Particle Scattering Focus Group

Report based on

inputs from FG members and review of literatures

A big “Thank You” to Stefan Kneifel

SUMMER SNOWFALL WORKSHOP

Scattering Properties of Realistic Frozen Hydrometeors from Simulations and Observations, as well as Defining a New Standard for Scattering Databases

Stefan Kneifel, José Dias Neto, Davide Ori, Dmitri Moisseev, Jani Tyynelä, Ian S. Adams, Kwo-Sen Kuo, Ralf Bennartz, Alexis Berne, Eugene E. Clothiaux, Patrick Eriksson, Alan J. Geer, Ryan Honeyager, Jussi Leinonen, and Christopher D. Westbrook

The International Summer Snowfall Workshop (ISSW) is a new workshop format for the international scientific community working on ground- and space-based observations, retrievals, and radiative transfer related to snowfall. This new snowfall workshop was inspired by the successful series of International Workshops on Space-based Snowfall Measurements (IWSSM; Bennartz et al. 2011), the latest of which (IWSSM-5) was held concurrently with the International Precipitation Working Group (IPWG) meeting in Bologna, Italy, in 2016. The new biennial ISSW is not intended to replace the IWSSM but rather to provide a forum to discuss

FIRST INTERNATIONAL SUMMER SNOWFALL WORKSHOP

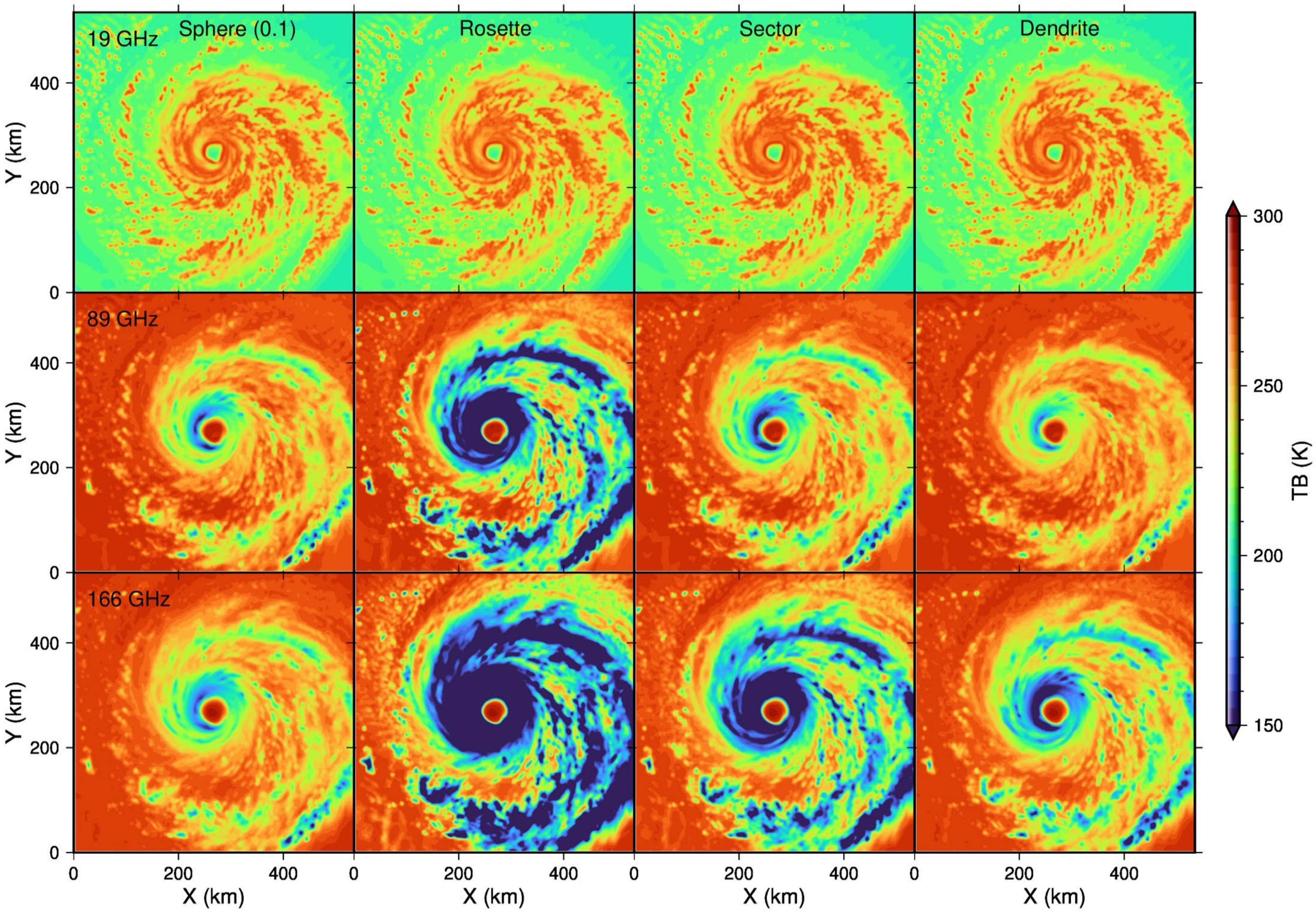
What: The workshop gathered almost 50 scientists from Europe and the United States to discuss the progress toward developing electromagnetic scattering databases for ice and snow particles in the microwave region, their applications, the physical approximations used to compute these scattering properties, and how remote sensing and in situ observations can be used to validate scattering datasets.

When: 28–30 June 2017

Where: Cologne, Germany

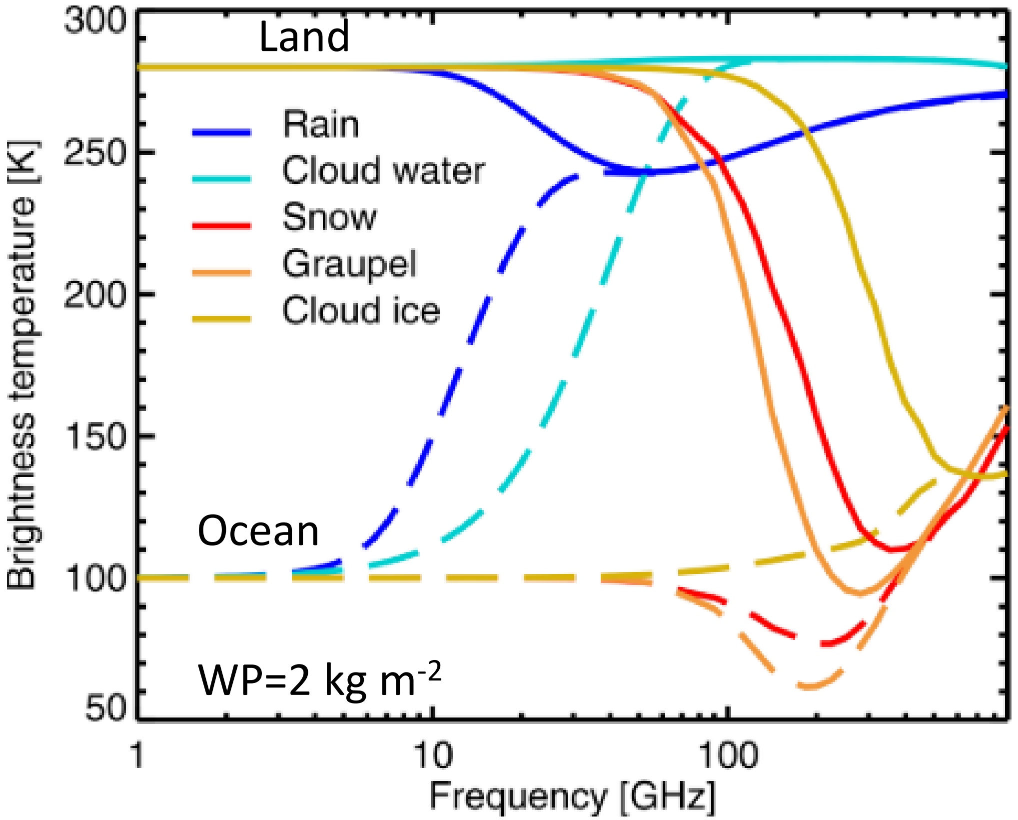
Importance for radiometer observations

TBs calculated from WRF simulation of hurricane Rita, assuming different particle shapes

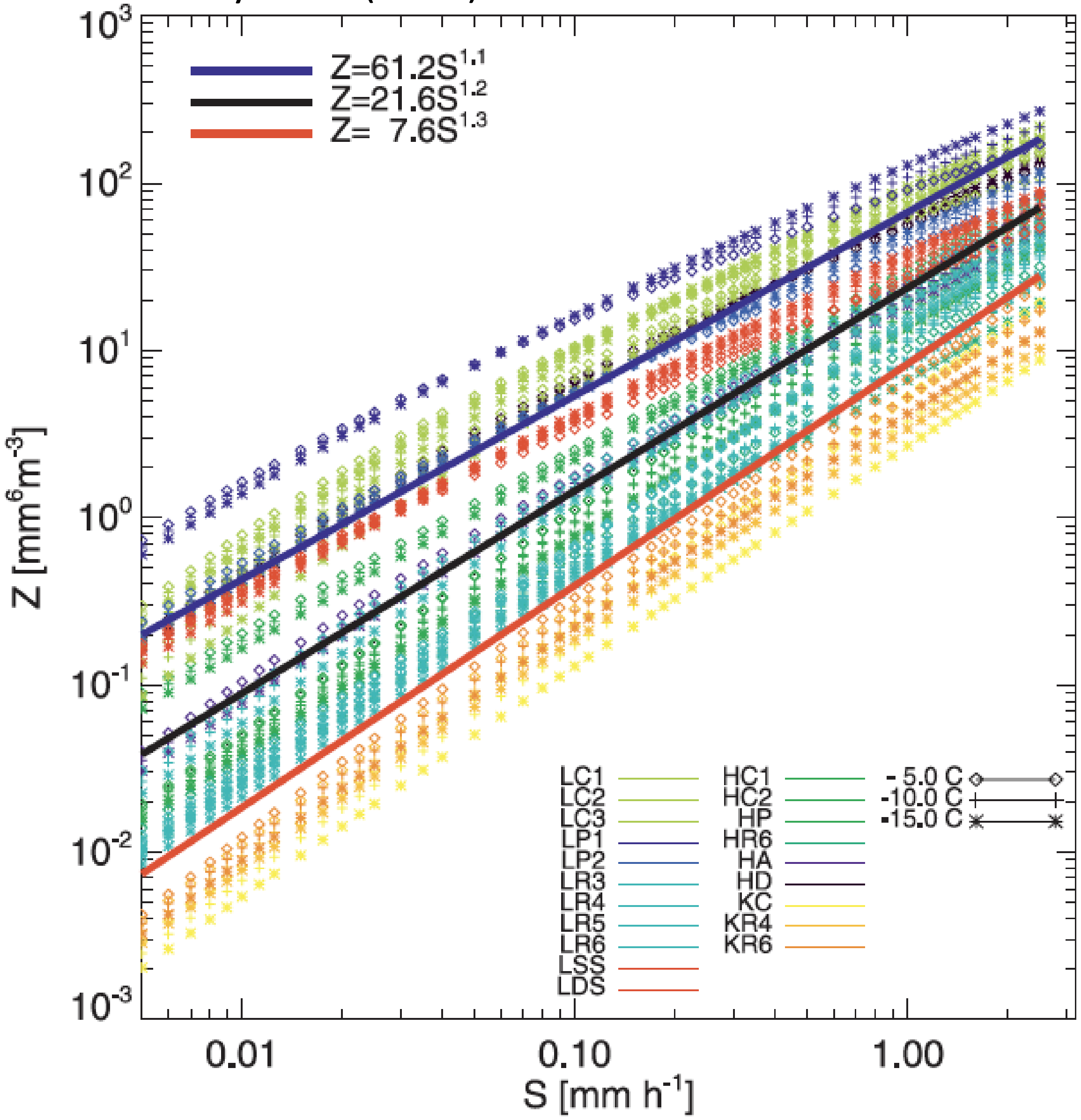


Importance for radiometer & radar observations

RTTOV-SCATT Simulated TBs, assuming different ice shape for snow, graupel and cloud ice (Geer et al. 2021)



Z-S relations, assuming different particle shapes Hiley et al. (2011)

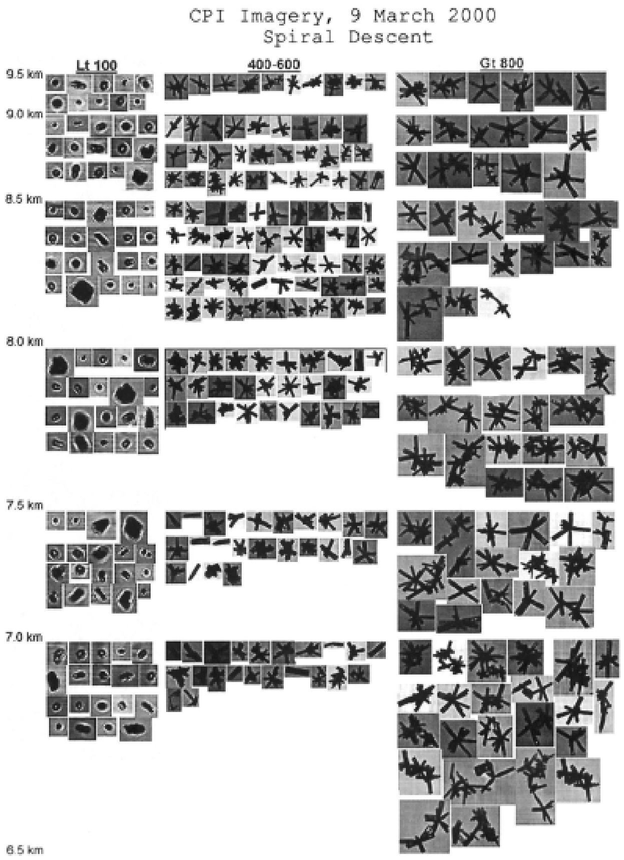


Particle Scattering Focus Group

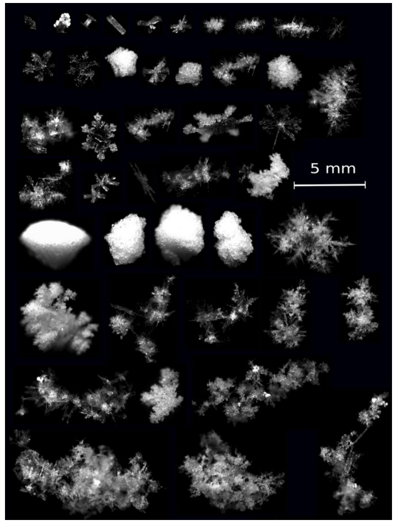
- Goal: Exchange ideas/work on:
  - How to build “radiatively” realistic particles (shape/density/structure/melting etc.) ?
  - How to efficiently compute/approximate their single scattering properties?
  - How to implement these properties in radiative transfer models or radar reflectivity computations?
  - What are the requests from algorithm development group regarding to scattering database?
- Activities:
  - Characterize ice particle shape/density/structure, etc.
  - Generate scattering database
  - Implement scattering database into radiative transfer models, constrained by observations
  - Want to hear: “I’d like to have scattering properties for such type(s) of particles”

Build “models” of particles

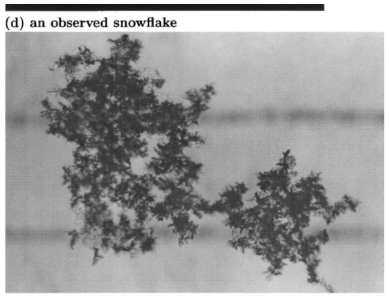
Real Worlds



Field & Heymsfield (2003)



MASC images
by Tim Garrett



Maruyama & Fujiyoshi (2005)

Idealized

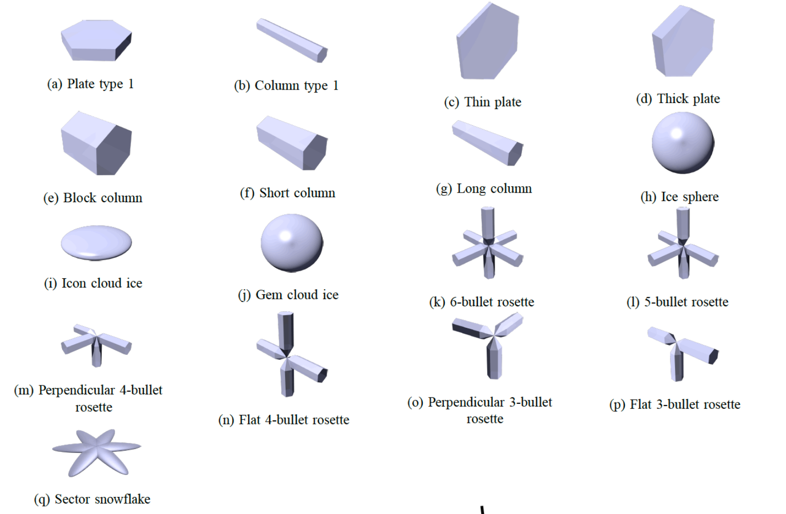
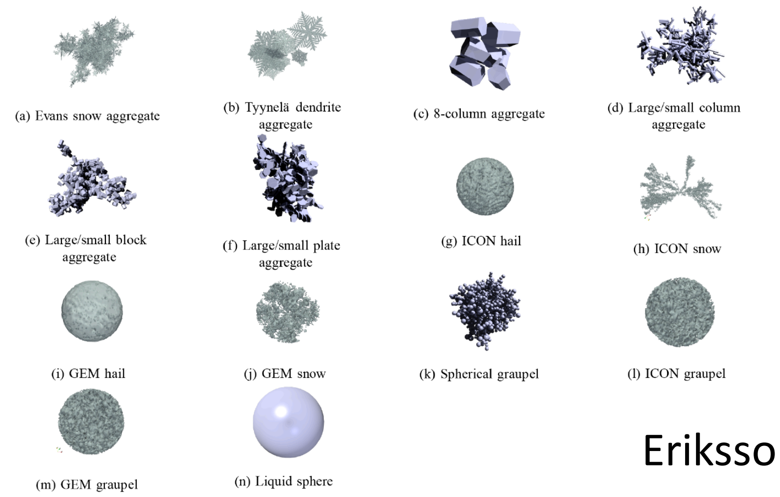


Figure 1. Single crystal habits included in the first database version. Shown particle orientation varies between the habits. Despite images **(h)** and **(j)** looking identical, they depict different particles; gem cloud ice **(j)** is a habit consisting of oblate spheroids with aspect ratio ≈ 0.92.

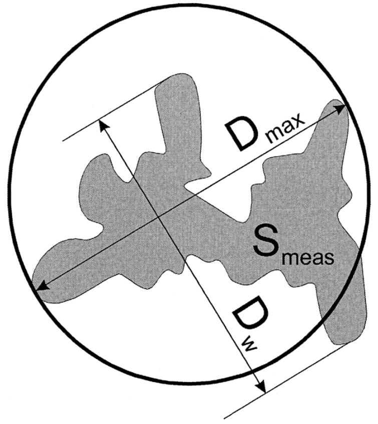


Eriksson et al. (2018)

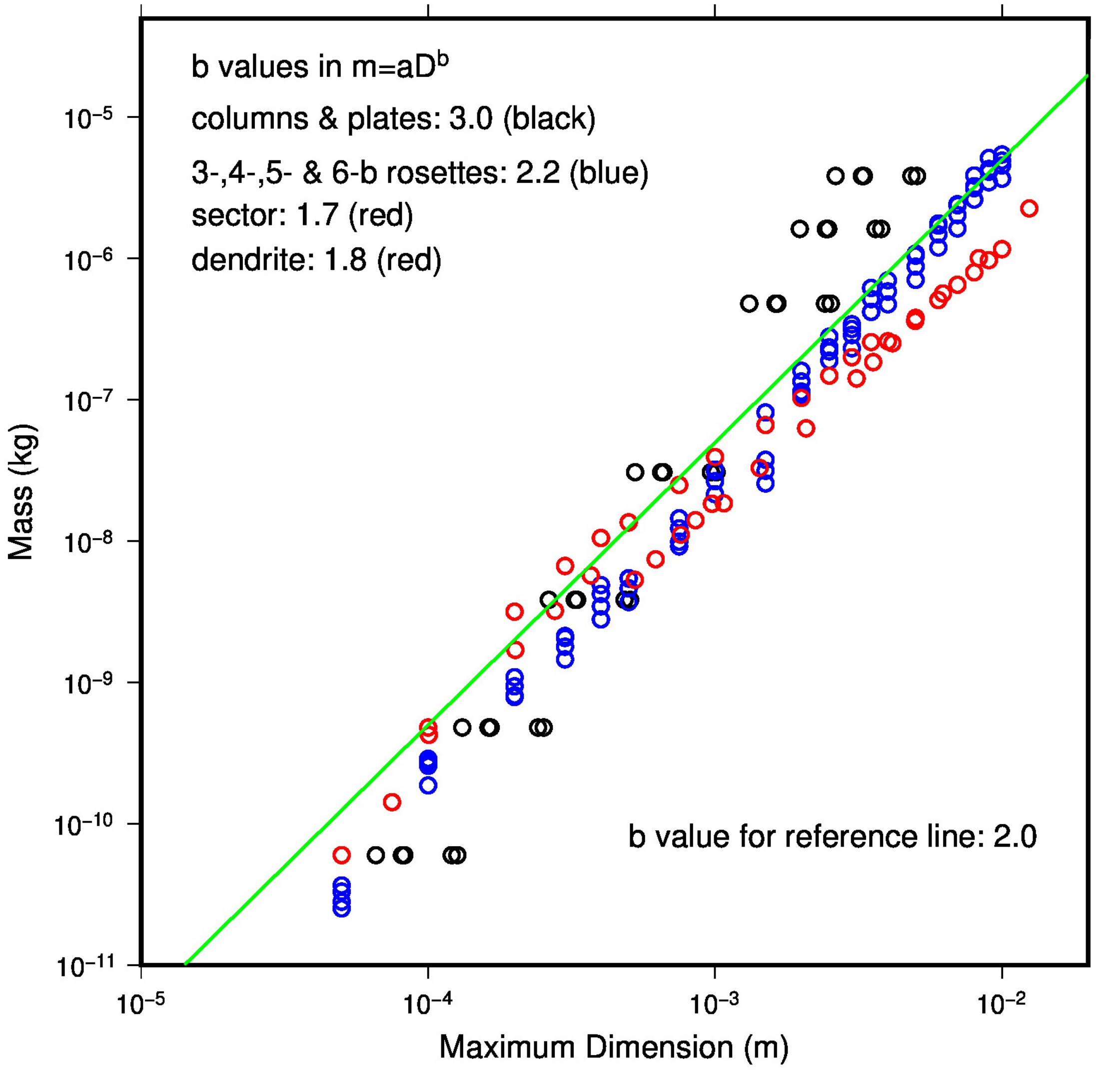
Figure 2. Aggregate and liquid habits included in the first database version. Shown particle orientation varies between the habits.

Constraints to “idealized” particles

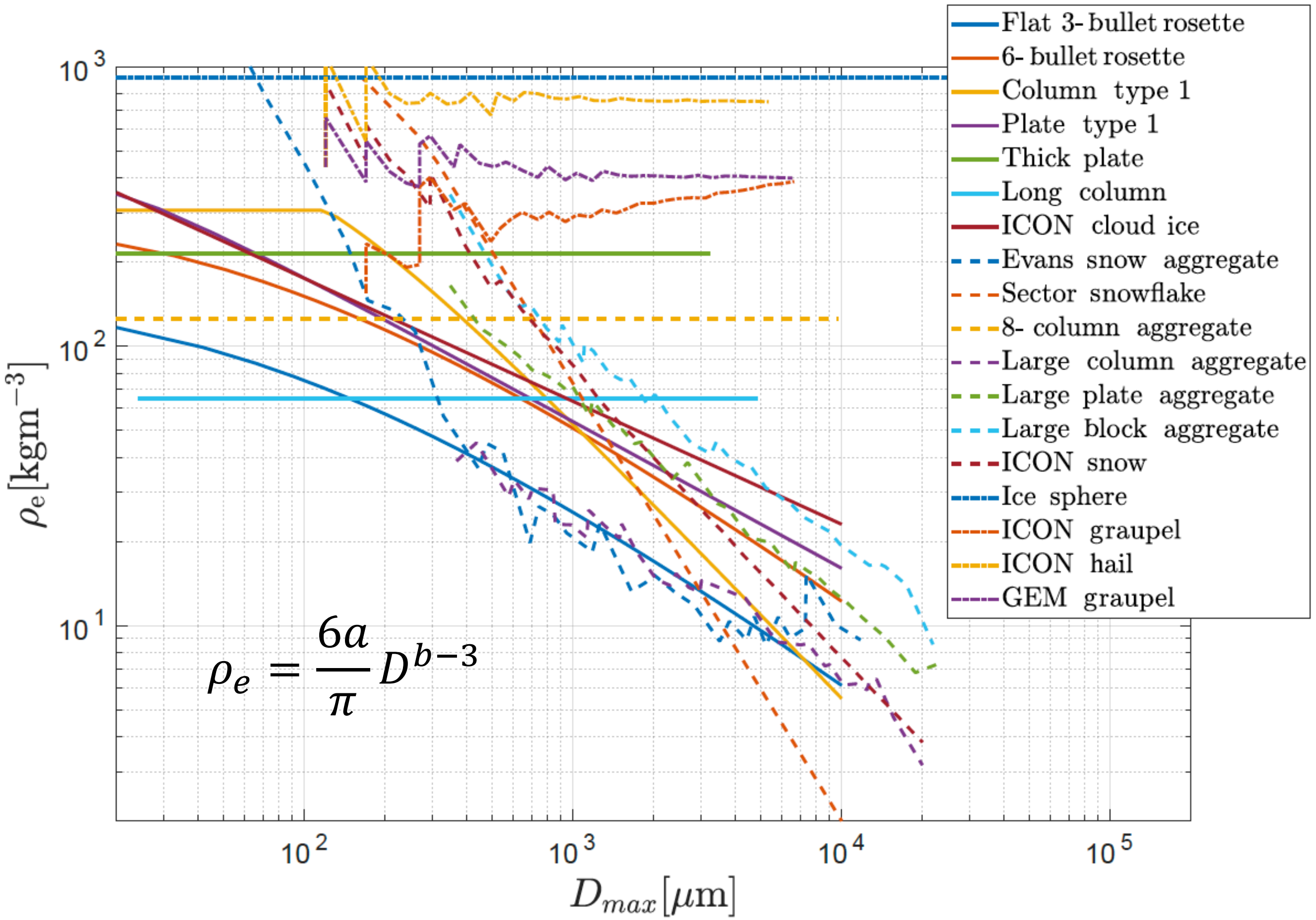
- Mass (m) – size (D) relation: $m = aD_{max}^{b}$
  - Controls how “dense” of a particle is. Typical values for b is 2 to 3, with compact particles b close to 3 while fluffy particles b close to 2.
  - Brown & Francis (1995), Francis et al. (1998), Heymsfield et al. (2013), Yang et al. (2000)
- Aspect ration: $\alpha = D_w / D_{max}$
  - Important for radar measurements of oriented particles
  - 0.6~0.8 (Korolev and Isaac, 2003)
  - Observations by MASC (Garrett et al., 2015)



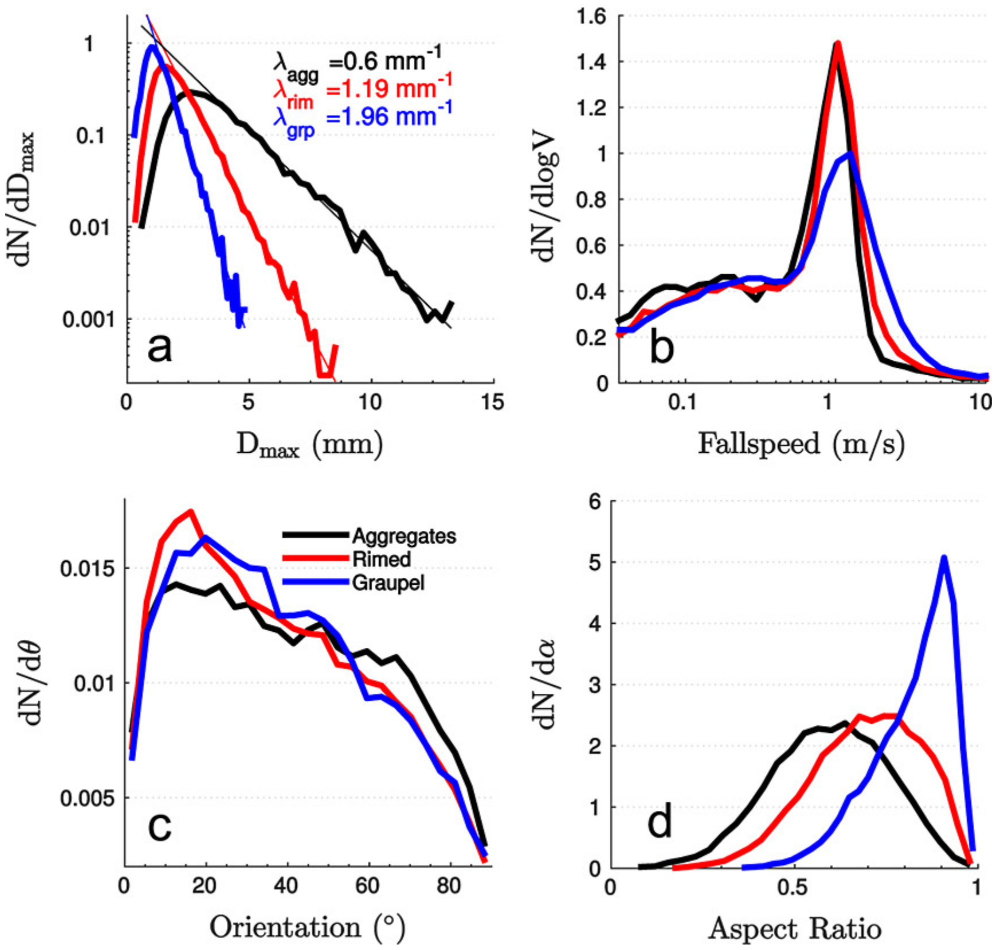
M-D relations for Liu (2008) particles

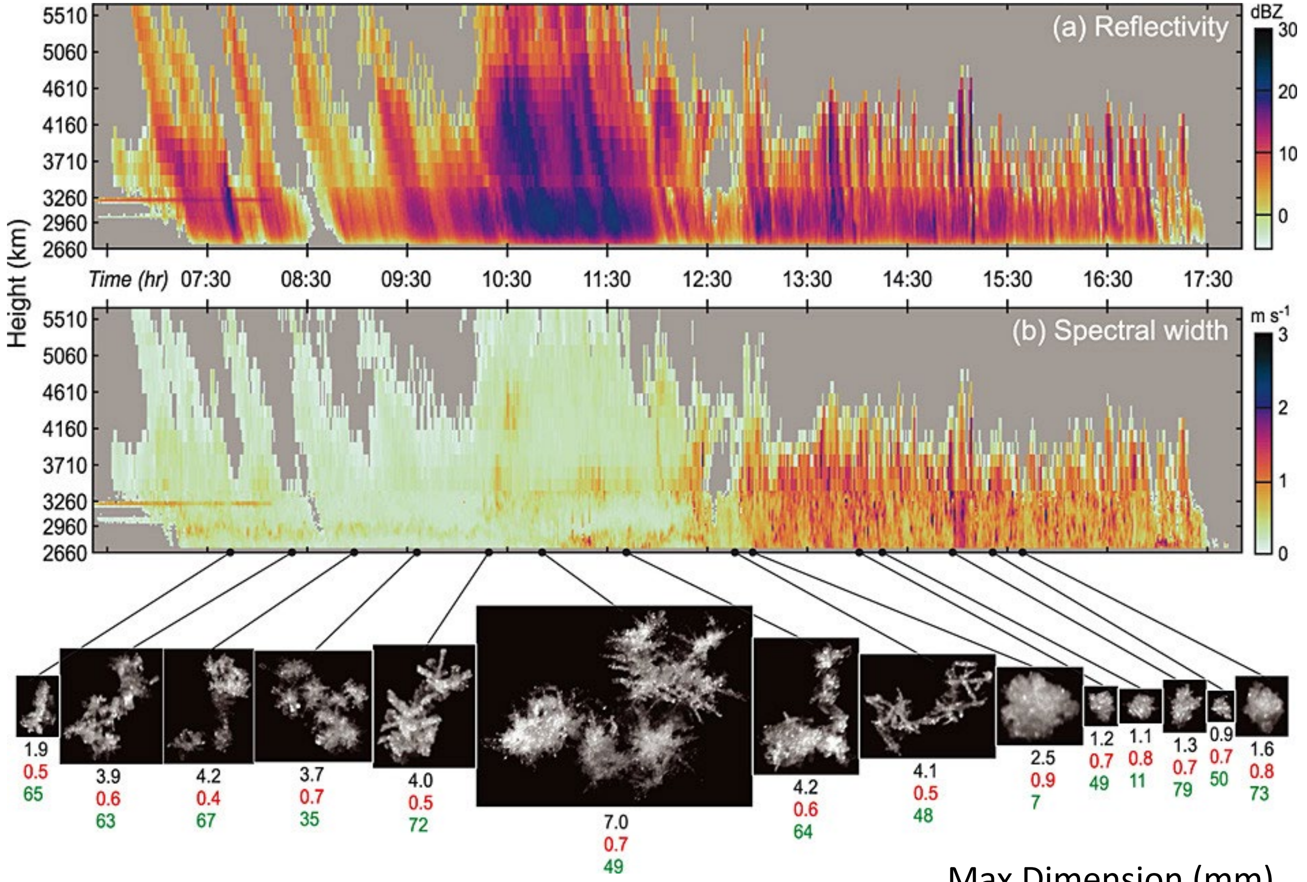


ARTS particles by Eriksson et al. (2018)



MASC obs of snowflakes' aspect ratio and orientations
Garrett et al. 2015 GRL





Max Dimension (mm)
Aspect Ratio
Orientation (degree)

A method to construct particle from images: 3D-GAN (generative adversarial network) by Jussi Leinonen et al. (2021, AMT)

From triplet MASC images, generate

- Total mass
- 3D structure
- Internal mass distribution

Useful for constructing realistic snow particles

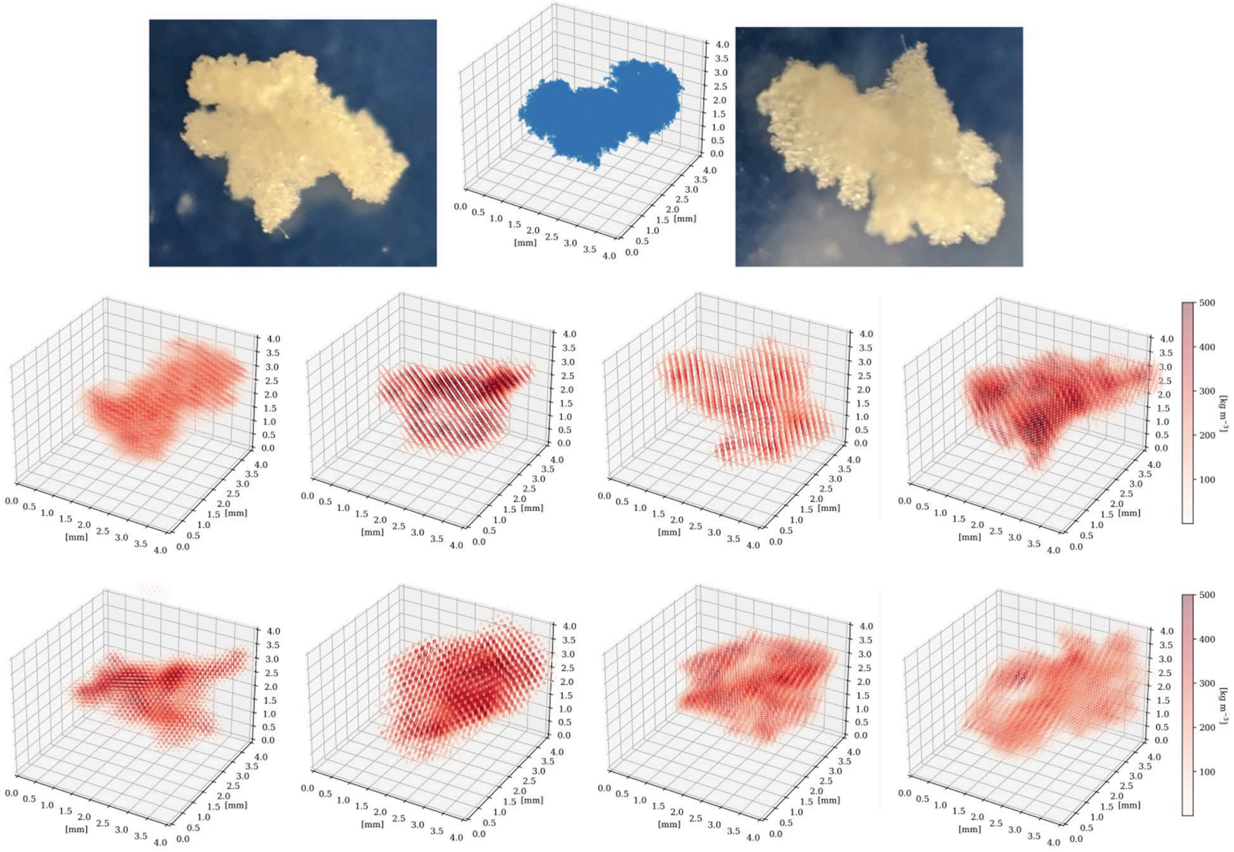


Figure 2. Example of the reconstruction outcome obtained while releasing eight consecutive times the same snowflake replica in the MASC measurement area. Top rows: actual photos of the replica and a pseudo-3D representation (every blue point represents a voxel filled with ice). Bottom rows: reconstructions obtained with 3D-GAN. Every point is color-coded according to the density (ice mass content) of each voxel.

M-D relations based on 3D-GAN ($m=aD^b$)

Table 4. Values of the parameters of the relation $m = a_m\, D_{max}^{b_m}$ estimated on the datasets of different field campaigns for various degrees of riming. m is estimated with 3D-GAN, while R_c is the normalized riming index as in Praz et al. (2017), averaged over the three camera views. D_{max} is the maximum dimension obtained from the triplet of images of the MASC.

R_c [-]	0.0−0.25	0.25−0.50	0.50−0.75	0.75−0.99	>0.99	**All**
Icegenesis 2020						
samples	183	552	386	392	257	
a_m [$\mathrm{kg\,m^{-b_m}}$]	0.014	0.017	0.09	1.457	49.582	**0.037**
b_m [-]	1.86	1.83	2.05	2.46	2.97	**1.91**
Davos 2015						
samples	1864	7509	8532	8973	3144	
a_m [$\mathrm{kg\,m^{-b_m}}$]	0.003	0.014	0.135	1.282	135	**0.025**
b_m [-]	1.58	1.80	2.13	2.43	3.13	**1.83**
APRES3 2015						
samples	285	674	642	715	257	
a_m [$\mathrm{kg\,m^{-b_m}}$]	0.012	0.021	0.158	2.156	16.199	**0.079**
b_m [-]	1.82	1.85	2.15	2.53	2.81	**2.04**
Valais 2016						
samples	444	2175	1928	2214	921	
a_m [$\mathrm{kg\,m^{-b_m}}$]	0.05	0.014	0.133	0.869	183.131	**0.02**
b_m [-]	1.66	1.79	2.13	2.37	3.17	**1.80**
Jura 2019						
samples	164	1313	1074	1026	1204	
a_m [$\mathrm{kg\,m^{-b_m}}$]	0.272	0.0234	0.169	0.786	155.926	**0.032**
b_m [-]	2.35	1.94	2.17	2.35	3.16	**1.84**

Type	AG	GR	COL	CPC	PC
Icegenesis					
samples	1060	458	110	5	137
a_m [$\mathrm{kg\,m^{-b_m}}$]	0.017	34.5	0.011	-	0.354
b_m [-]	1.78	2.93	1.84	-	2.27
Davos 2015					
samples	19343	7404	619	130	2526
a_m [$\mathrm{kg\,m^{-b_m}}$]	0.023	58.795	0.004	0.002	0.158
b_m [-]	1.82	3.02	1.67	1.54	2.14
APRES3 2015					
samples	1341	787	160	120	165
a_m [$\mathrm{kg\,m^{-b_m}}$]	0.03	10.8	0.026	0.016	0.277
b_m [-]	1.88	2.77	1.95	1.82	2.24
Valais 2016					
samples	5100	1946	172	18	446
a_m [$\mathrm{kg\,m^{-b_m}}$]	0.017	87.326	0.007	-	0.621
b_m [-]	1.77	3.07	1.76	-	2.37
Jura 2019					
samples	2940	1667	47	8	119
a_m [$\mathrm{kg\,m^{-b_m}}$]	0.030	126.612	-	-	0.465
b_m [-]	1.86	3.14	-	-	2.33

AG: aggregates, GR: graupel, COL: columns, CPC: combination of planar crystals and columns, PC: planar crystals. Results are reported only if at least 80 samples are available.

Ways to compute ice particle scattering

- Mie with some assumption of dielectric constant
- T-Matrix with some assumption of dielectric constant
- Variety of Rayleigh-Gans Approx.
- DDA
- …
- New method development - K.-S. Kuo’s poster

Scattering Databases

Compiled by Kneifel et al. (2020)

Table 15.1 Databases of scattering properties for snow particles at microwave frequencies

Publication	Particle habits	Morphology	Size range (μm)	Frequency range (GHz)	Orientations	Scattering Method	Availability
Liu (2008)	N1e, C1e, C1g, C2a, P1a, P1c, P1f	Pristine	50–10000	13.4–340	Random	DDA	https://github.cam/rhoneyagar/scatdb
Pelty and Huang (2010)	N1e, P1e	Aggregated	125–10000	13.4–89	Random	DDA	Author
Botta et al. (2010)	N1e	Aggregated, melted	500–11000	3, 35.6	Horizontal	GMM	Author
Tyynelä et al. (2011)	P1e, P1f	Aggregated	200–24000	5.6–94	Horizontal	DDA	http://helios.fmi.fi/~tyynelaj/
Tyynelä et al. (2013)	N1e, P1a, P1d, C2a	Pristine, aggregated	450–8500	3–220	Horizontal	DDA	http://helios.fmi.fi/~tyynelaj/
Nowell et al. (2013)	C2a	Aggregated	800-12000	10.7-183.3	Random	DDA	https://github.com/rhoneyager/scatdb
Ori et al. (2014)	Cle	Aggregated, melted	1000–15000	5.6–157	Random	DDA	Author
Tyynelä and Chandrasekar (2014)	Nle, Cle, Pla, P1e, P1f, C2a, R4b	Pristine. aggregated	100–24000	2.7–220	Horiz., random	DDA	http://helios.fmi.fi/~tyynelaj/
Leinonen and Szyrmer (2015)	P1e	Aggregated, rimed	700–20000	9.7–94	Gaussian	DDA	Author
Leinonen and Moisseev (2015)	Nle, Pla, P1e, C2a	Aggregated	200–10000	13.6–94	Gaussian	DDA	Author
Lu et al. (2016)	Nle, Cle, Pla, Plc, Pld, R4c	Pristine, aggregated	100–62000	9.4–94	Horizontal	GMM, DDA	https://www.arm.gov/data/data-sources/icepa.rt-mod-120
Kuo et al. (2016)	N1e, P1a, P1c, P1d, P1e, P1f, P2c	Pristine, aggregated	260–14000	3–190	Random	DDA	https://storm.pps.eosdis.nasa.gov/storm/OSSPTest.jsp
Johnson et al. (2016)	N1e, P1e	Aggregated, melted	100–14000	13.4–183	Random	DDA	Author
Ding et al. (2017)	Cle, C1f, Pla, C2a	Pristine, aggregated	2–10000	1–874	Random	II-TM, IGOM	Author
Eriksson et al. (2018)	N1e, Cle, C1g, P1a, C2a, P1c, P1f	Pristine, aggregated	10–22000	1–886	Random	DDA, Mie	https://doi.org/10.5281/zenodo.1175572

ARTS database

Particle habits are listed according to the classification by Magono and Lee (1966)
Note that some of the databases include also particle types that are not classified, such as soft/solid spheroids

The Atmospheric Radiative Transfer Simulator (ARTS) database

- The most complete one thus far – compiled existing ones and created new ones
- DDA method, Well documented, freely downloadable
- Implemented as “standard” in RTTOV-SCATT & CRTM
- Eriksson et al. (2018)

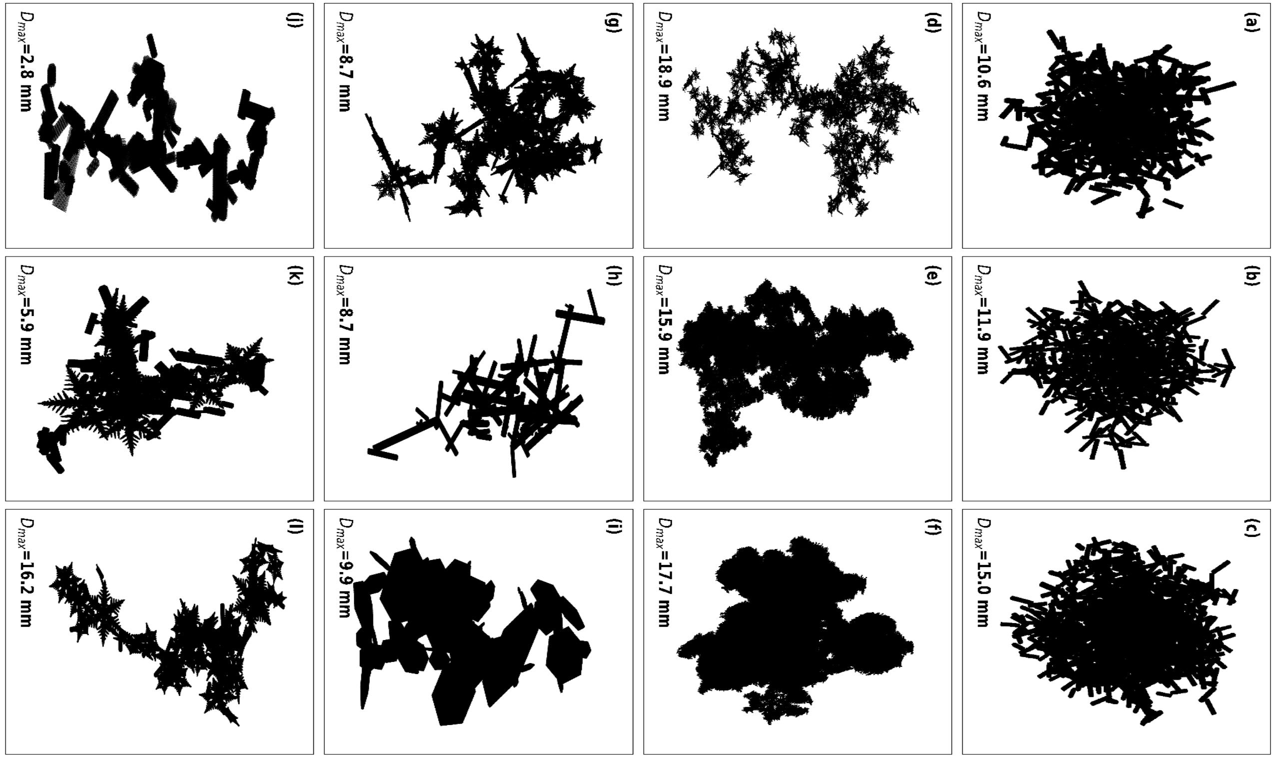
https://doi.org/10.5281/zenodo.1175572

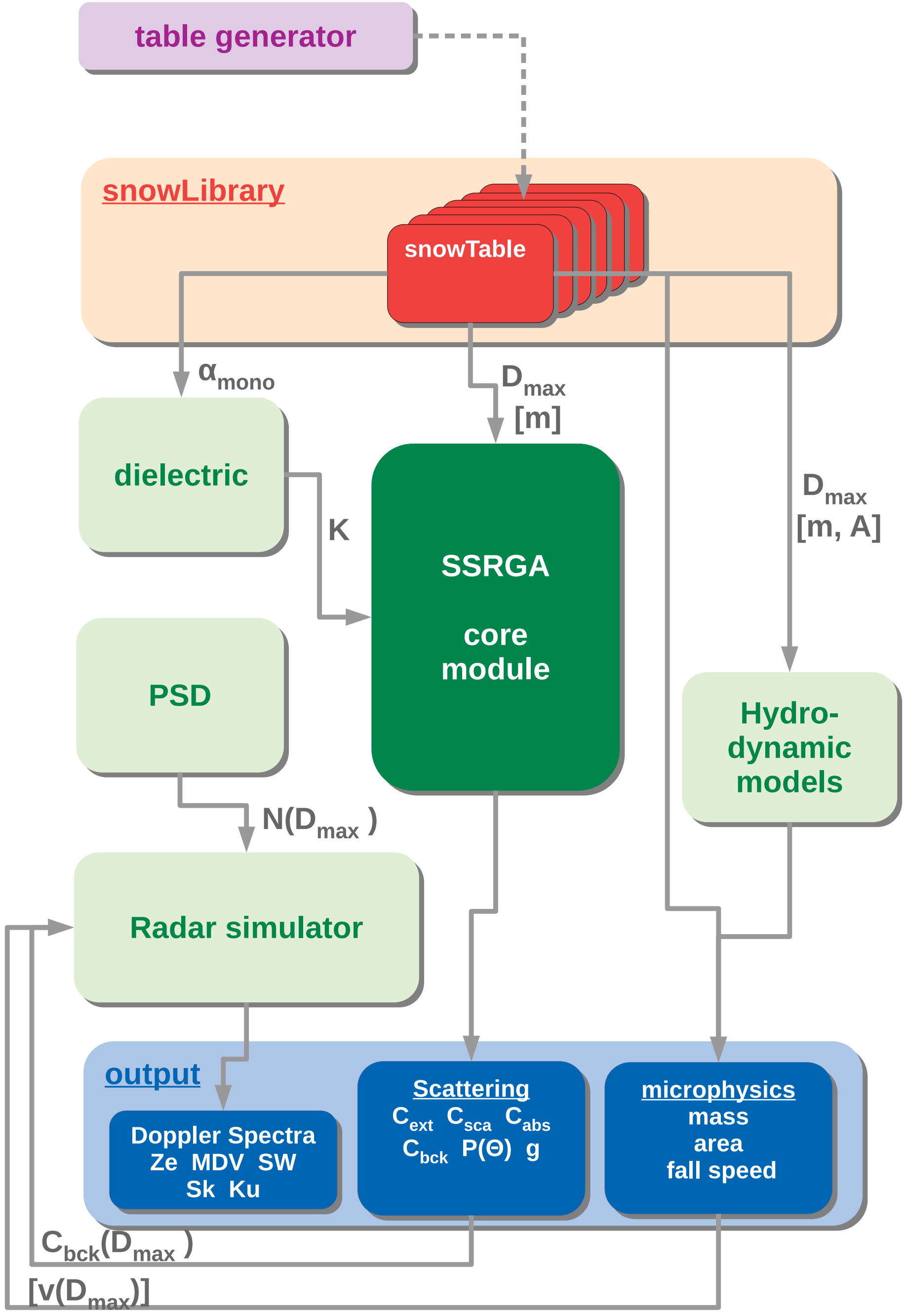
Table 1. Habits included in the first version of the database. Habits marked with * have scattering properties calculated using Mie theory. The last column displays the software or source used to create the shape data of the given habit, with abbreviations being SFTK (SnowFlake ToolKit, Sect. 3.1.1), RC (RimeCraft, Sect. 3.1.2), RSP (Recreated Shape Data, Sect. 4.2) and ESP (External Shape Data, Sect. 4.3.1). See the text for further details.

Habits	Id	D_{max} (µm)	D_{veq} (µm)	No. of sizes	a	b	Software used
Ice:							
Single crystals:							
Pristine:							
Plate type 1	9	13–10 000	10–2596	45	0.76	2.48	RSP
Column type 1	7	14–10 000	10–1815	45	0.037	2.05	RSP
Thin plate	16	25–5059	10–2000	35	30	3.00	RSP
Thick plate	15	16–3246	10–2000	35	110	3.00	RSP
Block column	12	13–2632	10–2000	35	210	3.00	RSP
Short column	13	17–3303	10–2000	34	110	3.00	RSP
Long column	14	24–4835	10–2000	35	34	3.00	RSP
Sector snowflake	3	20–12 000	20–1415	34	0.00081	1.44	RSP
Ice sphere*	24	1–50 000	1–50 000	200	480	3.00	Mie
ICON cloud ice	27	13–10 000	10–2929	45	1.6	2.56	SFTK
GEM cloud ice	31	10–3088	10–3000	45	440	3.00	SFTK
6-bullet rosette	6	16–10 000	10–2371	45	0.48	2.42	RSP
5-bullet rosette	2	17–10 000	10–2231	45	0.4	2.43	SFTK
Perpendicular 4-bullet rosette	10	18–10 000	10–2071	45	0.32	2.43	SFTK
Flat 4-bullet rosette	11	18–10 000	10–2071	45	0.32	2.43	SFTK
Perpendicular 3-bullet rosette	4	19–10 000	10–2137	45	0.44	2.47	SFTK
Flat 3-bullet rosette	5	20–10 000	10–1882	45	0.2	2.43	SFTK
Aggregates:							
Pristine:							
Evans snow aggregate	1	32–11 755	50–2506	35	0.20	2.39	ESP
Tyynelä dendrite aggregate	26	595–20 826	228–3328	35	0.10	2.25	ESP
8-column aggregate	8	19–9714	10–5000	39	65	3.00	RSP
Small column aggregate	17	105–3855	37–738	35	0.14	2.45	SFTK
Large column aggregate	18	368–19 981	128–3021	35	0.25	2.43	SFTK
Small block aggregate	21	100–7328	72–1665	35	0.21	2.33	SFTK
Large block aggregate	22	349–21 875	253–4607	35	0.35	2.27	SFTK
Small plate aggregate	19	99–7054	53–1376	35	0.077	2.25	SFTK
Large plate aggregate	20	349–22 860	197–4563	34	0.21	2.26	SFTK
ICON hail	30	120–5349	94–5000	35	380	2.99	RC
ICON snow	28	120–20 000	94–3219	35	0.031	1.95	RC
GEM hail	29	120–5031	94–5000	35	540	3.02	RC
GEM snow	32	170–10 459	94–5000	35	24	2.86	RC
Rimed:							
Spherical graupel	23	622–9744	454–5293	30	13	2.69	SFTK
ICON graupel	29	170–6658	94–5000	35	390	3.13	RC
GEM graupel	33	120–6597	94–5000	35	170	2.96	RC
Liquid:							
Liquid sphere*	25	1–50 000	1–50 000	200	523	3.00	Mie

snowScatt – Ori et al. (2021)

- Over 50,000 Aggregates particles, including rimed ones
- Self-similar Rayleigh-Gans Approx. (SSRGA)
- https://github.com/OPTIMICe-team/snowScatt





Melting particles – Johnson et al. (2015)

- Selected melting particles
- DDA computed scattering properties
- Showed significant difference of Z and TBs depending melting fraction

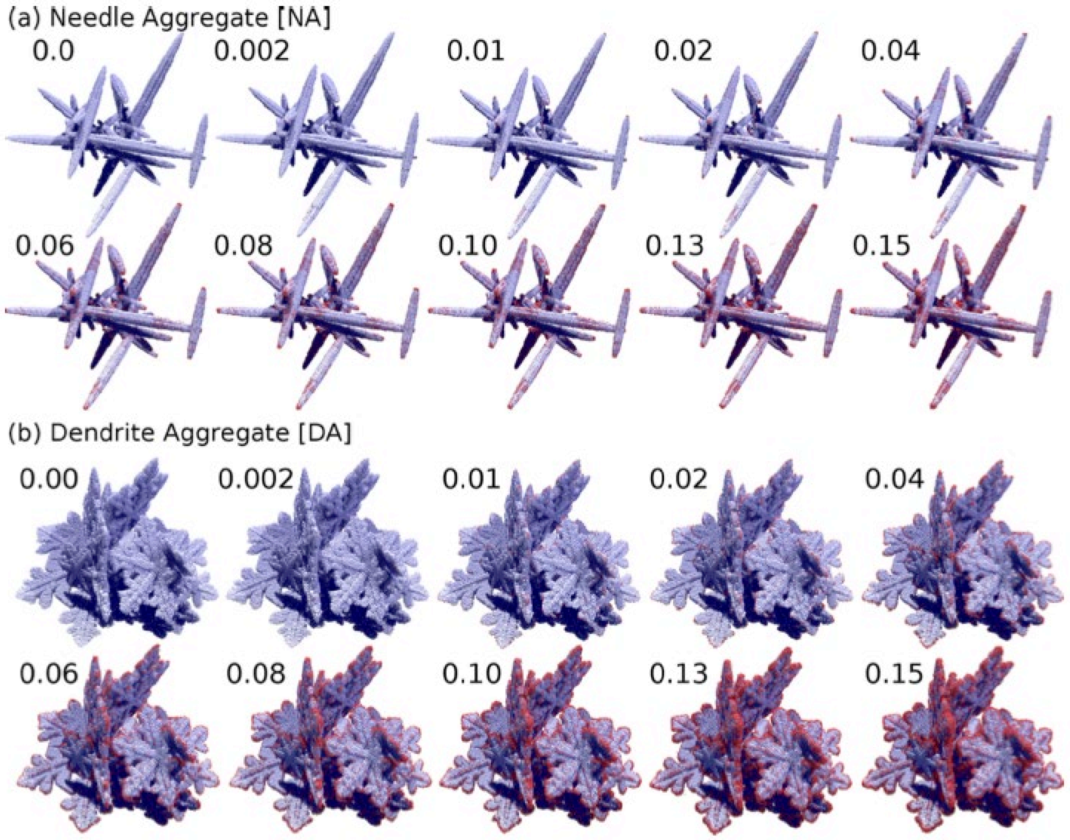


Figure 1. Selected steps in the onset of melting for **(a)** needle-aggregate (NA), and **(b)** dendrite-aggregate (DA). Blue regions are ice, red regions are liquid water; mass fraction of melt water is indicated at each step.

What are lacking?

- Need more understanding for riming and melting particles, particularly
  - Riming particles:
    - Need particle structure info
  - Melting particles
    - Need particle structure info
    - Need good scattering computation method
- Ultimate question: which particle(s) are suitable for a given cloud/precipitation type?
  - Consistency studies
  - Implementation to radar/radiometer simulators

Implementation to RTTOV-SCATT – Geer et al. (2021)

- Use RTTOV-SCATT with ECMWF environmental variables
- Compare with SSMIS OBS for 13-22 June 2019
- Consider other factors simultaneously (see right)
- Use a cost function to find best matches

Dimension	Index	Short name	Description or dimension name	Mean change in TB (K)
1. Cloud overlap	1	Land C_{av}	C_{av} effective cloud fraction over land	0.046
	2	Control (Land C_{max})	C_{max} effective cloud fraction over land	0
2. Convective snow mixing ratio	1	−half CV snow	Convective snow mixing ratio scaled by 0.5	0.057
	2	Control	Convective snow mixing ratio not scaled	0
	3	+half CV snow	Convective snow mixing ratio scaled by 1.5	−0.046
3. Convective snow PSD	1	Control (CV F07 T)	Field et al. (2007) tropical PSD for all snow	0
	2	CV MP48	Marshall and Palmer (1948)	−0.067
4. Convective snow particle shape	1	CV ARTS column agg.	ARTS large column aggregate	0.071
	2	Control (CV Liu sector)	Liu (2008) sector snowflake for all snow	0
	3	CV ARTS block agg.	ARTS large block aggregate	−0.029
	4	CV ARTS column	ARTS column type 1	−0.042
	5	CV Liu 3-bullet	Liu (2008) 3-bullet rosette	−0.072
	6	CV ARTS graupel	ARTS gem graupel	−0.187
5. Large-scale snow particle shape	1	LS ARTS sector	ARTS sector snowflake	0.054
	2	LS ARTS 6-bullet	ARTS 6-bullet rosette	0.043
	3	LS ARTS plate agg.	ARTS large plate aggregate	0.032
	4	Control (LS Liu sector)	Liu (2008) sector snowflake for all snow	0
	5	LS ARTS column	ARTS column type 1	−0.065
	6	LS ARTS block agg.	ARTS large block aggregate	−0.090
6. Ice cloud particle shape and PSD	1 ... 8	See Table 3		

Implementation to RTTOV-SCATT – Geer et al. (2021)

Cost function is “mean difference” and “skewness” between simulated and observed TBs

$$J(\boldsymbol{v}) = \frac{1}{m}\sum_j \left(0.5\frac{1}{n}\sum_l \left|\mathrm{Mean}\left(\mathrm{Bin}_l\left(d_{i,j,\boldsymbol{v}}\right)\right)\right| + 0.5\frac{1}{n}\sum_l \left|\mathrm{Skew}\left(\mathrm{Bin}_l\left(d_{i,j,\boldsymbol{v}}\right)\right)\right|\right).$$

Table 4. Results of parameter search.

Dimension/metric	Best
Cloud overlap	Land C_{av}
Convective snow mixing ratio	+half CV snow
Convective snow PSD	Control
Convective snow particle shape	CV ARTS column
Large-scale snow particle shape	LS ARTS sector
Ice cloud particle shape and PSD	CI gamma 2e4
Cost function (control = 0.925)	0.908

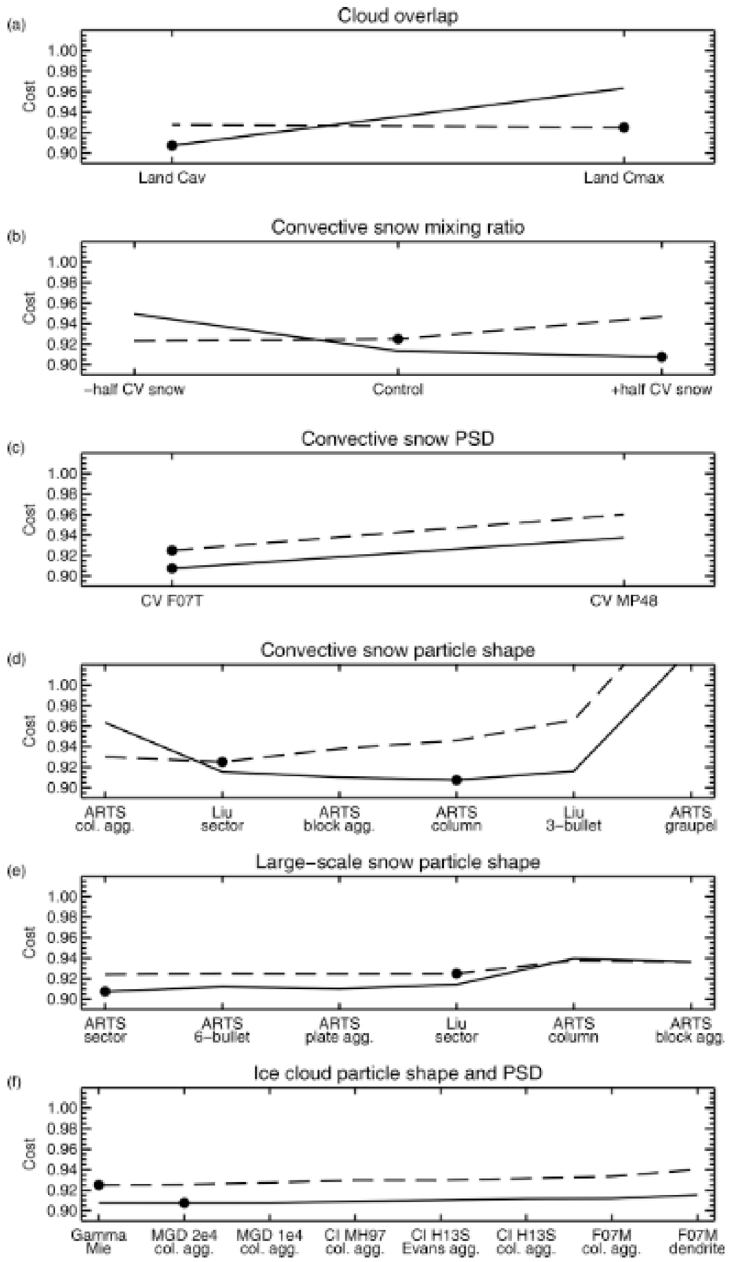
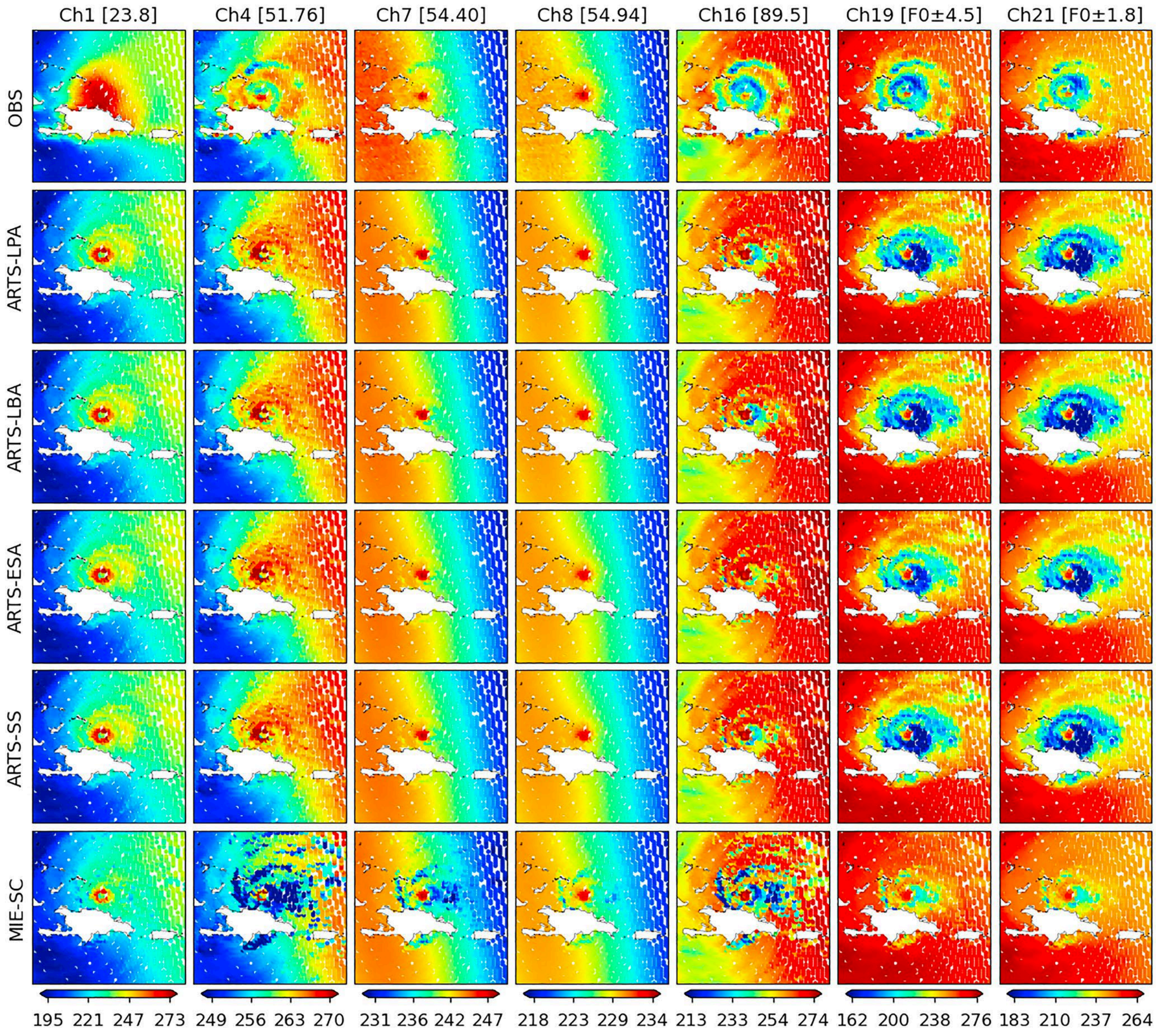


Figure 5. Slices through the six-dimensional cost function around the control configuration (dashed) and around the best configuration (solid; see also Table 4). The dimensions are ordered from least-scattering to most-scattering options. The dots indicate the parameter settings for the control and for the very best (lowest cost) configuration.

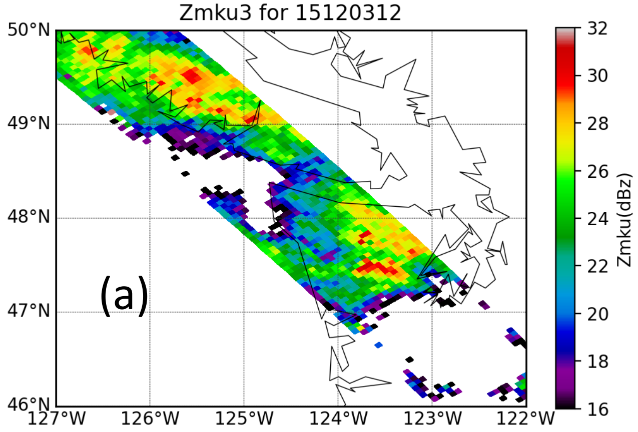
CRTM Implementation – Moradi et al. (2022)

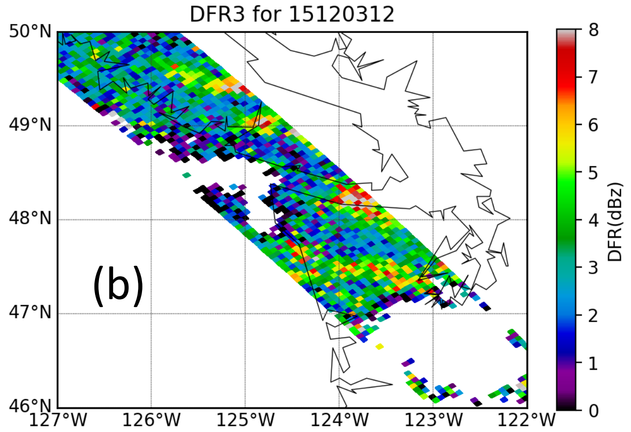
- ARTS scattering database
- Shape selectable, but defaults are:
  - LargePlateAggregates for snow
  - GemGraupel for graupel
  - GemHail for hail
  - IceSphere for cloud ice
- ATMS channels example (Hurricane Irma, IFS input)

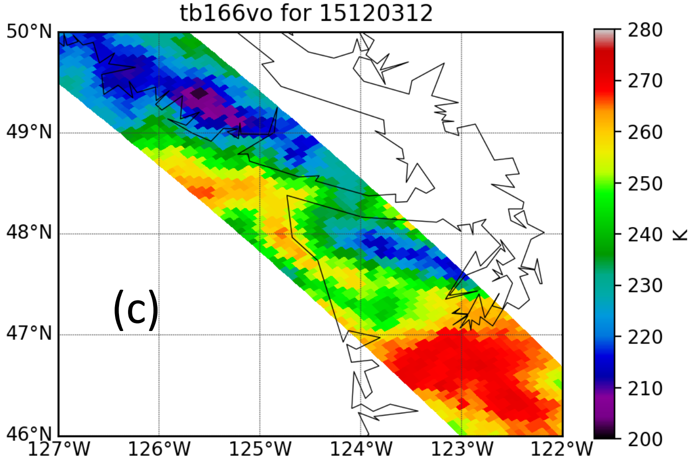


Radar – Radiometer OBS consistency
- Aonashi et al. (also see his presentation)

- Use collocated DPR Ku/Ka and GMI 89 and 166 GHz TBs.
- Four types of ice particles:
  - Sector snowflake (Liu 2008)
  - Lightly rimed aggregates (Ori et al. 2021)
  - Heavily rimed aggregates (Ori et al. 2021)
  - Graupel (sphere)
- Example of OLYMPEX 2015/12/03 Case







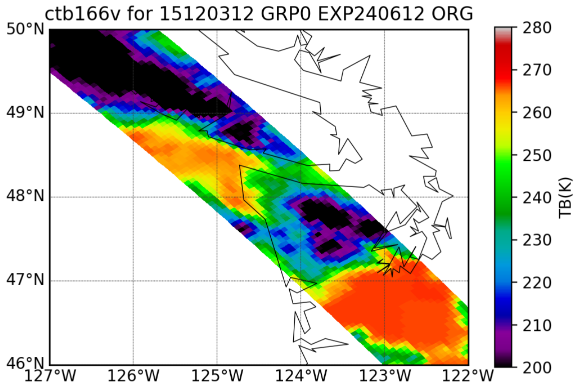
(a) DPR Zmku @3km (dBz)

(b) DPR DFR @3km (dBz)

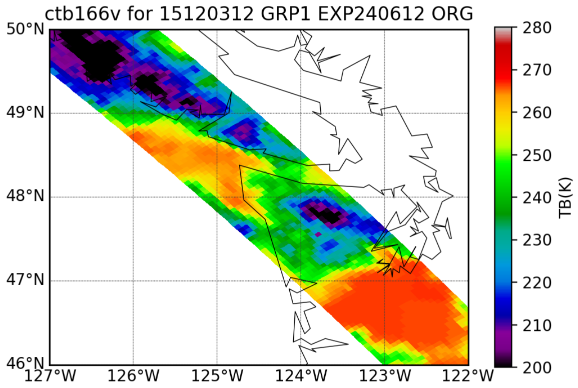
(c) GMI TB166v (K)

TB166v calculated from DPR Ze and DFR for (‘15/12/3/15 UTC) with particle models of (a) snowflake, (b)aggregates, (c)rimed aggregates, (d) graupels (sphere)

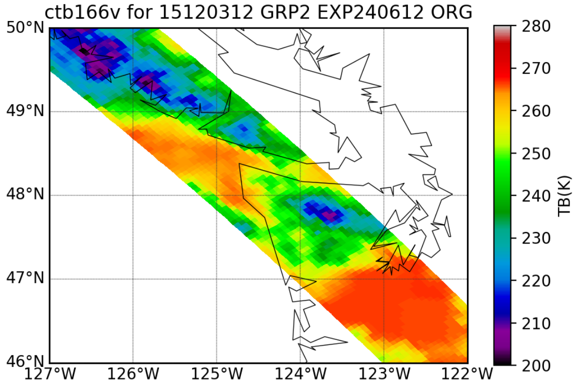
(a)



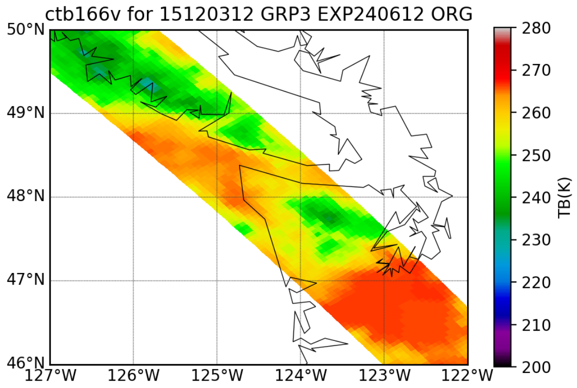
(b)



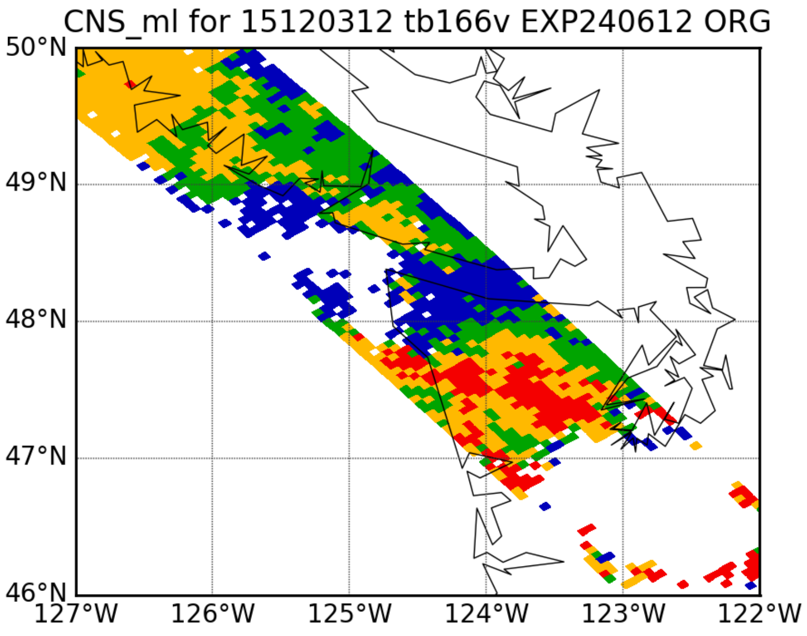
(c)



(d)



Most likely particle models estimated from GMI TB166v (TBo-TBc)



- Blue: Snowflakes
- Green: Aggregates
- Orange: Rimed aggregates
- Red: Graupels (Spheres)

Radiometer OBS consistency among different channels

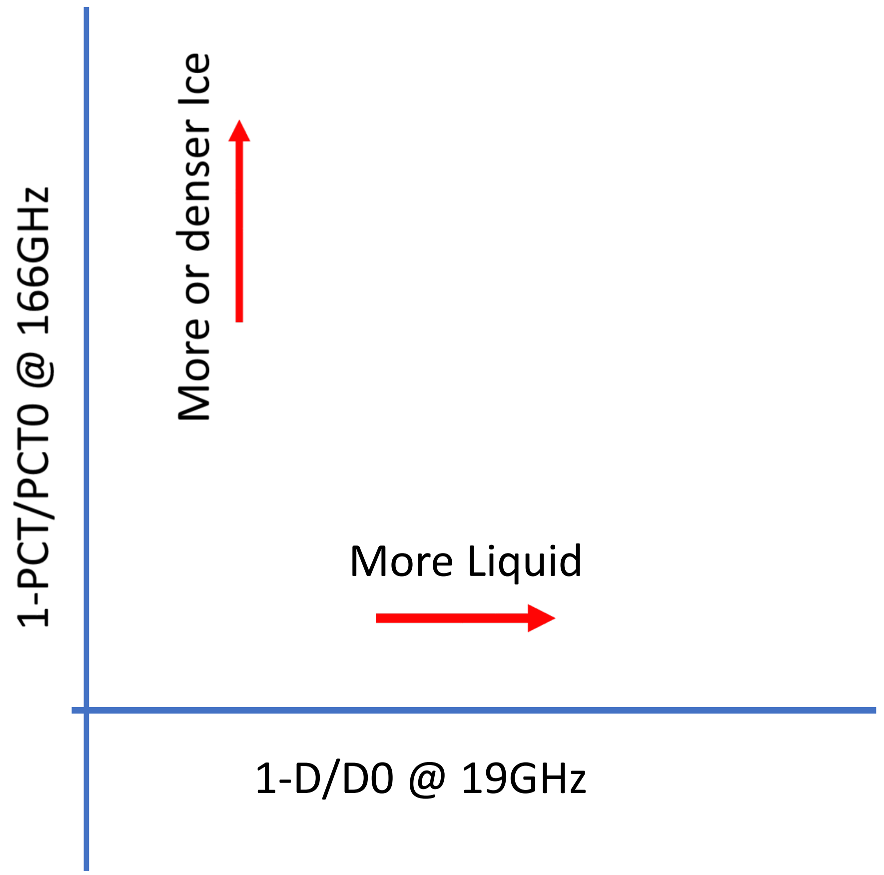
Microwave Obs over ocean:

- Low-freq Microwave: emission signal
  - GMI 19 GHz D=TBv-TBh

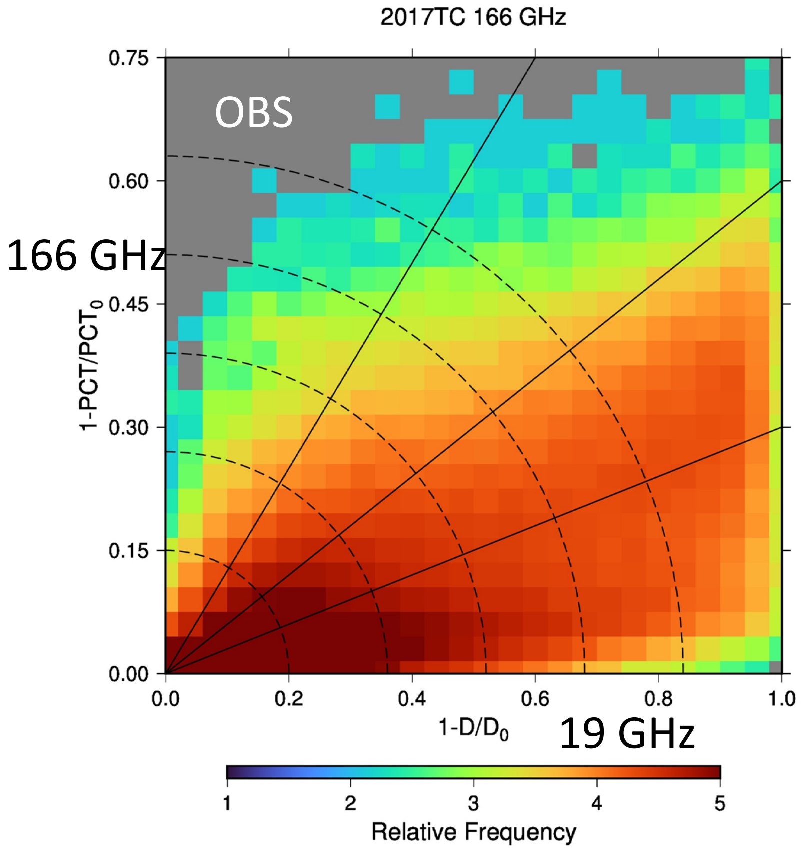
  Use: $1\text{-}D/D_0$ D_0: Clear-Sky D
- High-freq Microwave: scattering signal
  - GMI 166 GHz PCT=$(1+\alpha)$TBv-αTBh

  Use: $1\text{-}PCT/PCT_0$ PCT_0: Clear-sky PCT

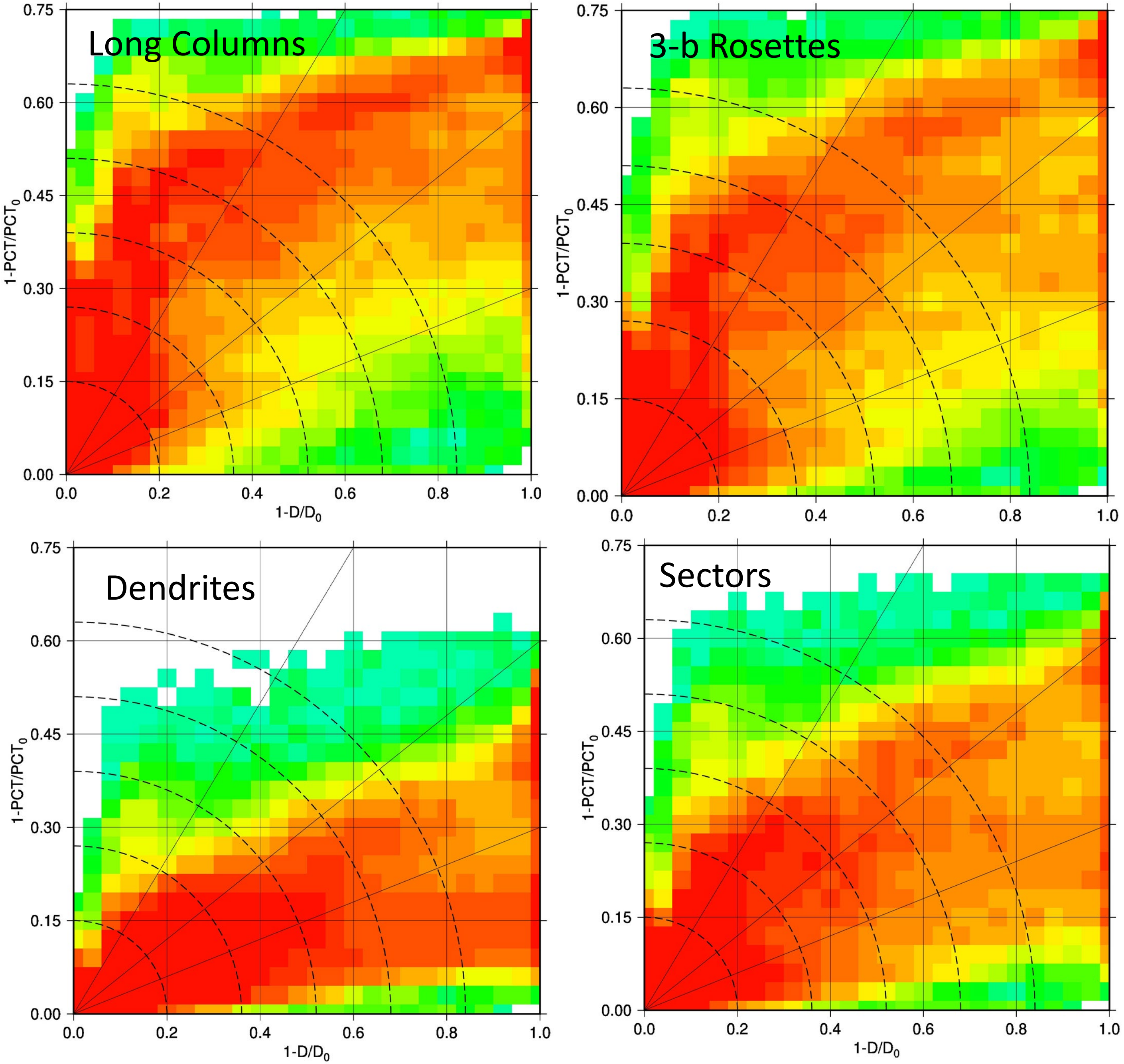
  Also, do this for 89 GHz



Which particle shape(s) leads to better distribution match?



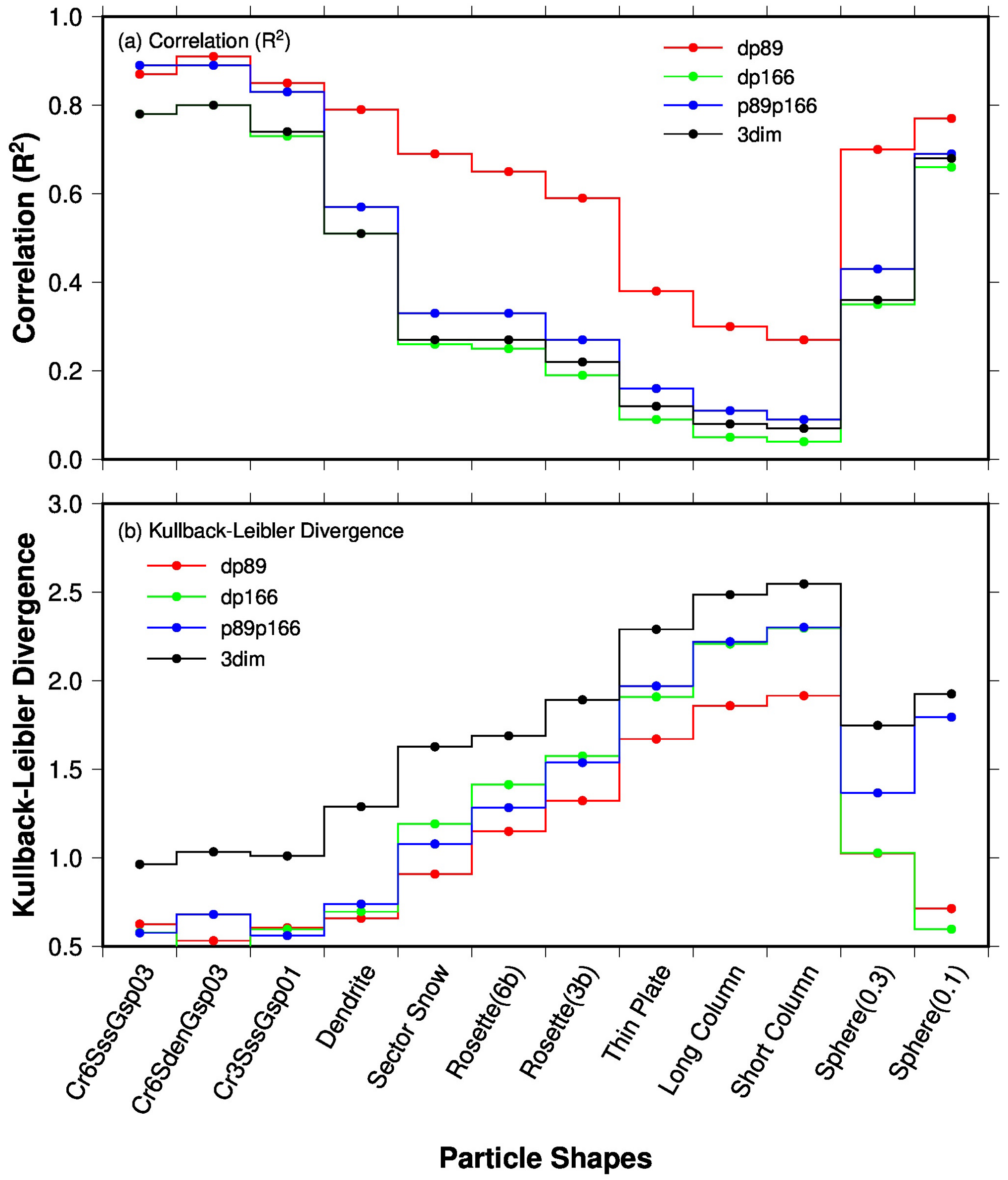
WRF Simulations w/ RT conversion



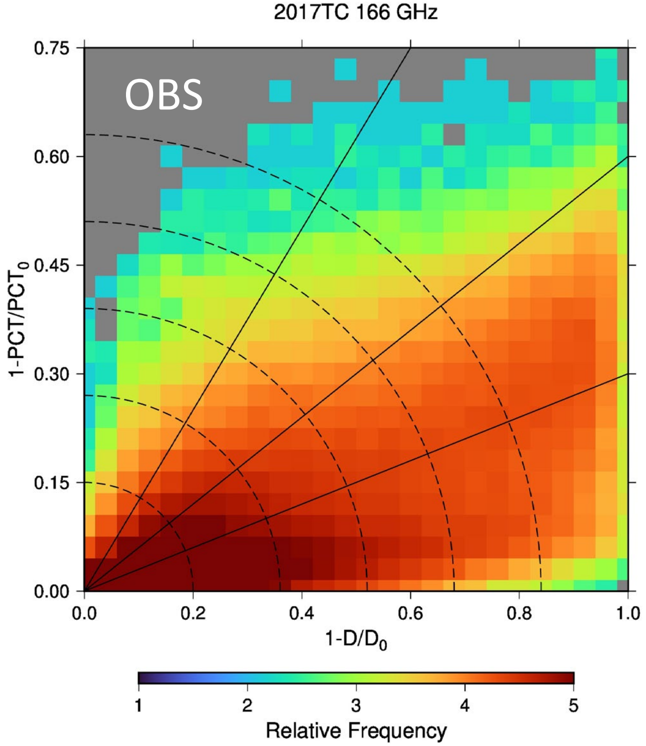
Composite PDF from 66 GMI observed hurricane/typhoon scenes during 2017 (based on JAXA tropical storm database)

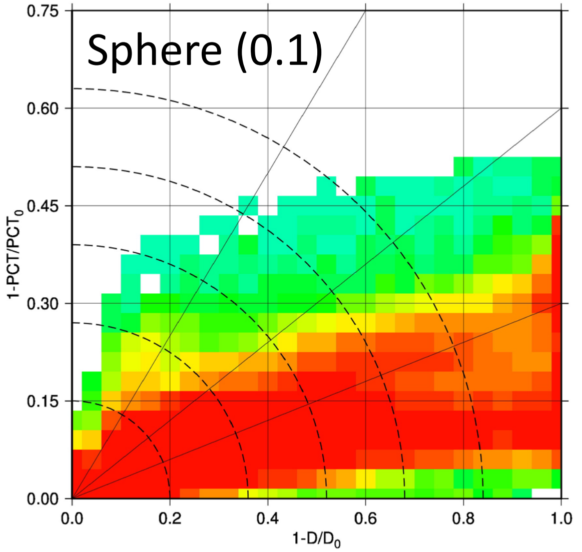
Find Good Matches

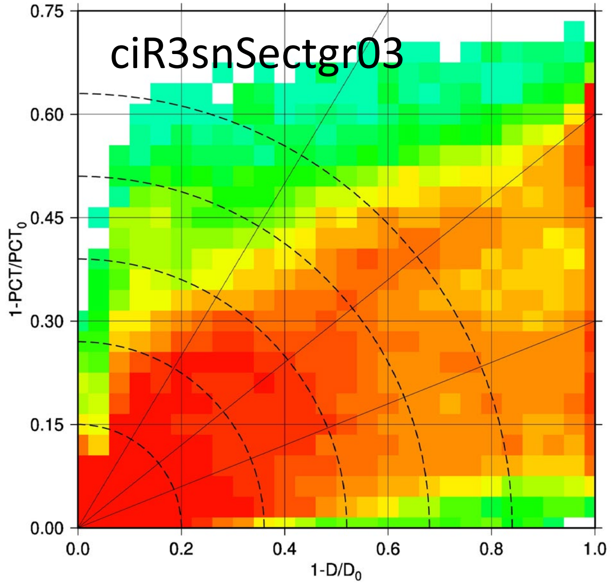
Disclaimer: Just Proof of Concept



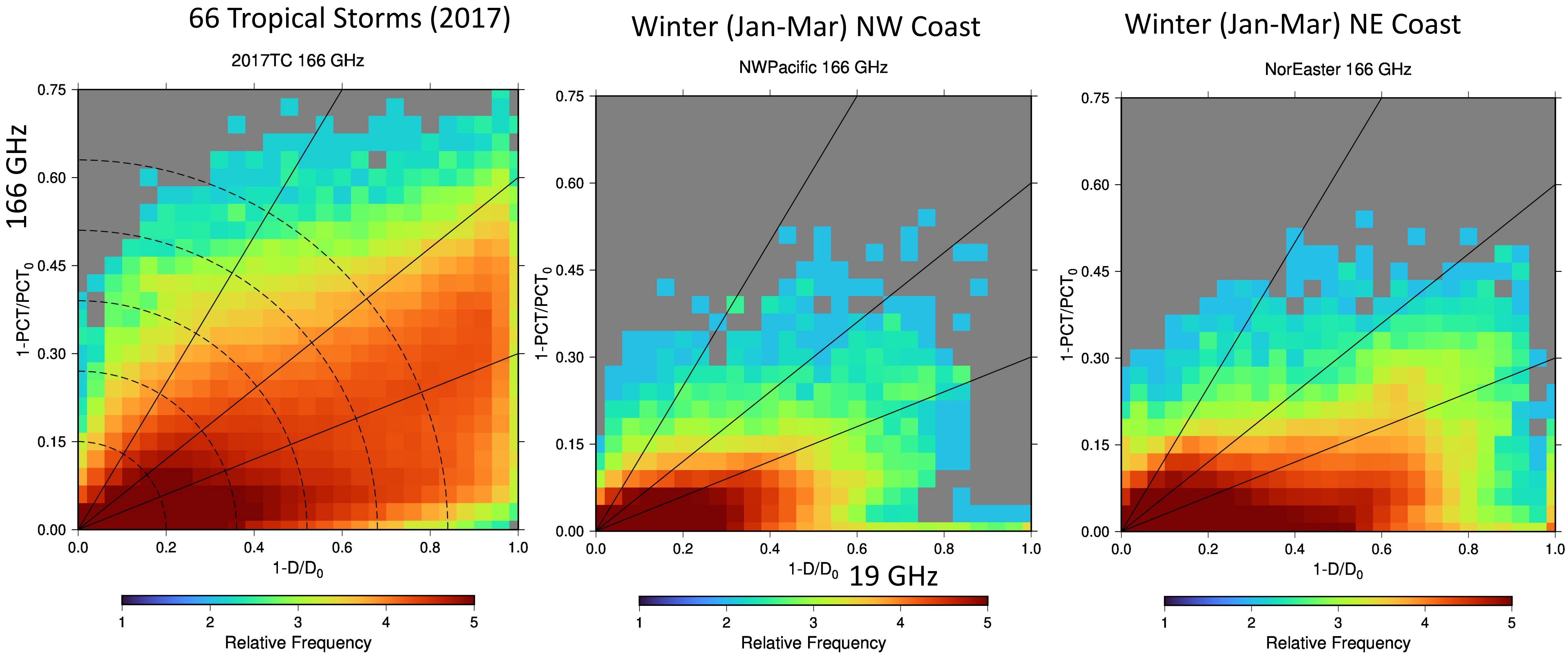
66 Cases of Tropical Storms







Cloud Type Dependent Considerations
GMI Observations



Moving forward
- Suggested for focus group discussions

- Identify gaps in the scattering database
  - Crystals/aggregates with low b values?
  - Riming particles
  - Melting particles
- Enhance simulators with realistic particles
  - Radiometer simulators: RTTOV-SCATT, CRTM,…
  - Radar simulators (melting layer, etc.)
- Consistency studies
  - Model – observation consistency; Radar-Radiometer consistency
  - What to use in simulators: Guidance for data assimilations, algorithm developers --- from “reality” to “idealized”, or “what should be used as defaults in popular simulators?”

Survey Questions

- What are your interests in particle scattering studies:
    1. Ice particle microphysics (morphology, structure, density, …)
    2. Scattering computation methods
    3. Radar/Radiometer simulators
    4. Application of ice scattering table in algorithm development/data assimilation etc.
    5. Other _________
- For scattering table developers, what are the challenges for you to generate scattering tables
    1. How to generate realistic particles
    2. Suitable computational method
    3. Don't know what users need
- For scattering table users,
    1. Couldn't find the particle shape I want in existing tables, such as _________
    2. Don't know what particle shapes are best suited for my study
    3. I'd like to have the scattering table arranged/archived in a way like _____________
- I have the following suggestions to better coordinate studies among members in our group