ML-Enhanced Unified Ice Microphysics Scheme Development

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February 14, 2024

CESM Atmosphere Working Group Meeting

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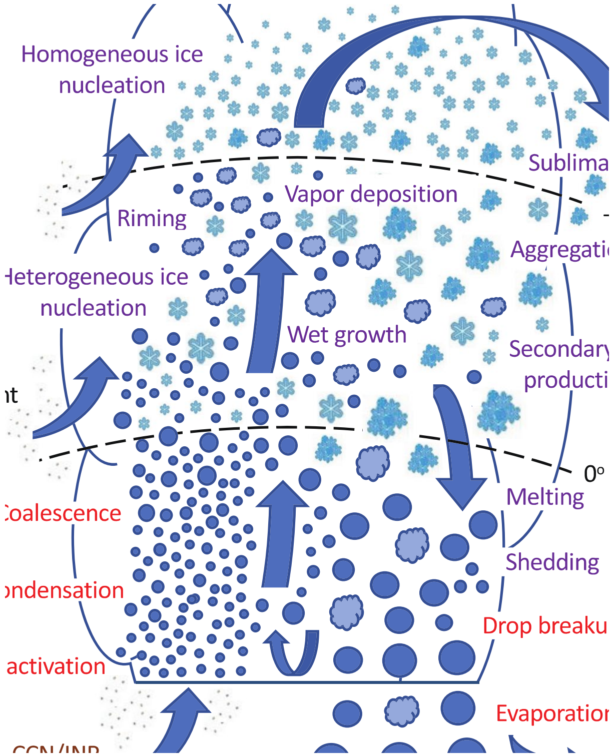
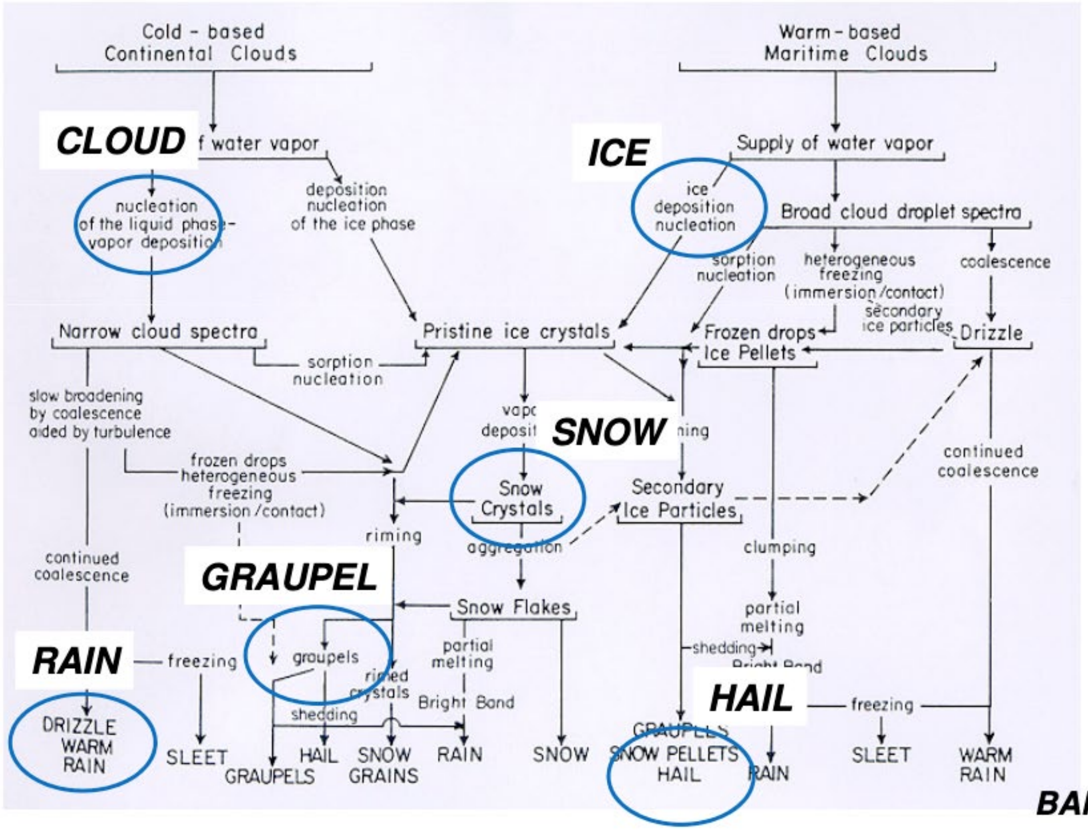
Issues with existing ice microphysics schemes

We don't know all of the physics



We don't know how to represent these processes in models

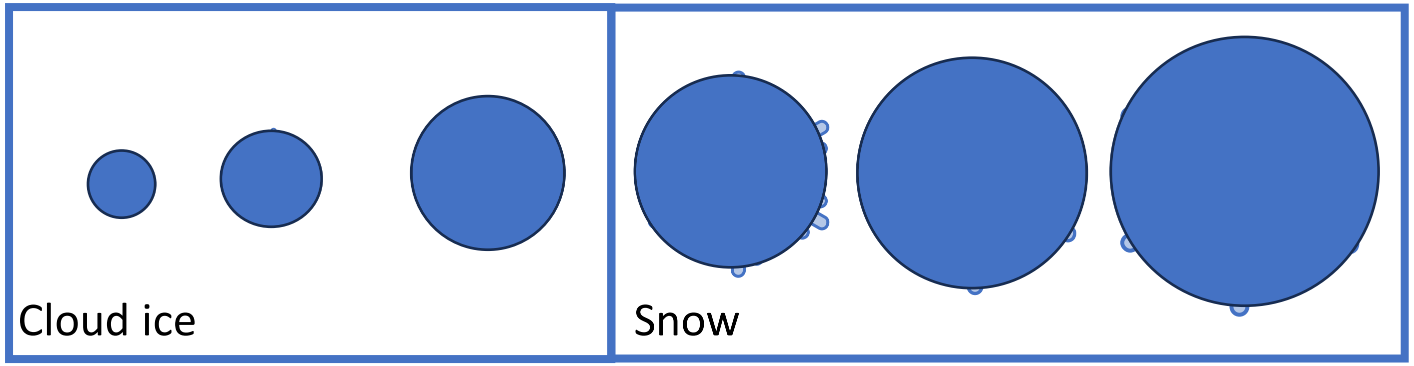


BAMS, 1967

Morrison et al. 2020, JAMES

Representation of ice microphysics in global models

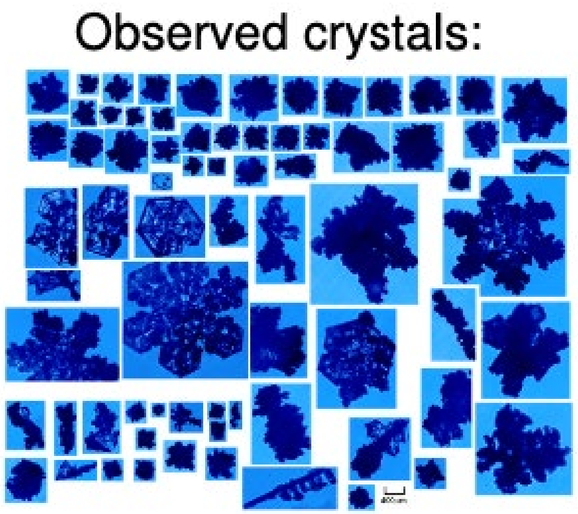
Traditional bulk approaches



- MG2 microphysics scheme [Gettelman and Morrison, 2015; Gettelman et al. 2015]
- 2 hydrometeor categories for ice (cloud ice & snow)
- Ice is assumed to be spherical with a fixed mass-dimensional relationship (m-D)

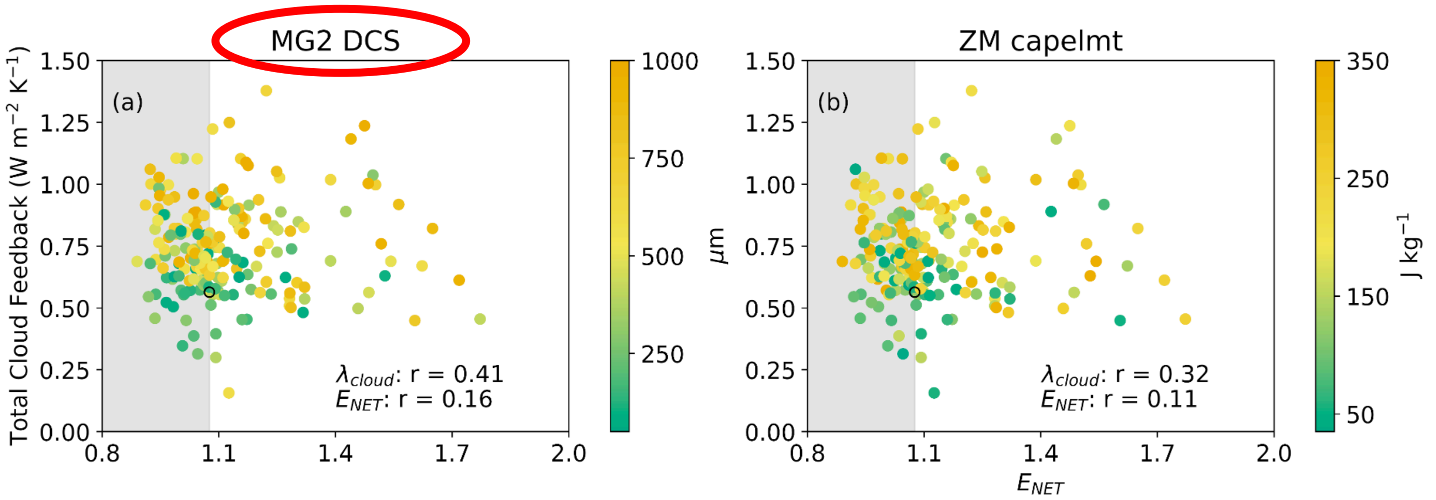
$$m = \alpha D^{\beta}$$

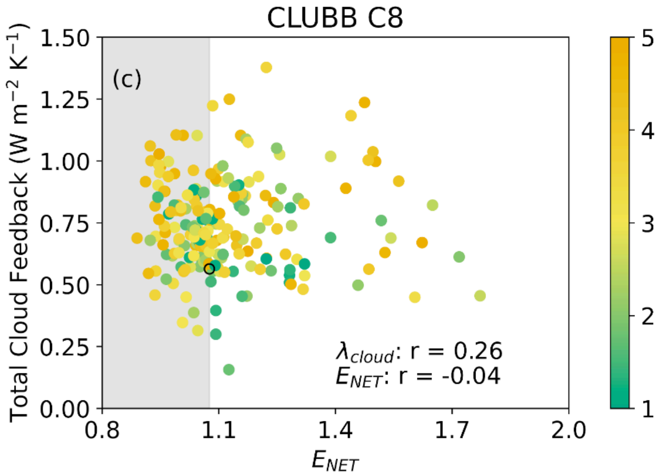
  - Problems:
    - Real ice particles have complex shapes
    - Discrete, abrupt changes in m-D in converting between ice categories
      - Ice-snow autoconversion parameter is unphysical
    - **α** and **β** are uncertain and unphysical over large parameter ranges
    - Constant m-D parameters cannot realistically capture particle growth histories



CESM currently demonstrates significant sensitivity to ice microphysics

- MG2 microphysics scheme [Gettelman and Morrison, 2015; Gettelman et al. 2015]
- Parametric and structural uncertainty
  - Ice to snow auto-conversion threshold is unphysical and poorly constrained by observations (D_{CS})
  - Particle mass, projected area, and terminal fall speed not treated consistently
  - Inconsistency between fall speeds, radiative effects of ice crystals
  - Significant sensitivity to ice fall speeds (~5 W/m²) [Mitchell et al. 2008]





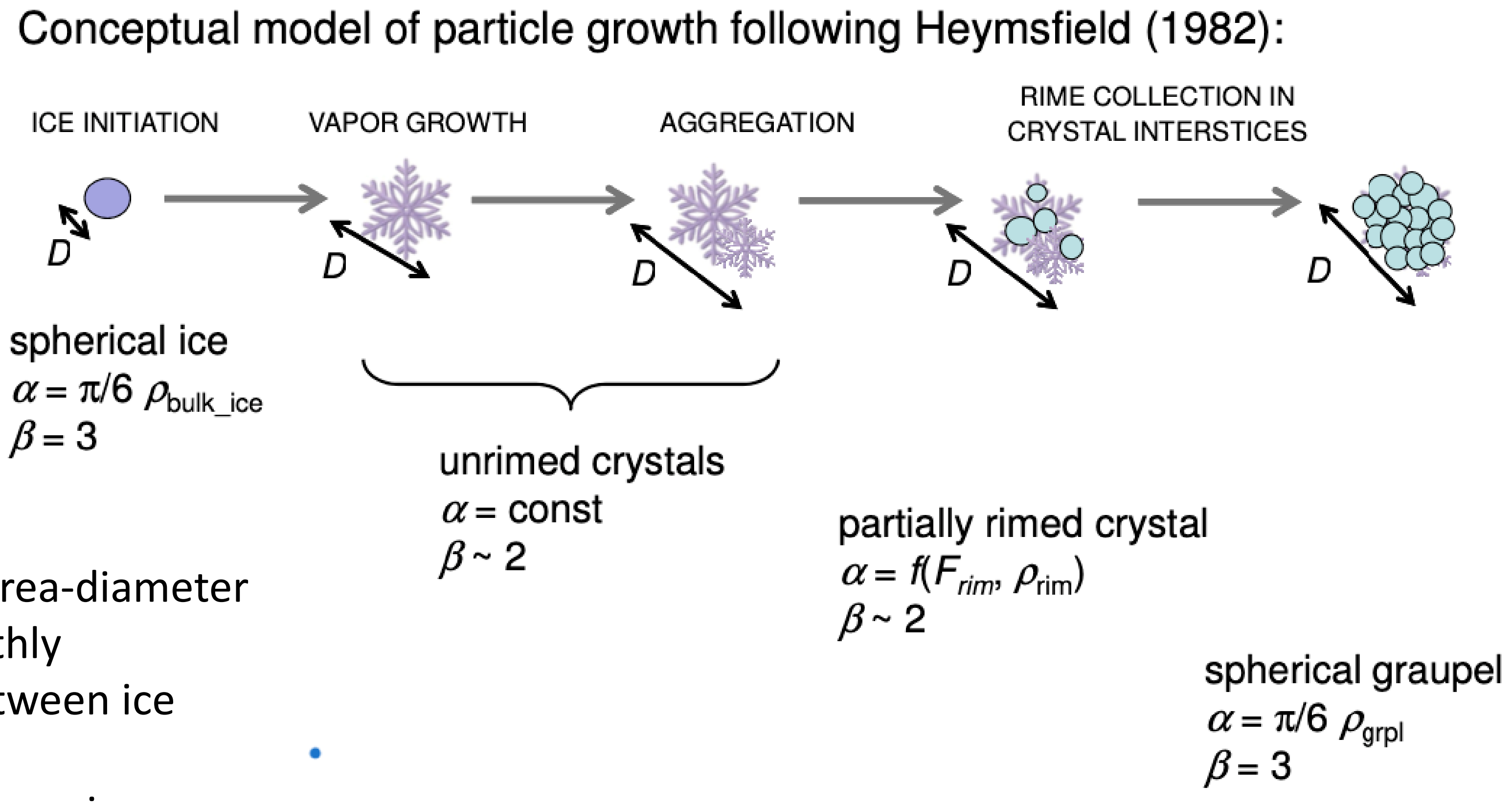
One of the 3 parameters with greatest influence on cloud feedbacks in CAM6 PPE [Duffy et al. 2024] –> need for improved observational and physical basis rather than tuning

E_{net} = scalar error metric of the impact of cloud errors on TOA radiation in the base state [Klein et al. 2013; Zelinka et al. 2022]

[Duffy et al. 2024]

Unified ice microphysics scheme predicts particle properties

Predict particle properties instead [P3 scheme - Morrison and Milbrandt, 2015]



- Allow mass-dimension (m-D) and area-diameter (A-D) relationships to evolve smoothly
- Removes unphysical separation between ice categories
- No abrupt changes due to auto-conversion processes

Figure: J. Milbrandt

Unified ice microphysics scheme implemented in CAM-5

- MG2 modified to be a unified ice microphysics scheme and implemented in CAM5 [Eidhammer et al. 2017]
- Microphysical parameters formulated in terms of m-D and A-D relationships that vary with particle size
- m-D, A-D relationships calculated two different ways:
  - Based on cirrus observations during SPARTICUS field campaign [Erfani and Mitchell, 2016]
  - P3 method [Morrison and Milbrandt, 2015]

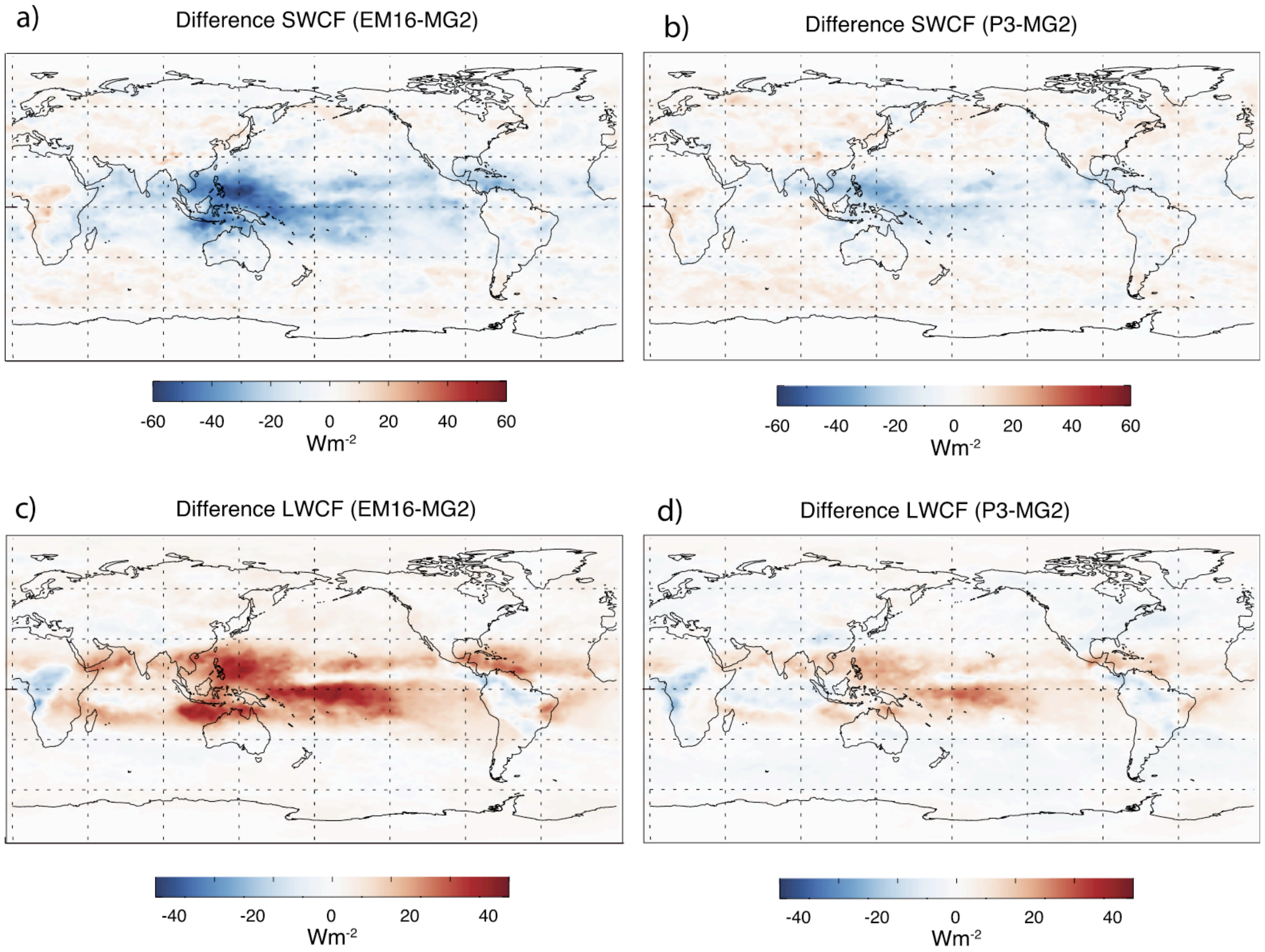
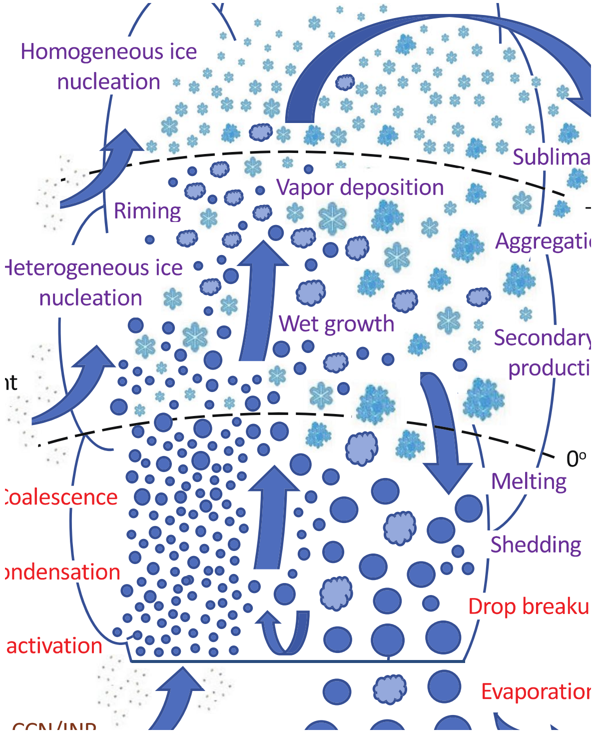


FIG. 2. Differences in zonal mean (a),(b) SWCF and (c),(d) LWCF between MG2 and either (left) EM16 or (right) P3.

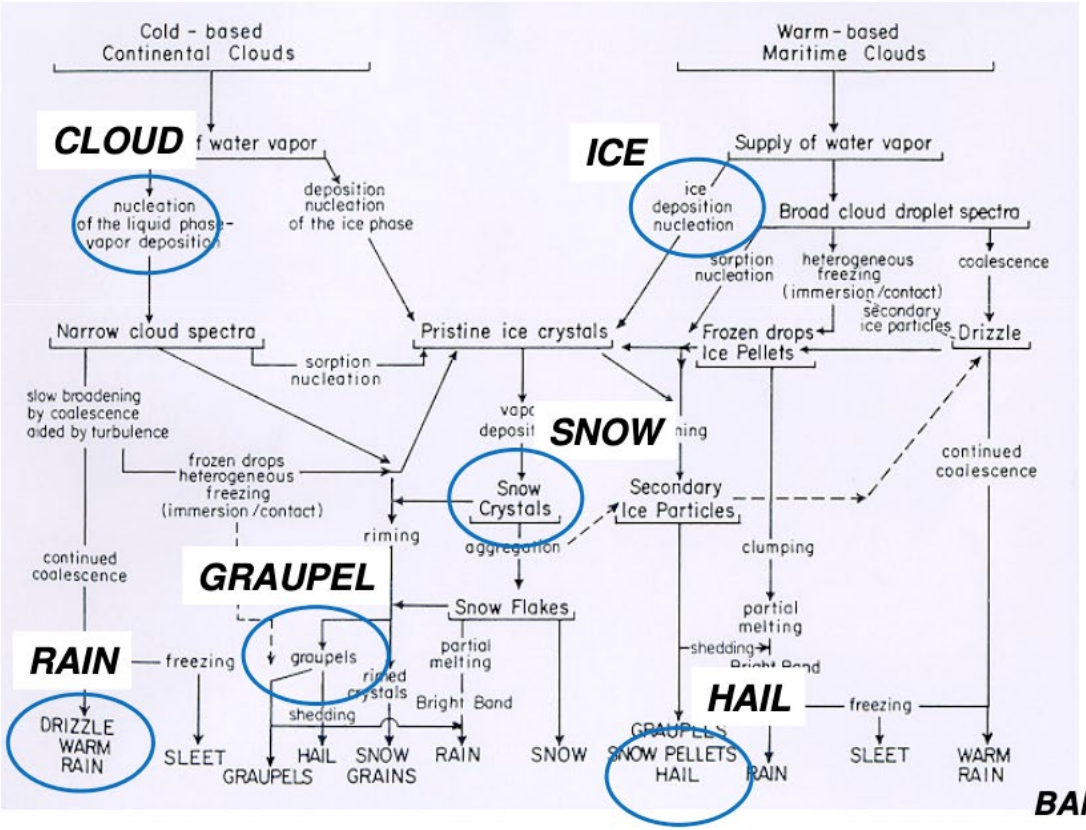
[Eidhammer et al. 2017]

Our work: ML-Enhanced Unified ice microphysics scheme

1. Improved physical basis for ice microphysical process rates based on *in situ* observations



2. Unified ice representation informed by *in situ* observations from 12 past aircraft campaigns



BAMS, 1967

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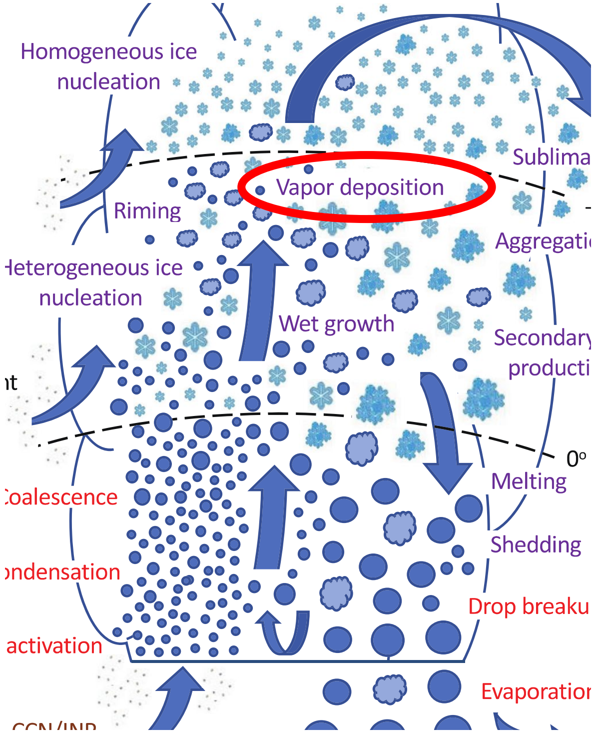

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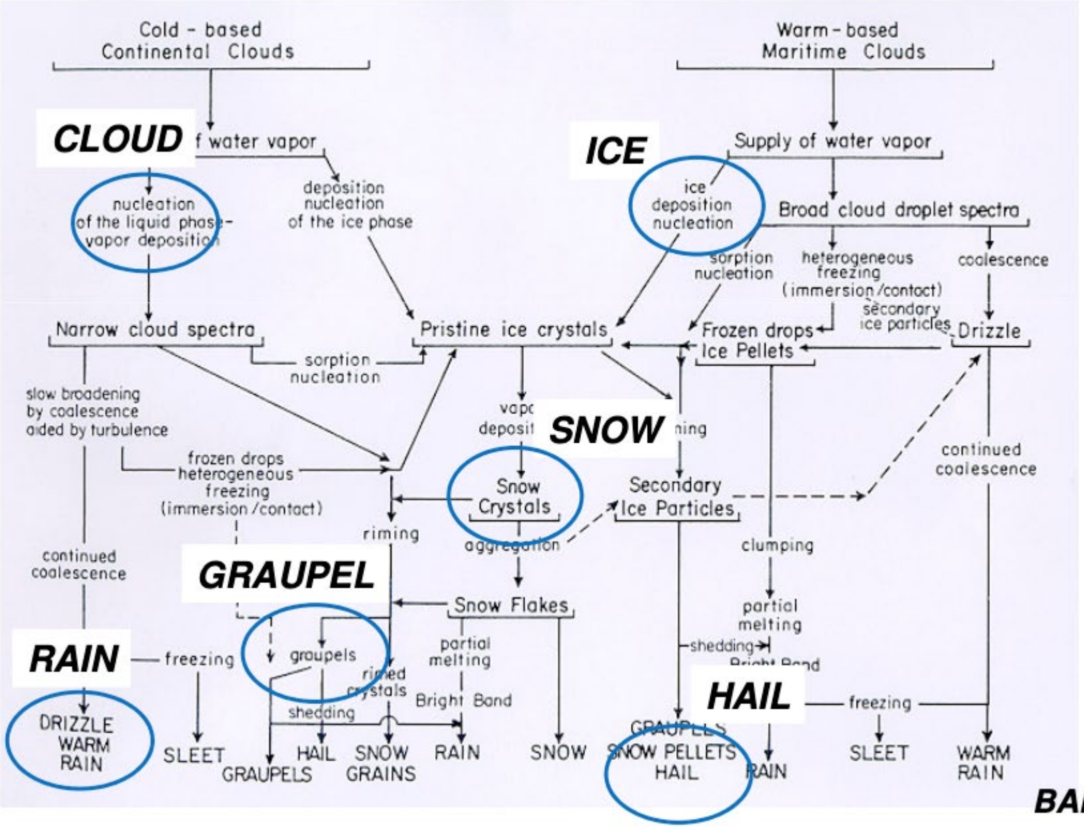


BAMS, 1967

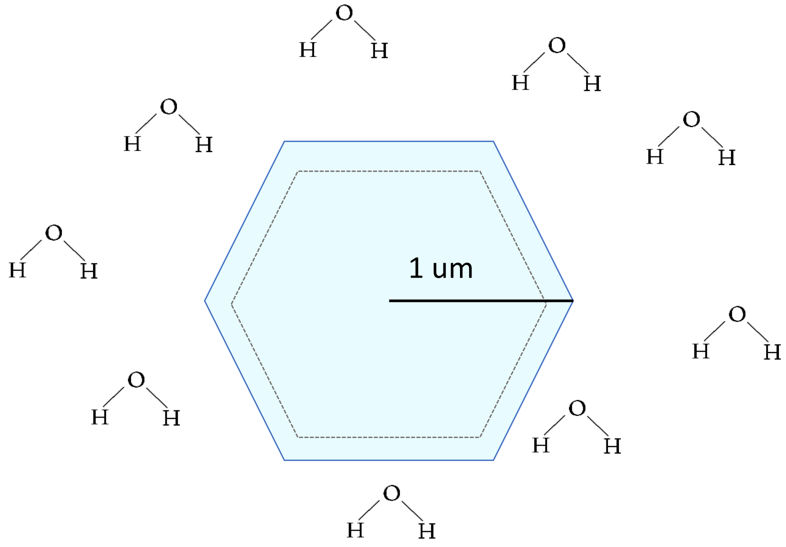
Diffusional growth of ice from vapor

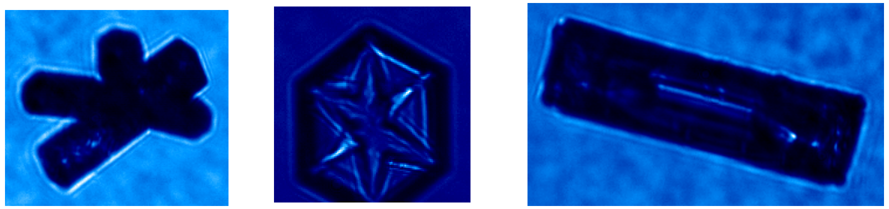
Single crystal ice growth rate for ice growing from vapor includes modifications for the deposition coefficient (through a modified water vapor diffusivity term)

$$\frac{dm_p}{dt} = \frac{4\pi C(S_{ice} - 1)}{\frac{RT_g}{\hat{e}_{ice}(T_g) D_w^* M_w} + LH}$$

$$D_w^* = \frac{D_w}{\frac{r}{(r+\Delta_v)} + \frac{D_w}{r\alpha_D}\left(\frac{w\pi M_w}{RT_a}\right)^{1/2}}$$

Deposition coefficient ($0 < \alpha_D < 1$) – how efficiently water molecules attach to growing ice crystal

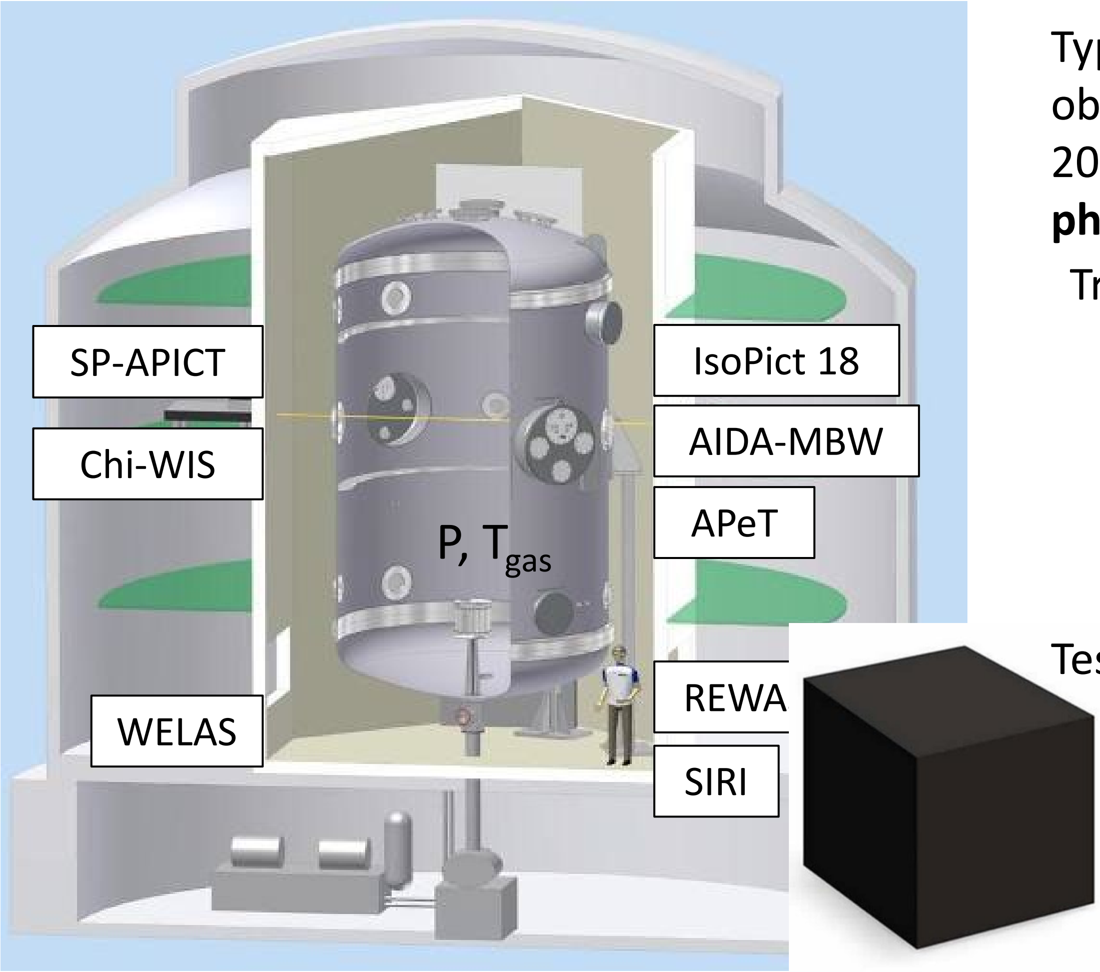




Pruppacher and Klett, 1997

IsoCloud Campaigns (ISOtopic fractionation in CLOUDs)

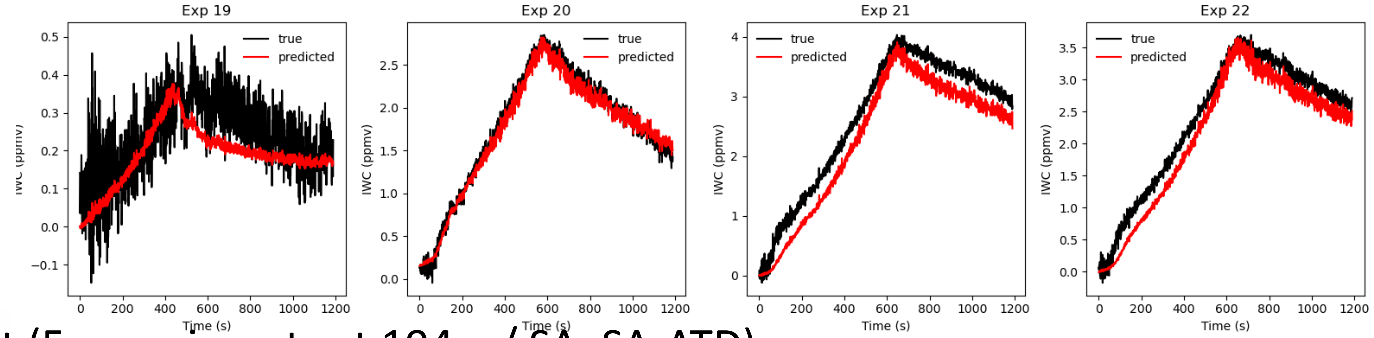
AIDA Aerosol and Cloud Chamber
Karlsruhe Institute of Technology



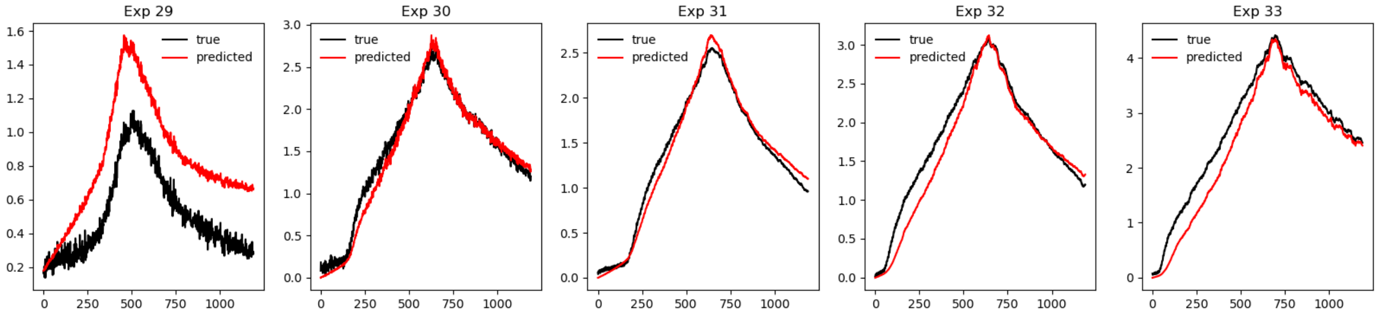
Data sets from 48 adiabatic expansions to form ice clouds (190 - 235 K) with a variety of heterogeneous and homogeneous IN

Typical approaches to evaluate models against cloud chamber observations requires assumptions about ice growth model [Skrotzki et al. 2013; Lamb et al. 2023]. **Can we use machine learning to learn unknown physics without a priori assumptions about the ice growth model**?

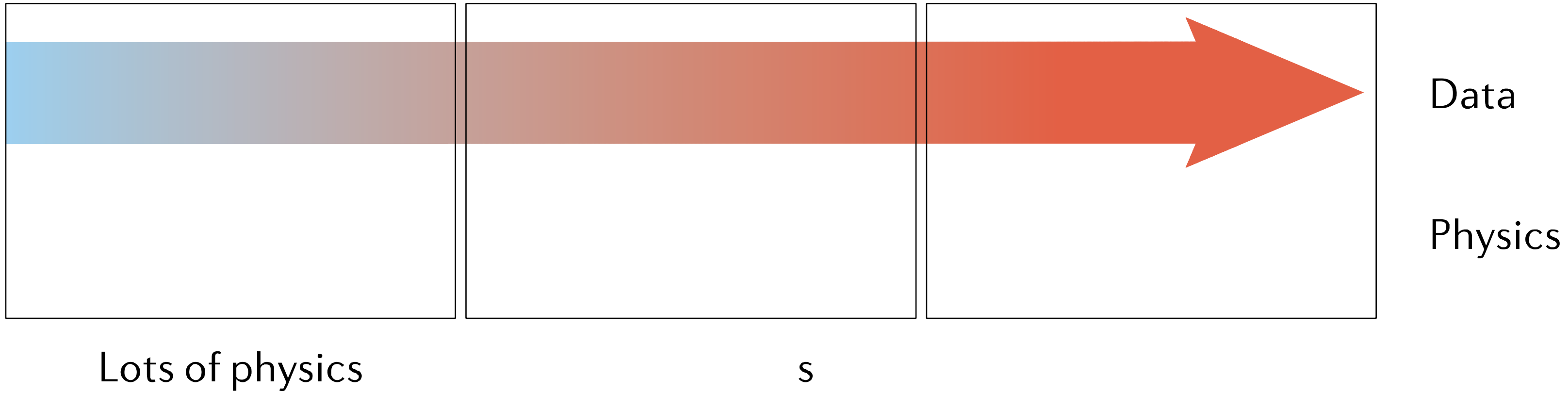
Train (4 experiments w/ ATD at 194 K)

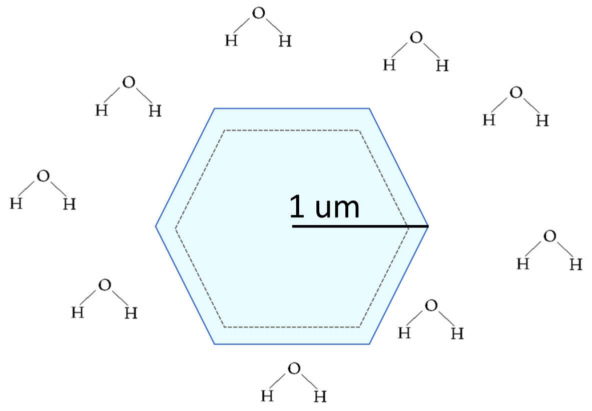


Test (5 experiments at 194 w/ SA, SA-ATD)

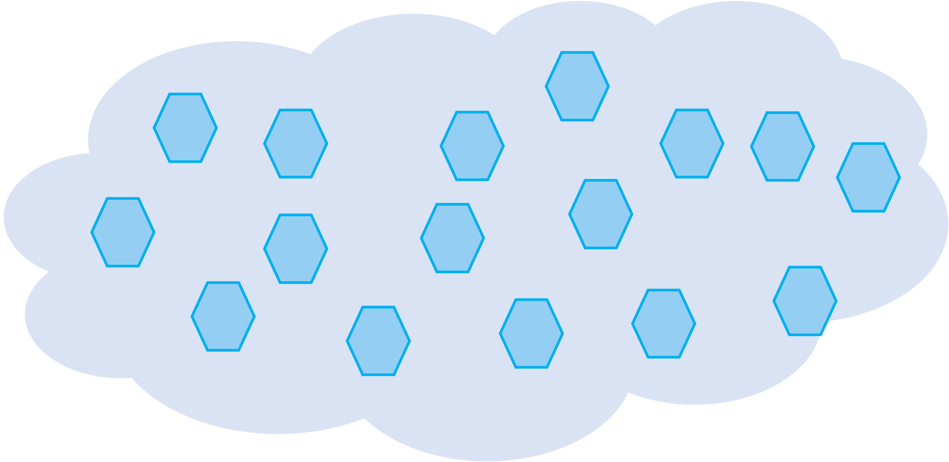


Add physics to machine learning model to improve interpretability!





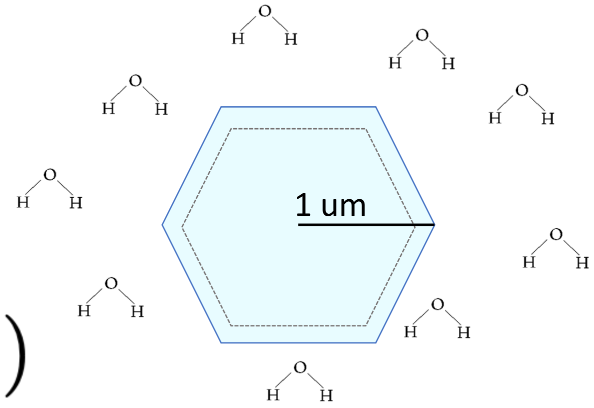
We want to know the structure of the **single particle mass growth rate** but observations only provide constraints on **integrated ice water mass per volume in the entire cloud**



Can we use a hybrid-physics machine learning model to directly learn about parameters in the single crystal ice growth equation?

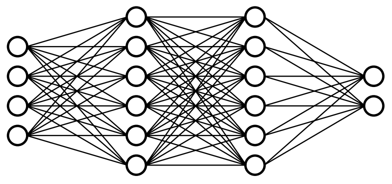
Figure from Karniadakis et al. Nat. Rev. Phys. 2021

Hybrid machine learning physics modeling for depositional ice growth



$$\frac{dm_p}{dt} = \frac{4\pi C(S_{ice} - 1)}{\frac{RT_g}{\hat{e}_{ice}(T_g) D_w^* M_w} + LH}$$

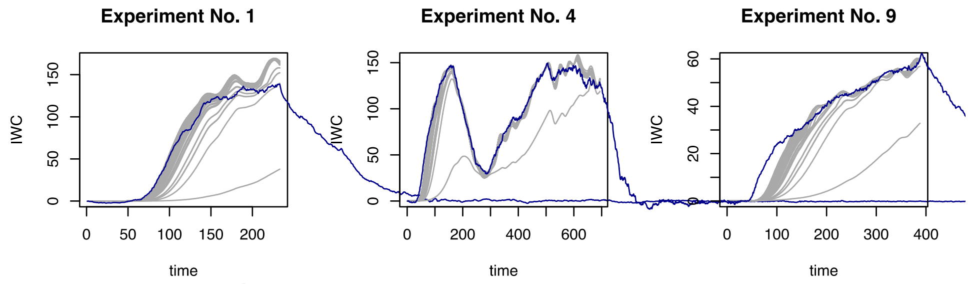
$$D_w^* = \frac{D_w}{\frac{r}{(r+\Delta_v)} + \frac{D_w}{r\alpha_D}\left(\frac{w\pi M_w}{RT_a}\right)^{1/2}}$$



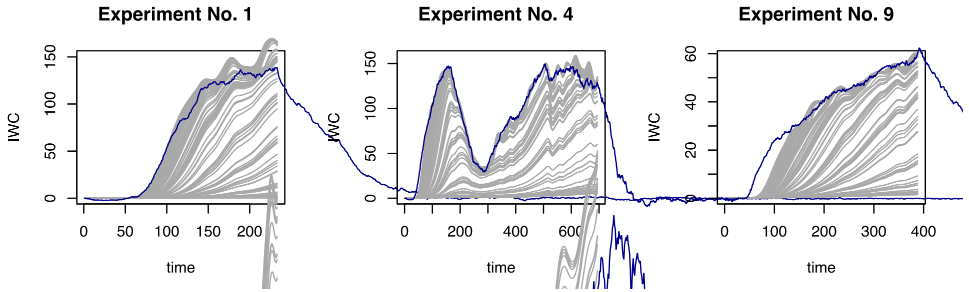
$$\alpha_D = f(S, T|\theta)$$

$$\log(\alpha_D) = f(S, T|\theta)$$

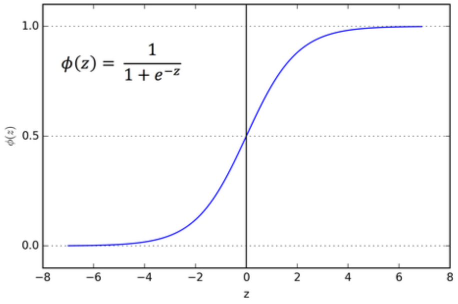
$\alpha \sim \mathscr{U}[0,1]$



$\log \alpha \sim \mathscr{U}[log(0.001), \log(1)]$



Sigmoid activation at final layer



K.D. Lamb, J.Y. Harrington, J. Mikhaeil, et al. "Reducing Structural Uncertainty in Depositional Ice Growth Models Using Neural Ordinary Differential Equations." In prep.

Neural ODE's to solve ODE's with an unknown functional form

- Parametrize derivative of a hidden state using a neural network (neural network acts a universal function approximator)

$$\frac{d\mathbf{h}(t)}{dt} = f(\mathbf{h}(t), t, \theta)$$

- NODE's perform efficient backpropagation through ODE solvers using adjoint sensitivity method [Pontryagin et al. 1962]

$$\begin{aligned} \mathbf{z}_{t_0} &\sim p(\mathbf{z}_{t_0}) \\ \mathbf{z}_{t_1}, \mathbf{z}_{t_2}, \ldots, \mathbf{z}_{t_N} &= \text{ODESolve}(\mathbf{z}_{t_0}, f, \theta_f, t_0, \ldots, t_N) \\ \text{each} \quad \mathbf{x}_{t_i} &\sim p(\mathbf{x}|\mathbf{z}_{t_i}, \theta_{\mathbf{x}}) \end{aligned}$$

Neural Ordinary Differential Equations

Ricky T. Q. Chen*, Yulia Rubanova*, Jesse Bettencourt*, David Duvenaud
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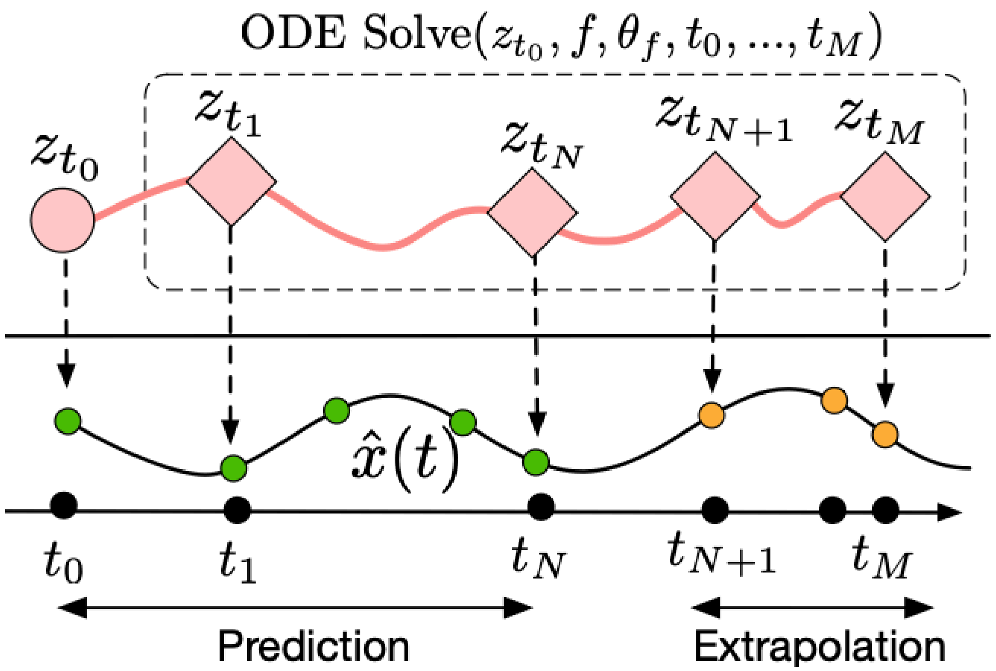
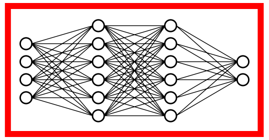
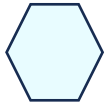


Integrate hybrid model for ice of different sizes growing simultaneously

N_1

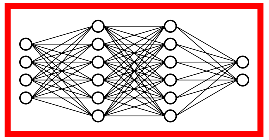
$$m_1(t) = \int_0^t \frac{dm_1}{dt} dt + m_1(t=0)$$





N_2

$$m_2(t) = \int_0^t \frac{dm_2}{dt} dt + m_2(t=0)$$



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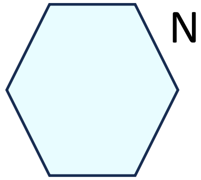
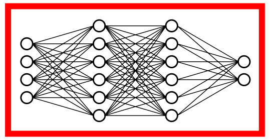
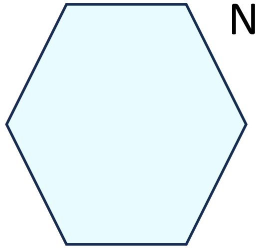


N_{n-1}

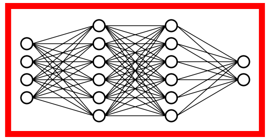
$$m_{n-1}(t) = \int_0^t \frac{dm_{n-1}}{dt} dt + m_{n-1}(t=0)$$





N_n

$$m_n(t) = \int_0^t \frac{dm_n}{dt} dt + m_n(t=0)$$



- Implemented in PyTorch
- NN for $\boldsymbol{\alpha}_D$ for each ice crystal share the same weights
- Back-propagation through all the ice bins to optimize NN weights for all ice crystals simultaneously

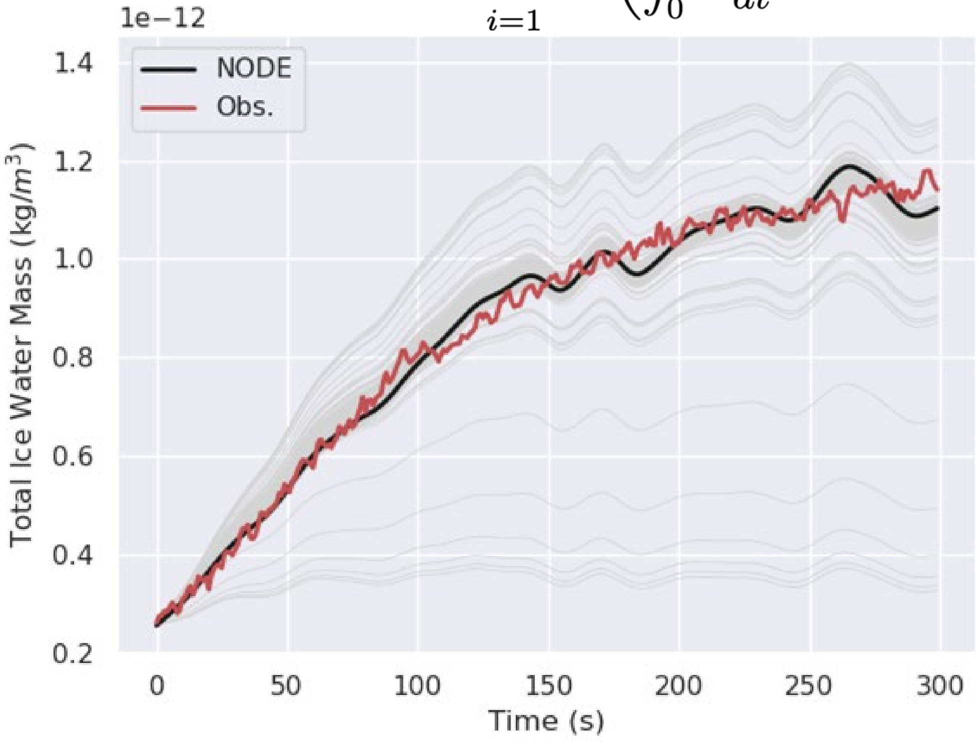
$$IWC = \sum_{i=1}^{n} N_i \left(\int_0^t \frac{dm_i}{dt} dt + m_i(t=0) \right)$$

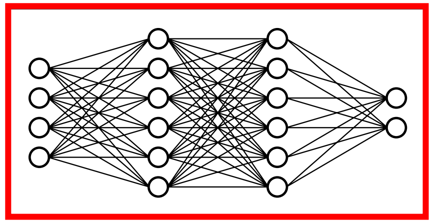
K.D. Lamb, J.Y. Harrington, J. Mikhaeil, et al. “Reducing Structural Uncertainty in Depositional Ice Growth Models Using Neural Ordinary Differential Equations.” In prep.

NODE model optimized to cloud chamber observations

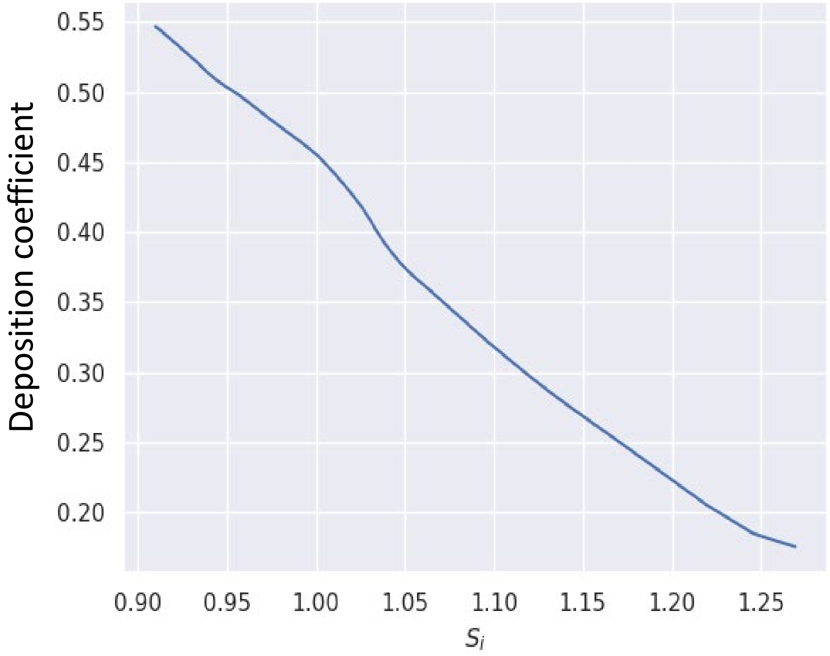
Use neural network with optimized weights to look at functional dependence of $\boldsymbol{\alpha}_D$ on S_i and T

$$IWC = \sum_{i=1}^{n} N_i \left(\int_0^t \frac{dm_i}{dt} dt + m_i(t=0) \right)$$





$$Log(\alpha_D) = f(S, T|\theta)$$



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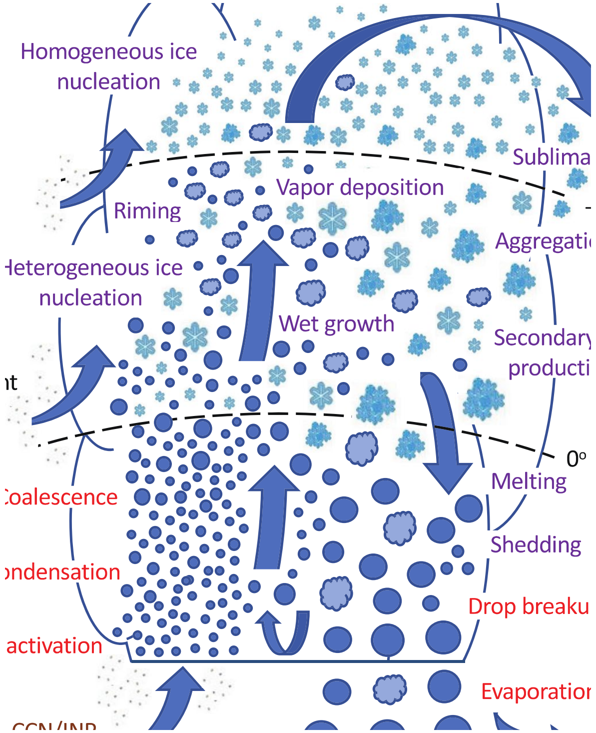
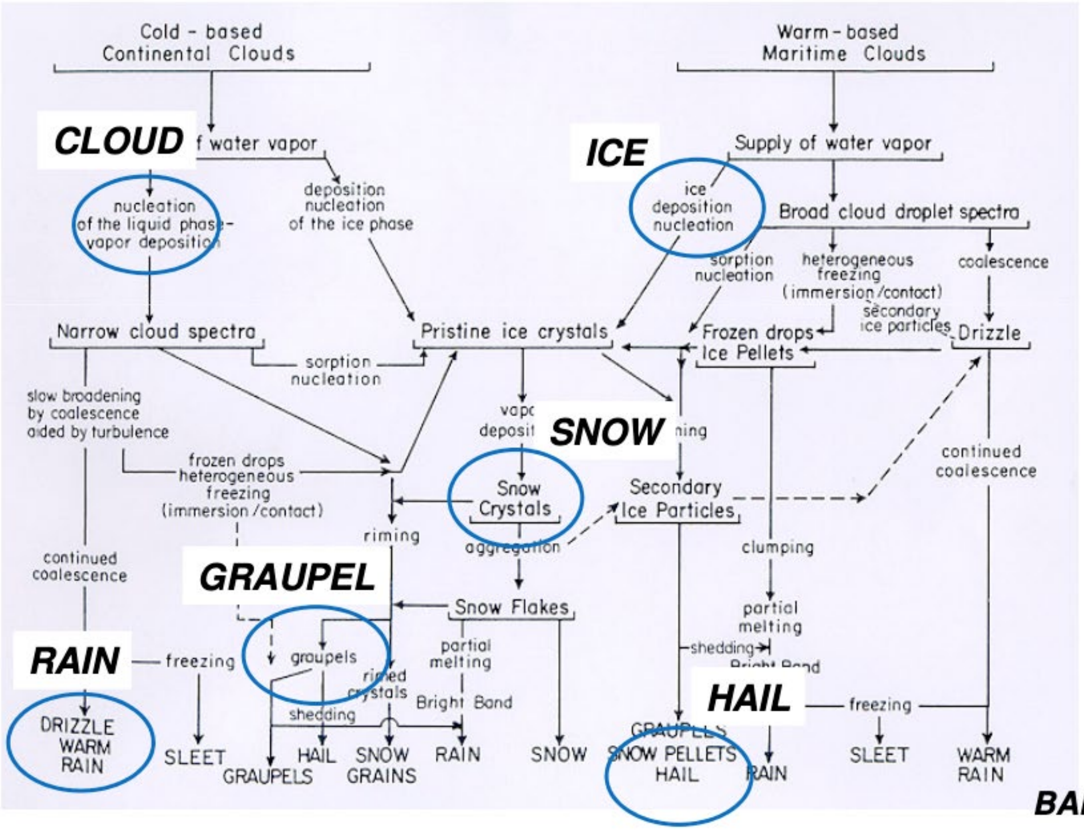
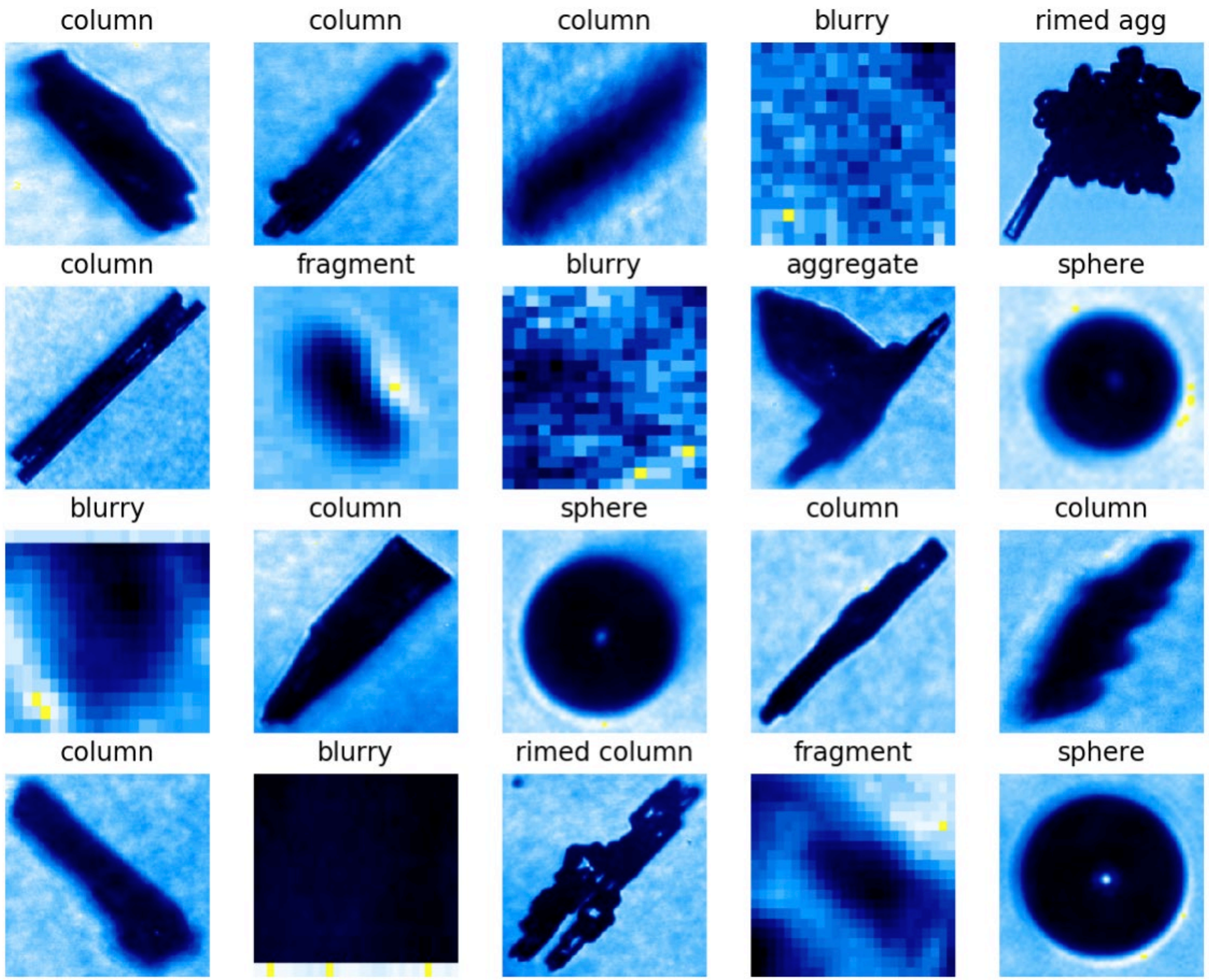


2. Unified ice representation informed by *in situ* observations from 12 past aircraft campaigns



BAMS, 1967

In situ observations from NASA & DOE aircraft campaigns



COCPIT - Classification of Cloud Particle Imagery and Thermodynamics

XCITE
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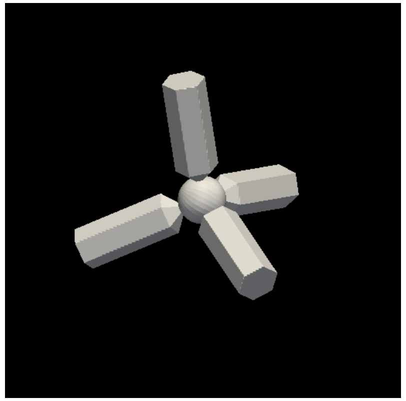
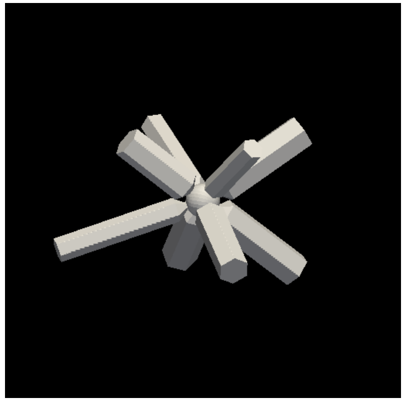
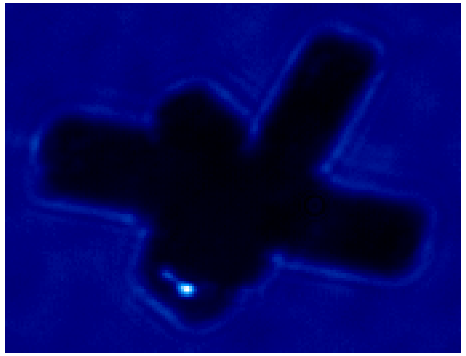
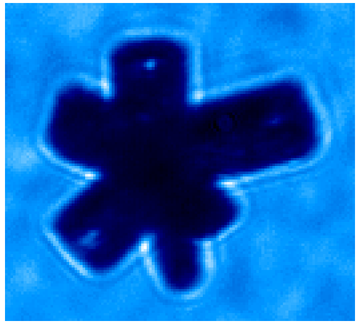
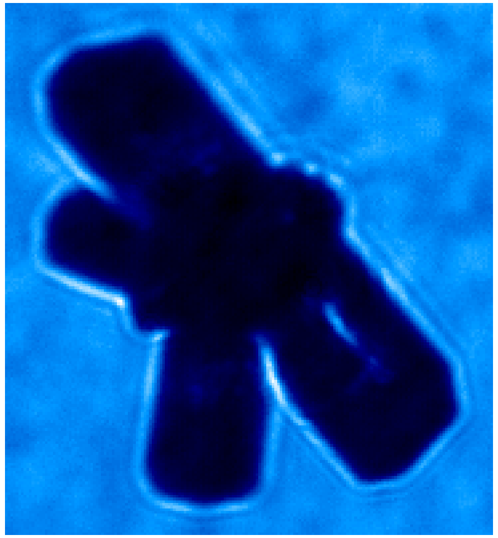
Computer vision methods applied to CPI images

- Consistent m-D and A-D relationships derived from observations
- Internally consistent particle fall-speeds and optical properties
- Significantly improved observational basis, including 12 flight campaigns
- Exploration of alternative approaches to characterize m-D, A-D (unsupervised learning of ice categories using data-driven approaches)

Outlook and Future Work

- Ice microphysical processes remain a major source of uncertainty in the CESM
- Both unknown physics and model representation need to be addressed
- We are re-evaluating past observations of ice processes to reduce structural uncertainty in microphysical processes using hybrid-physics machine learning approaches
- We are also developing updated mass-size and area-dimension relationships using computer vision methods applied to a data base of CPI images from past aircraft campaigns (See Joseph Ko's talk next!)

- Next steps: update unified ice microphysics scheme with expanded observational basis for ice processes
- Evaluation : compare PPE of updated CESM+ML-Enhanced Unified Ice Scheme with CESM-PPE [Eidhammer et al. 2024]

- Collaborations and ideas are welcome!

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