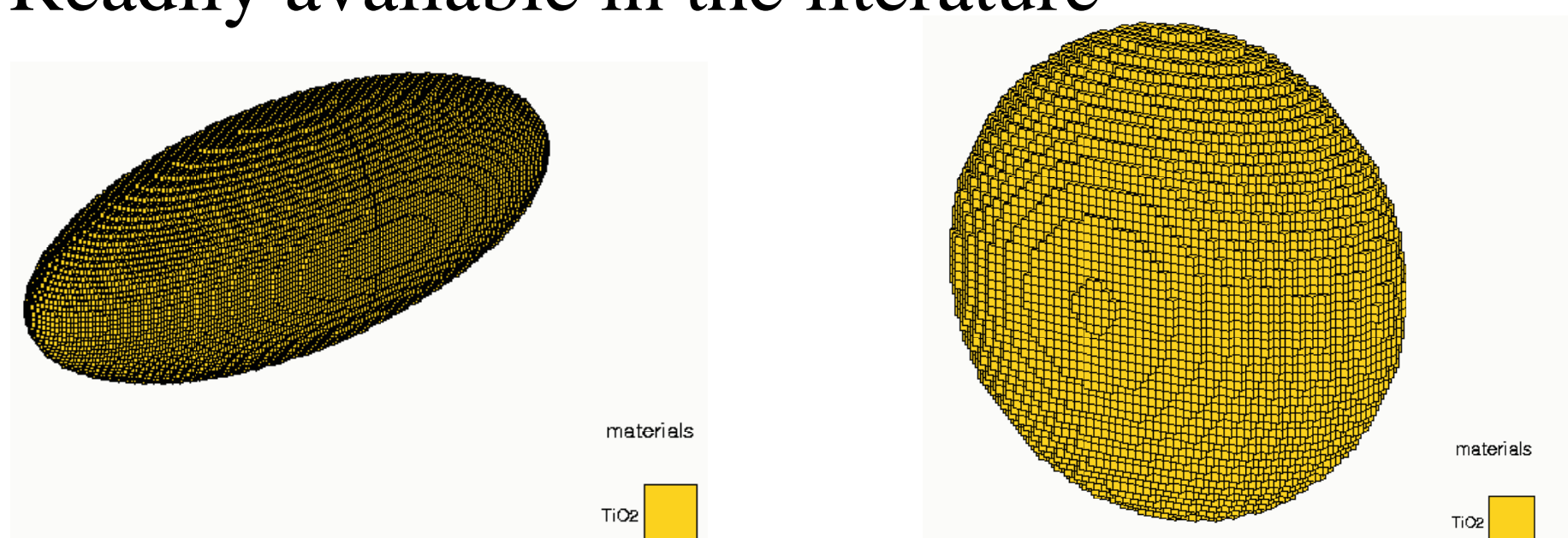


# COMPUTATIONAL OPTICS OF ANISOTROPIC SPHEROIDS

Alexander R. Hanuska, Roger H. French (CR&D, The DuPont Company)

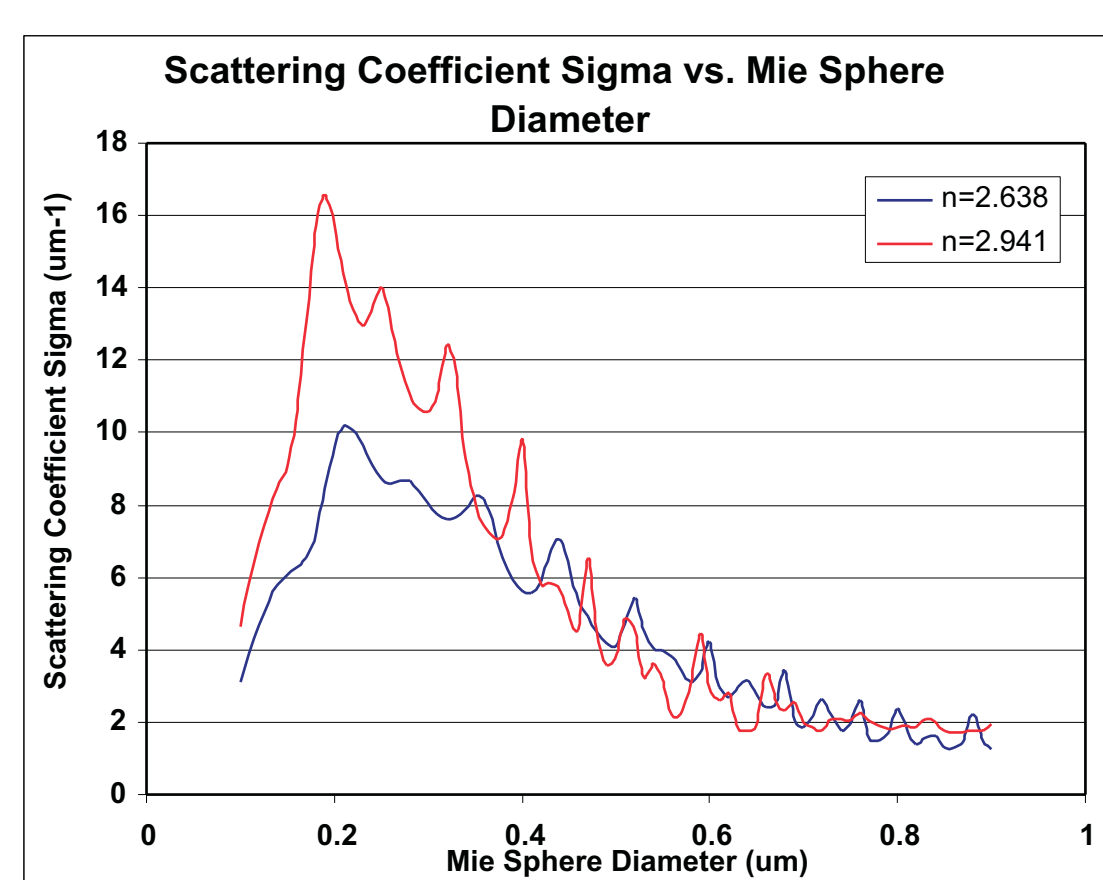
## Introduction

- Light scattering by complex geometric shapes
  - Spheroids, cubes, cylinders
  - Significant interest in paper, plastic, coatings
- For **Optically Anisotropic spheroids**,
  - Finite element approach for to determine
  - Optimal shape parameters
  - Maximum Scattering
- Interaction between **Optical** and **Geometrical** anisotropy of the particles is usually disregarded
- Solutions to Isotropic spheroids with varying shape parameters
  - Aspect ratio, volume, orientation
  - Readily available in the literature



## Mie & Intuition

- Analytical solutions to Maxwell's equations
  - Gustav Mie, 1908
- Single optically Isotropic sphere
- Angle-weighted scattering coefficient - Sigma
- Optimal TiO<sub>2</sub> sphere diameter varies with refractive index for maximum scattering
  - Diameter is 0.185um for n<sub>e</sub>=2.941
  - Diameter is 0.210um for n<sub>c</sub>=2.638



Is The Pancake The Ideal Scatterer For The Given Indices?

## Methods

- Finite element approach (EMFlex)
  - Time-domain solutions to Maxwell's equations
  - Solids modeled as meshed volumes
  - Anisotropic optical properties
  - Arbitrary microstructures and shapes
  - 20 million elements FEM models

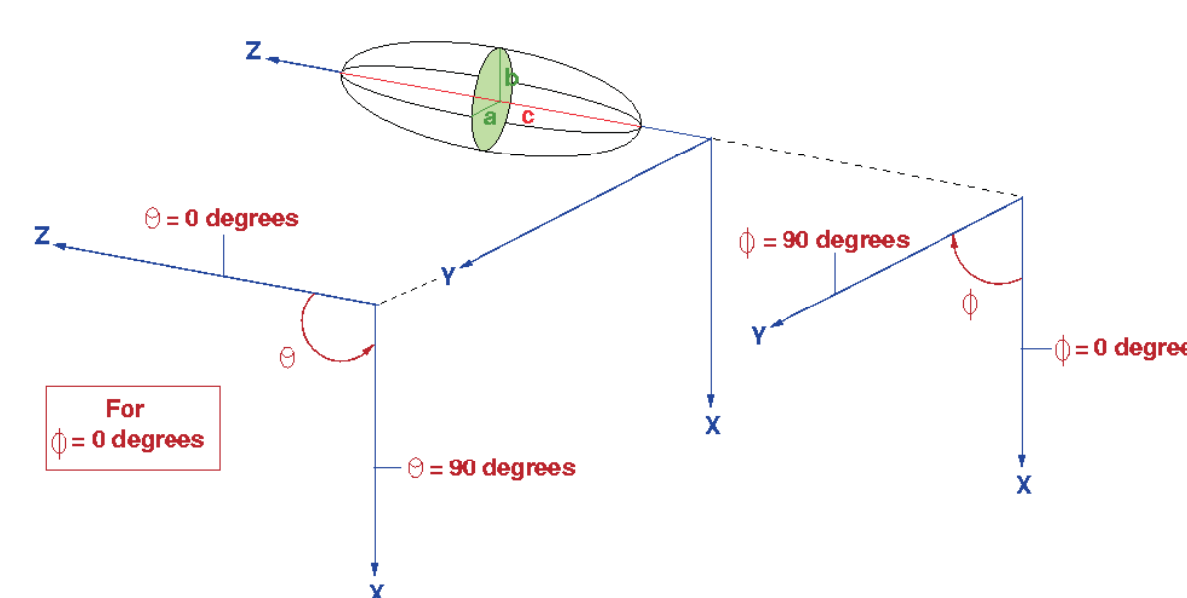
$$\nabla^2 \vec{E} - \epsilon\mu \frac{\partial^2 \vec{E}}{\partial t^2} = 0$$

- Platform: SGI Origin 2000 Compute Server
  - Fleets of 54 jobs, 30 minutes each
  - 40 R 10,000 Processors, 40 Gb Ram, 1 Terabyte file system

- Using optical constants of TiO<sub>2</sub>
  - n<sub>o</sub> =2.638
  - n<sub>e</sub> =2.941
- Vary aspect ratio from 0.5 to 4.5
- Far-field extrapolation
  - Forward hemisphere
  - Backward hemisphere
- Sphere diameters and volumes

	Equivalent Sphere Diameter (um)	Spheroid Volume (m3)
1	0.10	5.24E-22
2	0.18	3.05E-21
3	0.20	4.19E-21
4	0.22	5.57E-21
5	0.30	1.41E-20
6	0.40	3.35E-20

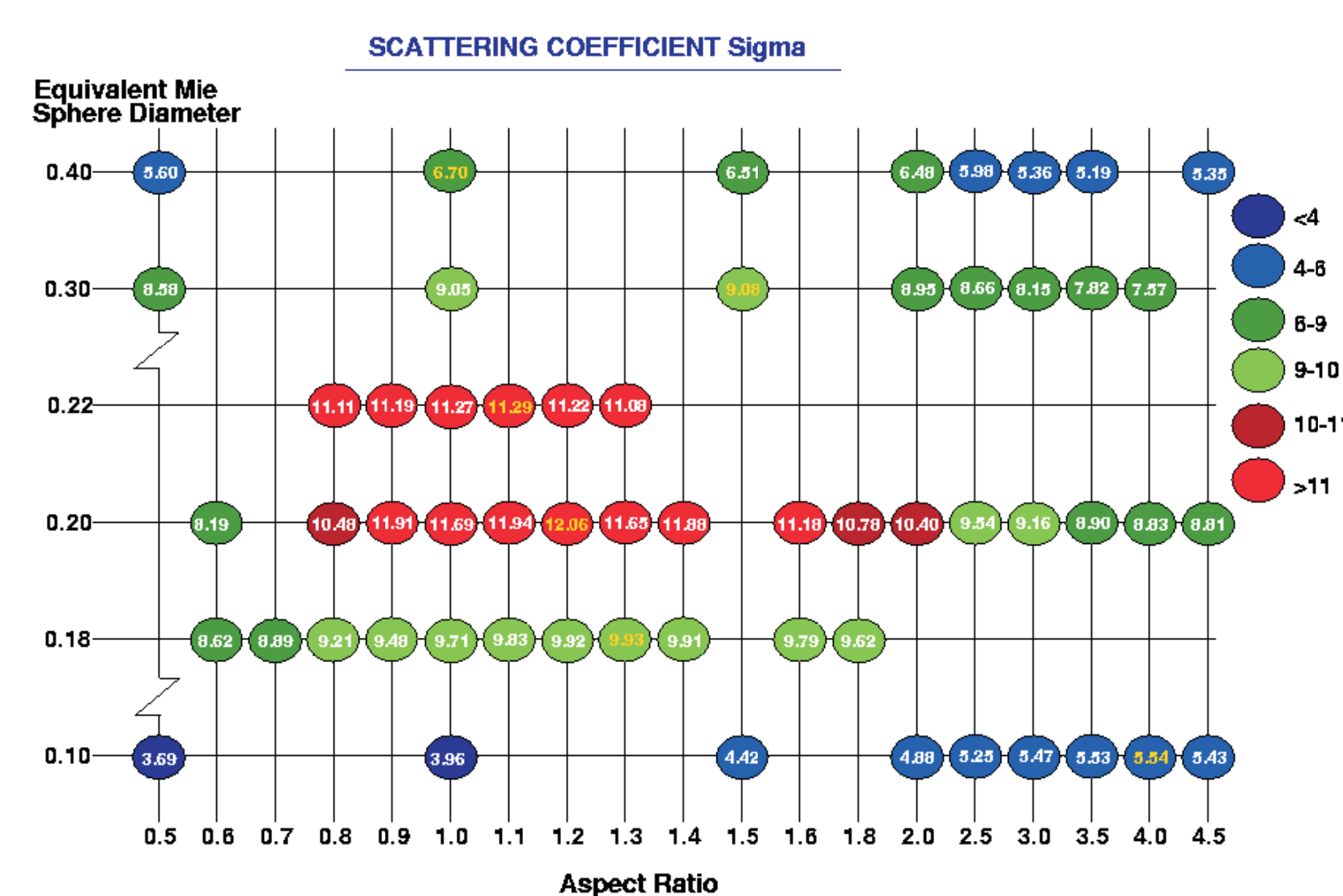
- Illumination conditions



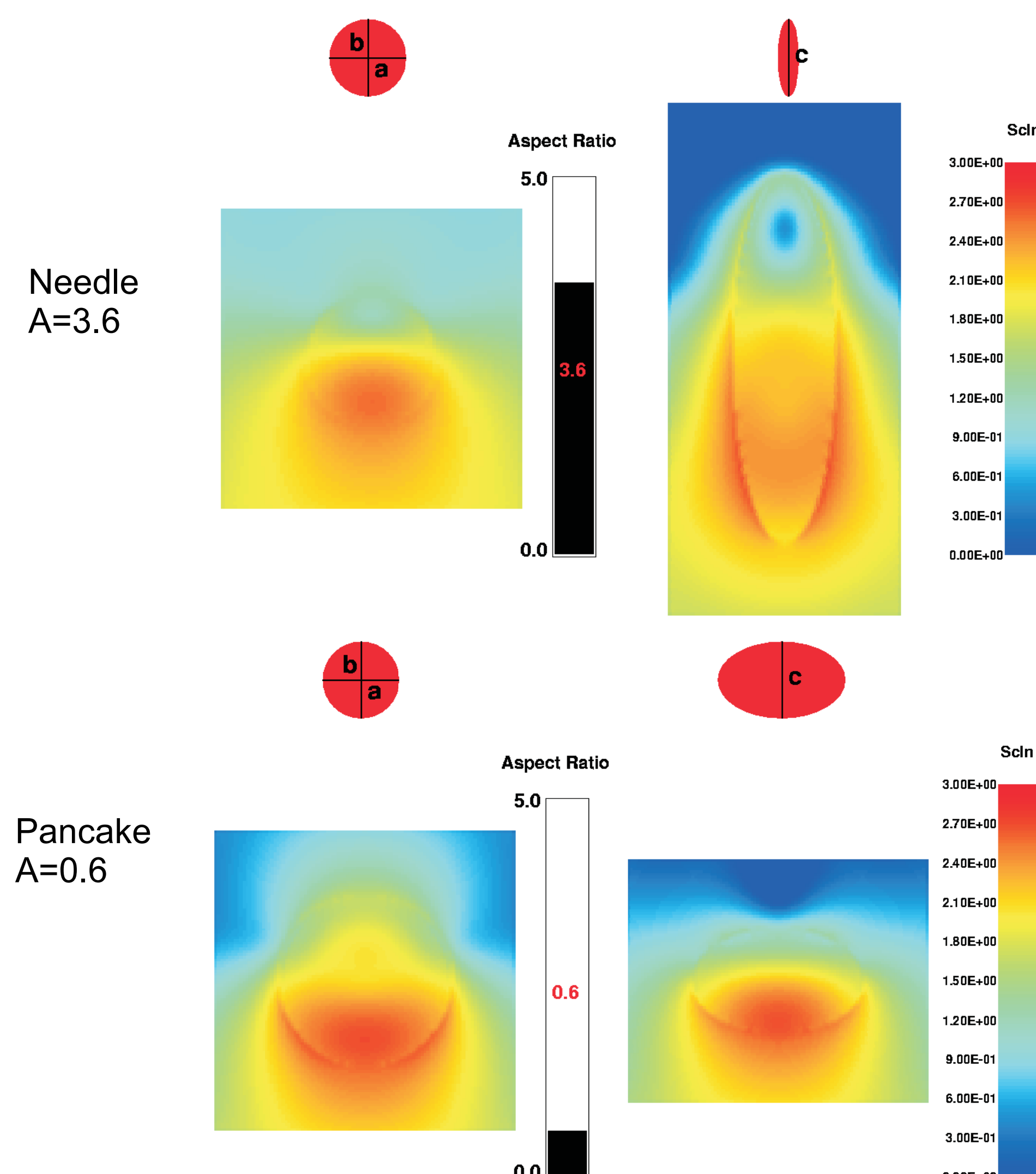
- Random Illumination from c-axis to ab-plane
- Theta from 5 to 85 degrees (9 illuminations)
- Sum up illuminations
- Wavelength: 560nm
- S&P polarizations added incoherently

## Results

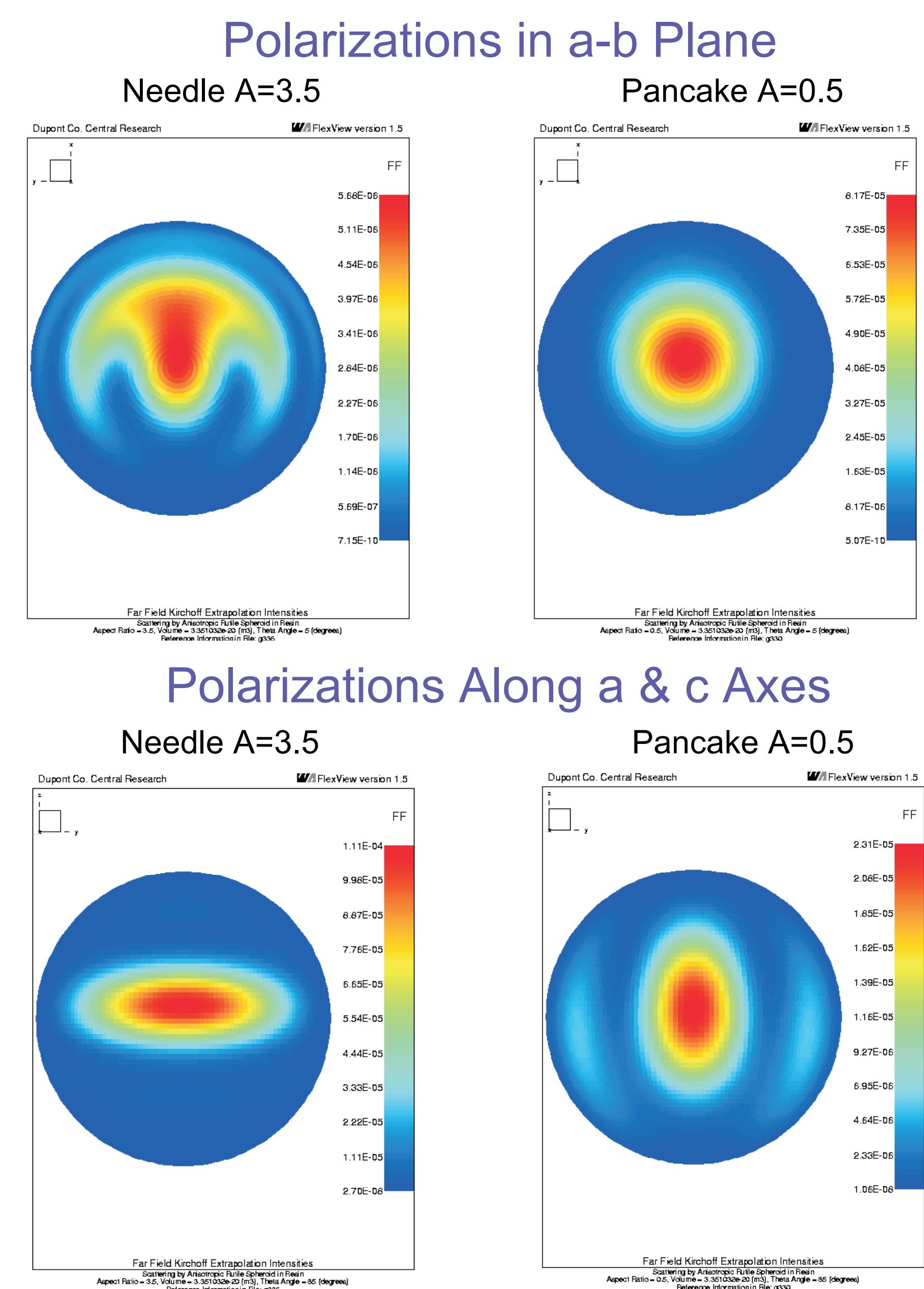
- Solution Matrix



## Near-Field Results



## Far-Field Results



## Discussion

- Maximum scattering coefficient Sigma
  - Occurs for different aspect ratios (A)
  - Vary with Equivalent Sphere Diameter (ESD)
  - Maximum Sigma=12.06 with A=1.2 and ESD=0.2um
- For optimally sized particles
  - Increasing A from 1 to 1.2 increases Sigma by 3%
  - Aspect ratio variation changes Sigma by up to 48%
- 20nm change in equivalent sphere diameter can change spheroid's scattering coefficient Sigma by up to 18%
- For sub-optimally sized particles
  - High aspect ratios can increase the scattering coefficient Sigma by up to 40%
- Anisotropic spheroids exhibit higher scattering than isotropic Mie spheres

## Conclusions

- Important coupling of **Optical** and **Geometrical** Anisotropy
- Needles (A>1) scatter more than Pancakes (A<1)
- Optimal aspect ratio (A=1.2) & volume (0.2 um) Scattering increased 3% more than for an anisotropic sphere
- Optimal particle volumes are still essential
- For sub-optimal volume particles increasing the aspect ratio increases the scattering coefficient Sigma