Enhanced Computational Capabilities of the Scattering Model NESCoP to Accurately Calculate SSPs of Large Realistic Hydrometeors

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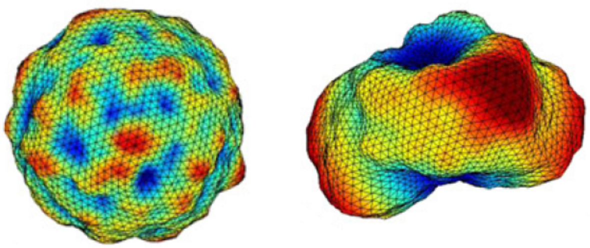
[4] L2E, Sorbonne Université, Paris, France

2019 PMM Science Team Meeting
November 4 – 8 2019, Indianapolis, IN

EM Scattering by arbitrarily shaped particles

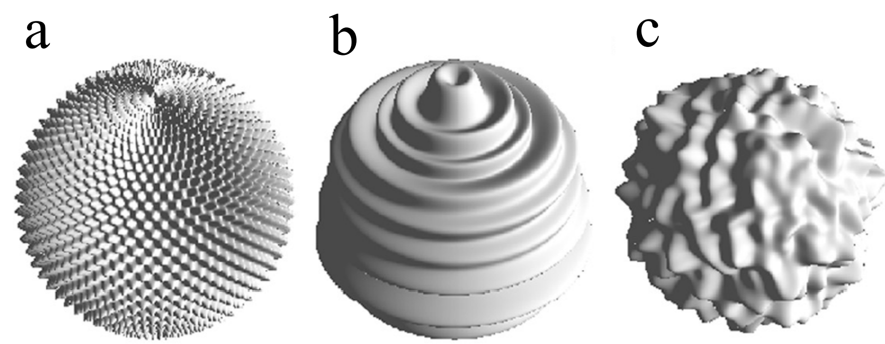
Mollon, Guilhem, and Jidong Zhao. "3D generation of realistic granular samples based on random fields theory and Fourier shape descriptors." Computer Methods in Applied Mechanics and Engineering 2014.



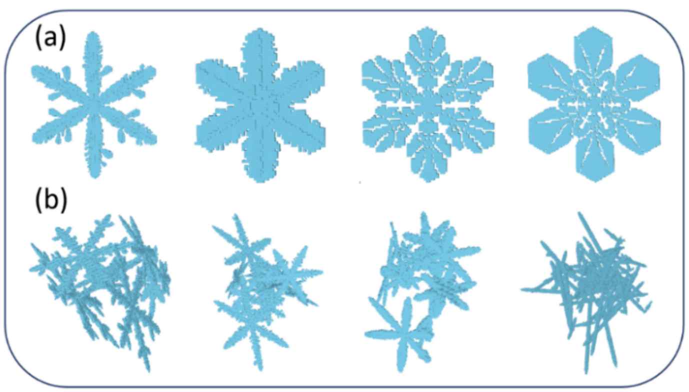
Single-scattering properties of particles with complex arbitrary geometries.

Kahnert, Michael, et al. "Light scattering by particles with small-scale surface roughness: comparison of four classes of model geometries." Journal of Quantitative Spectroscopy and Radiative Transfer, 2012.

Kuo, K.S, et al. 2016. The microwave radiative properties of falling snow derived from nonspherical ice particle models. Part I: An extensive database of simulated pristine crystals and aggregate particles, and their scattering properties. Journal of Applied Meteorology and Climatology



(a) 3D Chebyshev particles, (b) 2D and (c) 3D Gaussian random spheres

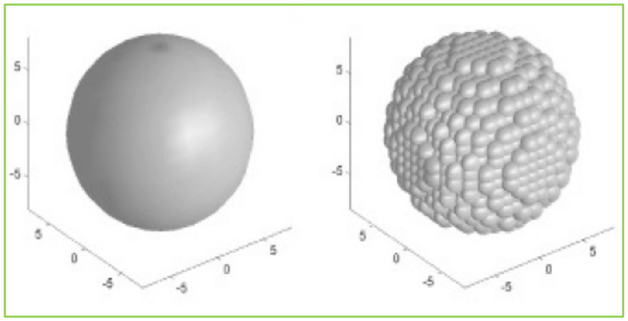


Pristine crystals (a) & aggregate (b) snow particles from OpenSSP database

Representative of different types of particles in nature : **mineral aerosol** particles in planetary atmospheres, **cosmic dust** particles, **regolith** particles on the surface of terrestrial planets and asteroids, **ice-cloud** particles…

EM Scattering by arbitrarily shaped particles

UCLA JIFRESSE



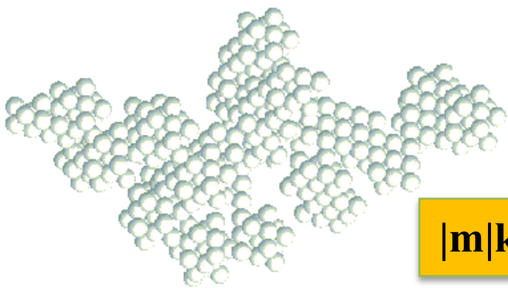
Discrete dipole approximation (DDA) representation of a sphere

NEED

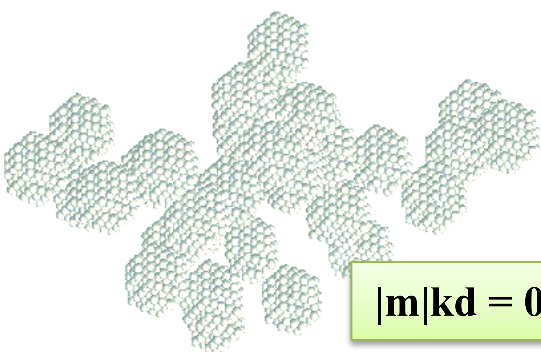
Single-scattering properties of particles with complex arbitrary geometries.

AVAILABLE NOW

Discrete Dipole approximation (DDA) : DDScat, ADDA, SIRRI, …



|m|kd = 0.6



|m|kd = 0.26

Validity criteria : |m|kd ≤ 1

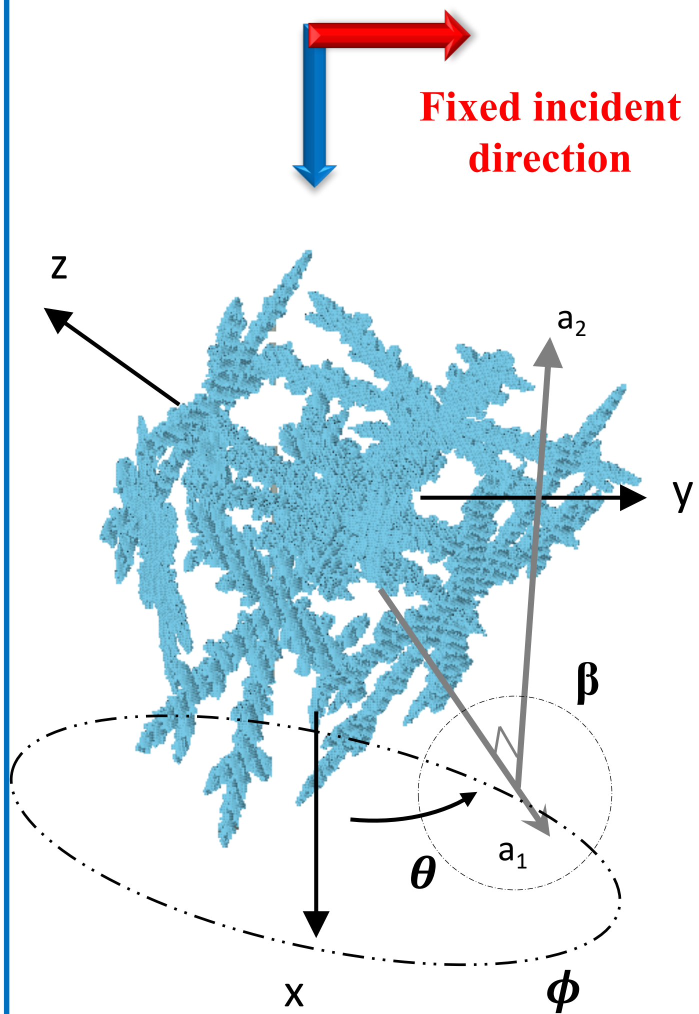
- **m** : complex refractive index
- **k** : wavelength number
- **d** : grid spacing

B.T. Draine and P.J. Flatau, "Discrete-dipole approximation for scattering calculations," in JOSA A, 1994.

Penttilä, Antti, et al. "Comparison between discrete dipole implementations and exact techniques." *JQSRT,* 2007

Zubko, Evgenij, et al. "Validity criteria of the discrete dipole approximation." Applied optics, 2010

EM Scattering by arbitrarily shaped particles



NEED

Single-scattering properties of particles with complex arbitrary geometries.

AVAILABLE NOW

Discrete Dipole approximation (DDA) : DDScat, ADDA, SIRRI, …

Iterative solvers : Krylov-space methods, such as conjugate gradient (**CG**), Bi-CG, Bi-CG stabilized (**Bi-CGSTAB**), CG squared (**CGS**), generalized minimal residual (GMRES),

Orientation averaging

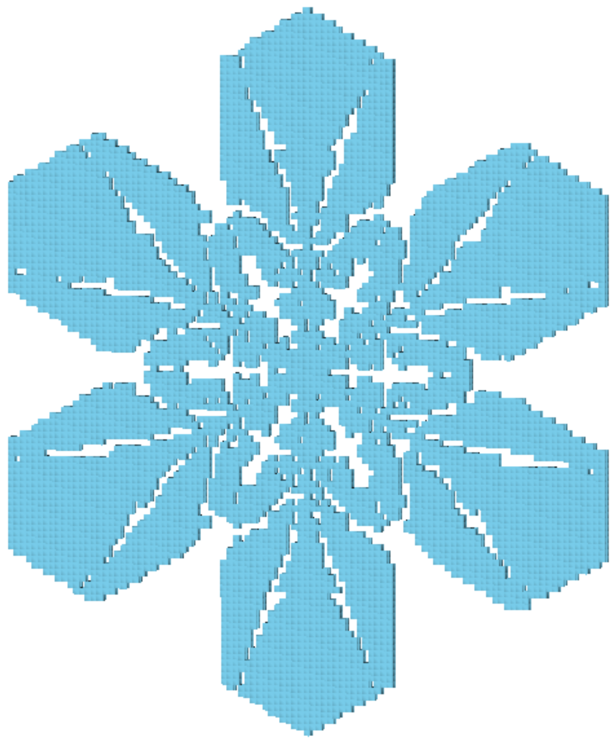
$$\langle Q \rangle = \frac{1}{8\pi^2}\int_0^{2\pi} d\beta \int_{-1}^{1} d\cos\theta \int_0^{2\pi} d\phi \; Q(\beta,\theta,\phi)$$

Yurkin, Maxim A., and Alfons G. Hoekstra. "The discrete dipole approximation: an overview and recent developments." Journal of Quantitative Spectroscopy and Radiative Transfer, 2007

VIEM/MoM-based 3D full-wave model

3D full-wave model, based on the volume integral equation method (VIEM)

Pristine crystal particle discretized into Nb_c elementary cubic cells



$$\bar{\bar{\Gamma}}\bar{E}(\bar{r}) = \bar{E}^{ref}(\bar{r})$$

Method of Moments

The particle is discretized into **Nbc** cubic cells Ω_n ,of side S_c

$$S_c \le \frac{\lambda_s}{10} ; \lambda_s = \frac{\lambda_0}{\sqrt{Re(\varepsilon_r)}}$$

$$D_\lambda = \lambda_s / S_c$$

Z is the **$3Nb_c$** x **$3Nb_c$ full** matrix representing the **interactions** between the different cells.

$$\bar{E}(\bar{r}) = \sum_{n=1}^{N} \sum_{q=1}^{3} E_q^n \, \bar{F}_q^n(\bar{r})$$

Use of piecewise constant basis functions

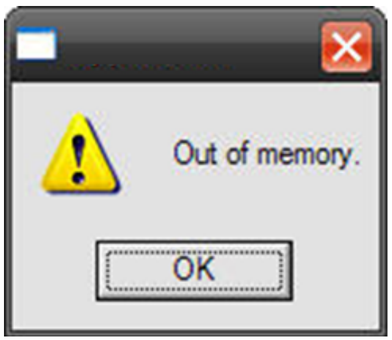
$$Z\,E = E^{inc}$$

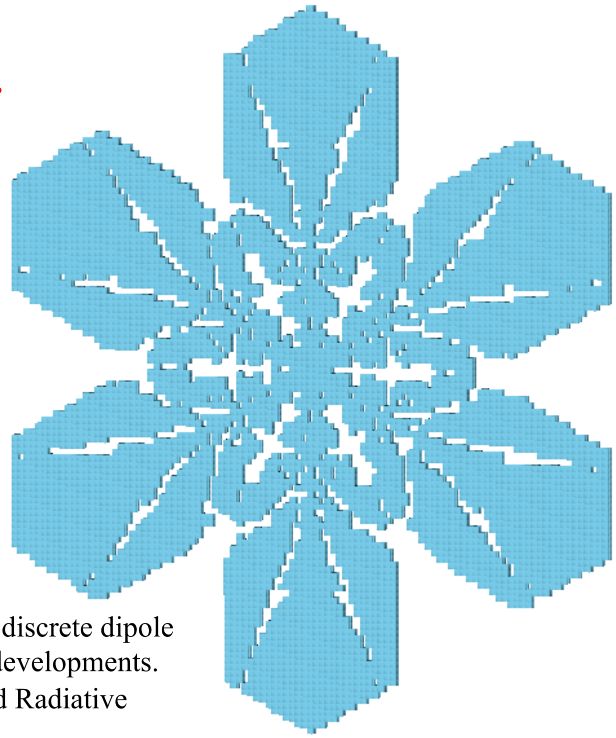
Direct solver

VIEM/MoM-based 3D full-wave model

3D full-wave model, based on the volume integral equation method (VIEM)

Storage of the entire matrix is prohibitive for direct methods





Yurkin Maxim, Hoekstra Alfons G. The discrete dipole approximation: an overview and recent developments. Journal of Quantitative Spectroscopy and Radiative Transfer. 2007 Jul 1;106(1-3):558-89.

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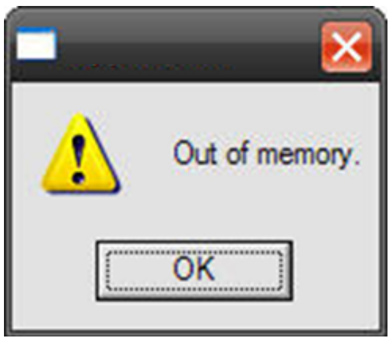

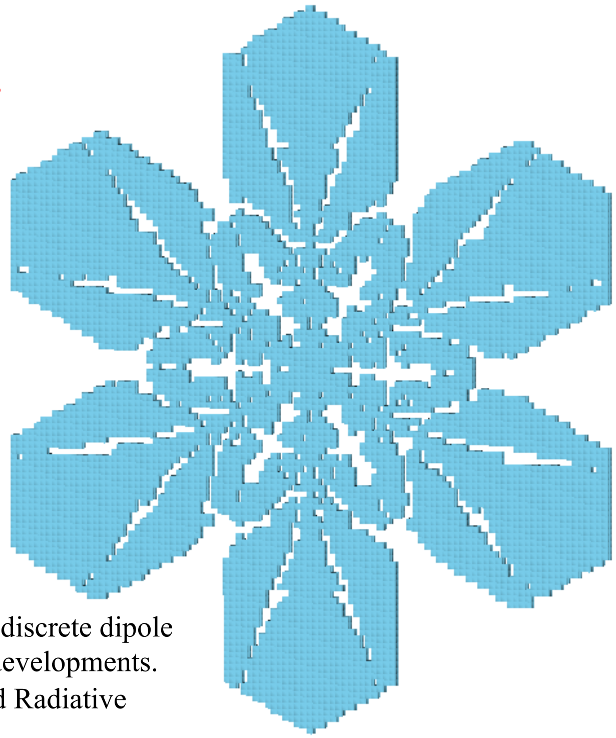

Yurkin Maxim, Hoekstra Alfons G. The discrete dipole approximation: an overview and recent developments. Journal of Quantitative Spectroscopy and Radiative Transfer. 2007 Jul 1;106(1-3):558-89.

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$$D_\lambda = \lambda_s / S_c$$

$$Z\,E = E^{inc}$$

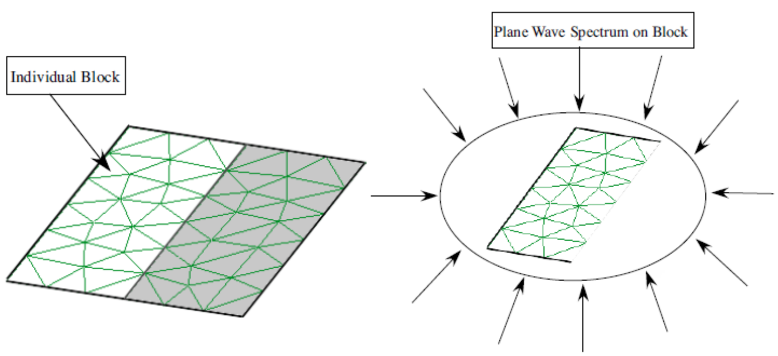
CBFM

Direct solver

The Characteristic Basis Function Method (CBFM)

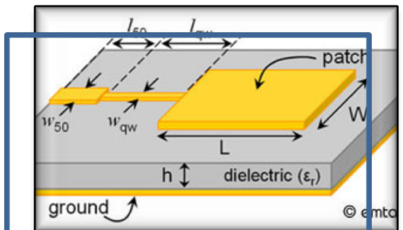
Direct solver-based

- **Better** adapted to **multiple right-hand** side problem
- Subject to a wide variety of enhancement techniques
- **T**unable depending on to the needs (memory or CPU) through the size of the blocks (h_B or $N_{b,max}$).
- **H**ighly amenable to **MPI** parallelization

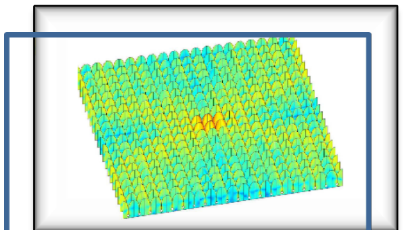


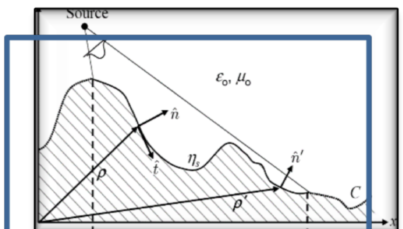
Spectrum of plane waves incident on a single block

The **CBFM** which has been proven to be accurate and efficient when applied to large-scale EM problems, even when the computational resources are limited

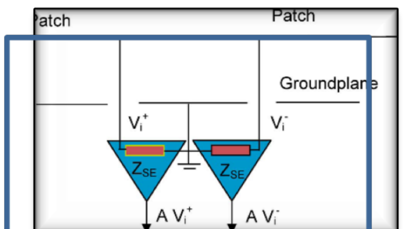


Microstrip circuits

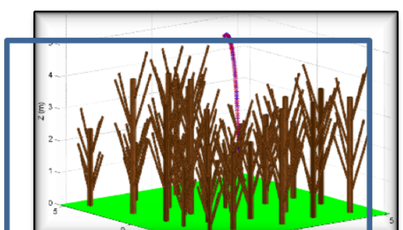

Large antenna arrays



Rough terrain profiles



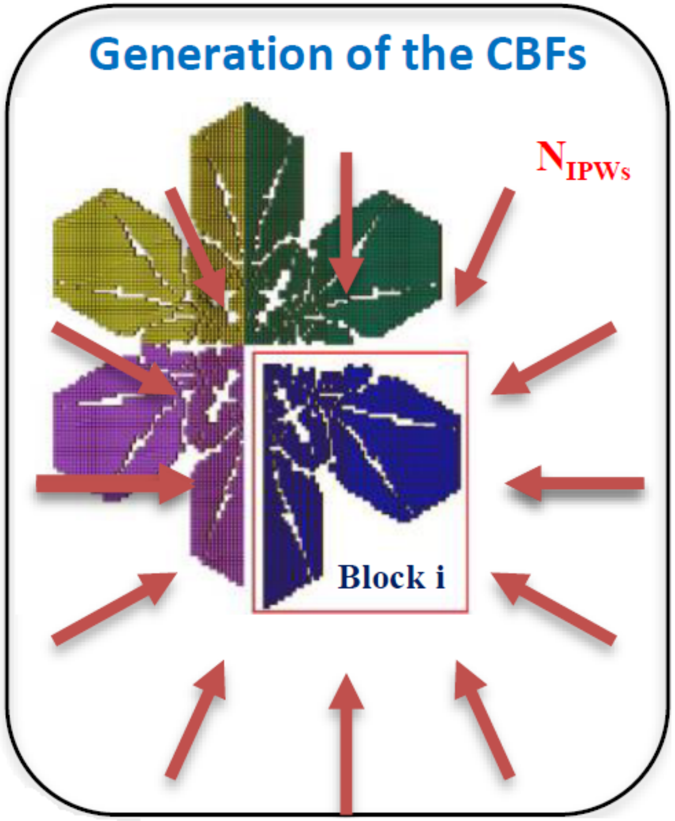
Connected patch arrays

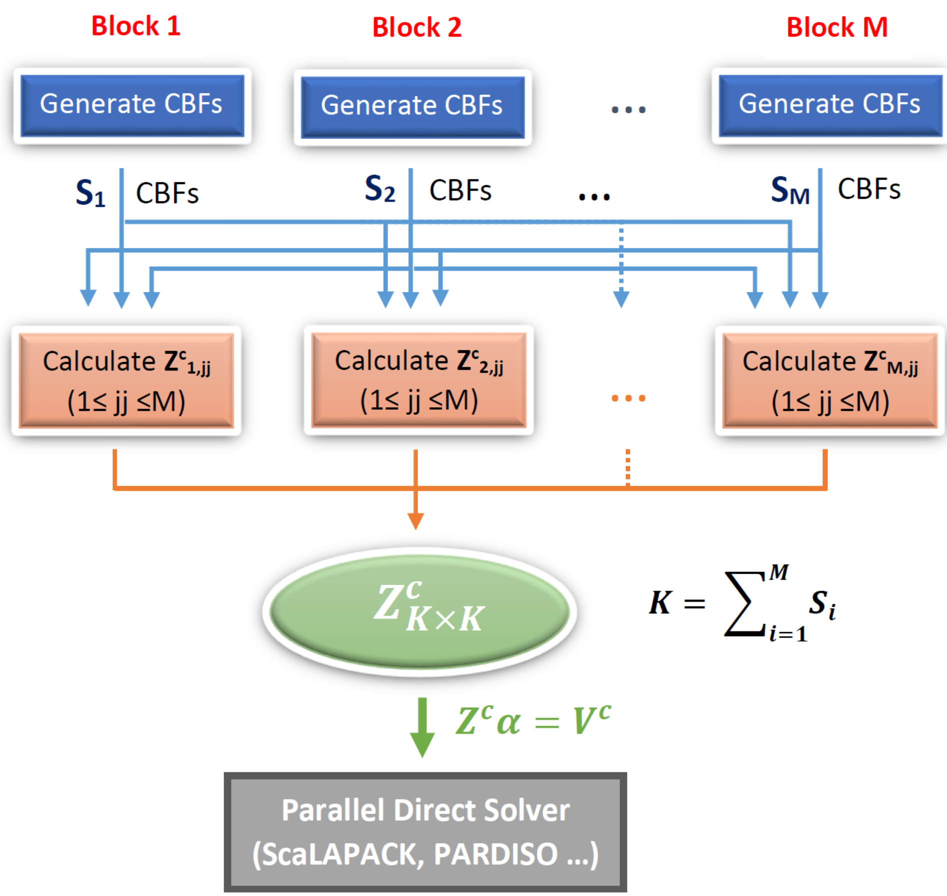

Large forest patches

R. Maaskant, R. Mittra, A. Tijhuis, "Fast Analysis of Large Antenna Arrays Using the Characteristic Basis Function Method and the Adaptive Cross Approximation Algorithm", IEEE Transactions on Antennas and Propagation, 2008.

Jaime Laviada et al,"Solution of Electrically Large Problems With Multilevel Characteristic Basis Functions", IEEE Trans. on Antennas Propagation, 2009.

Application of the domain decomposition-based CBFM





Multilevel

Sparse

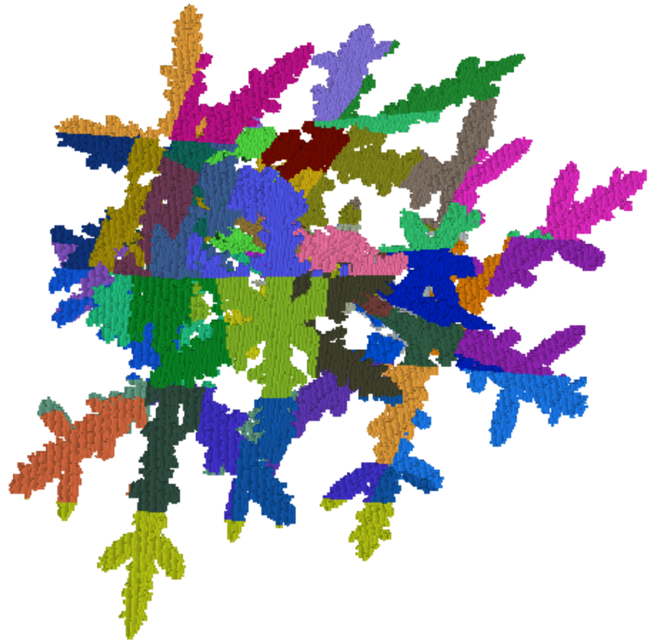
MPI

ACA/FMM

Efficient direct

The main steps of the CBFM in a distributed memory parallel configuration

Validation of the CBFM-based NESCoP



OpenSSP database

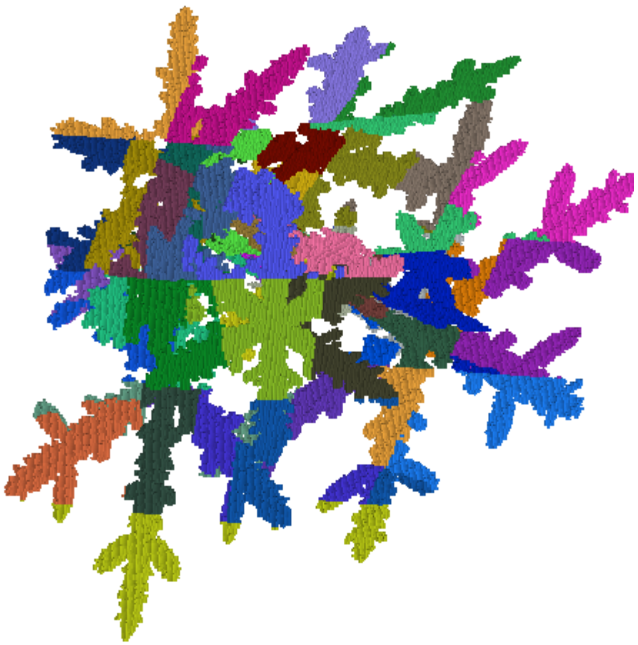
- 6646 particles : single pristine crystals and aggregate snow particles
- 50 µm resolution

$a_p = 1.61$ mm;
$d_m = 11.45$ mm;
@ $\lambda = 6$ mm : $x_p = 1.68$; $x_{p,dmax} = 6$;
$|m|kd = 0.0935$
$Nb_c = 140896$ cells

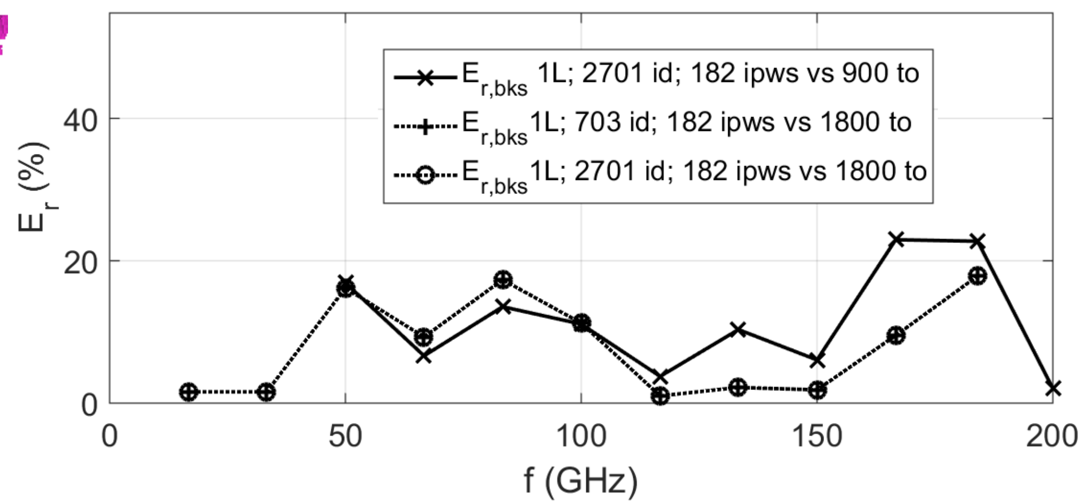
CPU time by NESCoP and DDScat as function of the number of target orientations for DDScat and incident directions for NESCoP

DDScat		NESCoP		
1 to	180 to	**190 id**	**703 id**	**1891 id**
4 hours	59 days	5 hours	12 hours	23 hours

Validation of the CBFM-based NESCoP



Relative difference in $\langle \boldsymbol{Q} \rangle = \frac{1}{4\pi} \int_0^{2\pi} \boldsymbol{d\phi_i} \int_0^{\pi} \textbf{sin}\, \boldsymbol{\theta_i}\ \boldsymbol{d\theta_i}\ \boldsymbol{Q}(\boldsymbol{\phi_i}, \boldsymbol{\theta_i})$



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Efficient Calculation of Averaged Scattering Quantities

$a_p = 1.61$ mm;
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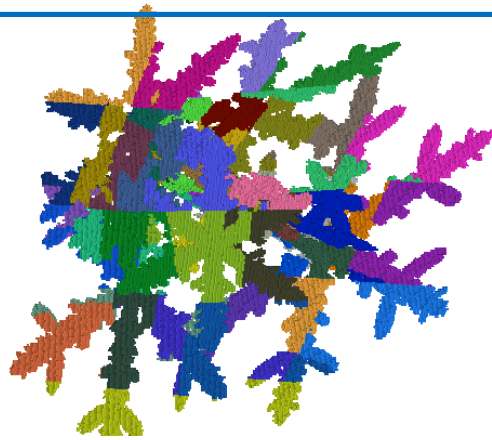
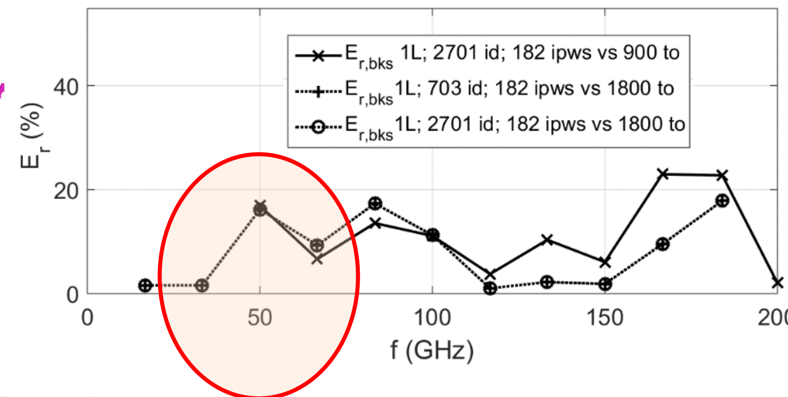
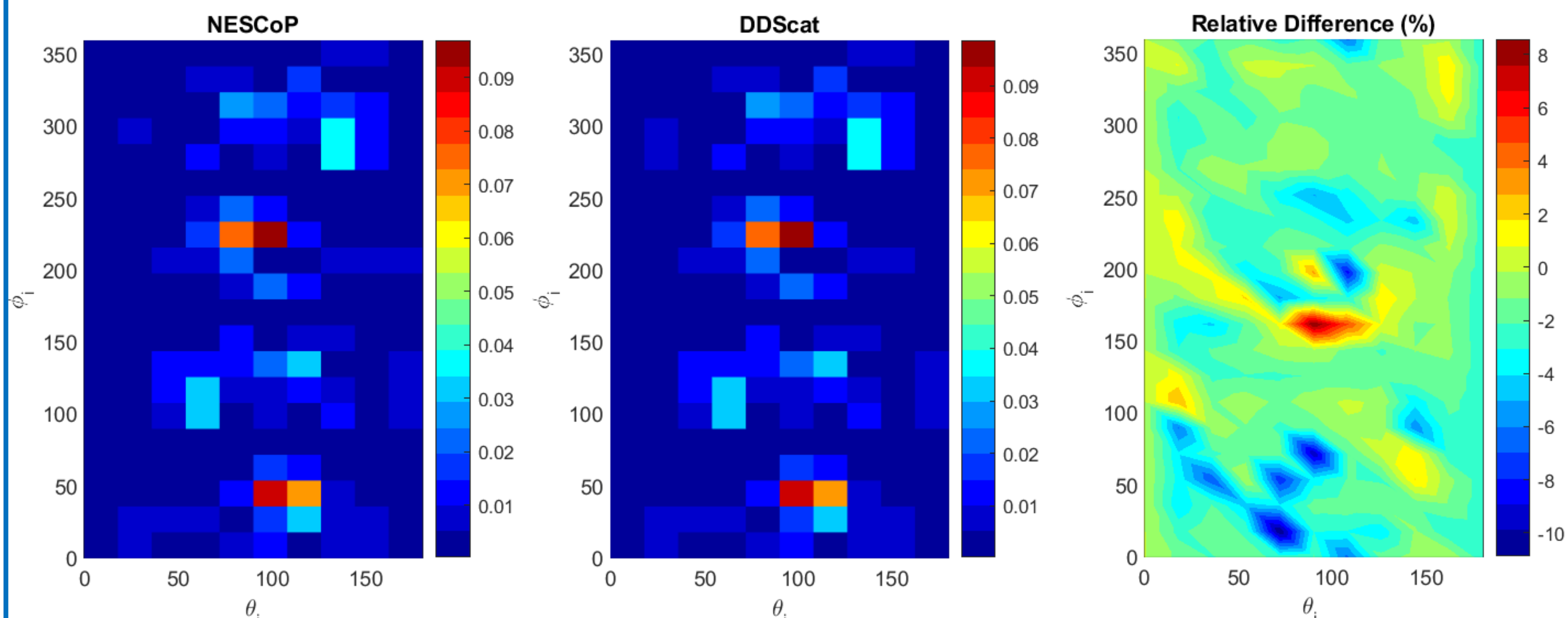




Qbks @ 50 GHz



Efficient Calculation of Averaged Scattering Quantities

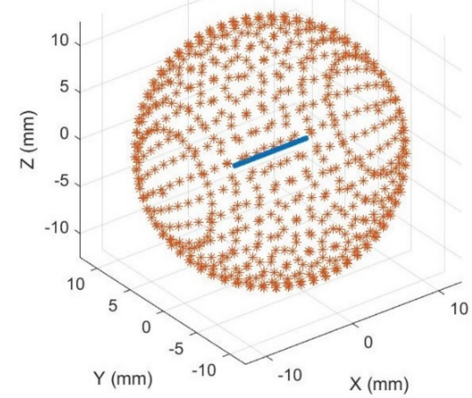
For an efficient & accurate orientation-averaging

- We investigate several quadrature schemes for integration over a spherical surface such as Lebedev quadratures and spherical designs, and numerically test their performance on different particle shapes.

$$\int_{\mathbb{S}^2} f(\mathbf{x})\,\mathrm{d}\Omega = \int_0^{2\pi}\int_0^{\pi} f(\varphi,\theta)\sin\varphi\,\mathrm{d}\varphi\,\mathrm{d}\theta$$

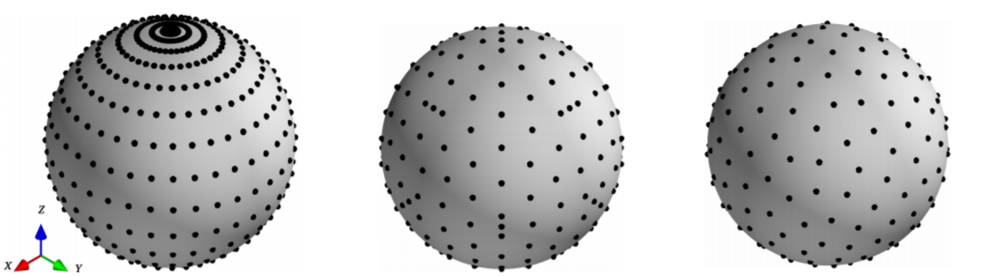
Beentjes, C.H., 2015. Quadrature on a spherical surface. http://people. maths. ox. ac. uk/beentjes/Essays.

Simpson's rule over cosθ



DDSCat

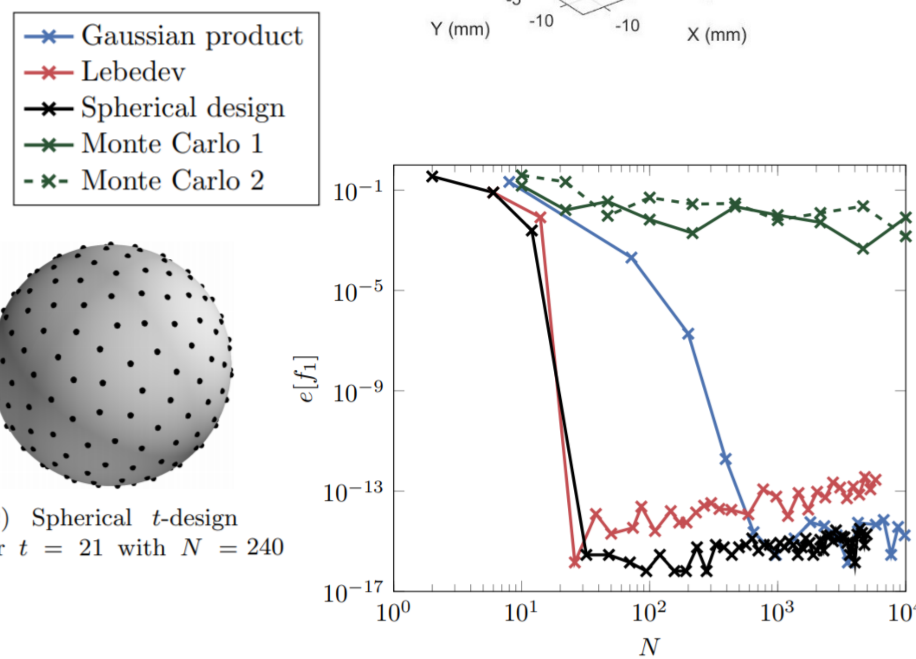
NESCoP



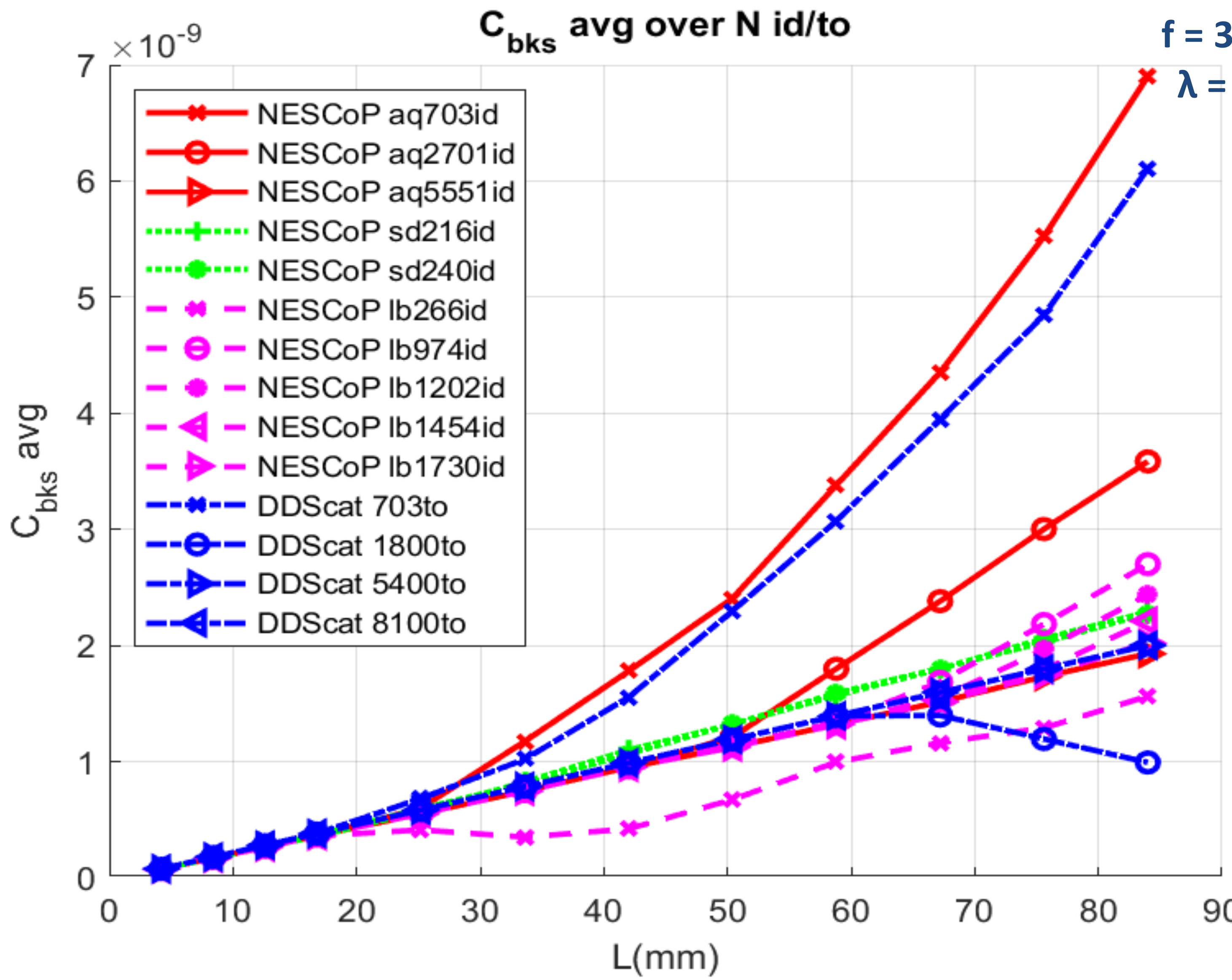
(A) Gaussian product grid with $N = 800$.

(B) Lebedev grid with $N = 266$.

(C) Spherical t-design for $t = 21$ with $N = 240$

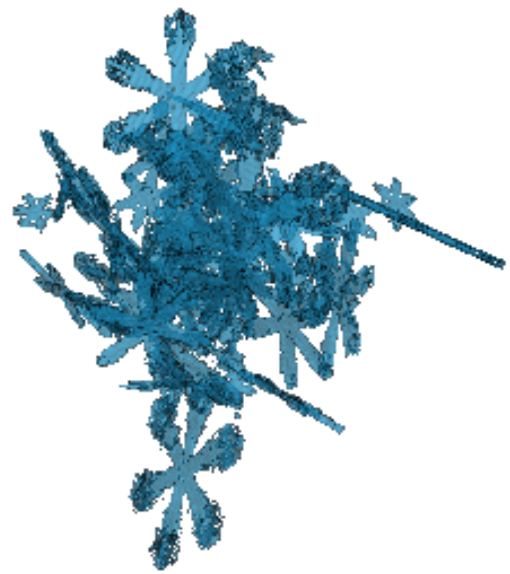


Efficient Calculation of Averaged Scattering Quantities

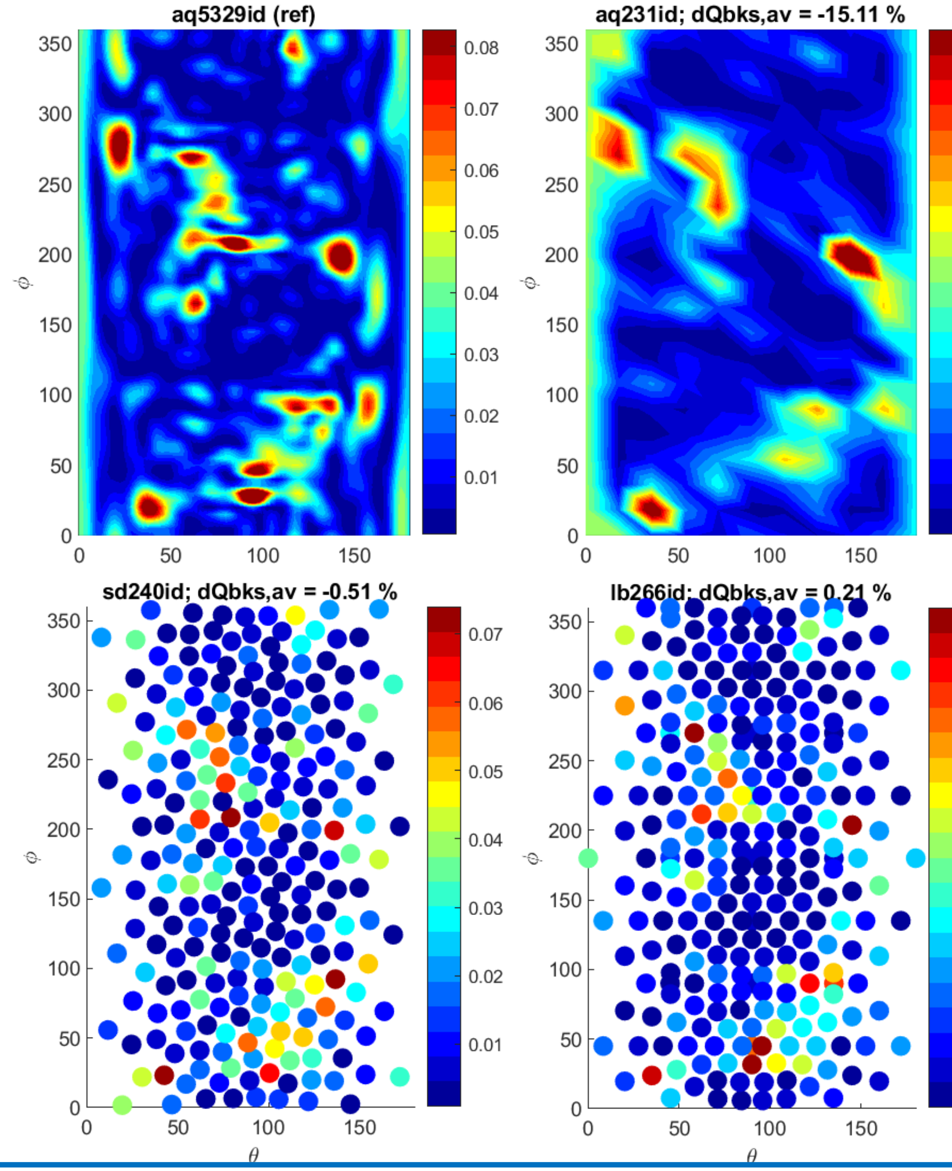


f = 35.75 GHz
λ = 8.39 mm

Efficient Calculation of Averaged Scattering Quantities



a_p = 1.4246 mm;
d_m=11.75 mm;
@ 94 GHz x_p =2.81;
$x_{p,max}$ =6; $x_{p,dmax}$=11.6
|m|kd = 0.17
Nb_c =96898 cells



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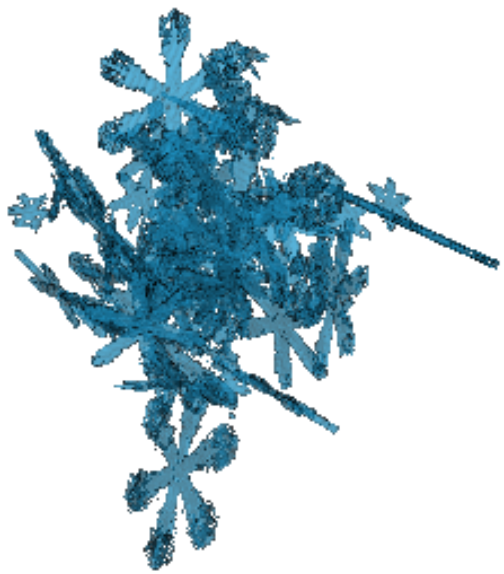

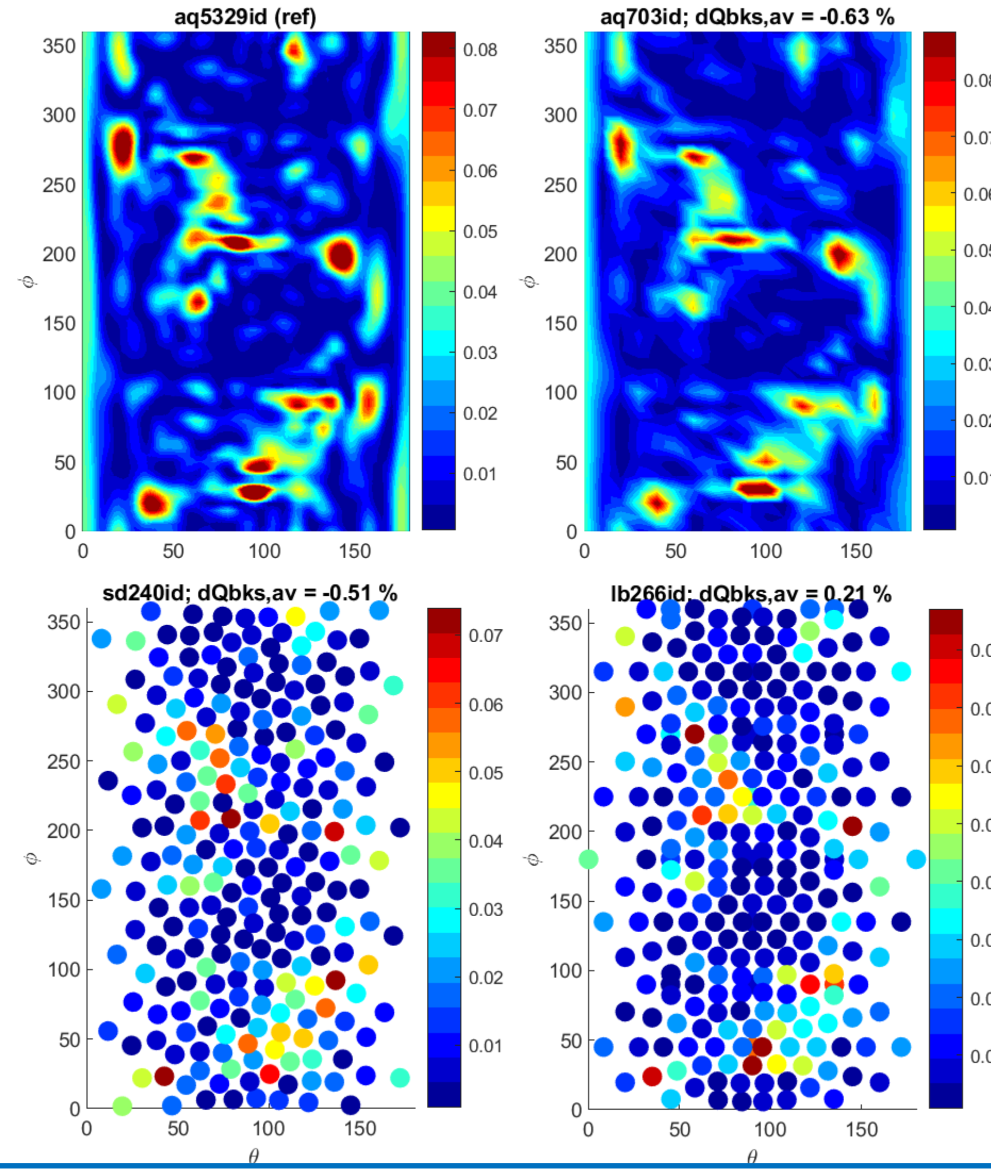

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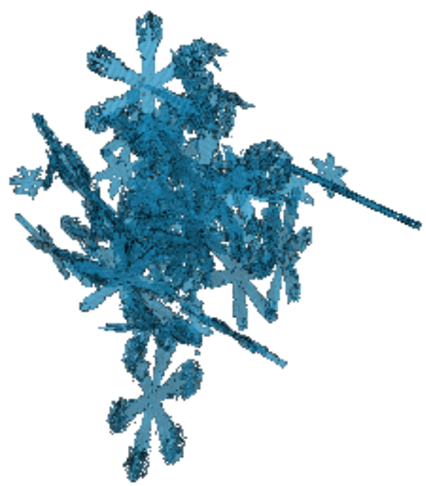
Efficient Calculation of Averaged Scattering Quantities

UCLA JIFRESSE

OpenMP 16 CPUs & 64GB RAM



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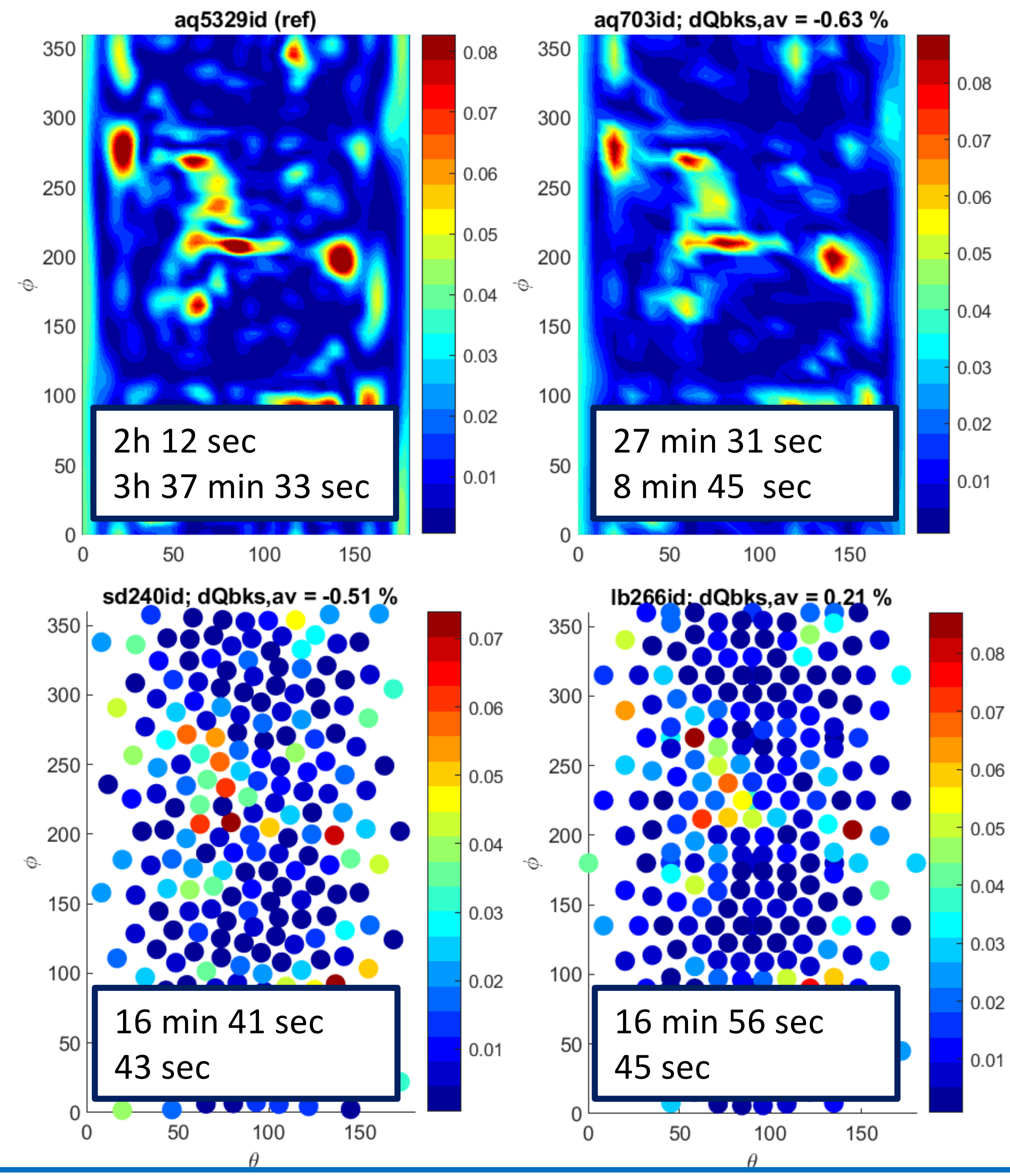
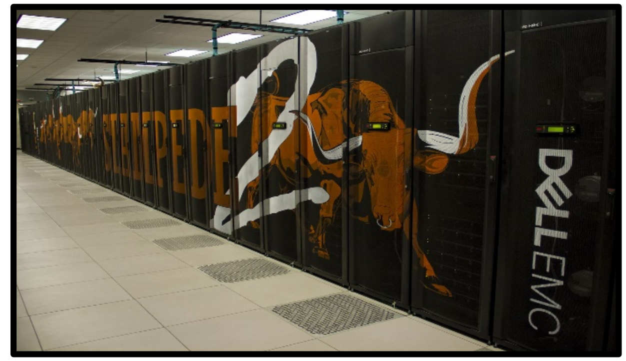
DDScat : 81 to calculated in 24 hours !
(30 min per target orientation)



MPI Parallelization of NESCoP

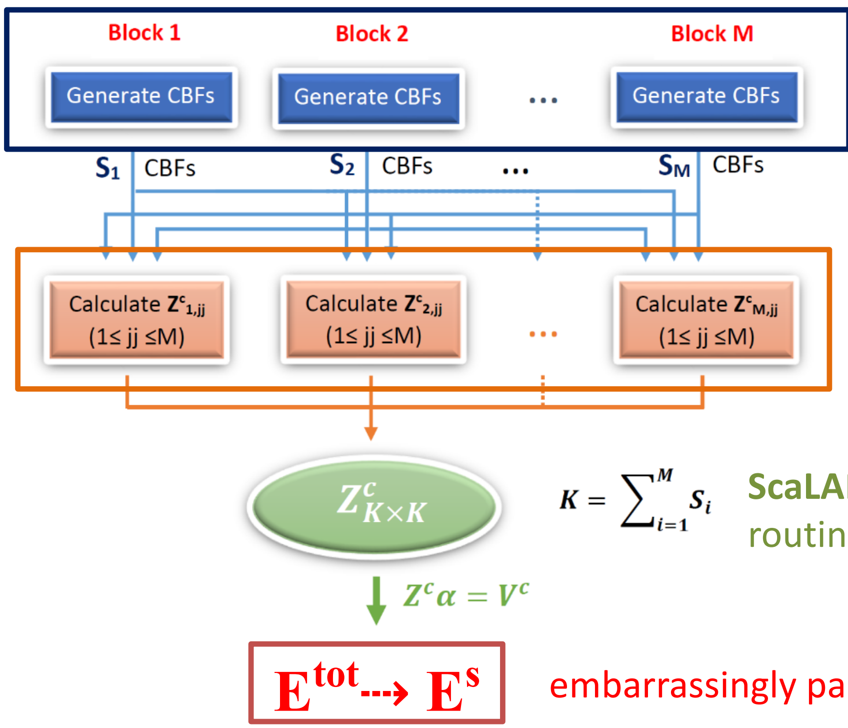
UCLA JIFRESSE

Goal : Increase the simulated particle size parameter envelope AND/OR its numerical size as much as the available computational resources allow.



TACC Stampede2

TEXAS ADVANCED COMPUTING CENTER



embarrassingly parallel

Major point of communication between MPI jobs

$$K = \sum_{i=1}^{M} S_i$$

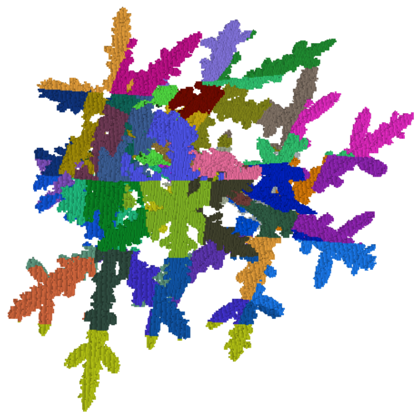
ScaLAPACK : high-performance linear algebra routines for parallel distributed memory machines

embarrassingly parallel

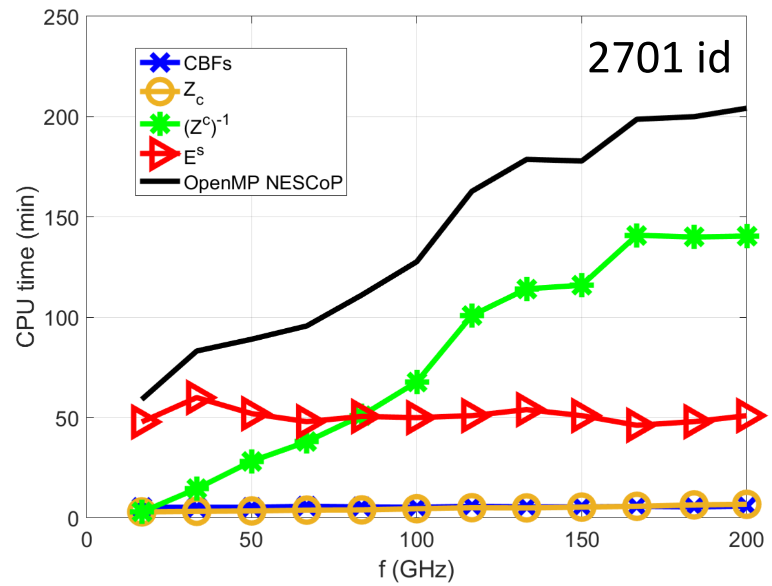
MPI Parallelization of NESCoP

UCLA JIFRESSE

a_p = 1.61 mm;
d_m=11.45 mm;
$0.56 \leq x_p \leq 6.74$
$|m|kd \leq 0.37$
Nb_c =140896 cells

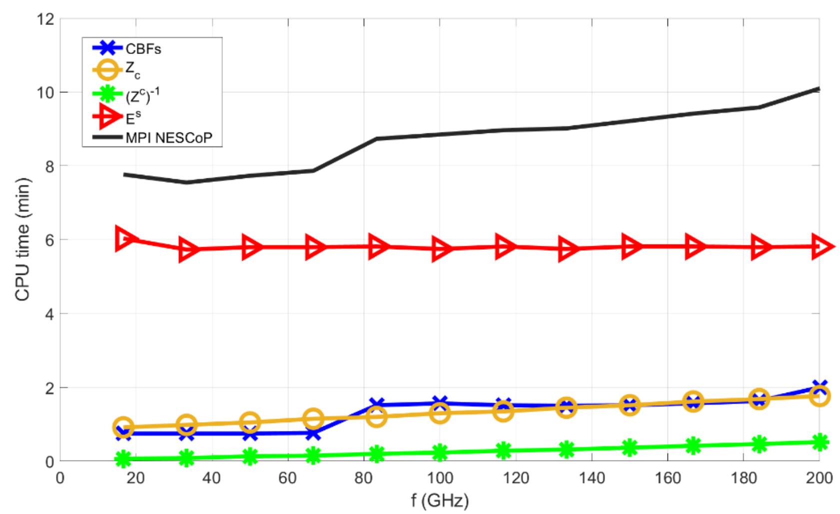


12 λ & 2701 incident directions



OpenMP : 16 CPUs with 64 GB RAM

Total : 28 h 26 min

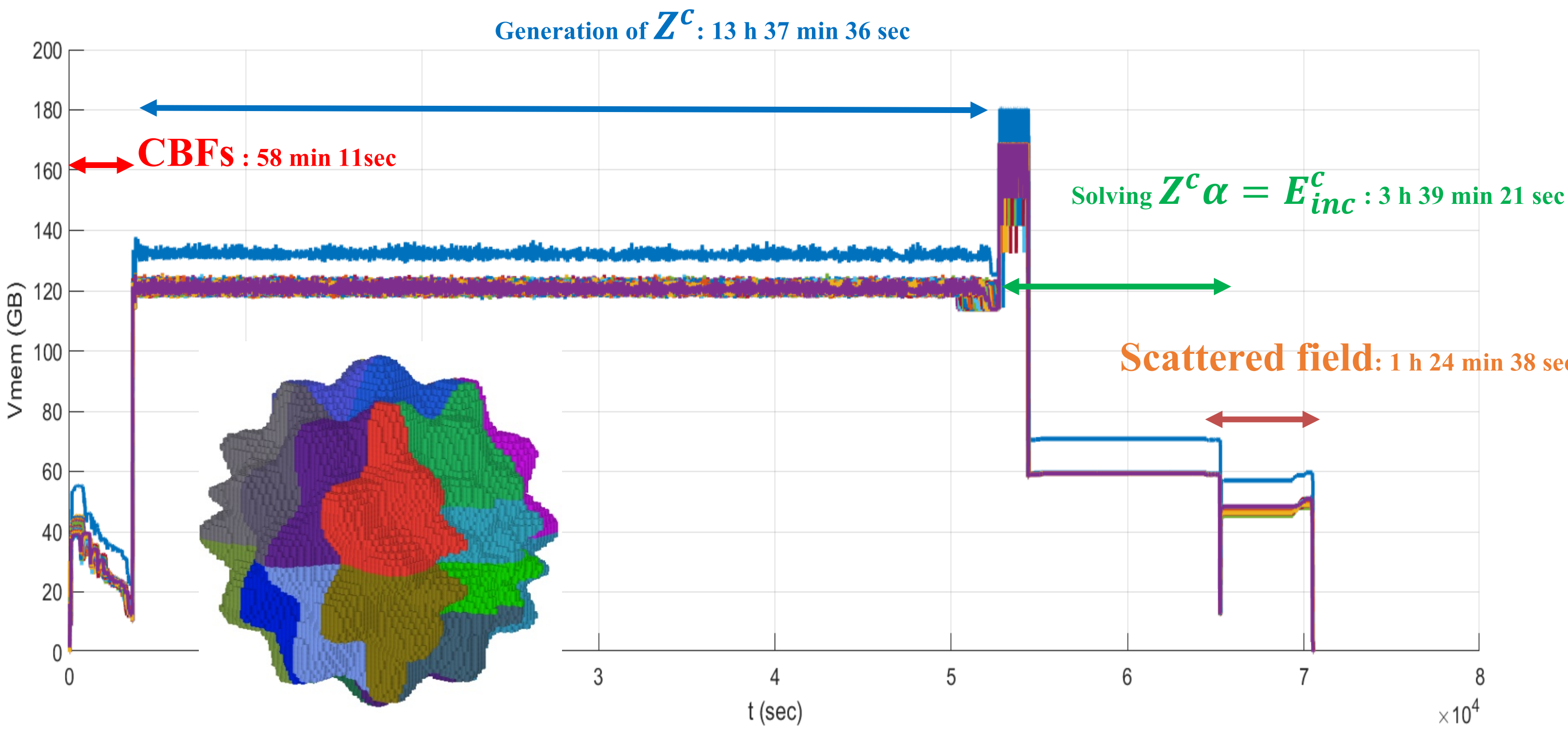


MPI : 96 MPI tasks; 2 SKX nodes on **TACC Stampede 2 with 48 cores & 192GB RAM each**

Total : 1 h 56 min

MPI Parallelization of NESCoP

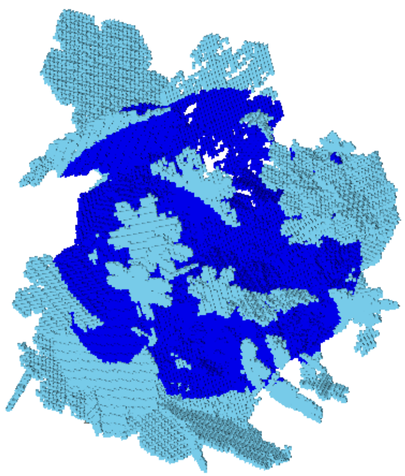
30 SKX nodes & 360 MPI jobs



Variations of virtual memory (GB) as function of time for the calculation on 60 SKX nodes (each plot color represents a node) of the EM scattering by a Chebyshev particle of size parameter 50.26 composed of Nb_c = 8,426,060 cells for 2701 both incident and scattering directions (7,295,401 total combinations). The size of the compressed matrix Z^c is 435,471 (1.72 % of the initial MoM matrix).

Inhomogeneity and Adaptive mesh

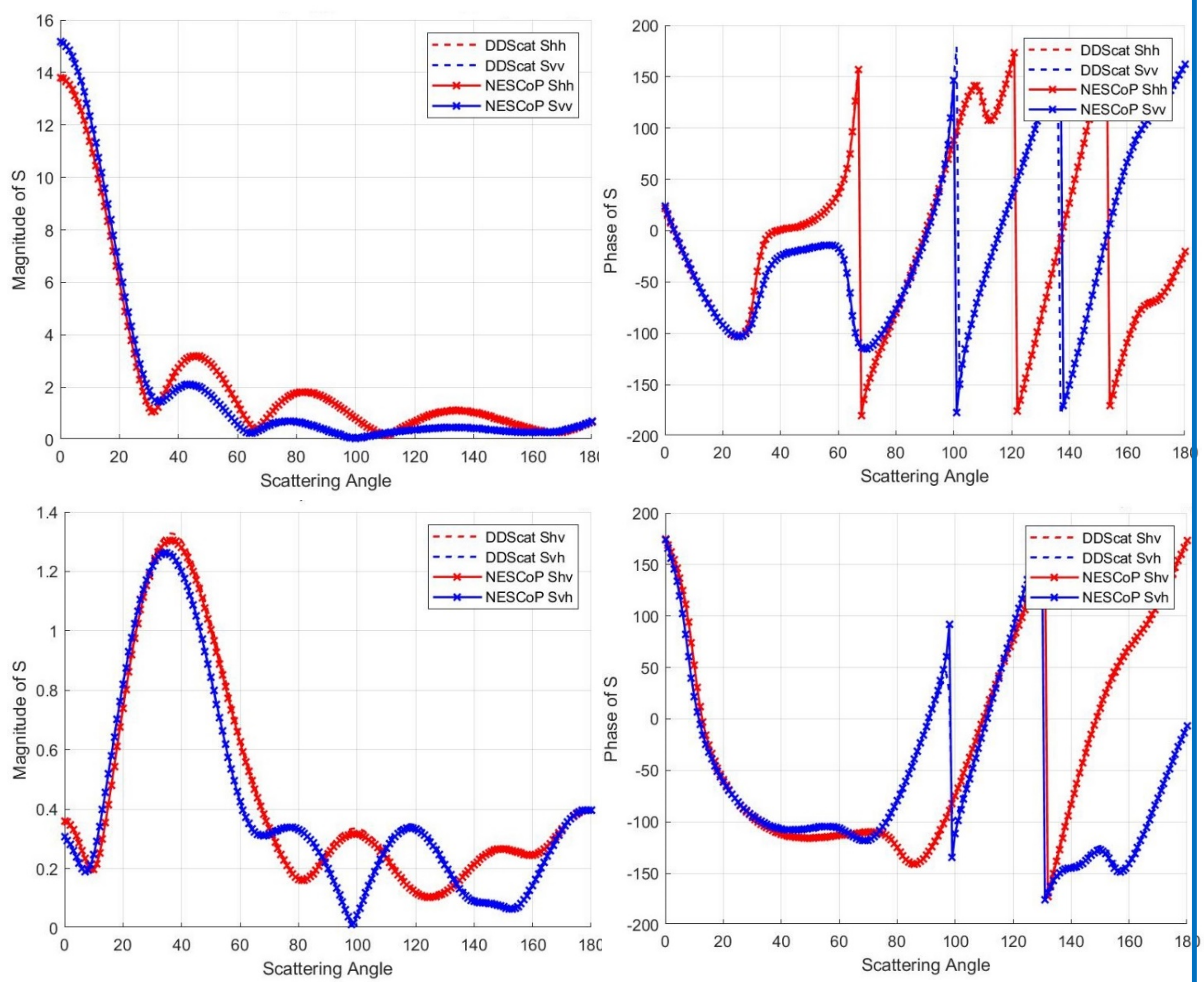
Melting Hydrometeor



a_p = 1.36 mm;
d_m=8.20 mm;
Nb_c =86164 cells

@ f = 94 GHz
$|m_w| \approx 2.8$

d = 50 µm
⇢ $|m|kd_{max} = 0.27$



Inhomogeneity and Adaptive mesh

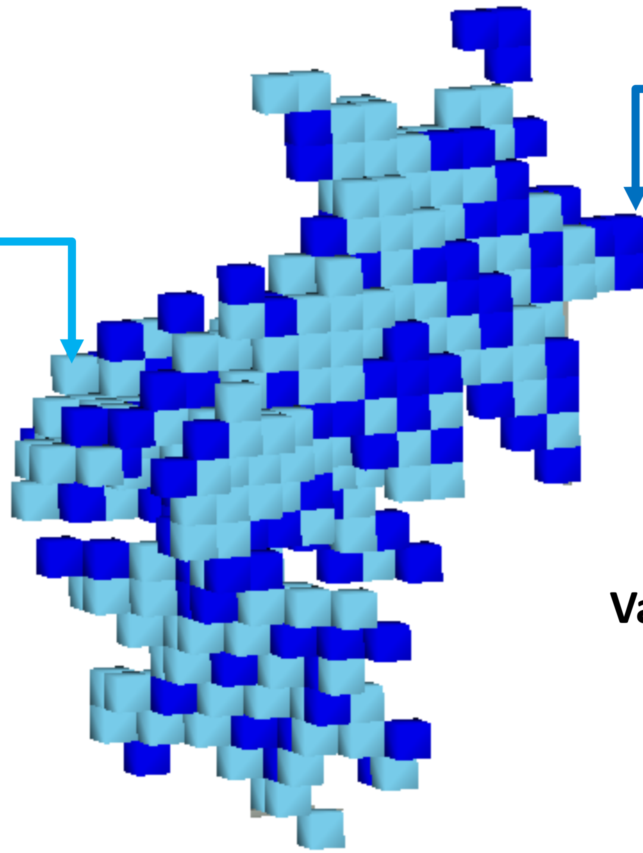
UCLA JIFRESSE

Melting Hydrometeor

Low-resolution uniform mesh

f = 250 GHz

d = 50 µm



Water 30%

m = 2.8+i*0.0021

|m|kd = 0.7854

70% Ice

m = 1.33+i*0.01

|m|kd = 0.3482

Validity criteria : |m|kd ≤ 1

- **m** : complex refractive index
- **k** : wavelength number
- **d** : grid spacing

Method of Moments

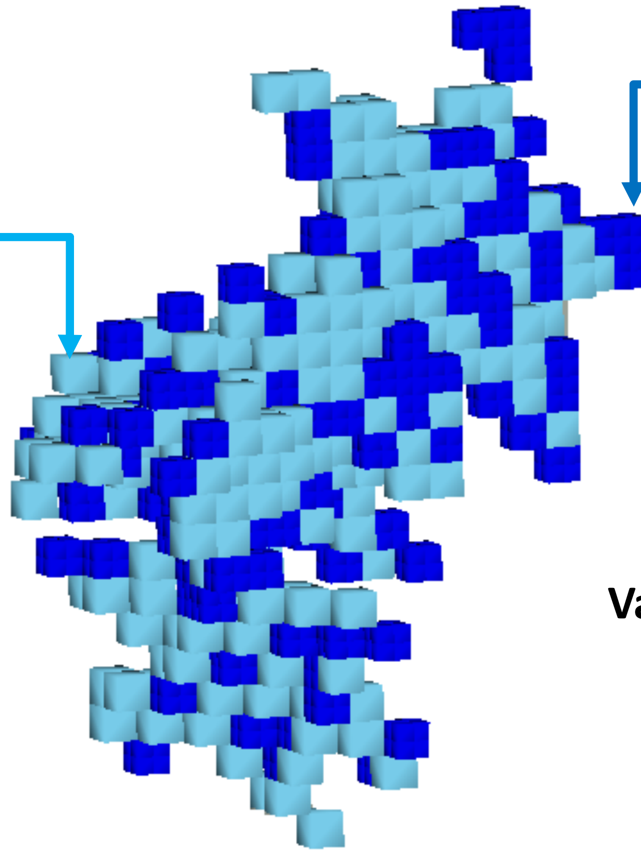
$$d \leq \frac{\lambda_s}{10} \; ; \lambda_s = \frac{\lambda_0}{\sqrt{Re(\varepsilon_r)}}$$

Inhomogeneity and Adaptive mesh

Melting Hydrometeor

Adaptive mesh

f = 250 GHz



70% Ice

m = 1.33+i*0.01

|m|kd = 0.3482

d = 50 µm

Water 30%

m = 2.8+i*0.0021

|m|kd = 0.3927

d = 25 µm

Validity criteria : |m|kd ≤ 1

- **m** : complex refractive index
- **k** : wavelength number
- **d** : grid spacing

Method of Moments

$$d \leq \frac{\lambda_s}{10}\ ;\ \lambda_s = \frac{\lambda_0}{\sqrt{Re(\varepsilon_r)}}$$

Conclusions and Perspectives

NESCoP

3D full wave model comparable to the DDA in terms of accuracy & providing **higher computational performance** particularly with orientational averaging of the EM scattering.

- Adaptive Mesh
- Hail Simulations
- Melting Hydrometeors
- Optimized MPI parallelization
- Large Size parameter
- NASA Github ?


Thanks for your attention