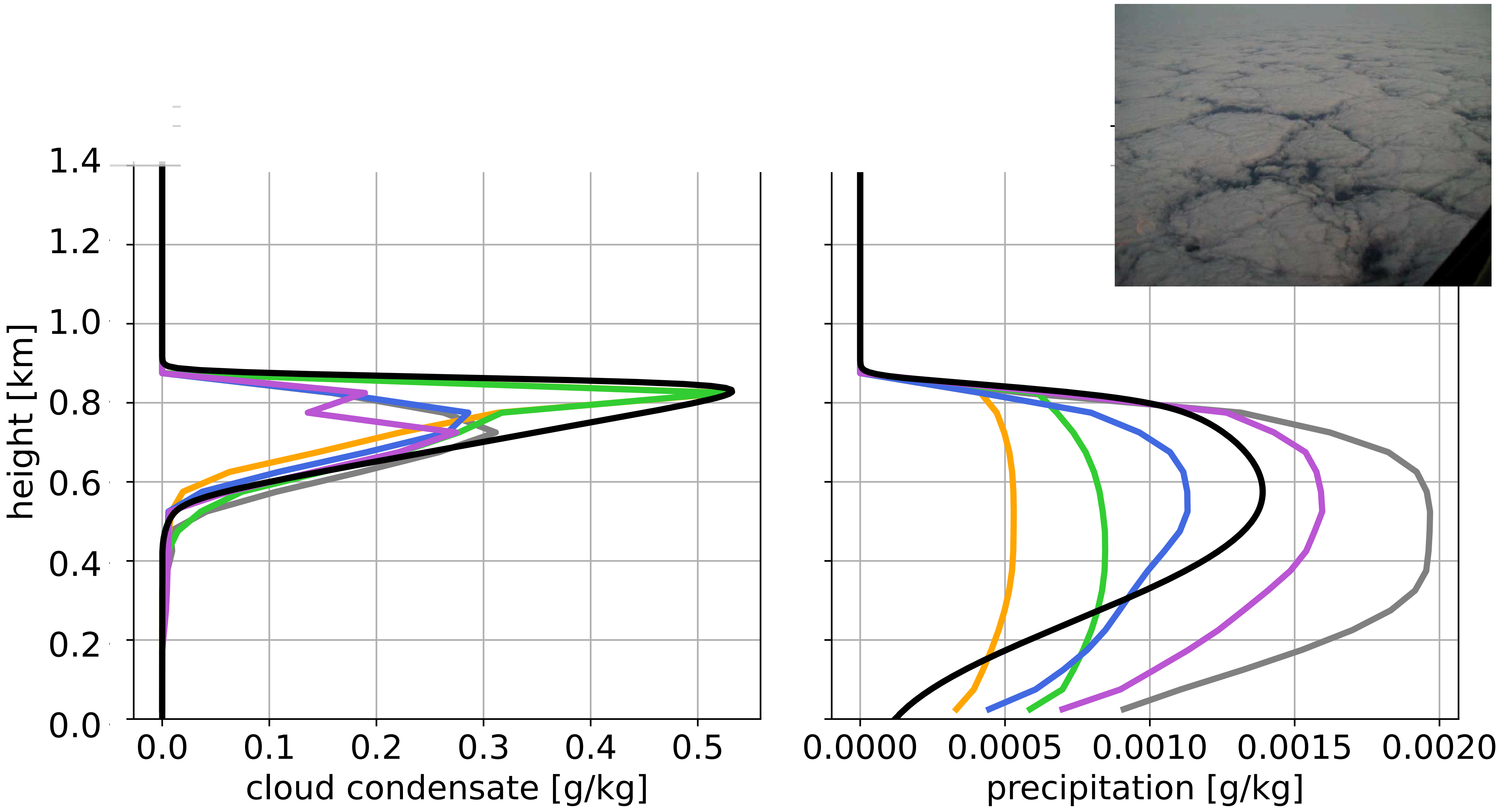
TRMM LBA
Development of deep convection over Amazon

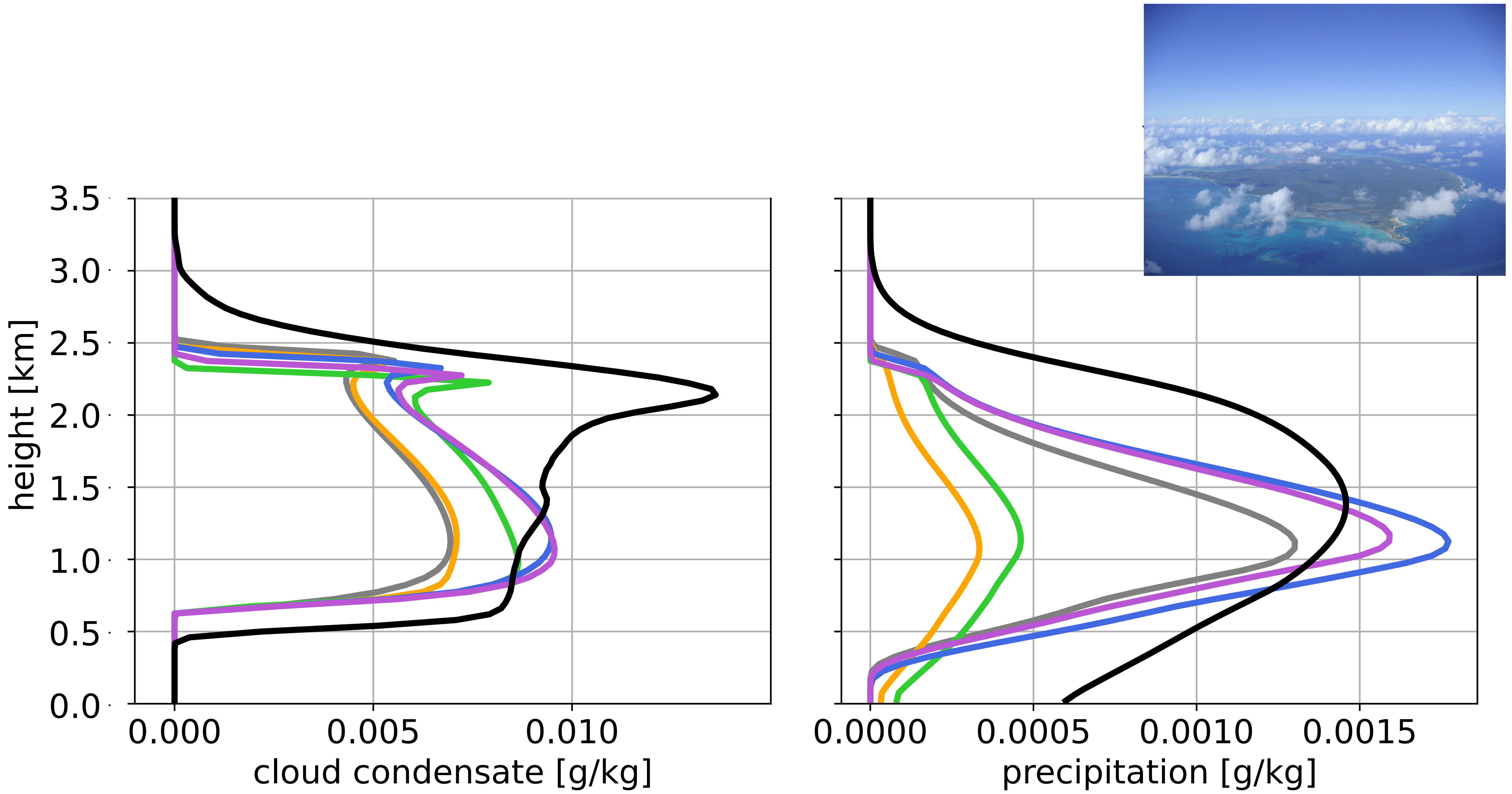
Grabowski et. Al., *JQRMS* 2006: Daytime convective development over land: A model intercomparison based on LBA observations

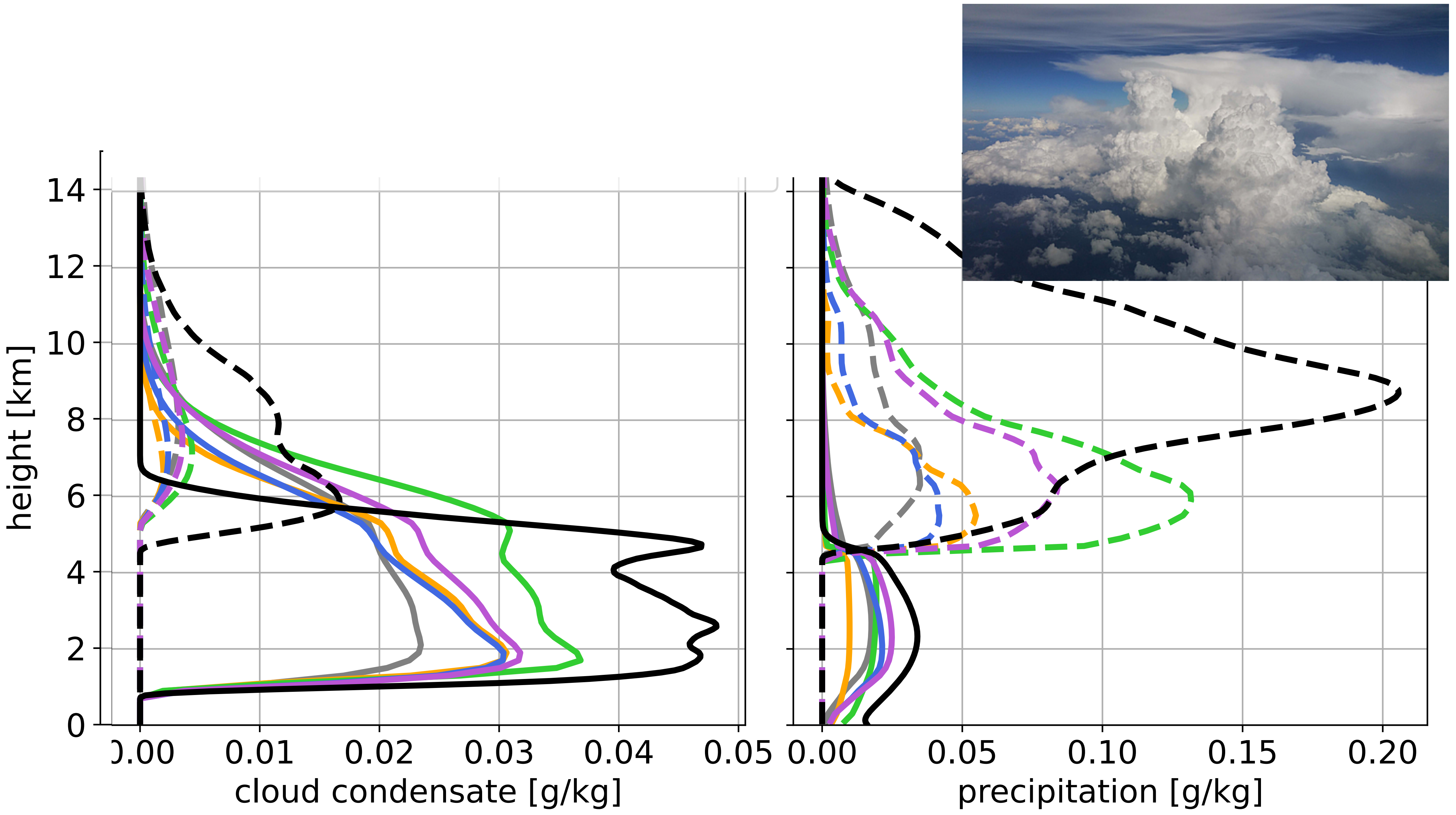
Individual test cases

3D LES data (observations)

Calibrated SGS model



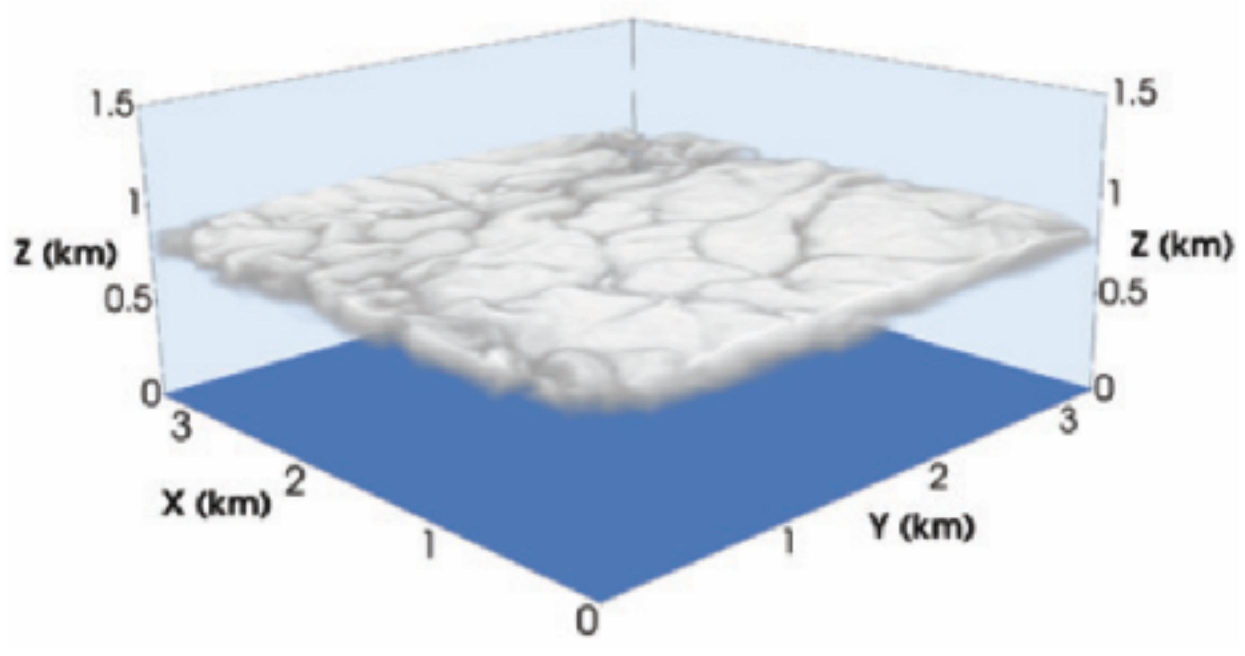




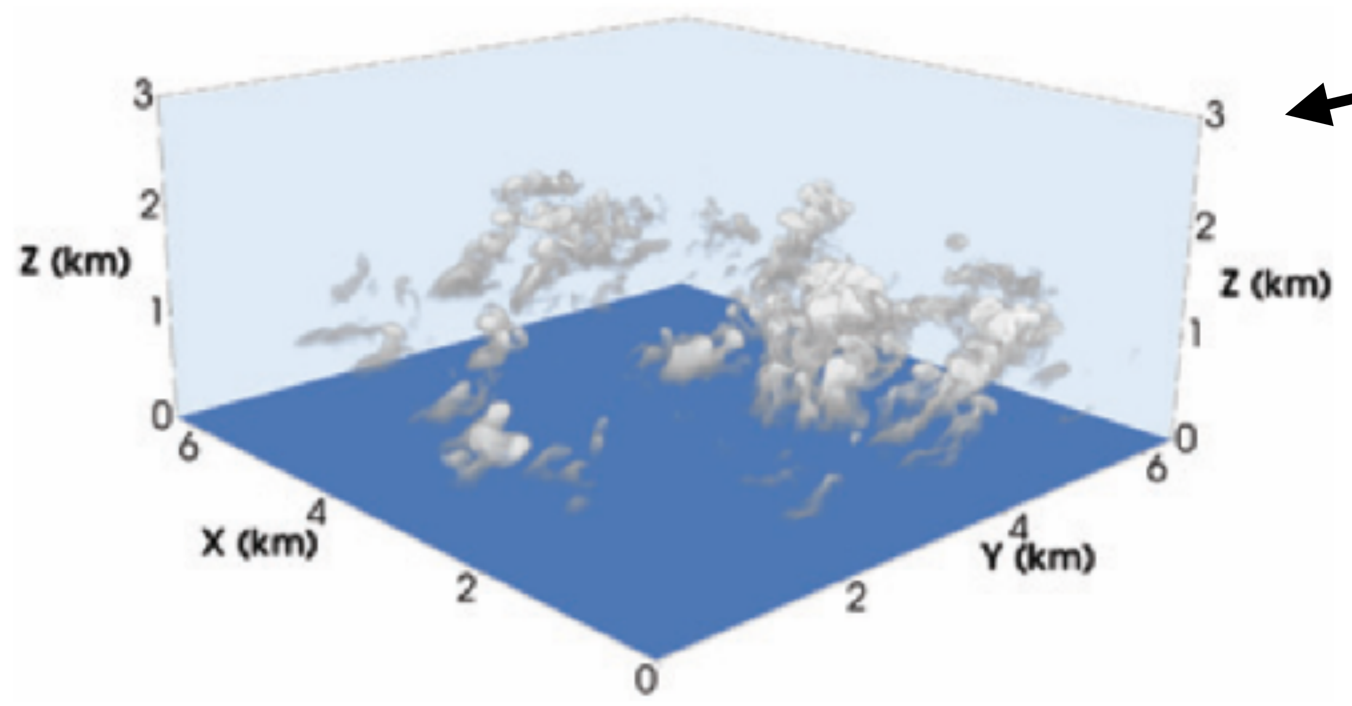
Jaruga et al. in prep.

Libraries of cases

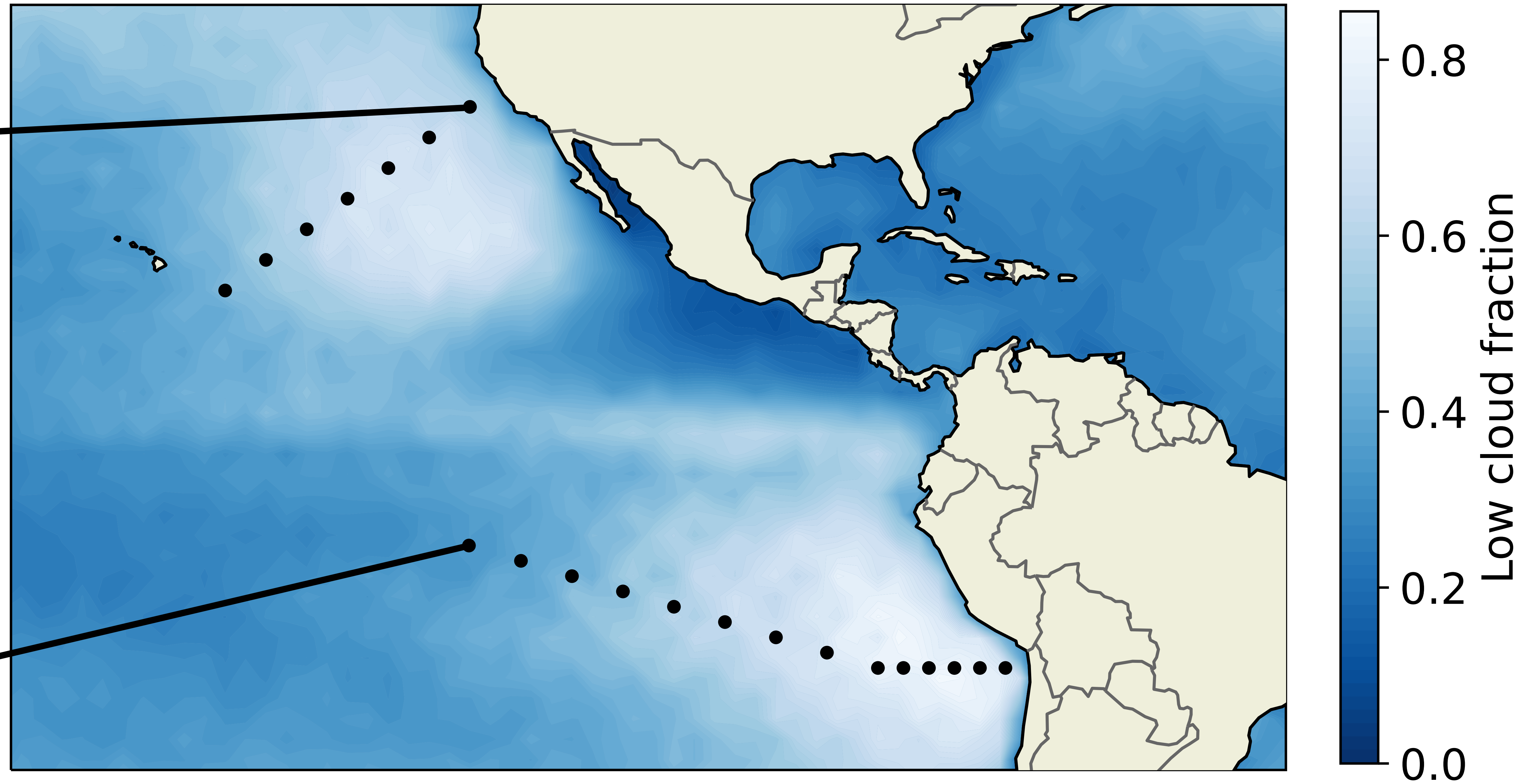
Stratocumulus



Shallow cumulus

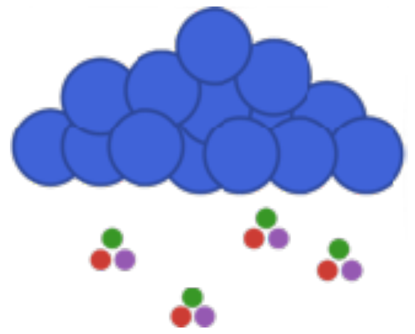


Synthetic data generation in different seasons and climates

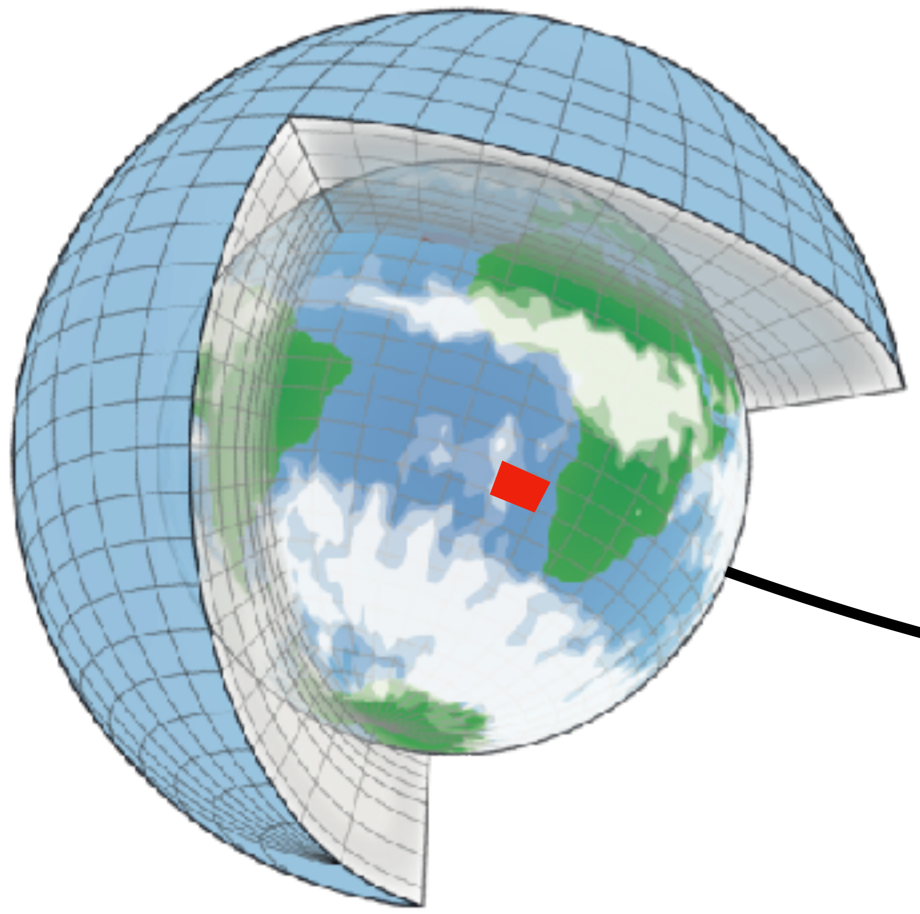


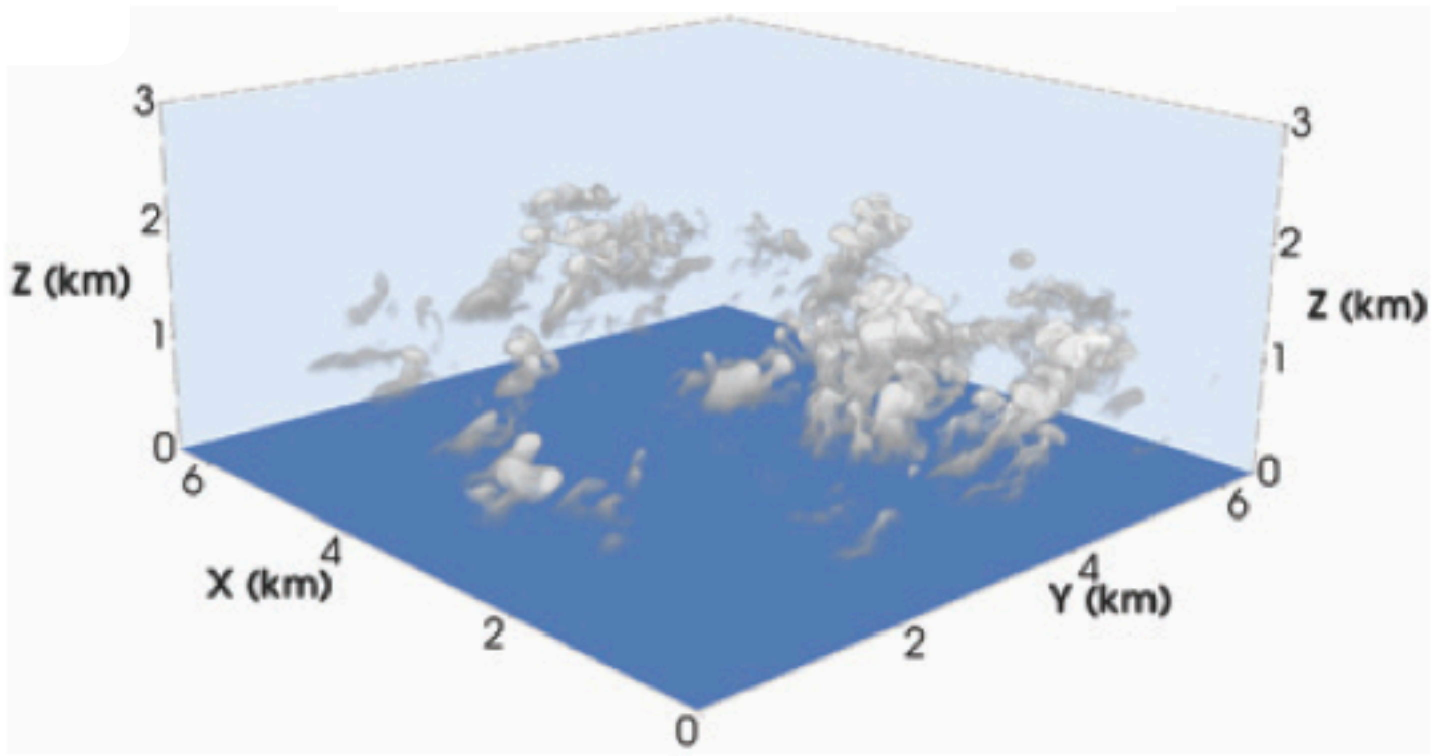
Shen et al., *JAMES* 2022: A Library of Large-Eddy Simulations Forced by Global Climate Models

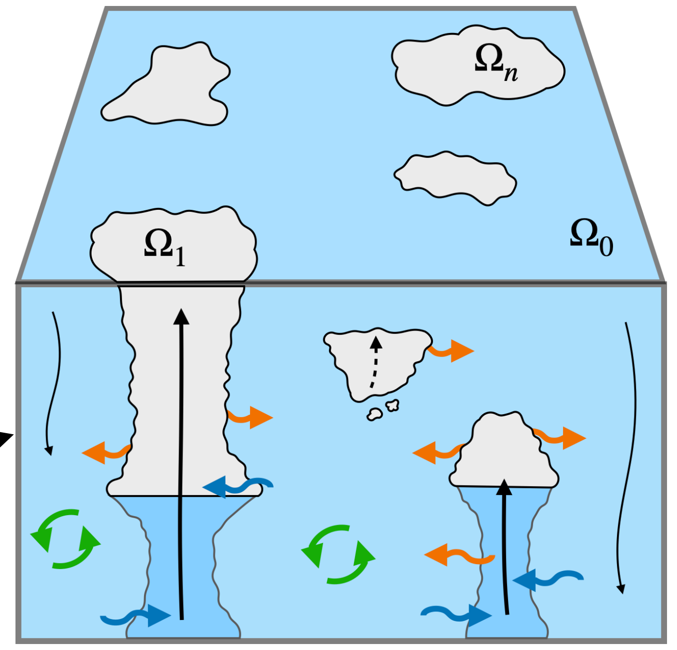
Generate data computationally, to machine learn unknown closure functions in coarse-grained model



The same microphysics scheme
used in high-res LES
and SGS models







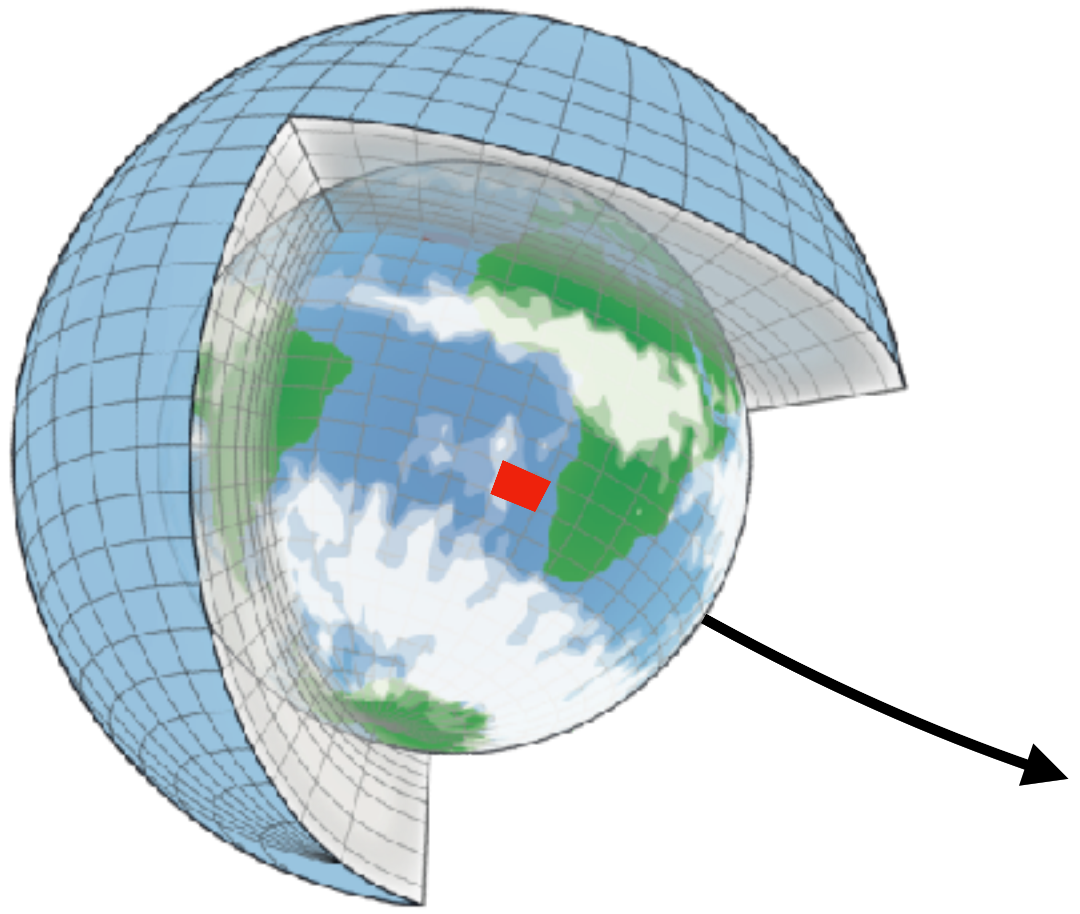
Targeted data
acquisition

3D LES high resolution simulations
of turbulence and convection

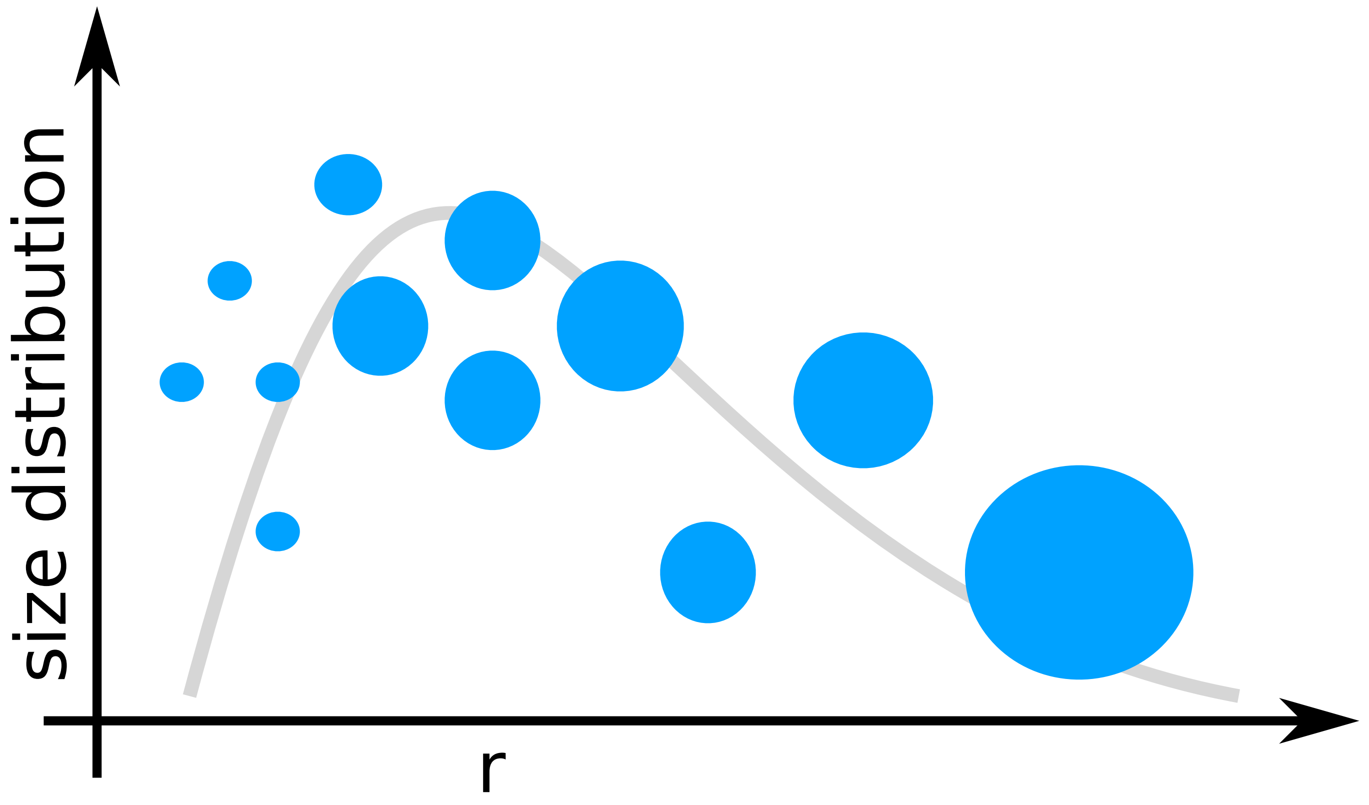
Process-level learning
Uncertainty quantification

CliMA
CLIMATE MODELING ALLIANCE

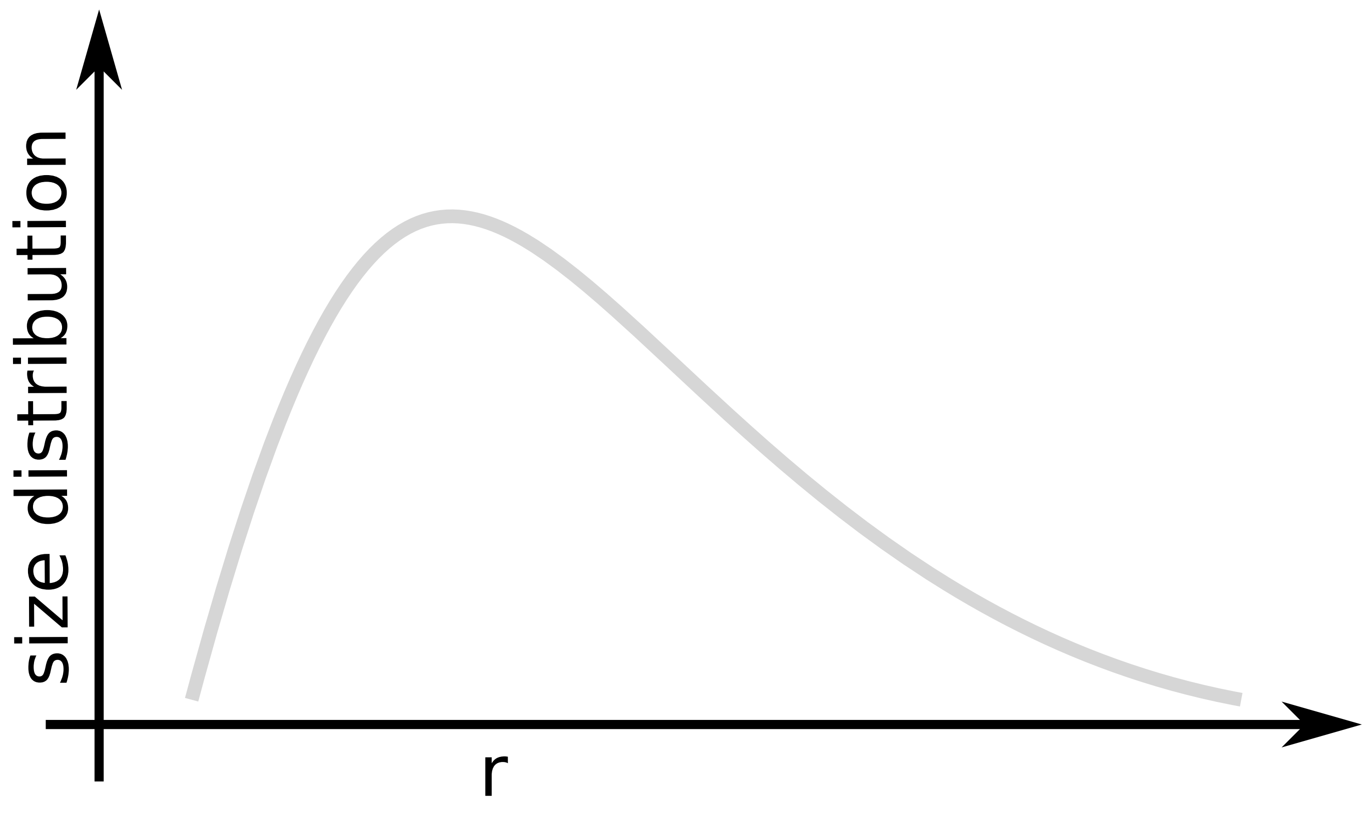
Generate data computationally, to machine learn unknown closure functions in coarse-grained model



Targeted data
acquisition

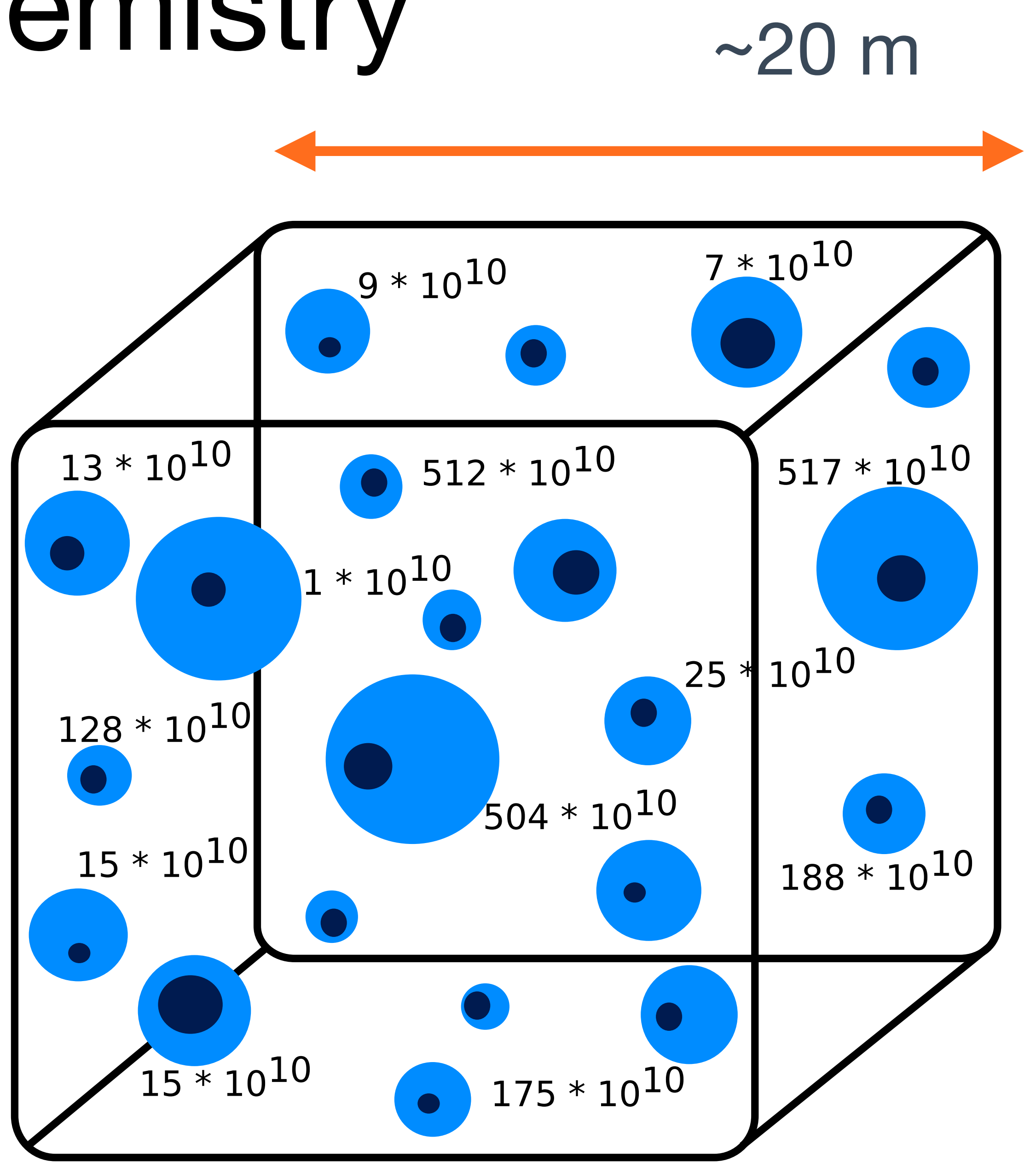


Lagrangian particle-based
high resolution simulations
of cloud microphysics



Process-level learning
Uncertainty quantification

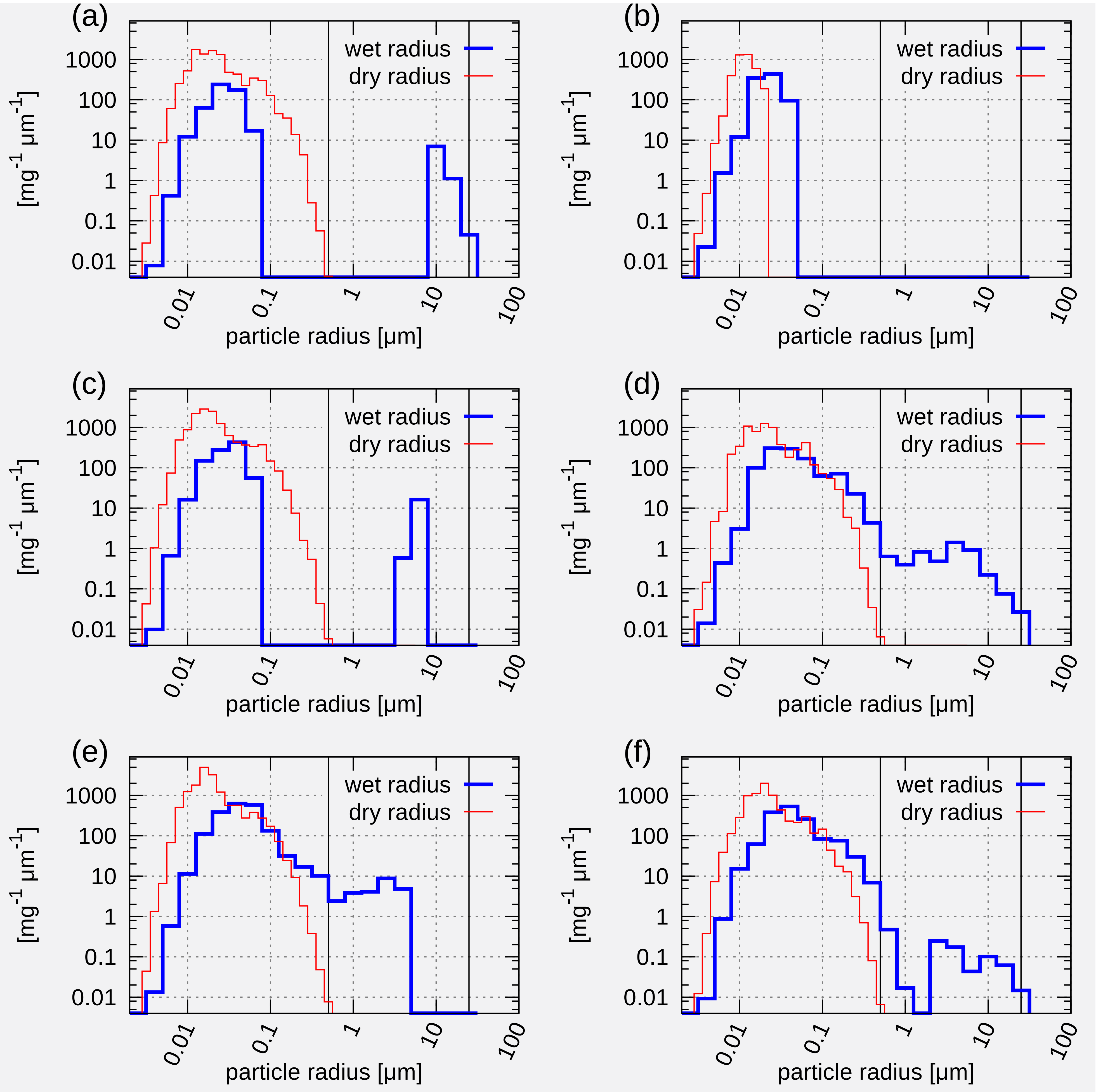
Particle-based (Lagrangian) microphysics and aqueous chemistry



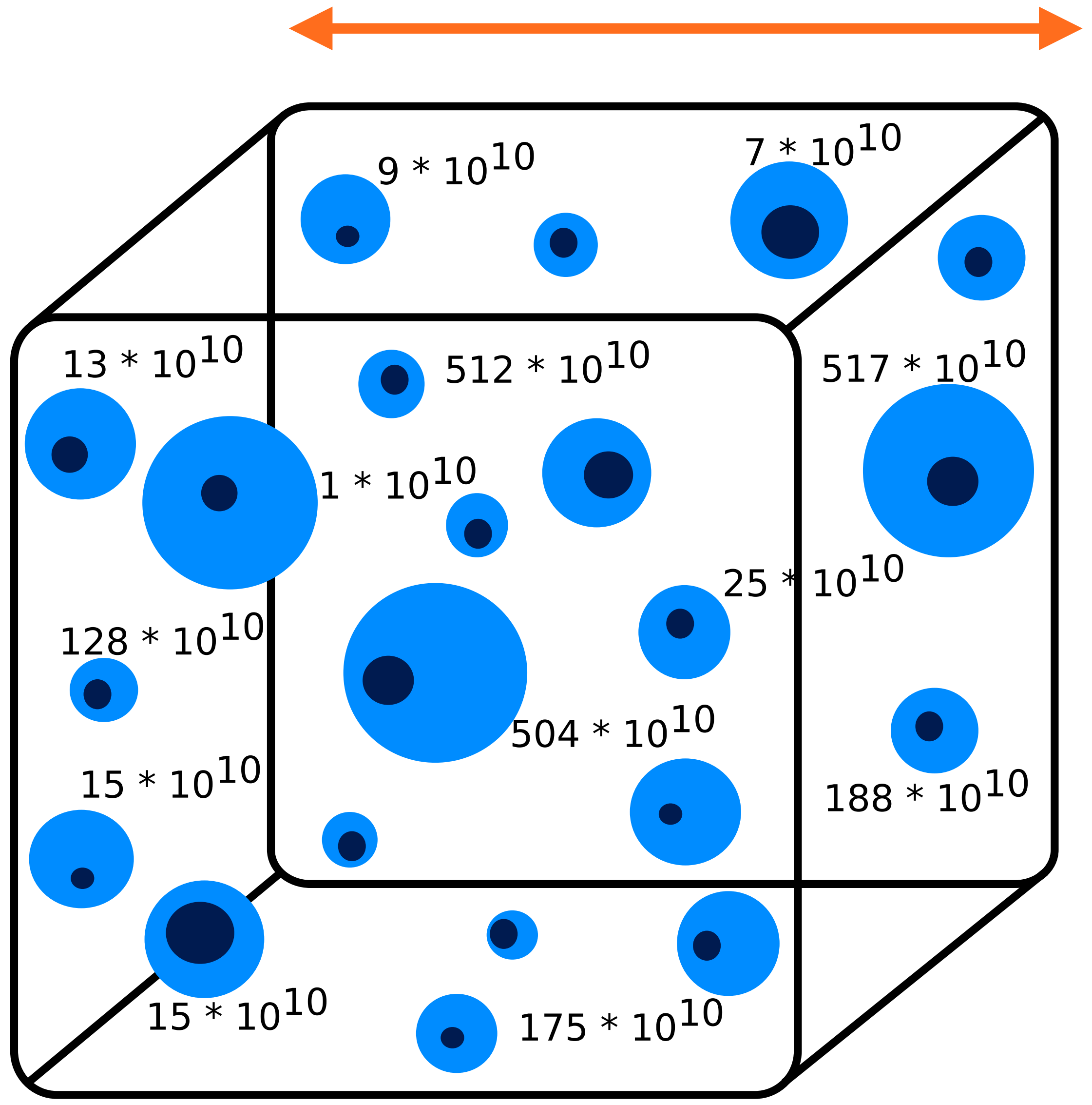
- location (x,y,z)
- wet and dry radius (r_w, r_d)
- higroscopicity (kappa)
- **multiplicity (n)**
- mass of dissolved chemical compounds

Shima et. al., *QJRMS* 2009: The super-droplet method for the numerical simulation of clouds and precipitation: A particle-based and probabilistic microphysics model coupled with a non-hydrostatic model
Arabas et. al., *GMD* 2015: libcloudph++ 1.0: a single-moment bulk, double-moment bulk, and particle-based warm-rain microphysics library in C++
Jaruga and Pawlowska, *GMD* 2018: libcloudph++ 2.0: aqueous-phase chemistry extension of the particle-based cloud microphysics scheme
Shima et. al., *GMD* 2020: Predicting the morphology of ice particles in deep convection using the super-droplet method: development and evaluation of SCALE-SDM 0.2.5-2.2.0/2.2.1

Particle-based (Lagrangian) microphysics and aqueous chemistry



~20 m

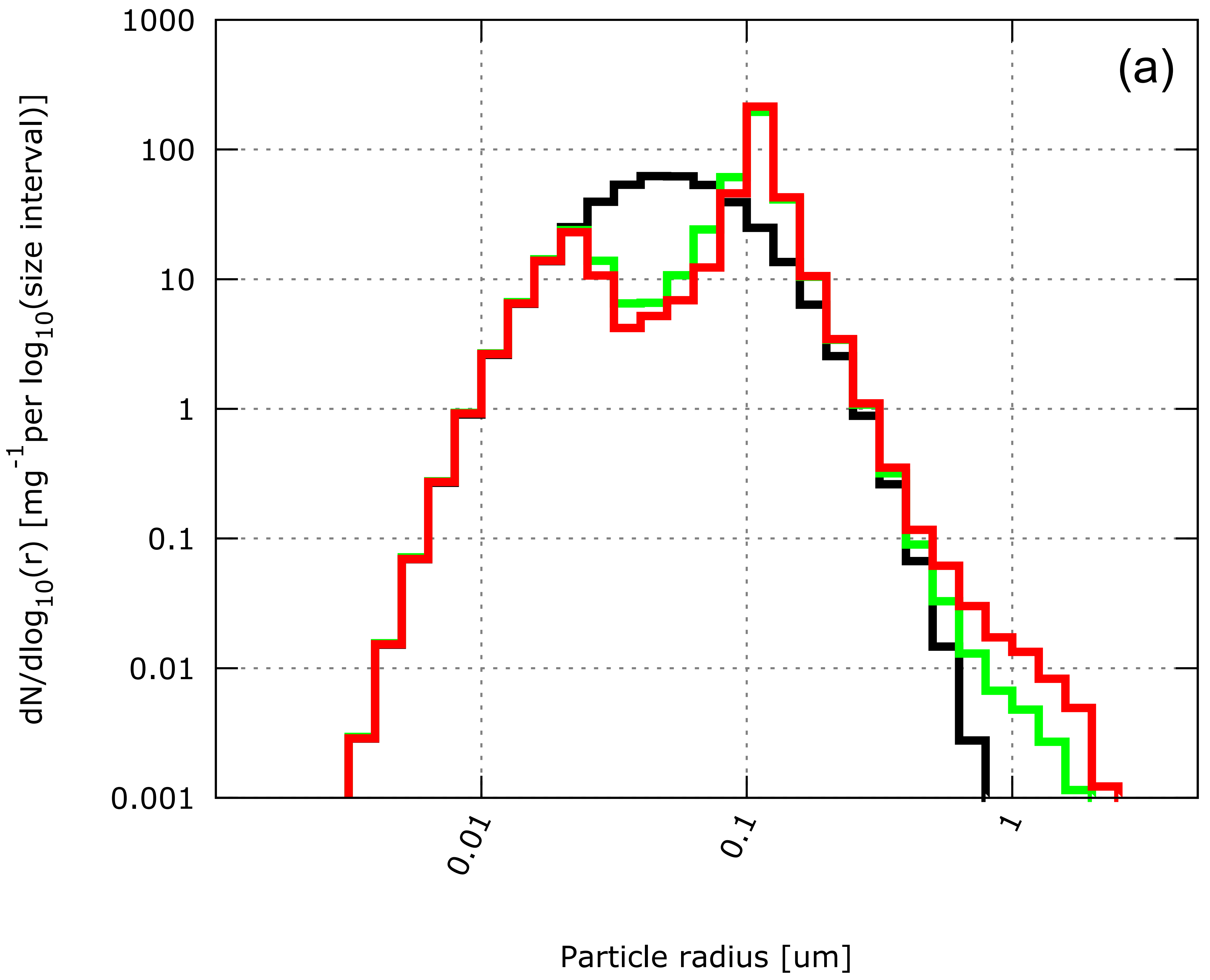


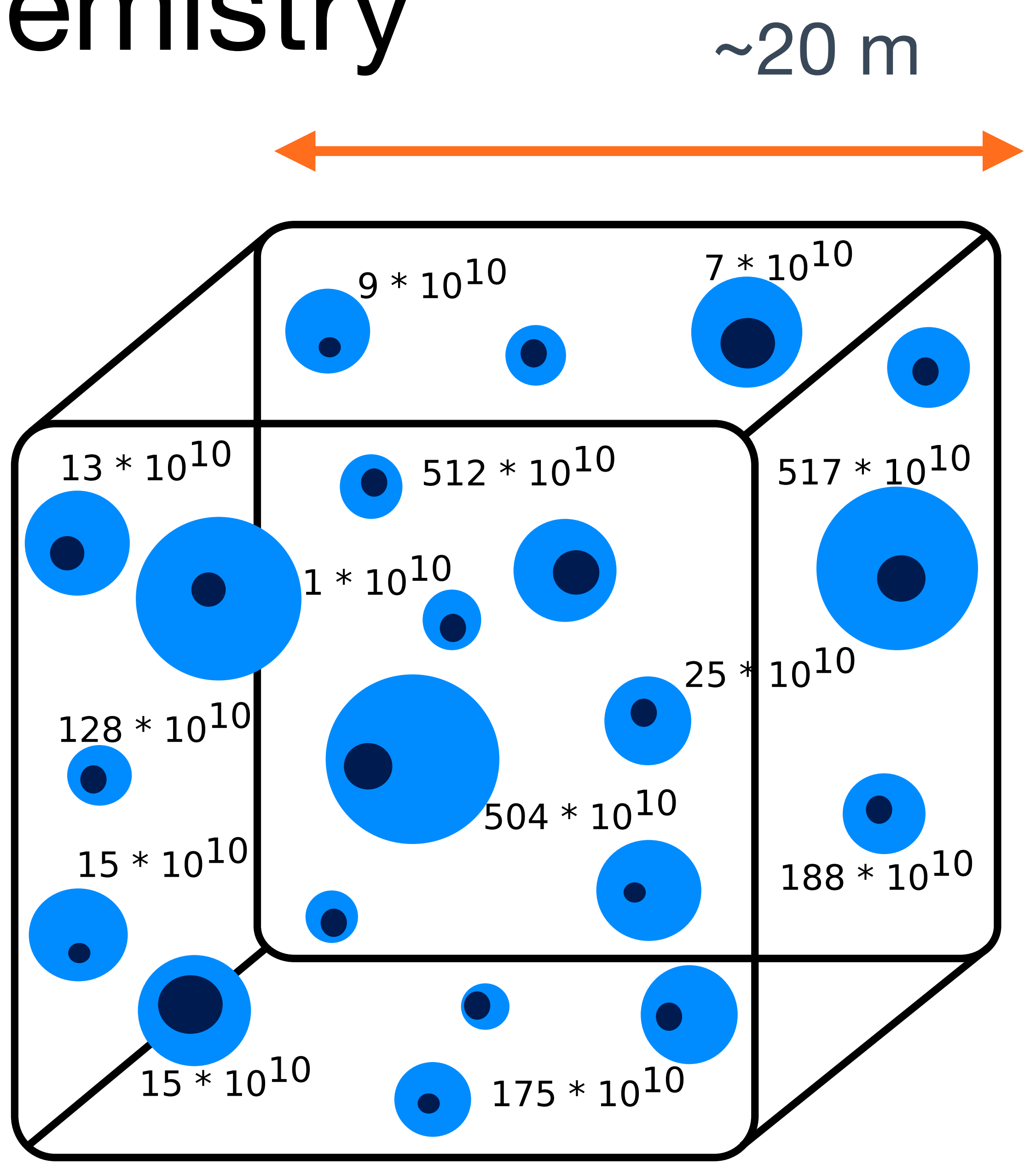
- location (x,y,z)
- wet and dry radius (r_{w}, r_{d})
- higroscopicity (kappa)
- **multiplicity (n)**
- mass of dissolved chemical compounds

Shima et. al., *QJRMS* 2009: The super-droplet method for the numerical simulation of clouds and precipitation: A particle-based and probabilistic microphysics model coupled with a non-hydrostatic model
Arabas et. al., *GMD* 2015: libcloudph++ 1.0: a single-moment bulk, double-moment bulk, and particle-based warm-rain microphysics library in C++
Jaruga and Pawlowska, *GMD* 2018: libcloudph++ 2.0: aqueous-phase chemistry extension of the particle-based cloud microphysics scheme
Shima et. al., *GMD* 2020: Predicting the morphology of ice particles in deep convection using the super-droplet method: development and evaluation of SCALE-SDM 0.2.5-2.2.0/2.2.1

CliMA CLIMATE MODELING ALLIANCE

Particle-based (Lagrangian) microphysics and aqueous chemistry





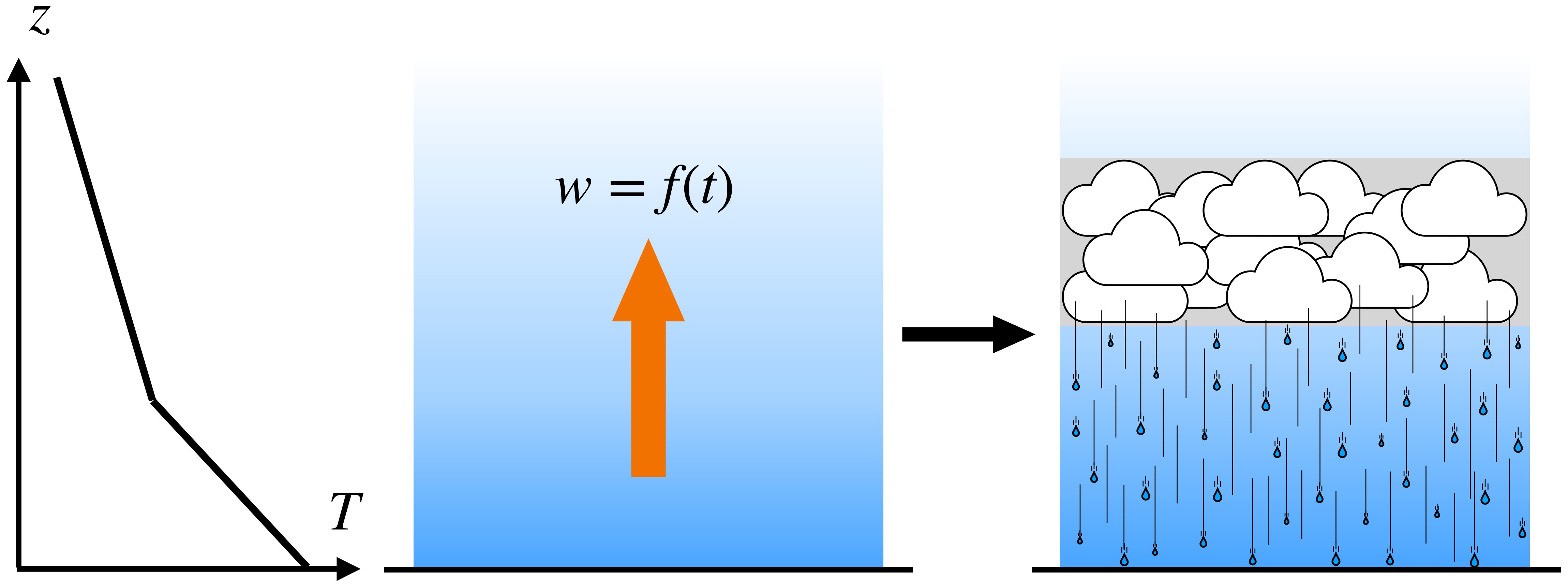
- location (x,y,z)
- wet and dry radius (r_w, r_d)
- higroscopicity (kappa)
- **multiplicity (n)**
- mass of dissolved chemical compounds

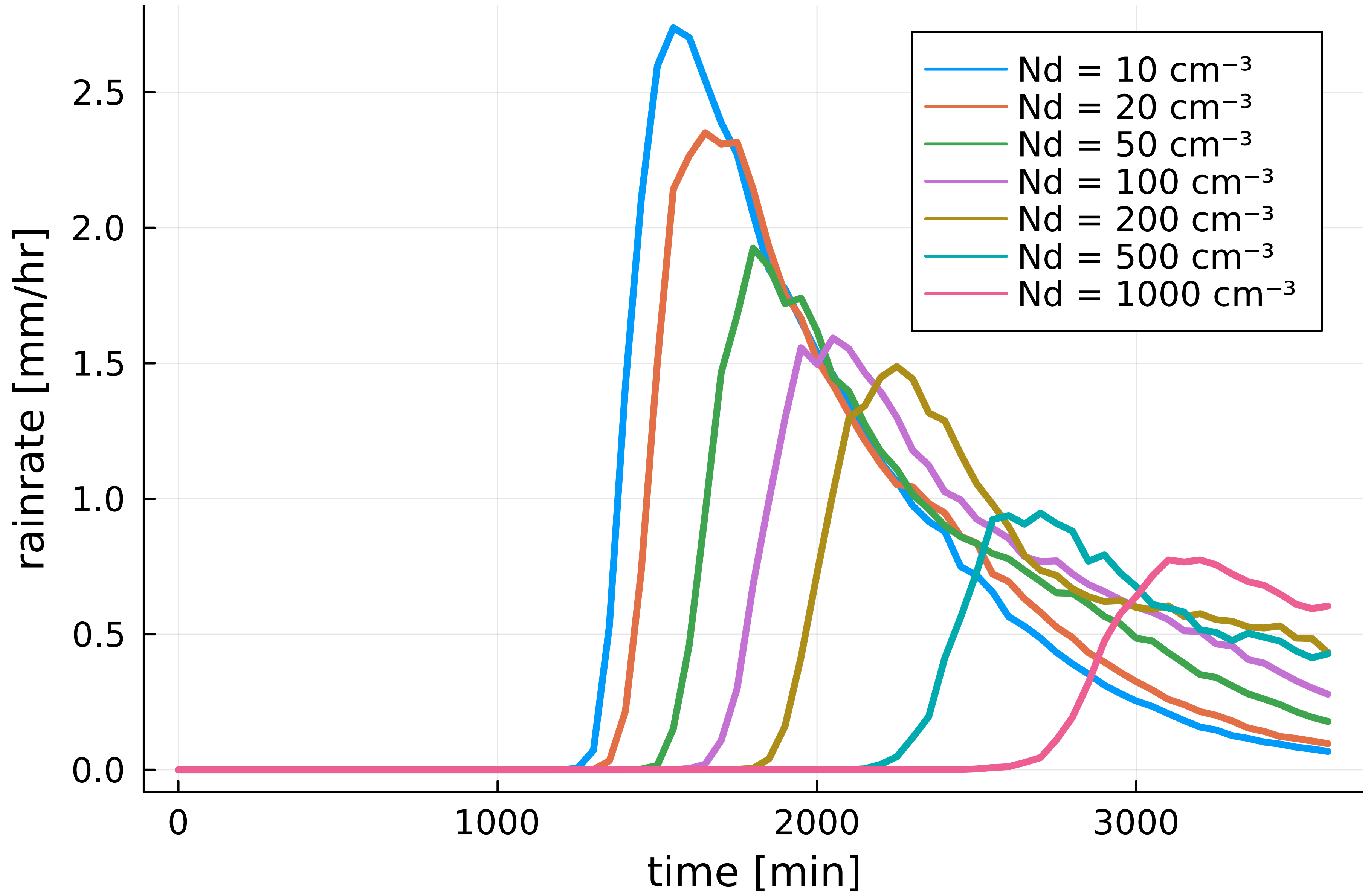
Shima et. al., *QJRMS* 2009: The super-droplet method for the numerical simulation of clouds and precipitation: A particle-based and probabilistic microphysics model coupled with a non-hydrostatic model
Arabas et. al., *GMD* 2015: libcloudph++ 1.0: a single-moment bulk, double-moment bulk, and particle-based warm-rain microphysics library in C++
Jaruga and Pawlowska, *GMD* 2018: libcloudph++ 2.0: aqueous-phase chemistry extension of the particle-based cloud microphysics scheme
Shima et. al., *GMD* 2020: Predicting the morphology of ice particles in deep convection using the super-droplet method: development and evaluation of SCALE-SDM 0.2.5-2.2.0/2.2.1

Machine learning for cloud microphysics

Sajjad Azimi
Postdoc Caltech

- 1D rain shaft with prescribed updraft speed and fixed temperature profile
- A library of rainshaft particle-based simulations with varying updraft speed and droplet concentration



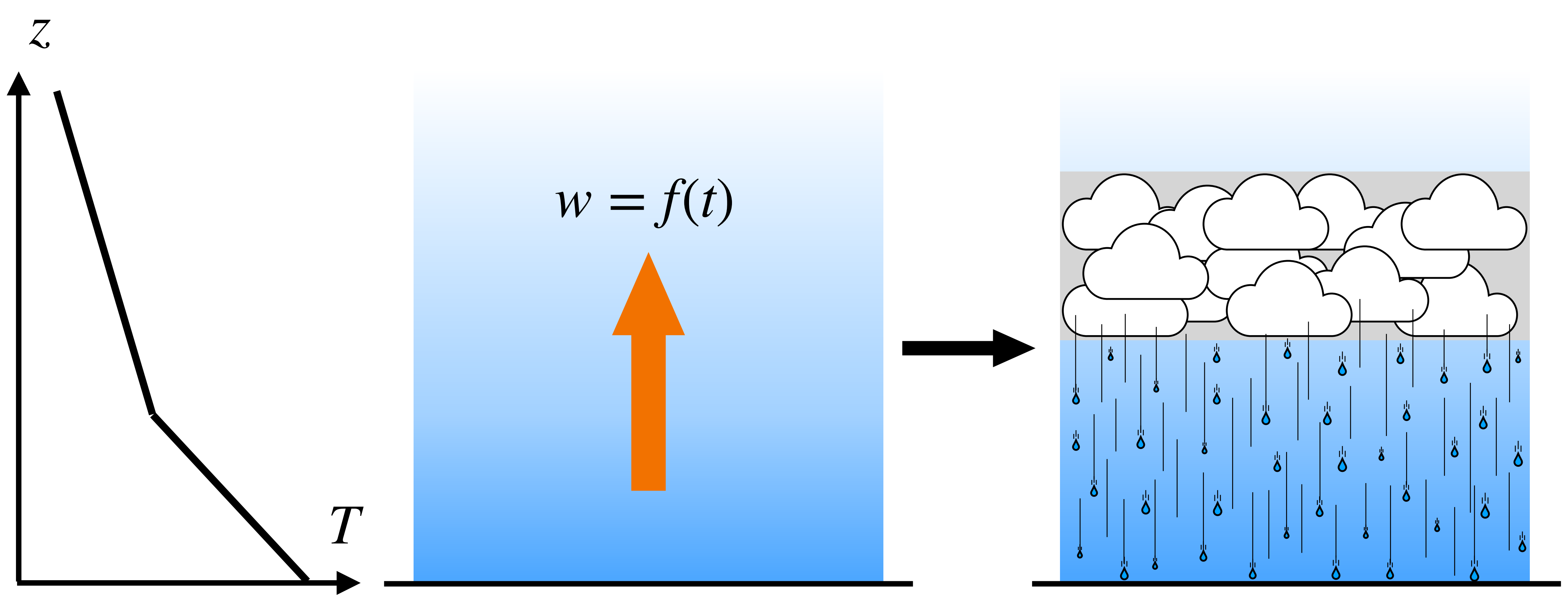


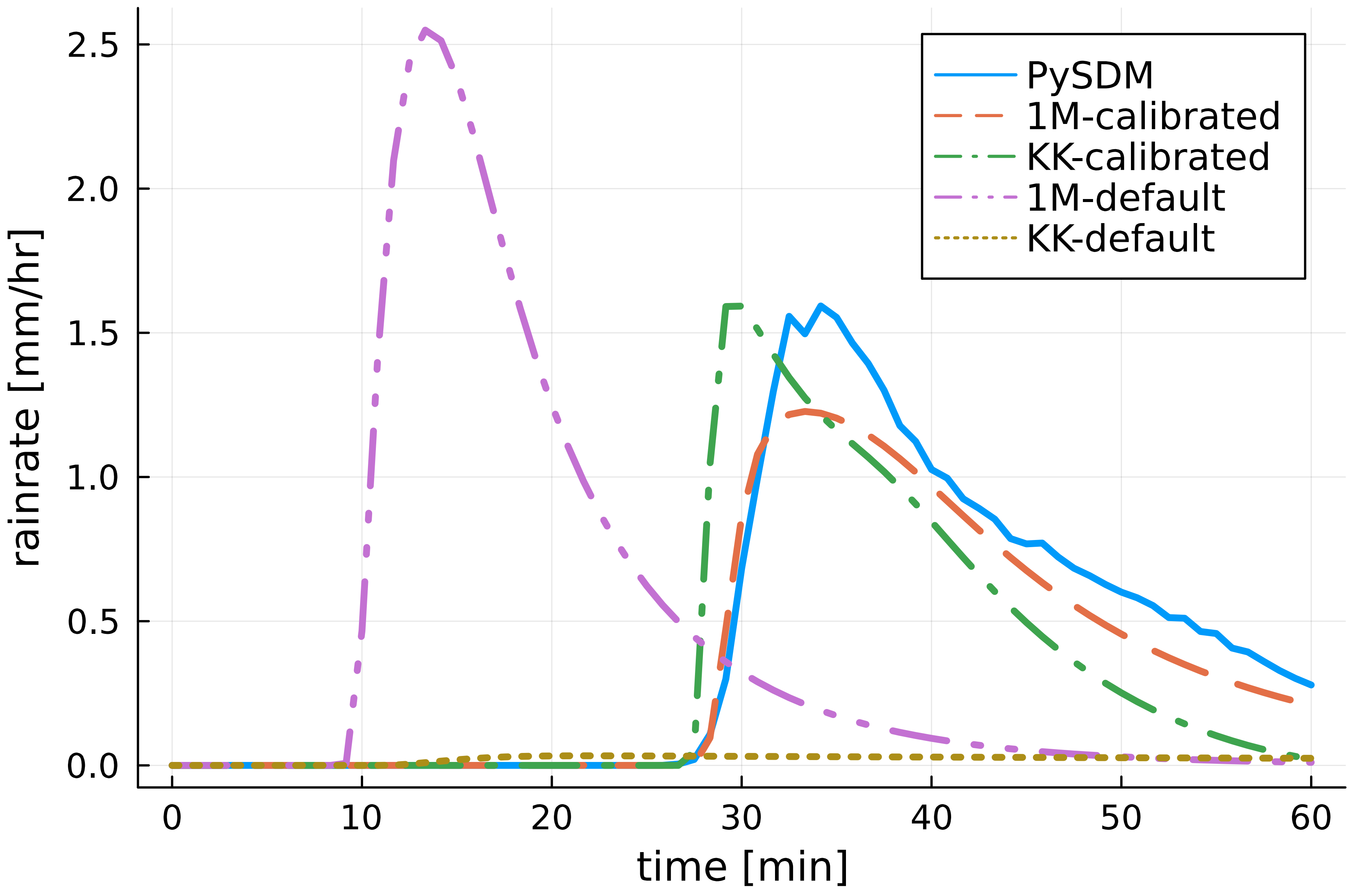
Bartman et al *JOSS* 2021: PySDM v1 particle-based cloud modeling package for warm-rain microphysics and aqueous chemistry
Shipway and Hill *QJRMS* 2012: Diagnosis of systematic differences between multiple parametrizations of warm rain microphysics using a kinematic framework

Machine learning for cloud microphysics

Sajjad Azimi
Postdoc Caltech

- 1D rain shaft with prescribed updraft speed and fixed temperature profile
- A library of rainshaft particle-based simulations with varying updraft speed and droplet concentration
- Working on calibrations of 1M and 2M schemes





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

- **CLIMAParameters.jl** - storage for our free parameters
- **Thermodynamics.jl** - thermodynamics relations, saturation adjustment
- **CloudMicrophysics.jl** - aerosol activation, 0 and 1 moment microphysics
- **TurbulenceConvection.jl** - SGS turbulence, single column simulations setup
- **CalibrateEDMF.jl** - pipeline for calibrating TurbulenceConvection.jl
- **EnsembleKalmanProcesses.jl** - UQ and optimisation algorithms
- **Kinematic1D.jl** - testing sandbox for microphysics
- **Cloudy.jl** - multi-moment cloud microphysics

- **PySDM** - super-droplet algorithm implementation
- **PySDM-examples** - example PySDM simulation setups (0D, KiD-1D, KiD-2D)

Thank you for your attention!

Anna Jaruga KITP 2022

Caltech

CliMA
CLIMATE MODELING ALLIANCE