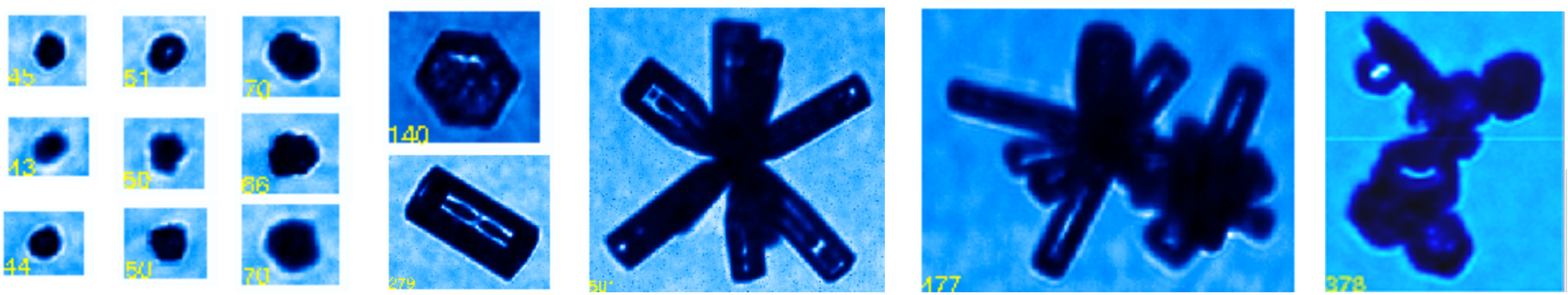
Scattering calculations of atmospheric ice crystals: Studies on orientation average & atmospheric halo



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NCSA

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- Blue Waters
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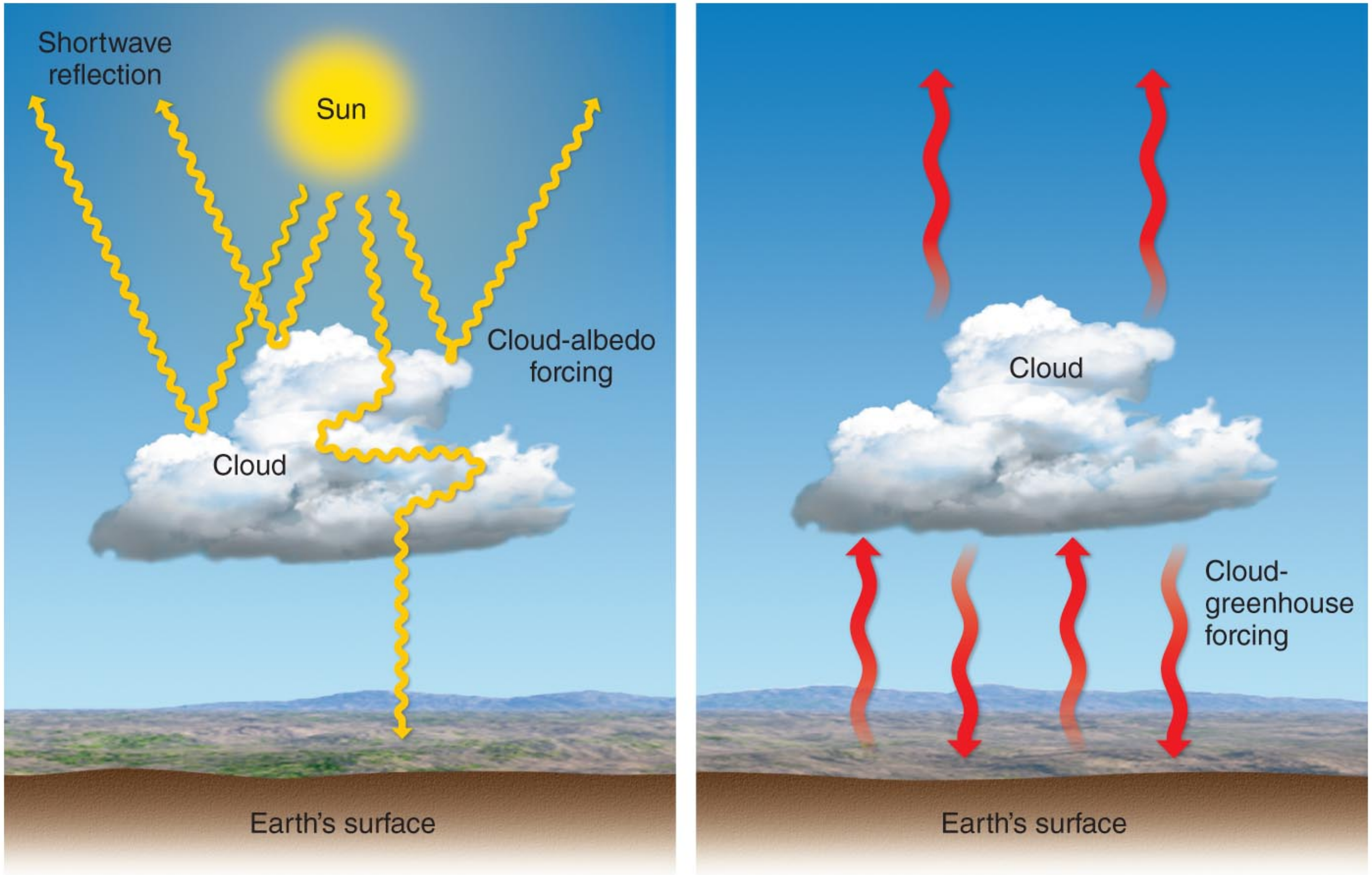
- Andreas Macke, GOM

Outline

- **Motivation**
- **Challenging problems**
- **Orientation average**
- **Atmospheric halo formation**
- **Summary**

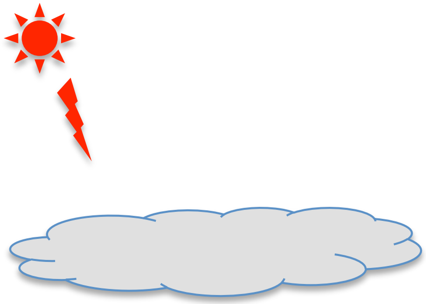
I. Motivation



(a) Shortwave radiation (b) Longwave radiation

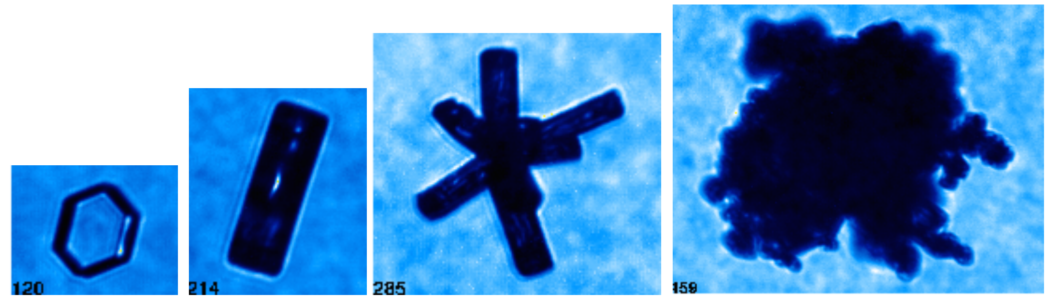
- **Clouds crucial regulator of Earth's radiation budget**
- **Knowledge of cloud radiative properties required**

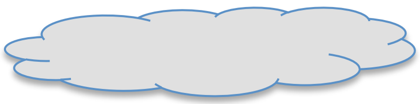
II. Challenging Problems



Ice cloud

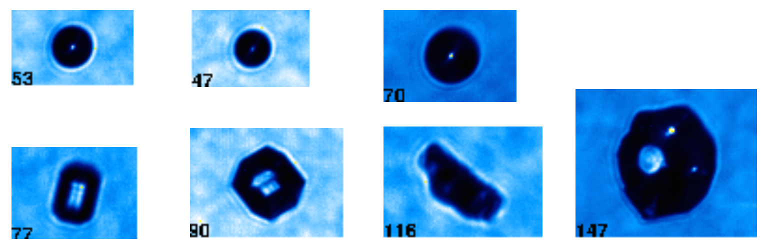
Non-spherical particles

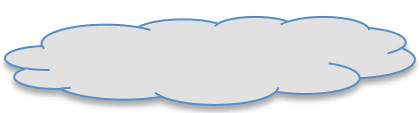




Mixed-phase cloud

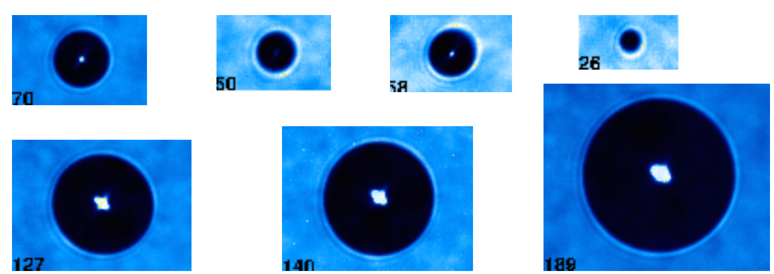
Spherical
+
Non-spherical



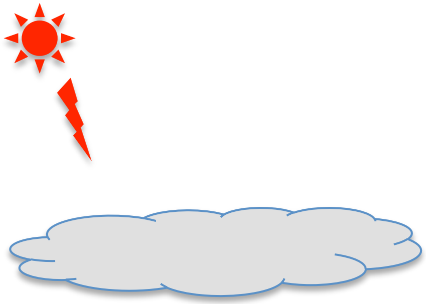


Liquid cloud

Spherical

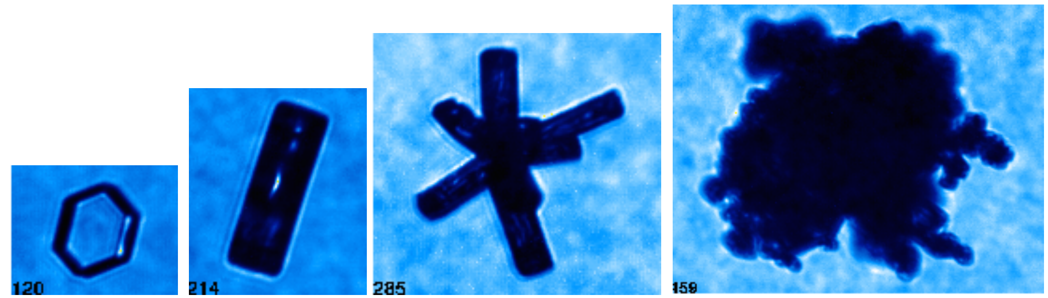


II. Challenging Problems



Ice cloud

Non-spherical particles



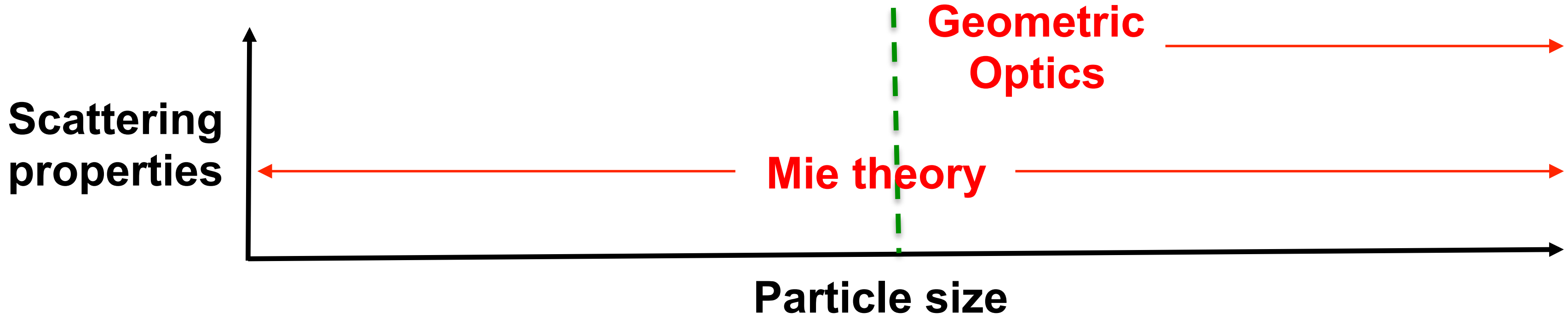
Wide variety of non-spherical shapes !!!

II. Challenging Problems

Finding methods to compute scattering properties of particles

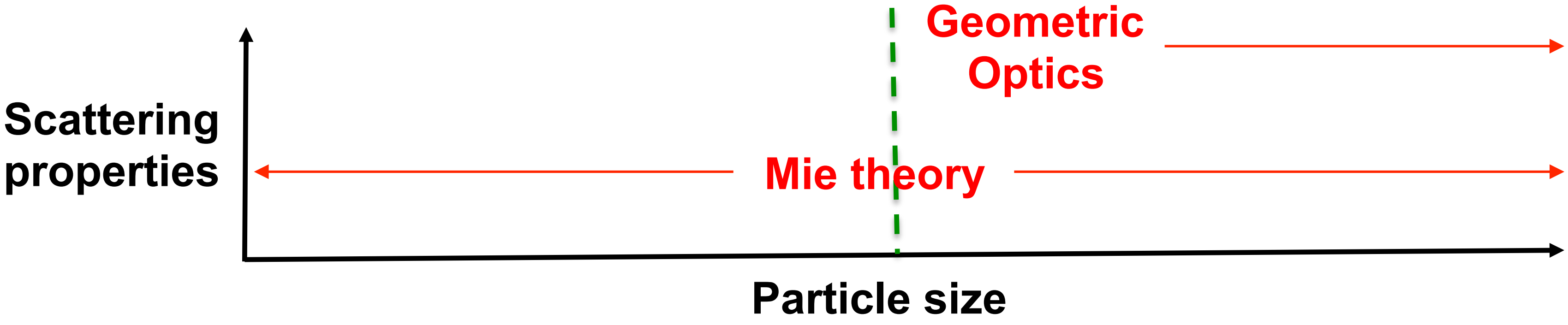
II. Challenging Problems

Spherical particles

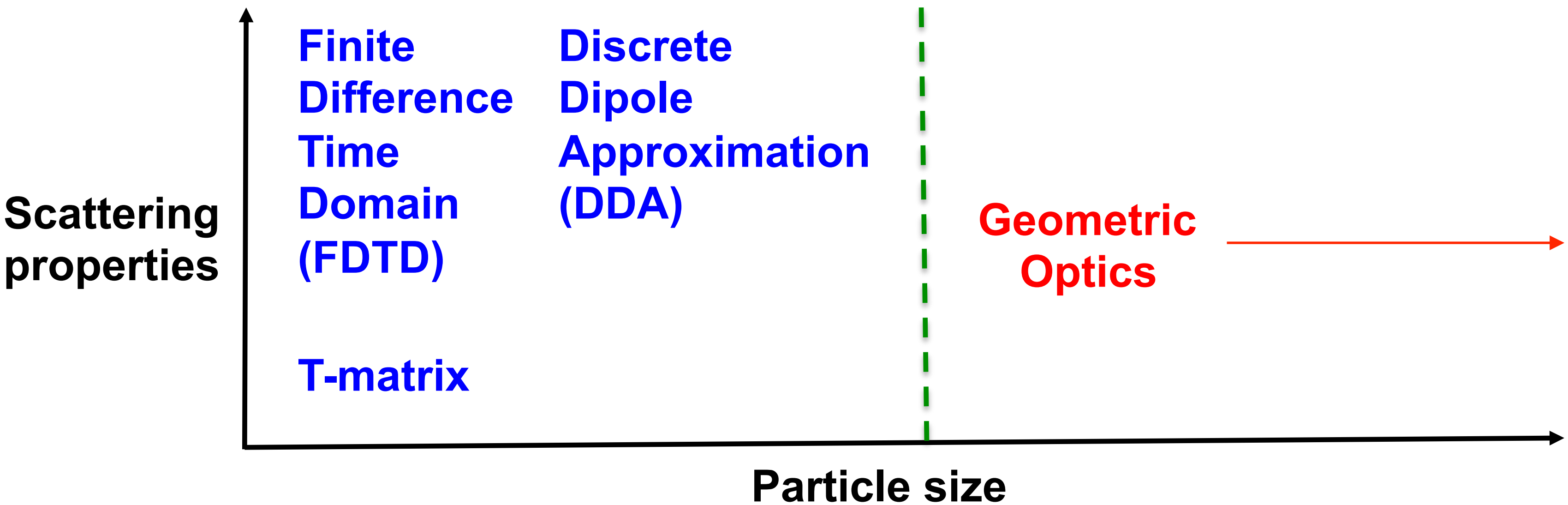


II. Challenging Problems

Spherical particles



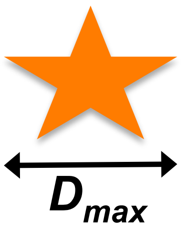
Non-spherical particles



II. Challenging Problems

Light scattering solution | **Non-spherical particles**

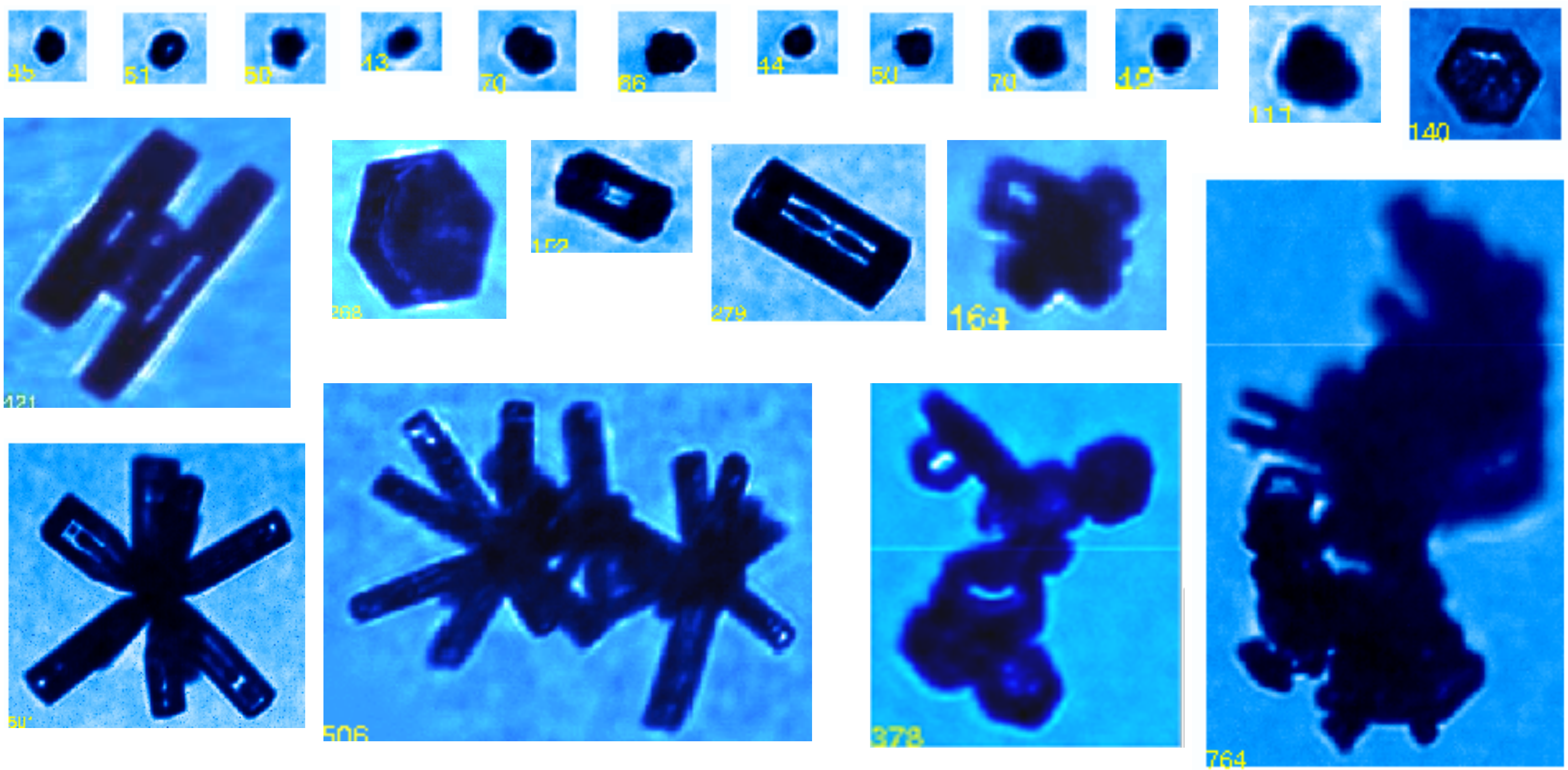
- **Geometric Optics for large particles**
  - Computationally cheap
  - Approximation
  - Only valid when particle is much larger than λ of incident light
  - Size parameter $\chi = \pi D_{max}/\lambda >>> 1$



- **Exact solutions for small particles**
  - Solve Maxwell's equations
  - ADDA, FDTD, T-matrix, etc.
  - Computationally expensive
  - Resources required increases with particle size
  - Applicability of upper limit is not well known
  - Theoretically, possible with large resources

II. Challenging Problems

Shape & Size

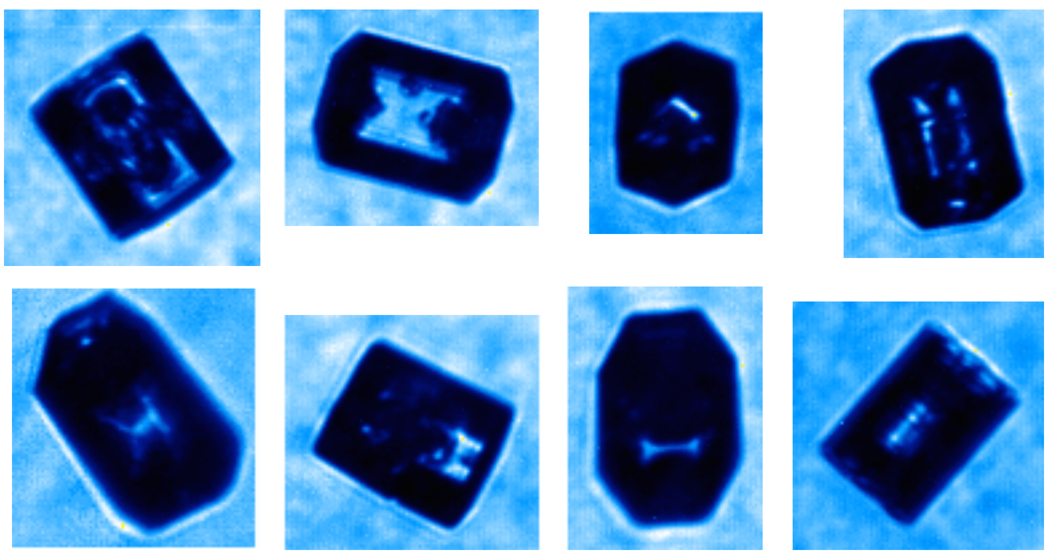


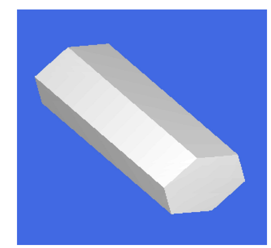
Various shapes and sizes of ice crystals !!!
From ~ 5 to 1000s of μm

II. Challenging Problems

Orientations

- Most ice crystals do not have preferred orientation
- Orientation average required to compute scattering properties needed for models/retrieval schemes
- Random orientations have been assumed in scattering calculations

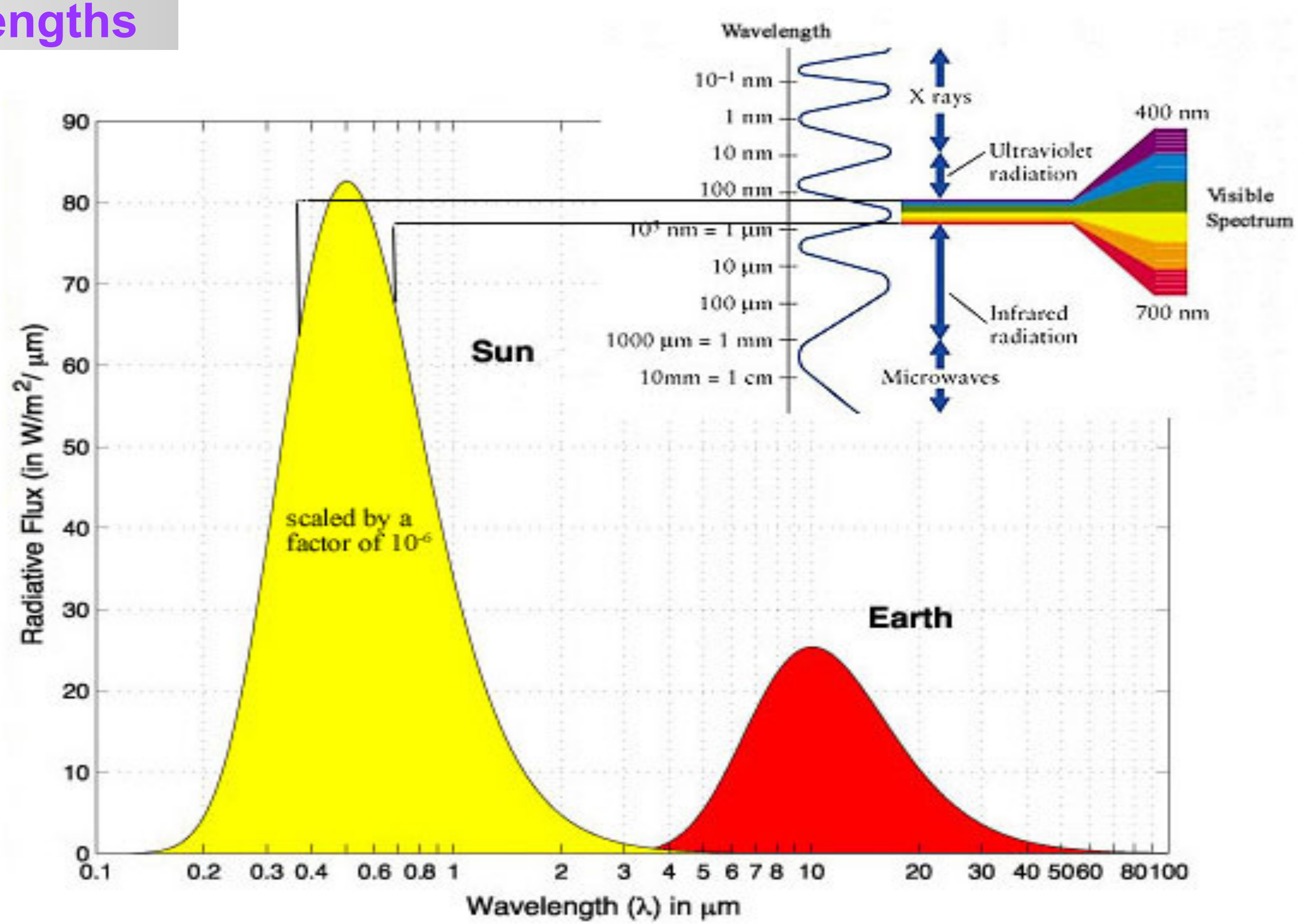




Column

II. Challenging Problems

Wavelengths



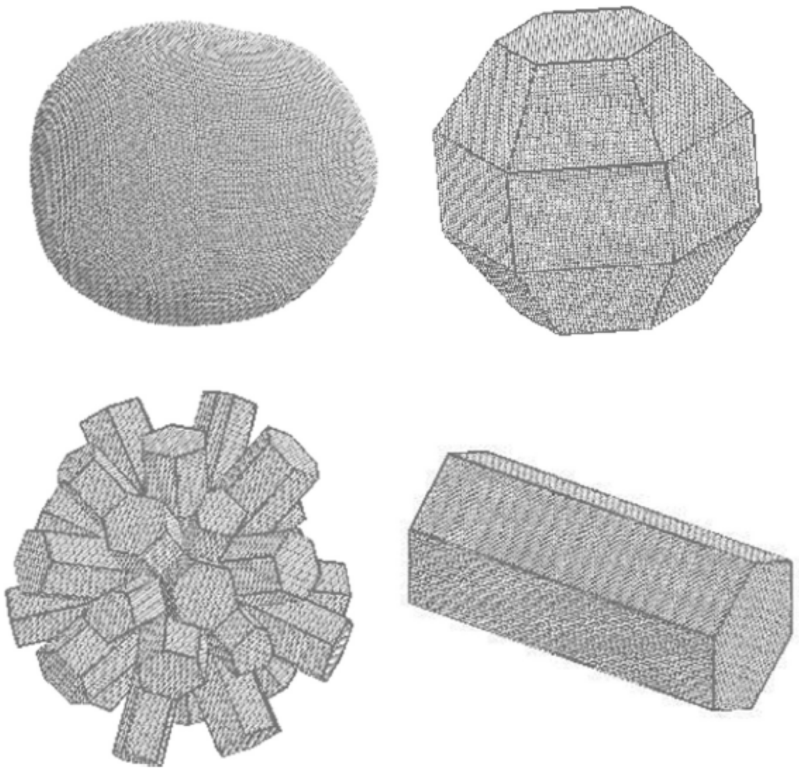
- Calculations required across large spectrum
- Refractive index of ice crystals vary with λ

II. Challenging Problems

- Light scattering solutions for non-spherical particles require large computing resources (increase with size)
- Various shapes and sizes
- Across large spectrum ranges
- Orientation average is required
- NICS Kraken & TACC Stampede
- Using BW, large scattering database is being built
- Input for radiative transfer models, climate models, and satellite retrieval algorithms

II. Challenging Problems

Discrete dipole approximation (DDA) by Purcell and Pennypacker (1973)



- Represent crystals by *N* dipoles
- *N* linear equations for *N* fields exciting *N* dipoles

- Discretization of integral equations using Green's function of the surrounding medium

- Any shape
- Faster than FDTD
- Free source code
- ADDA V1.3b4

III. Orientation Average

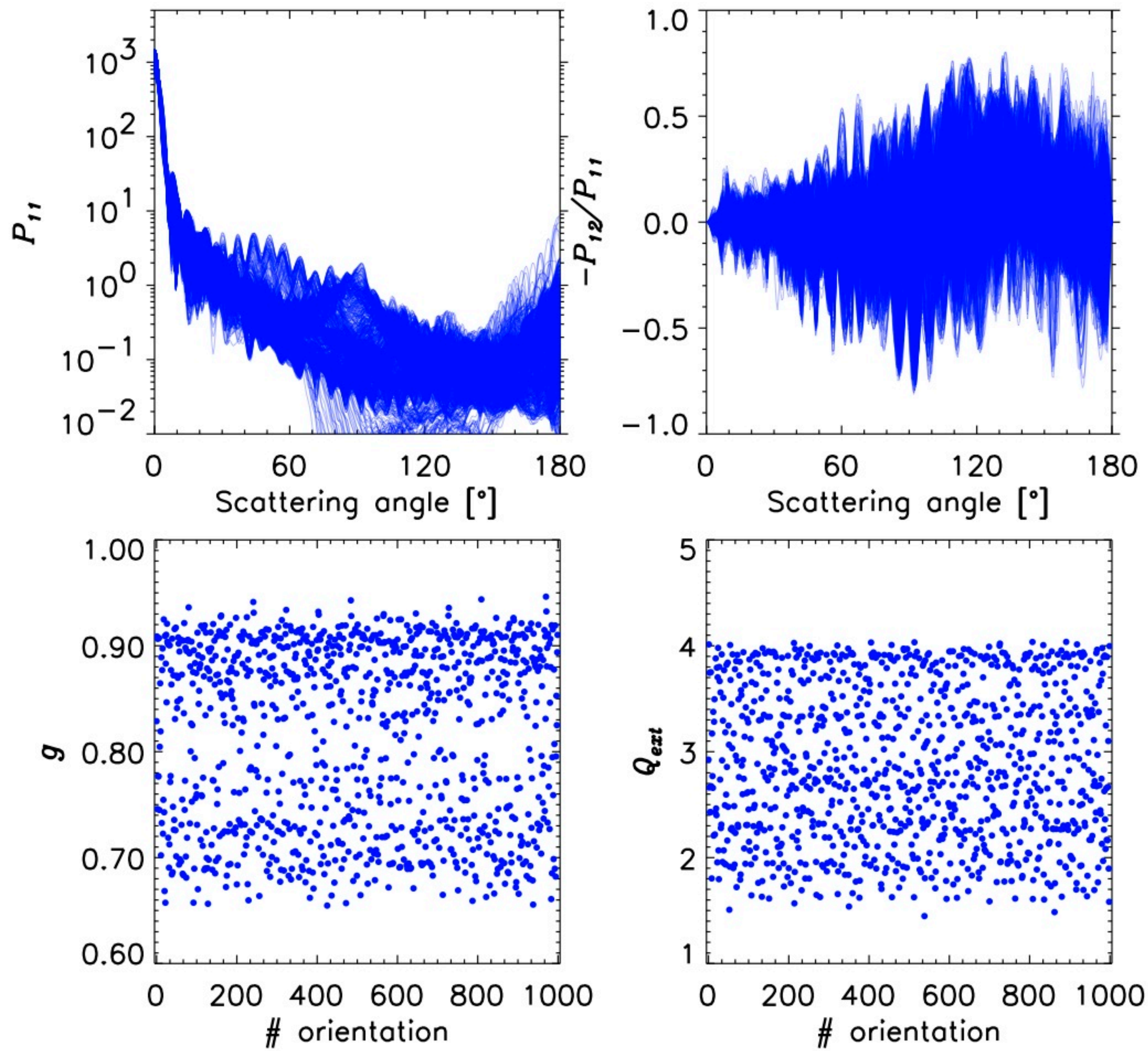
Orientations

Column, *D*=10 μm
λ= 0.55 μm

DDA
1000 orientations

Wide range of variations !

How many orientations are required for accurate results (e.g., 1.0%) ?

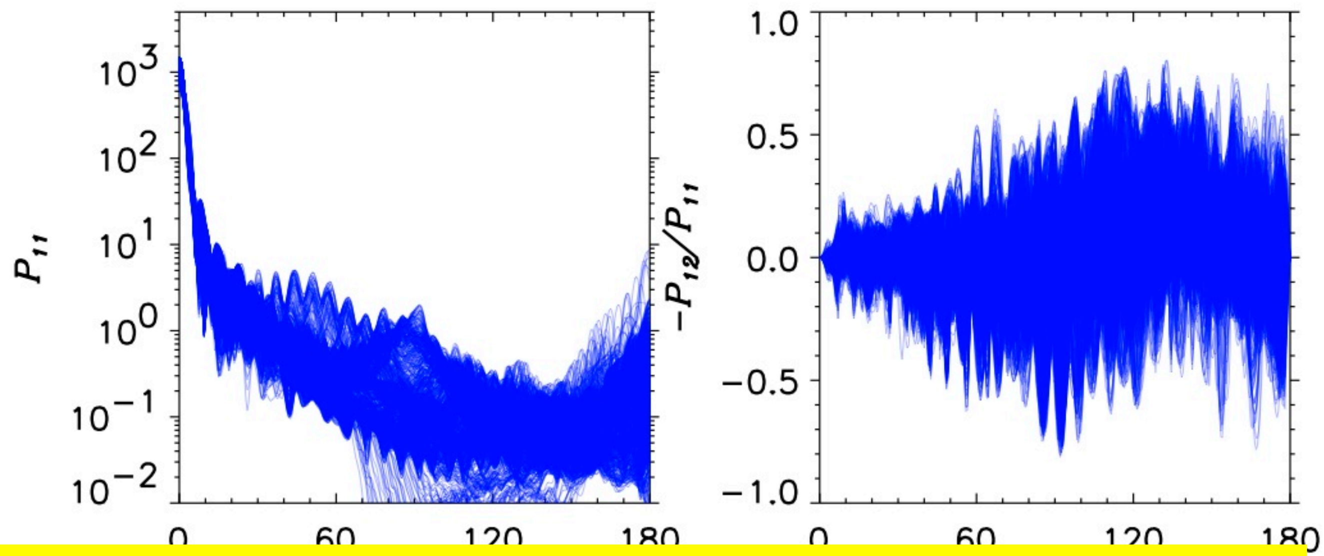


III. Orientation Average

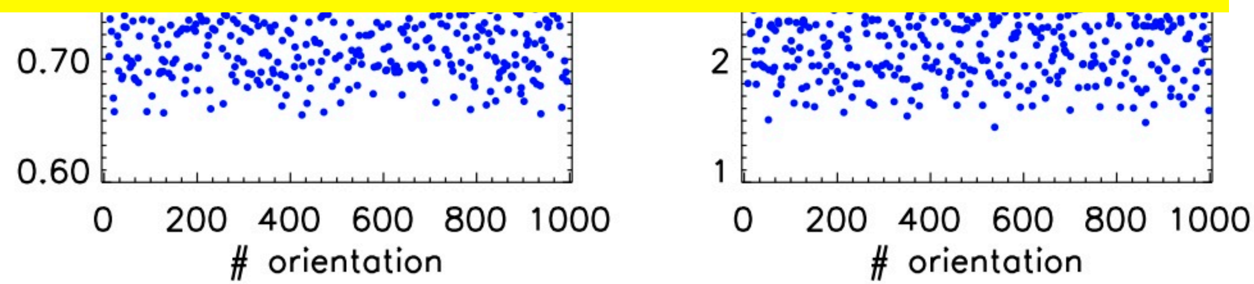
Orientations

Column, *D*=10 μm
λ= 0.55 μm

DDA
1000 orientations



Using 10 BW nodes
~ 5.6 hr. each orientation
~ 56,000 node hr. total



III. Orientation Average

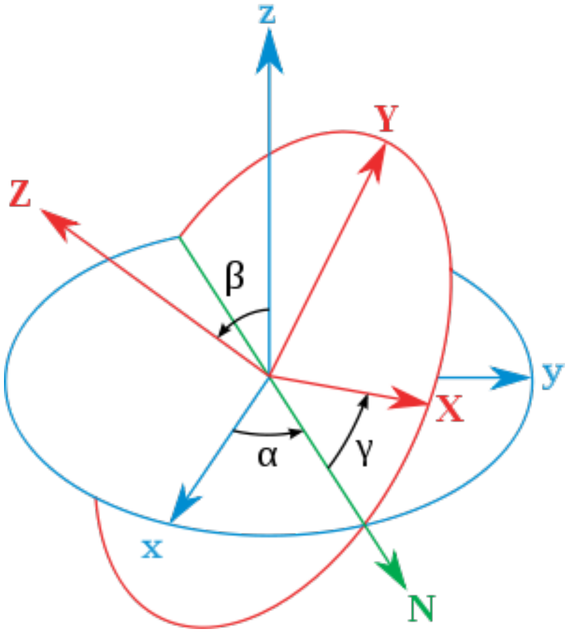
Orientations

- Orientation average for mean scattering properties
  - Phase matrix (e.g., P_{11} and degree of linear polarization)
  - Asymmetry parameter (g)
  - Single-scattering albedo (ω_o)

- Euler angles, α, β, γ, define particle orientations

  1. Lattice grid
     - equal spaced over Euler angles

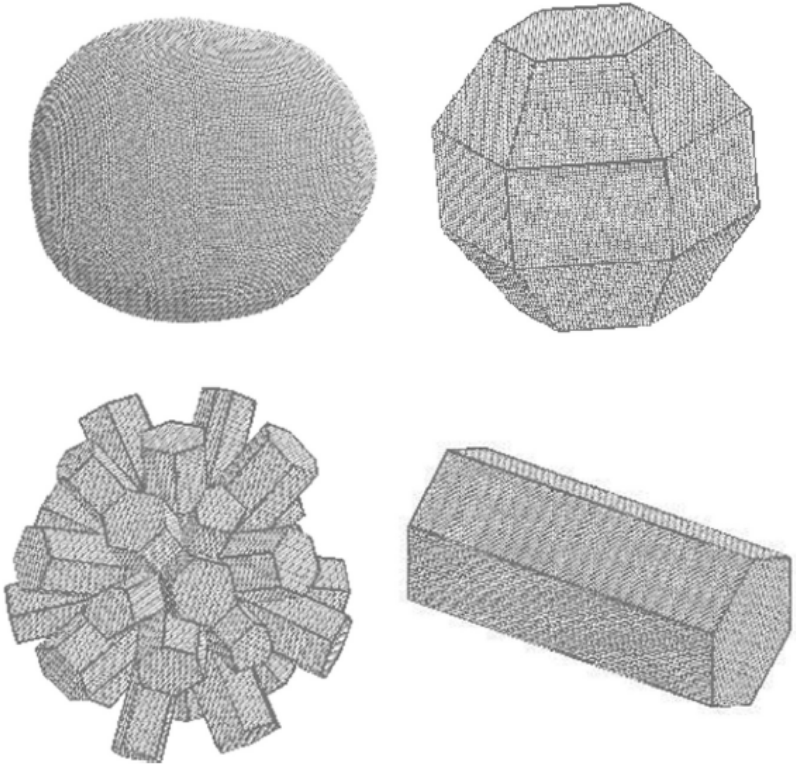
  2. Quasi Monte Carlo (QMC)
     - efficiently choose Euler angles



III. Orientation Average

Ice Crystals

- **4 crystals models**
  - Gaussian random sphere (GS)
  - Droxtal (DX)
  - Budding Bucky ball (3B)
  - Column (COL)

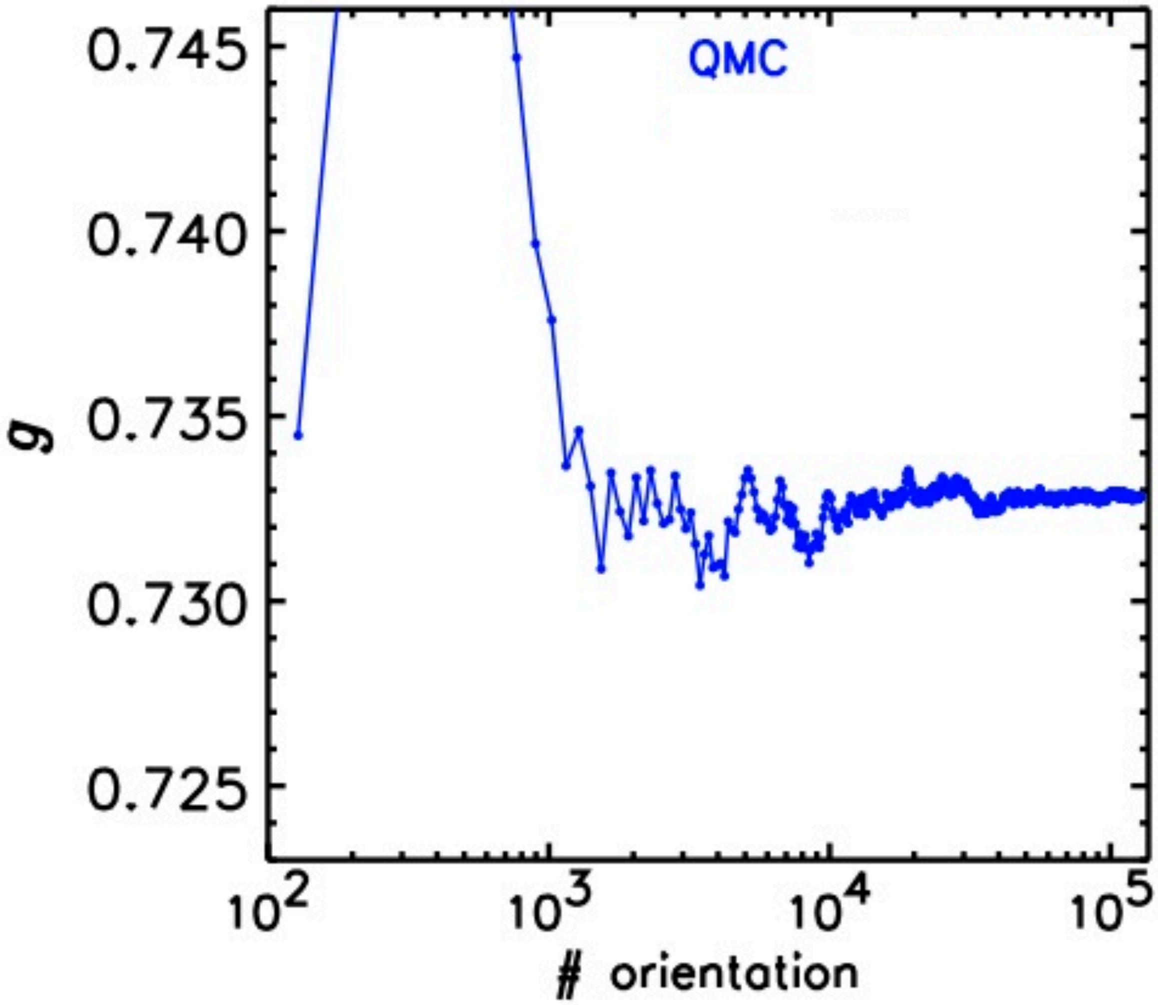


- D_{max} = 10 μm
- ADDA
- Lattice grid & QMC
- λ=0.55, 3.78, and 11.0 μm

III. Orientation Average

GS

λ = 3.78 μm

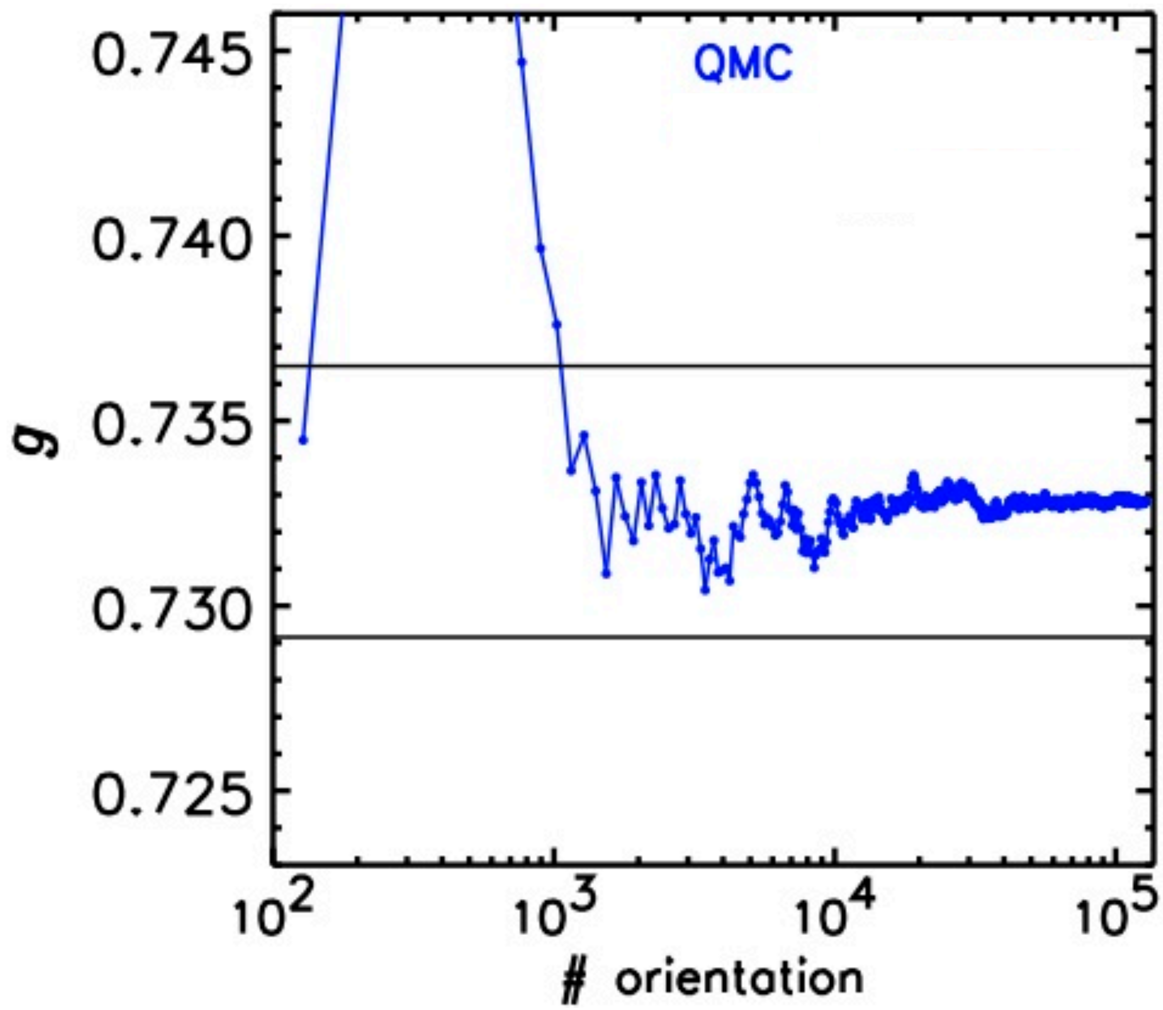


Average converges with number of orientations

III. Orientation Average

GS

λ = 3.78 μm



+ 0.5 %

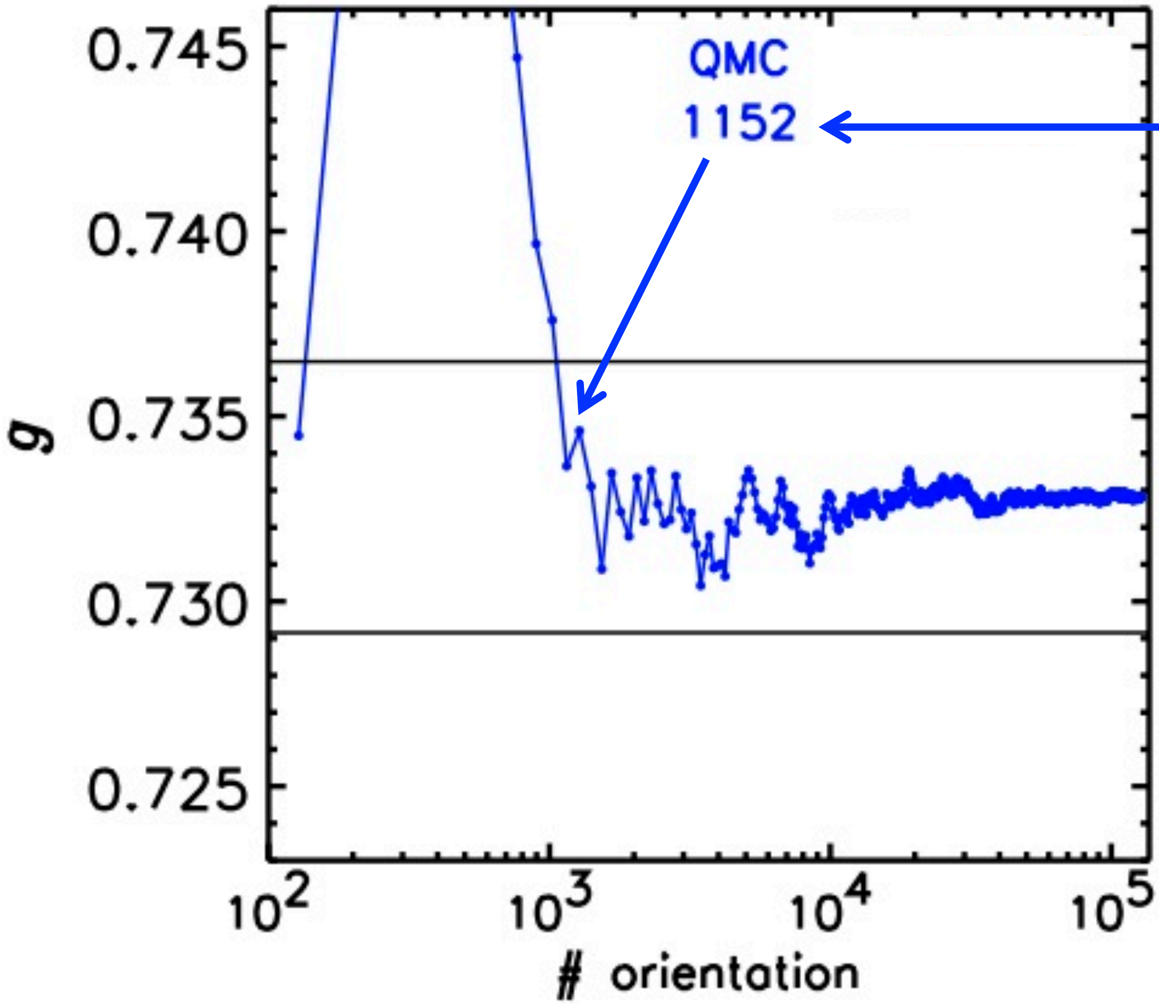
1.0% accuracy

- 0.5 %

III. Orientation Average

GS

$\lambda = 3.78\ \mu m$



QMC needs
1152 orientations
for 1.0 %
accuracy in average

+ 0.5 %

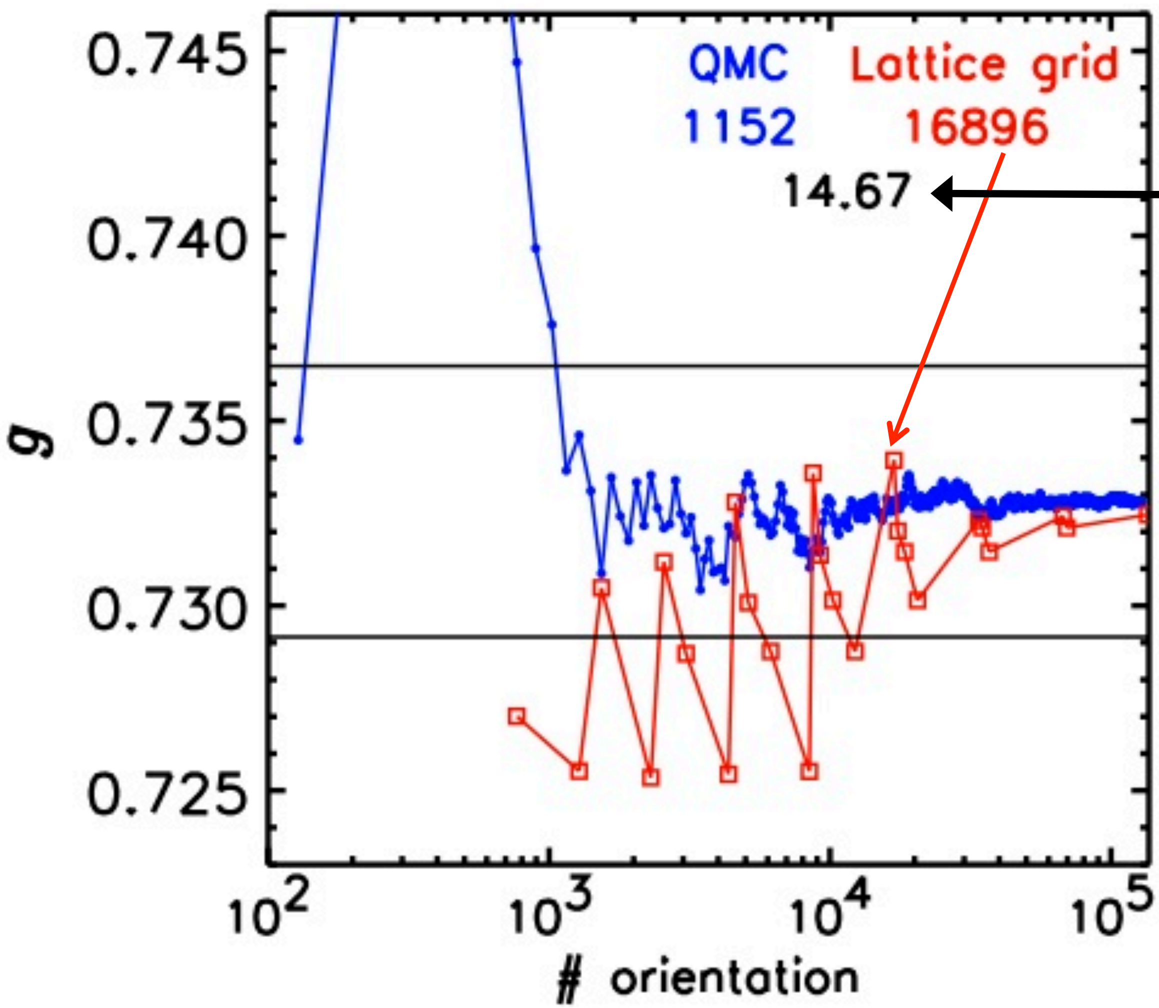
1.0%
accuracy

- 0.5 %

III. Orientation Average

GS

λ = 3.78 μm



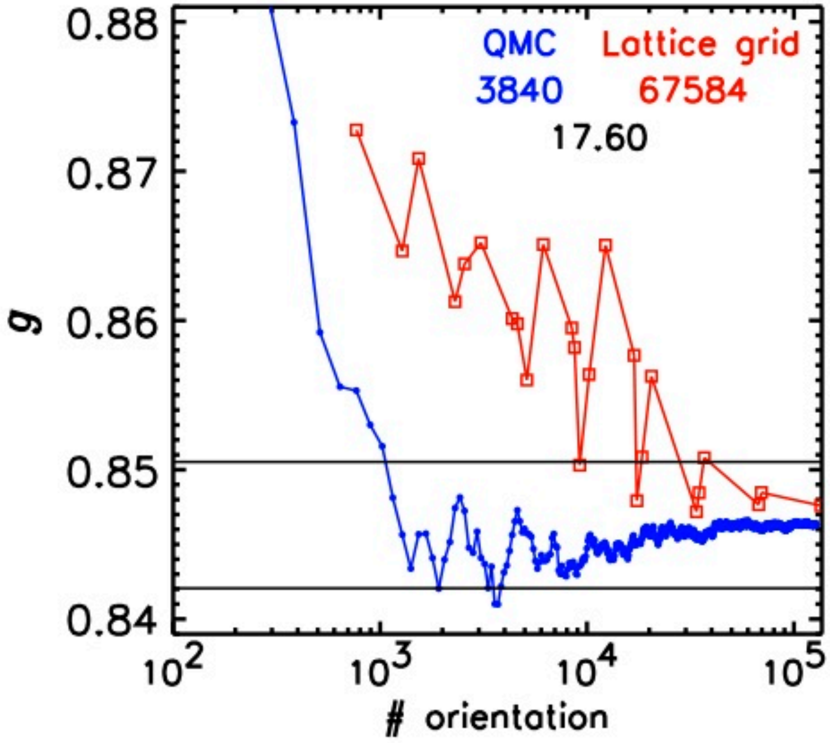
Min. # ratio
Lattice grid/QMC

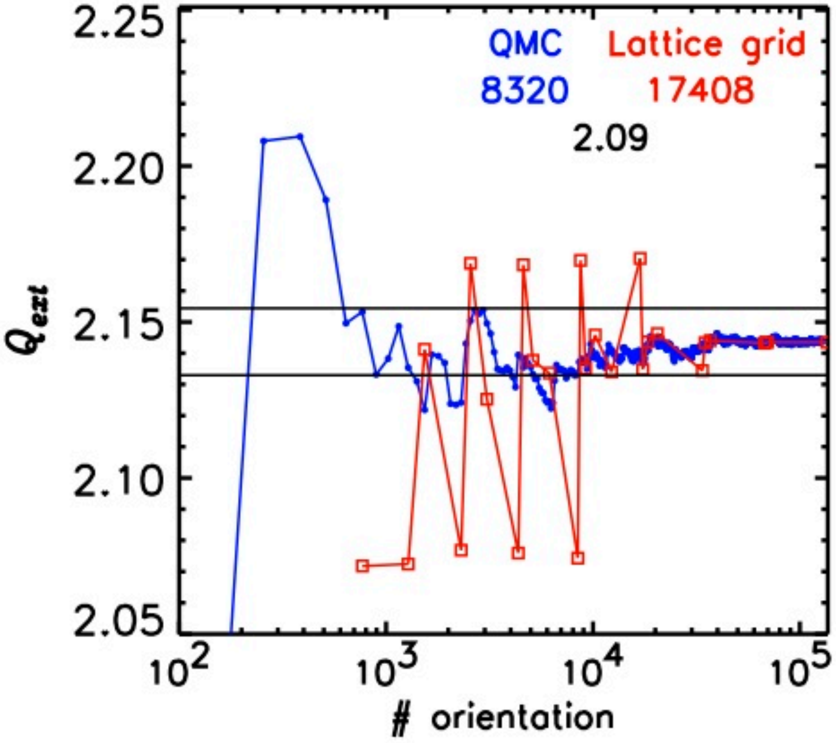
- **Lattice grid** needs 14.67 times more computing time than **QMC**

III. Orientation Average

GS

λ = 0.55 μm



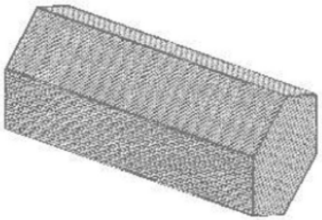


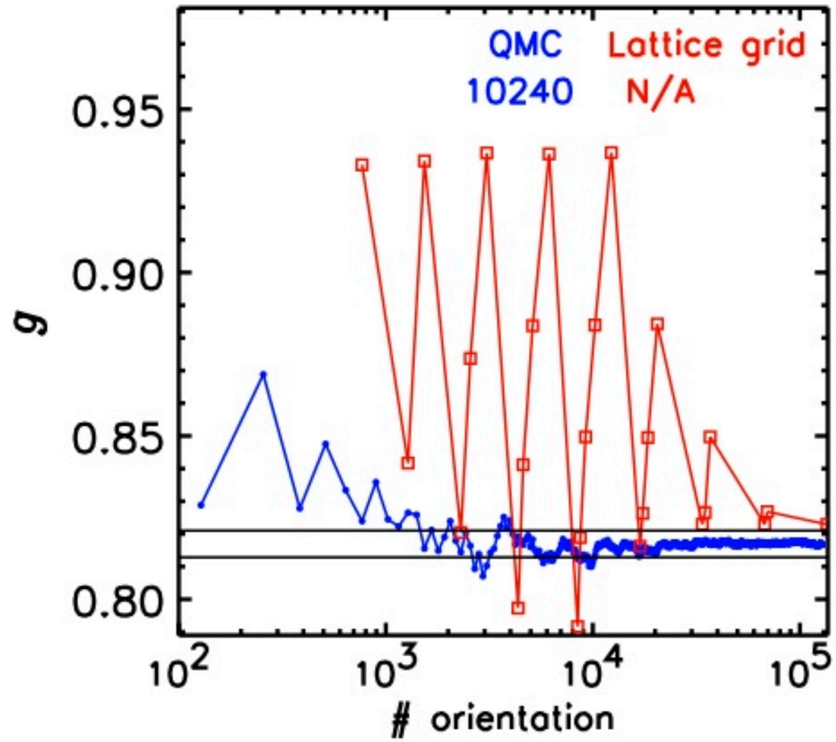
More orientations are required at non-absorbing λ !!!

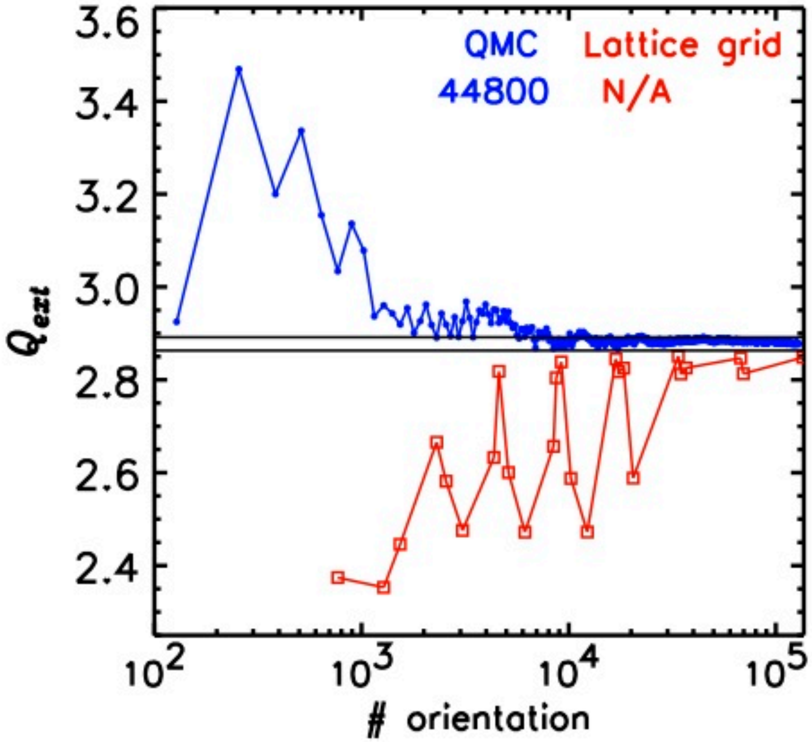
III. Orientation Average

COL

λ = 0.55 μm







More orientations are required than for GS !!!

III. Orientation Average

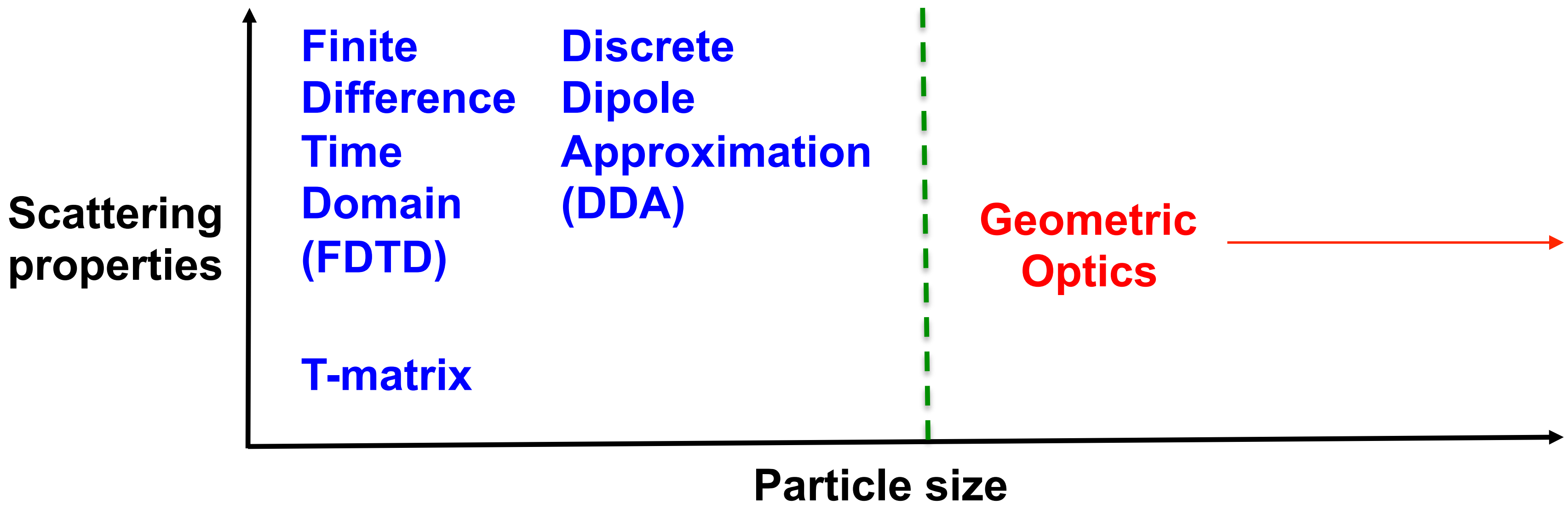
- **QMC requires fewer orientations than lattice grid for nonspherical atmospheric particles & less computing time (more than 50% less)**
- **Single-scattering properties & MIN # orientations depend on particle shapes**
- **Required MIN # of orientations depends on λ**
- **Convergence of scattering properties has to be checked when an exact solution is not available**

Um and McFarquhar (2013, *JQSRT*)

IV. Atmospheric Halos

- Scattering calculations of small ice crystals requires large computing resources

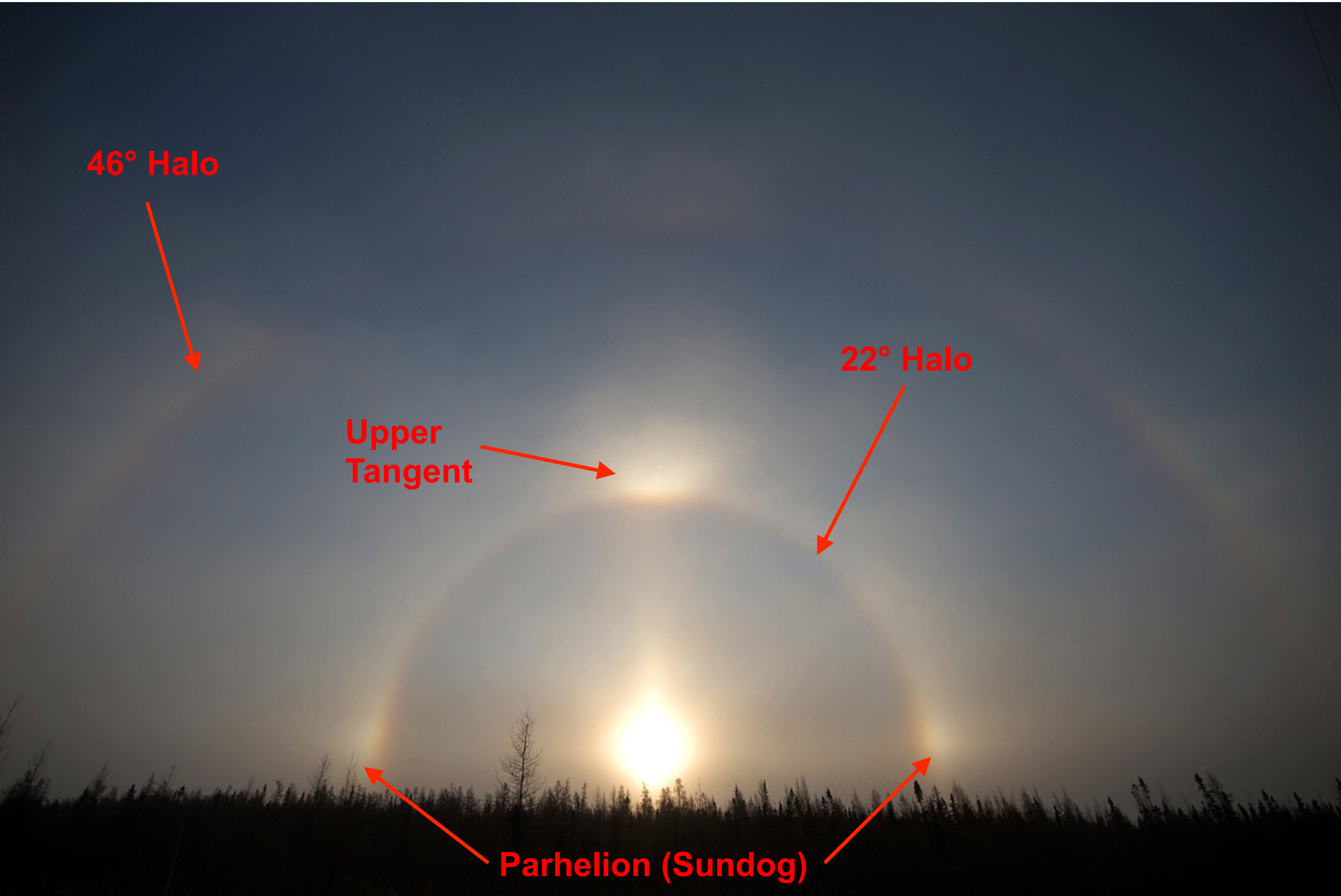
- GOM for large particles needs less resources



- Find threshold size where can switch to GOM

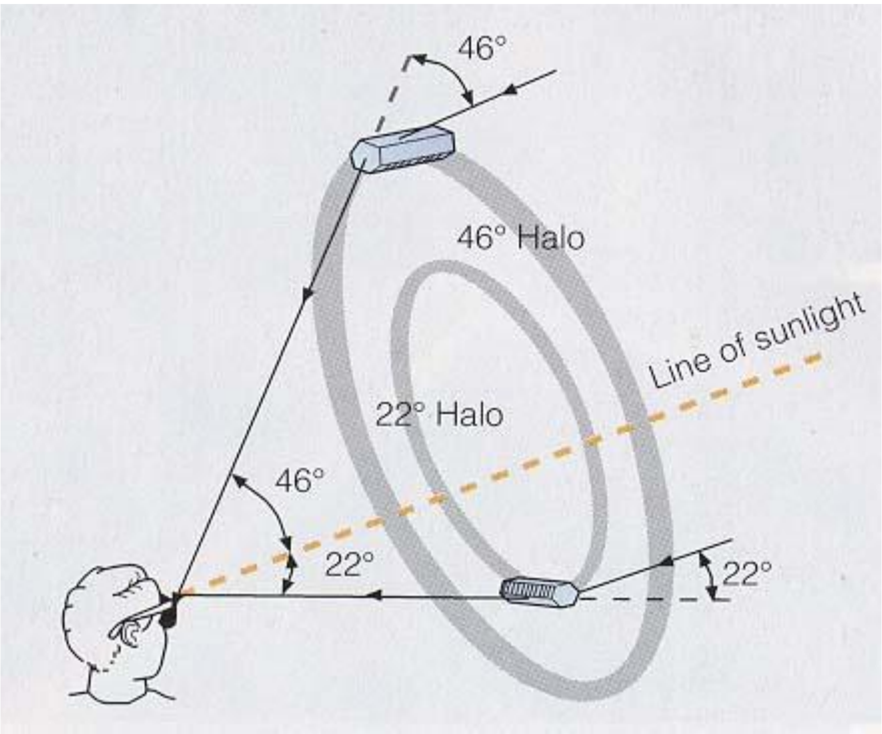
IV. Atmospheric Halos

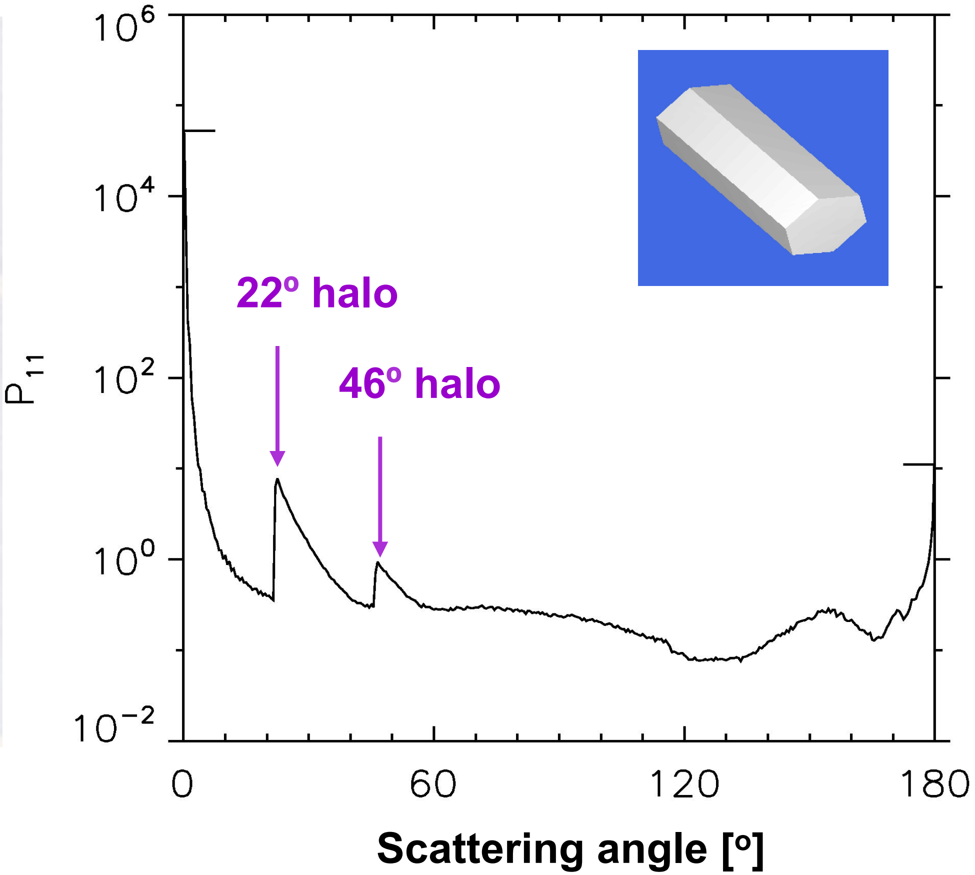
IV. Atmospheric Halos



IV. Atmospheric Halos

Circular Halos





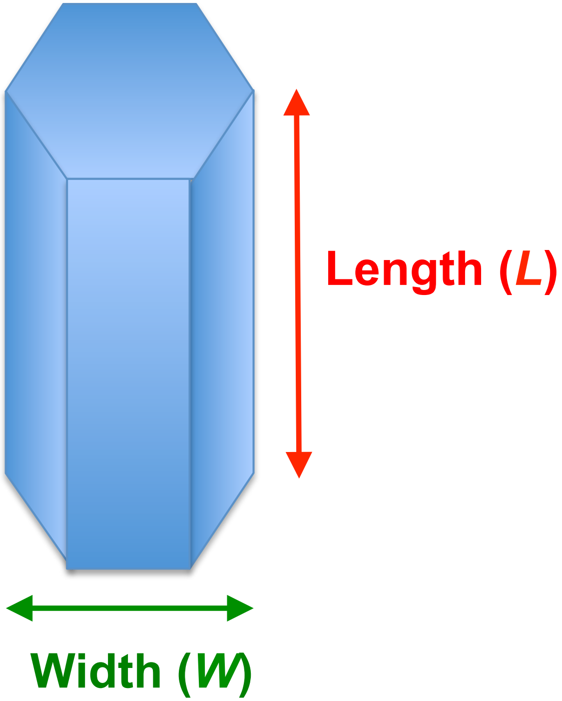
- Halos appear in geometric optics regime
- Finding size at which ADDA calculations produce halos

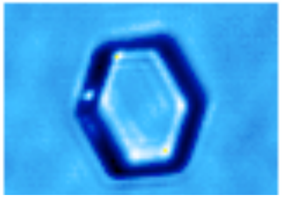
IV. Atmospheric Halos

Simulations

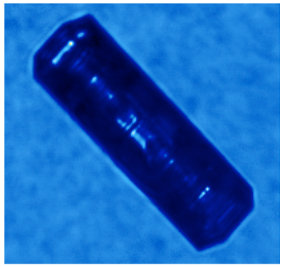
Aspect Ratio (*AR*) = *L* / *W*

***AR* = 0.10, 0.25, 0.50, 1.00, 2.00, 4.00**





Thin Plate



Long Column

***W* : up to 20 μm**

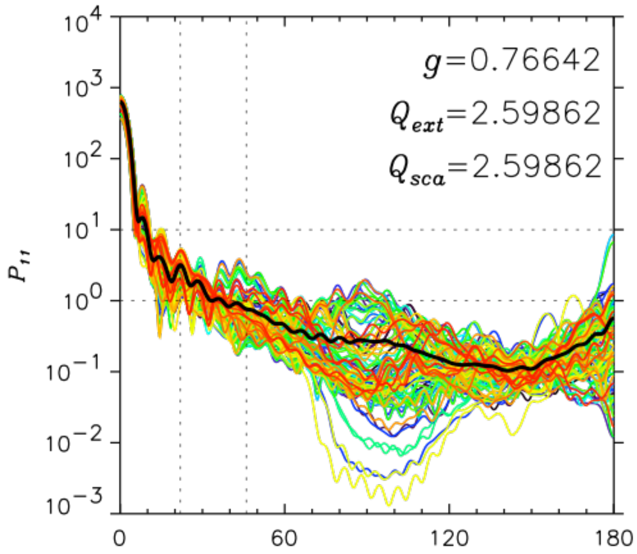
***L*: up to 48 μm**

@ λ=0.55 μm using ADDA & QMC

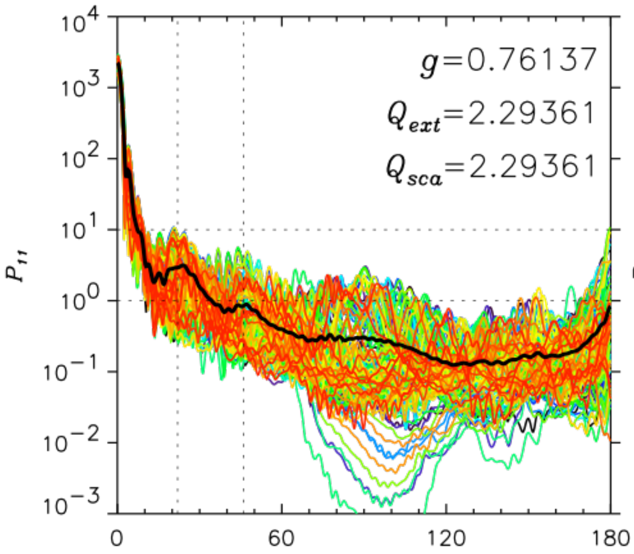
IV. Atmospheric Halos

AR = 1.0

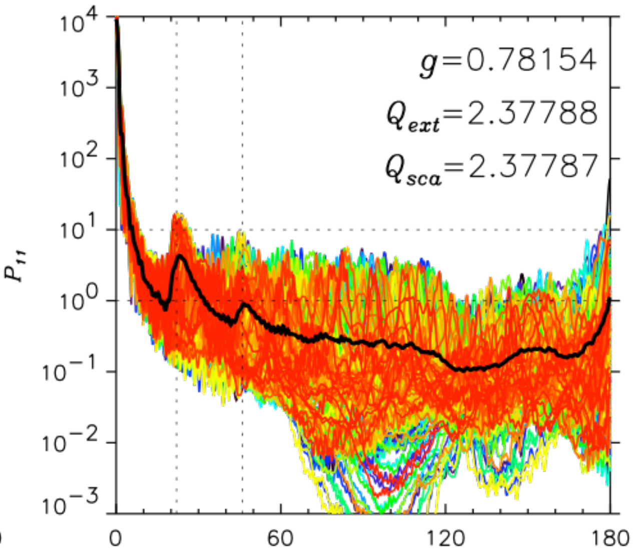
Scattering Phase function P_{11}



W **=5 μm** ***L*** **=5 μm**
χ =28.6 χ_{veq} **=30.7**



W **=10 μm** ***L*** **=10 μm**
χ =57.1 χ_{veq} **=61.4**

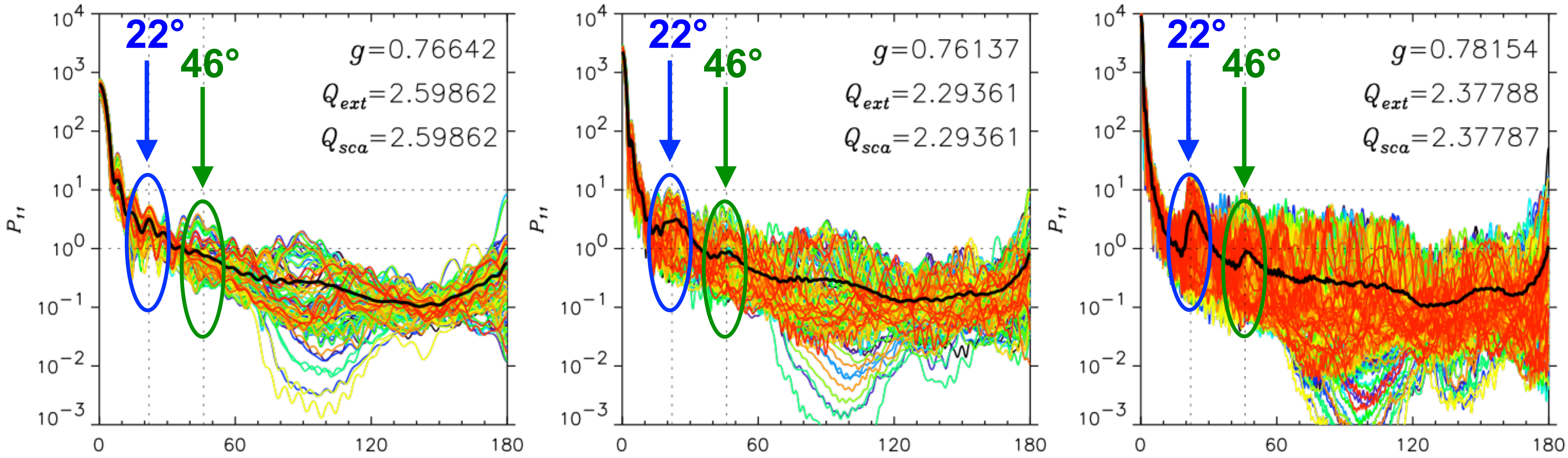


W **=20 μm** ***L*** **=20 μm**
χ =114.2 χ_{veq} **=122.7**

Size increases

IV. Atmospheric Halos

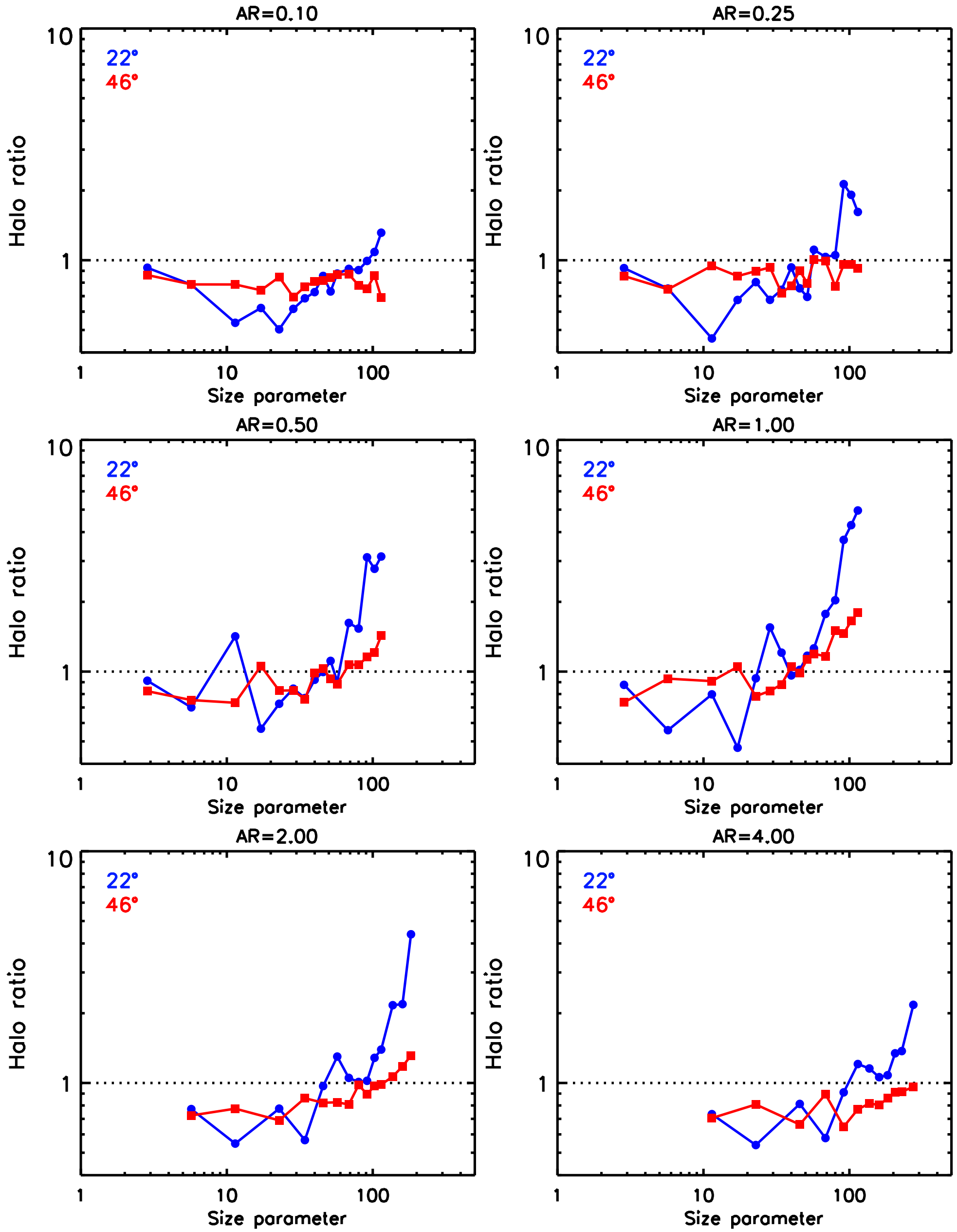
AR = 1.0



W **=5 μm** ***L*** **=5 μm**	***W*** **=10 μm** ***L*** **=10 μm**	***W*** **=20 μm** ***L*** **=20 μm**
χ **=28.6** χ_{veq} **=30.7**	χ **=57.1** χ_{veq} **=61.4**	χ **=114.2** χ_{veq} **=122.7**

- **Halos form as particle size increases**

IV. Atmospheric Halos



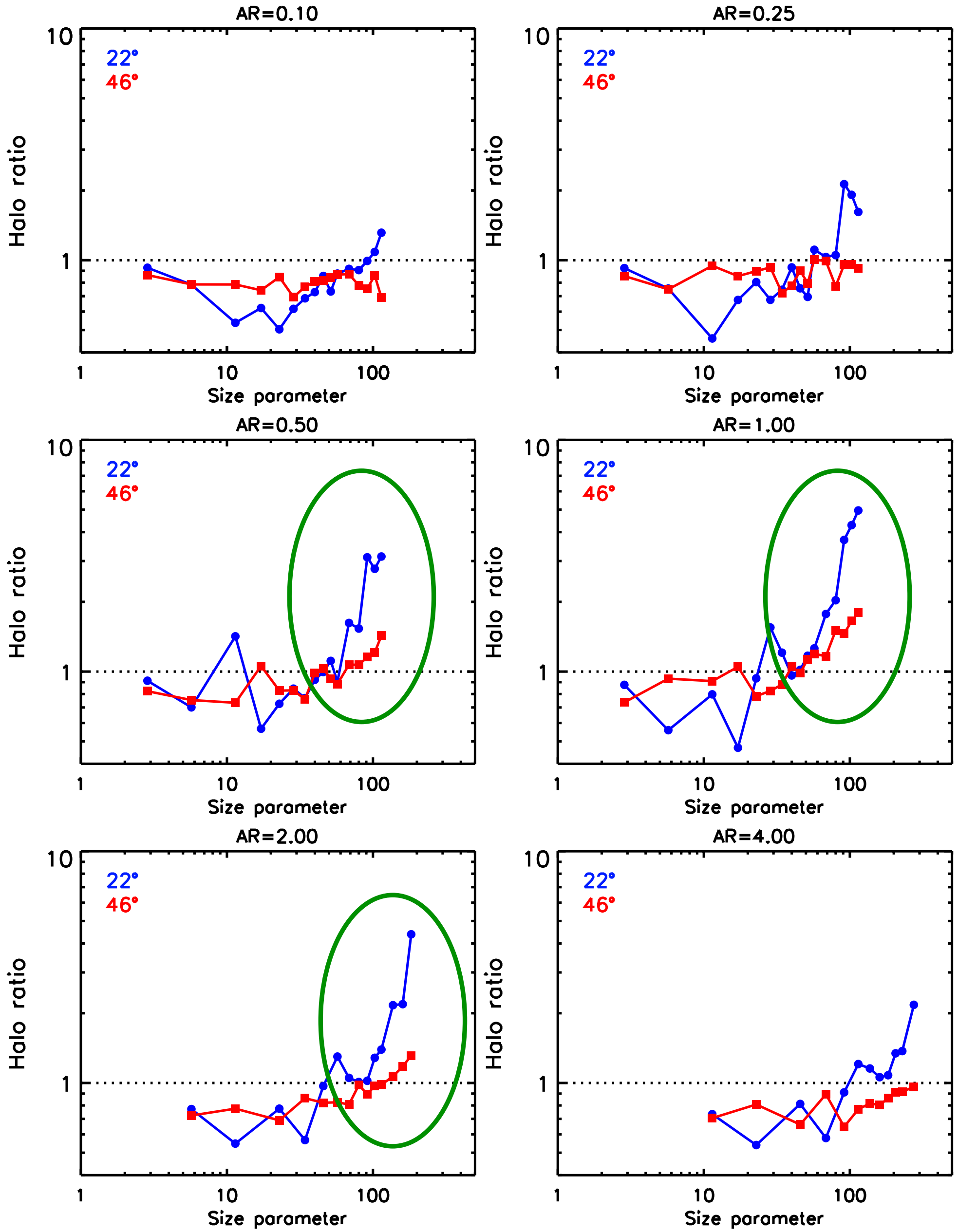
- Halo Ratio (*HR*) = $P_{11}(\theta_1)/P_{11}(\theta_2)$

- 22°
  - $P_{11}(22°)/P_{11}(18°)$

- 46°
  - $P_{11}(46°)/P_{11}(42°)$

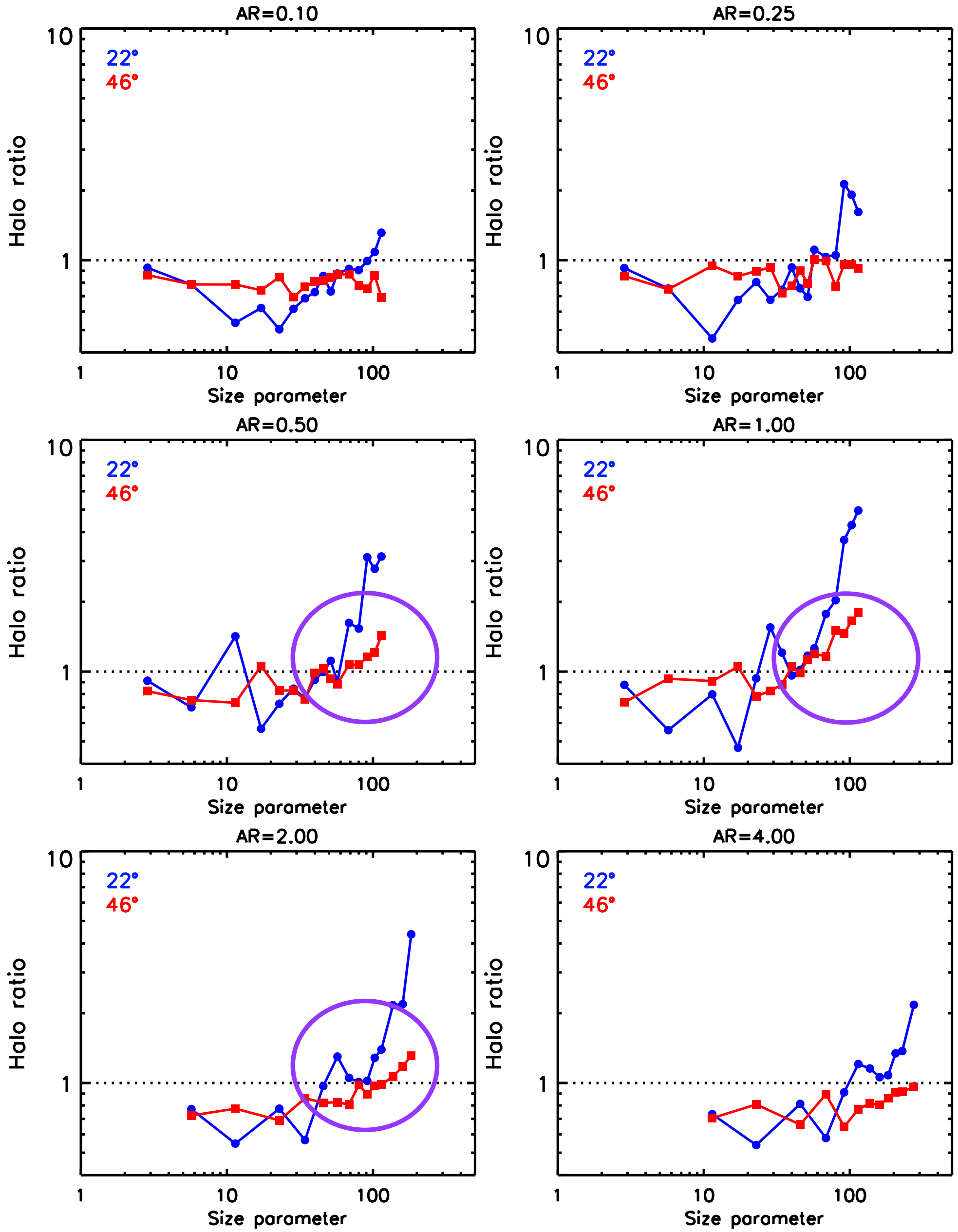
- Halo formed when *HR* > 1.0

IV. Atmospheric Halos



- Halo Ratio (*HR*) = $P_{11}(\theta_1)/P_{11}(\theta_2)$
- 22°
  - $P_{11}(22°)/P_{11}(18°)$
- 46°
  - $P_{11}(46°)/P_{11}(42°)$
- Halo formed when *HR* > 1.0
- Compact shape (*AR* ~ 1.0)
  22° and 46°

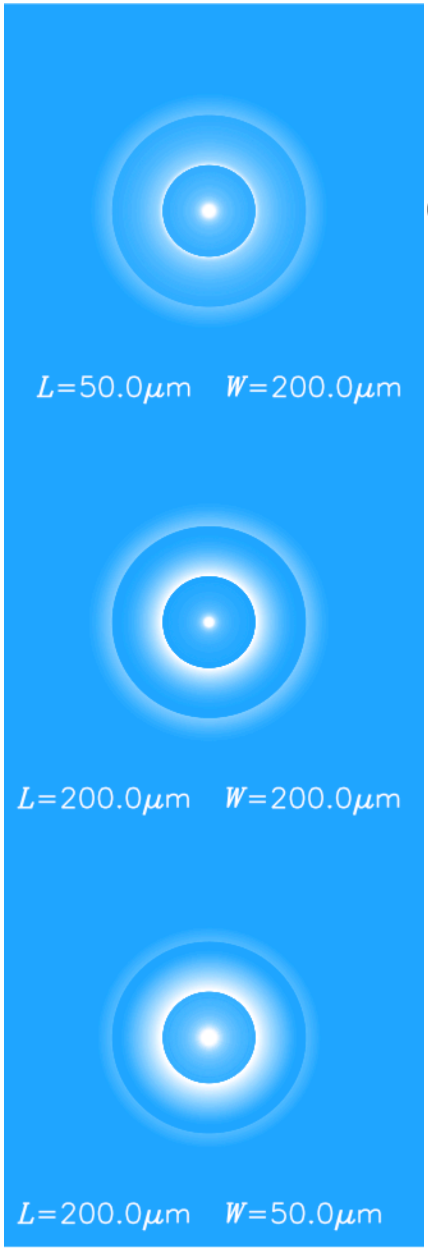
IV. Atmospheric Halos



- Halo Ratio (*HR*) = $P_{11}(\theta_1)/P_{11}(\theta_2)$
- 22°
  - $P_{11}(22°)/P_{11}(18°)$
- 46°
  - $P_{11}(46°)/P_{11}(42°)$
- Halo formed when *HR* > 1.0
- Compact shape (*AR* ~ 1.0) 22° and 46°
- *AR*=0.5, 1.0, and 2.0 for 46°

- Polar coordinate plots of P_{11}
- Large particles with GOM
- *AR* = 0.25 (top)
- *AR* = 1.00 (middle)
- *AR* = 4.00 (bottom)

GOM *AR*



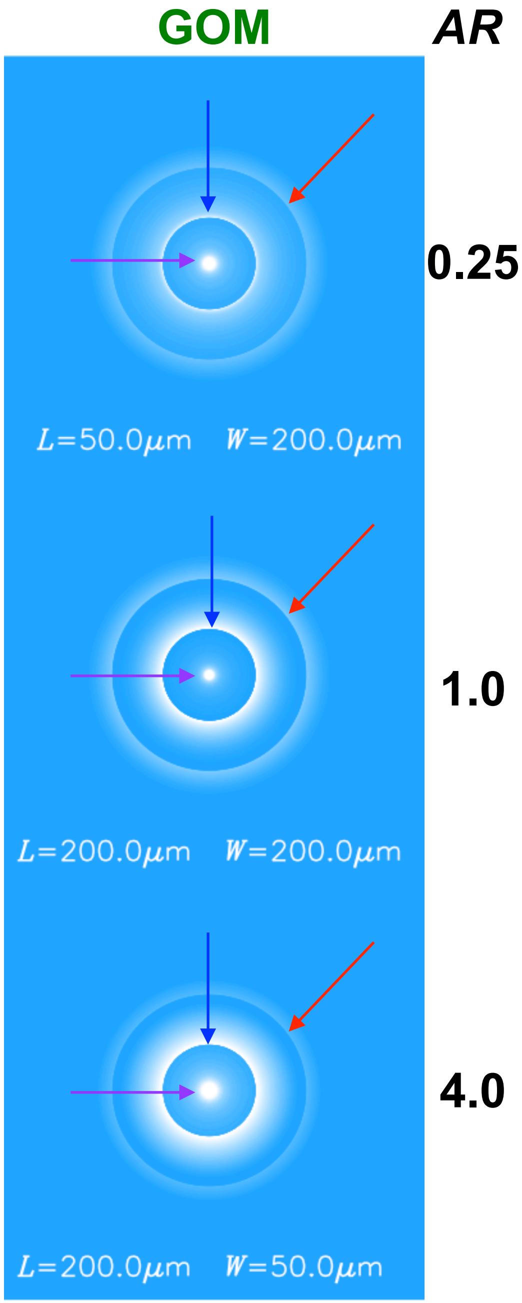
0.25

1.0

4.0

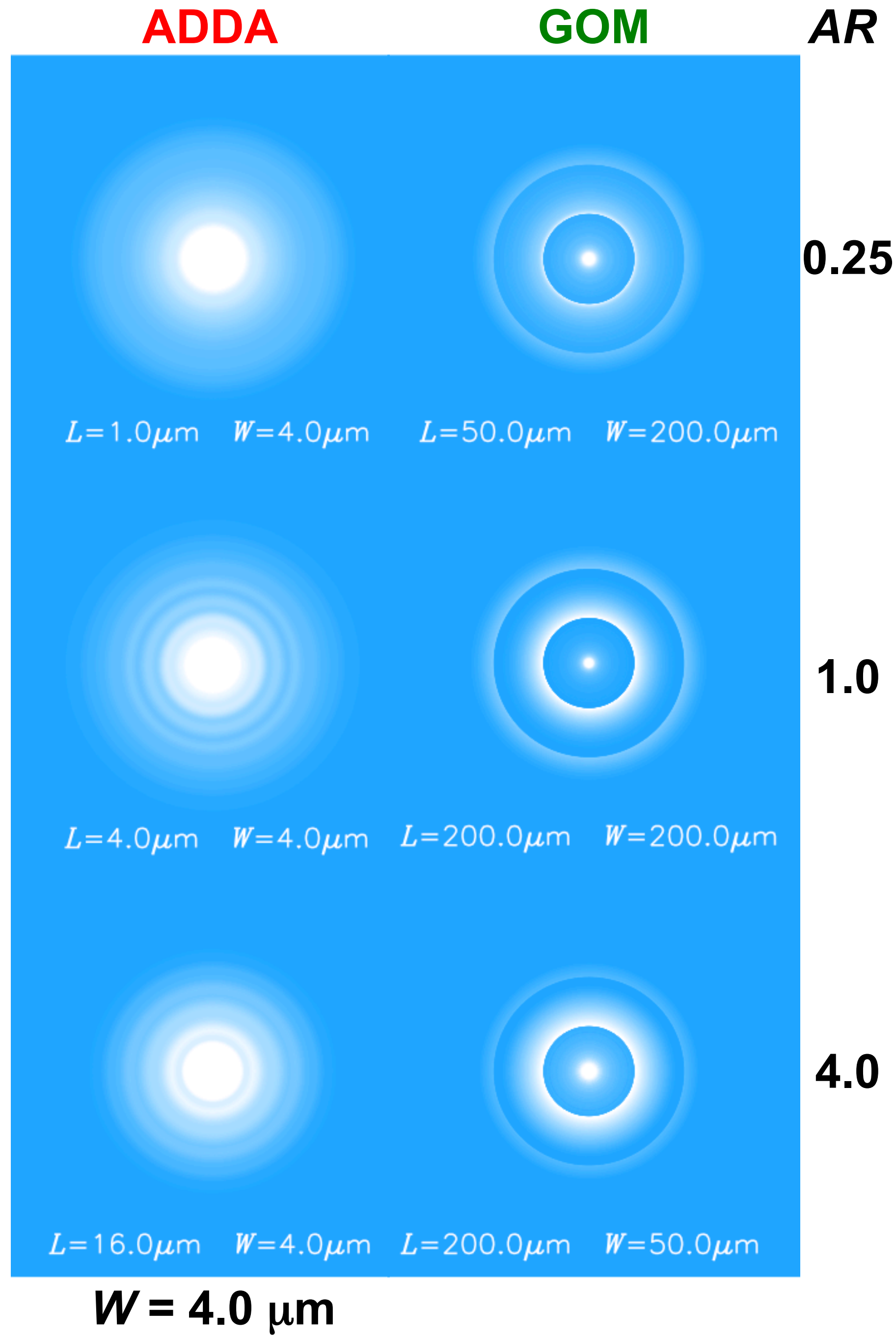
- Polar coordinate plots of P_{11}
- Large particles with GOM
- *AR* = 0.25 (top)
- *AR* = 1.00 (middle)
- *AR* = 4.00 (bottom)

- What we see in sky
- Filled circle is Sun
- Inner bright ring is 22° halo
- Outer bright ring is 46° halo



- Small particles,
- *W* = 4.0 μm with ADDA

- No distinct halos
- Diffraction dominant

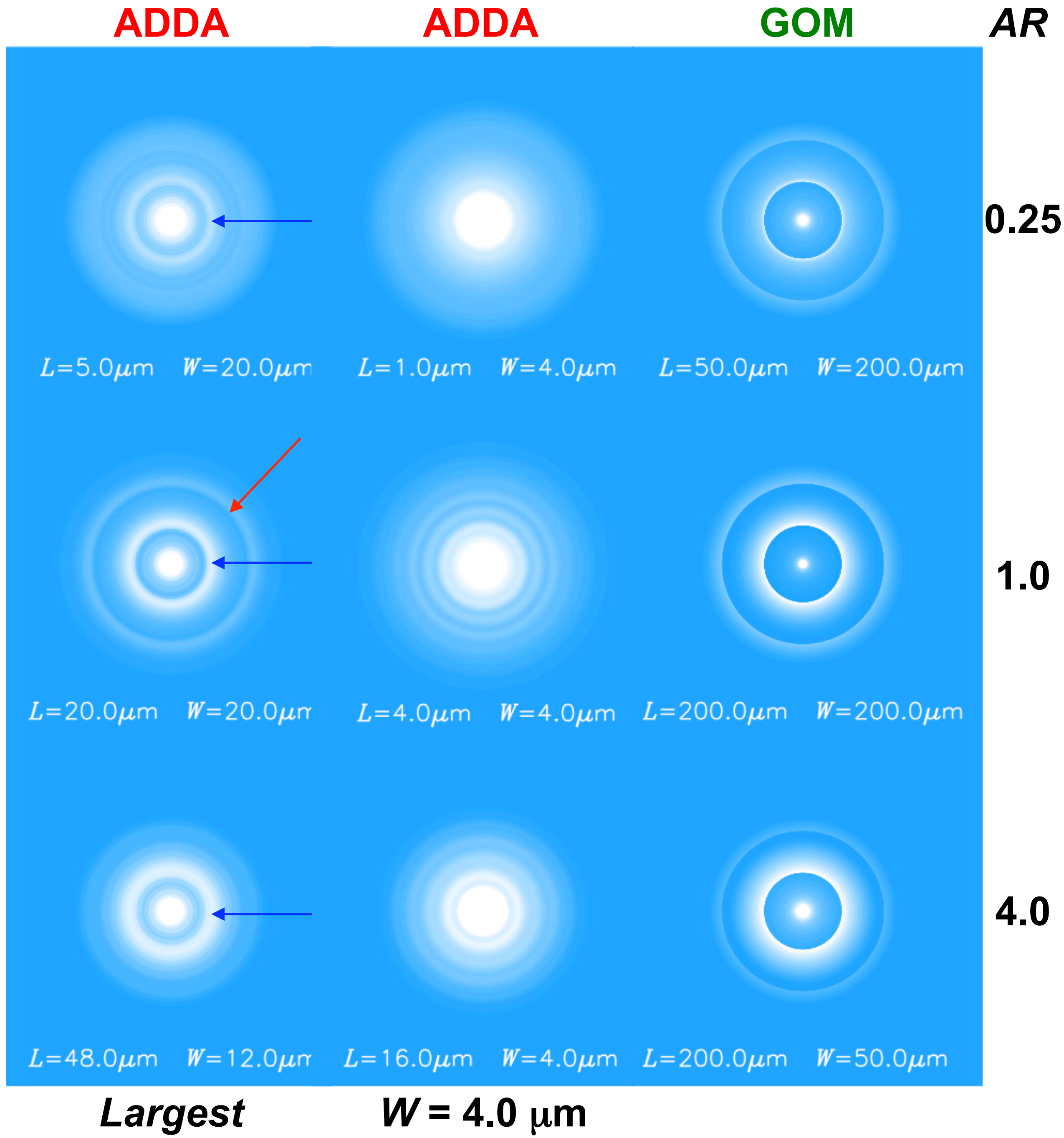


- Largest particles in each *AR* with ADDA

- 22° halo for all *AR*
- 46° for *AR*=1.0

- Compact shape (*AR*=1.0) produces clear & sharp halos

- More larger size is required



V. Summary

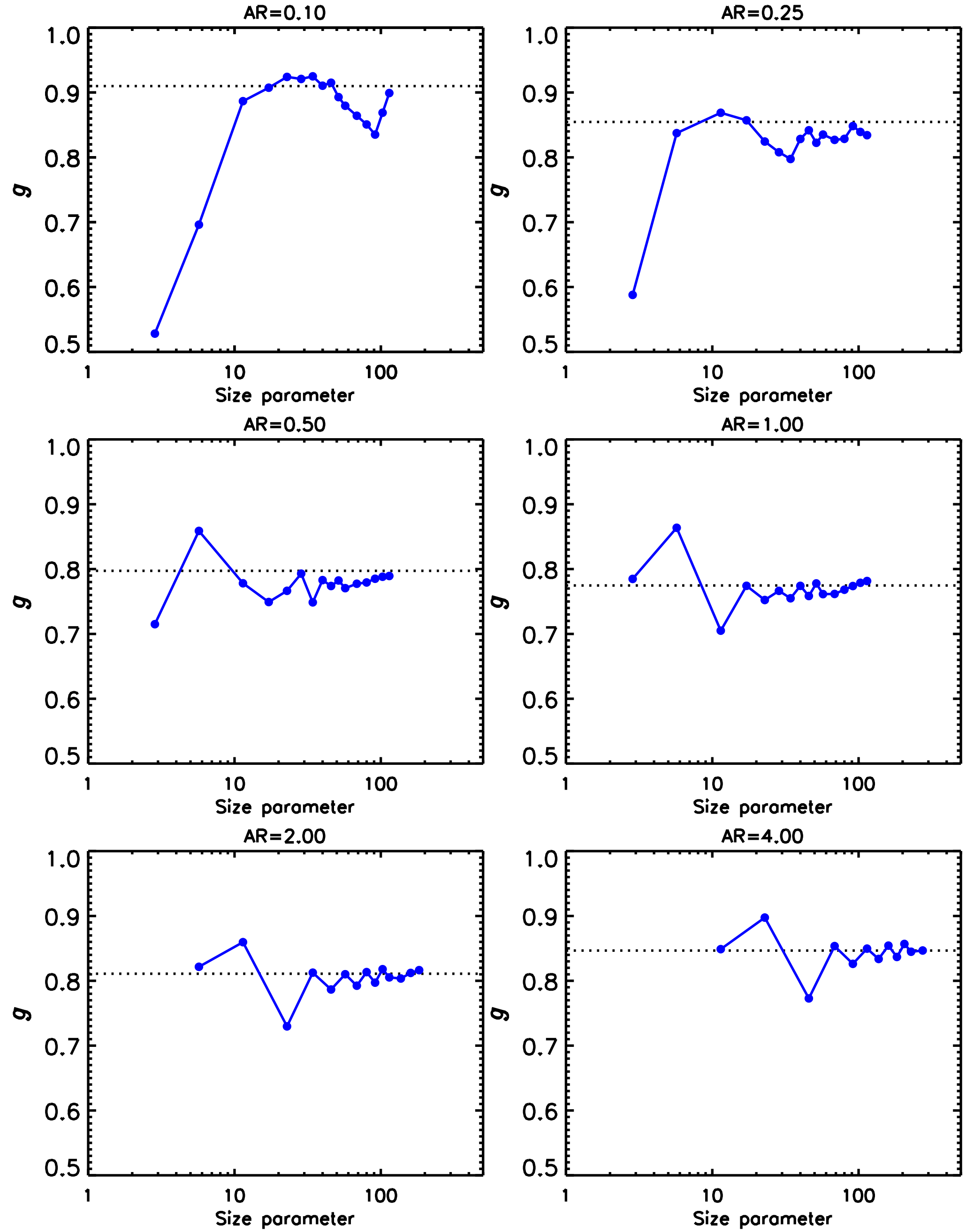
- Advanced orientation average scheme (i.e., QMC) can save significant amount of computing time (more than 50%) compared to conventional scheme (i.e., equal spaced)
- Atmospheric halos form @ size parameter of ~60, depending on aspect ratio of ice crystal
- Calculations with larger size required to be in geometric optics regime
- Scattering database being built for radiative transfer models, climate models, & satellite retrieval algorithms

Asymmetry parameter (g)

- **Convergence was made**
  - ***AR*** **= 0.5, 1.0, 2.0, 4.0**

- **For AR = 0.1 & 0.25**
  - **more larger sizes are required for convergence**

- **ADDA**
- **GOM (dot line)**



I. Mo


circumzenithal arc
supralateral
46° halo
suncave parry
sunvex Parry
upper tangent
22° halo
Moilanen arc
parhelion (sundog)
parhelic circle
helic arc
Parry supralateral
sun pillar