Systematic comparison of dust scattering codes: Insights from automated cross-validation using POMELO

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Background

Dust scattering calculations - determining extinction, scattering, and polarization cross-sections for aspherical particles - are fundamental to multiple research domains:

- **Astrophysical observations**: Dust opacity calculations for JWST, ALMA, VLT facility interpretations
- **Atmospheric modeling**: Aerosol studies and climate research applications
- **Radiative transfer**: Essential input for protoplanetary disk and stellar wind modelling

Current Limitations

- **Multiple methods available**: DDA (DDSCAT), TMM (MISH), SVM (HOM6, SPVV), spheroidal TMM (SoMSP) with different computational approaches
- **No systematic validation**: Published dust models lack cross-method comparison
- **Method selection by tradition**: Choices based on convenience rather than evidence
- **Unknown reliability regimes**: Size parameter limits and systematic differences unquantified

Critical Need

- **Quality assurance protocols**: Systematic validation required for computational dust research
- **Evidence-based selection**: Method performance assessment across parameter regimes
- **Community standards**: Cross-validation framework for model reliability
- **Uncertainty quantification**: Systematic error detection and propagation prevention

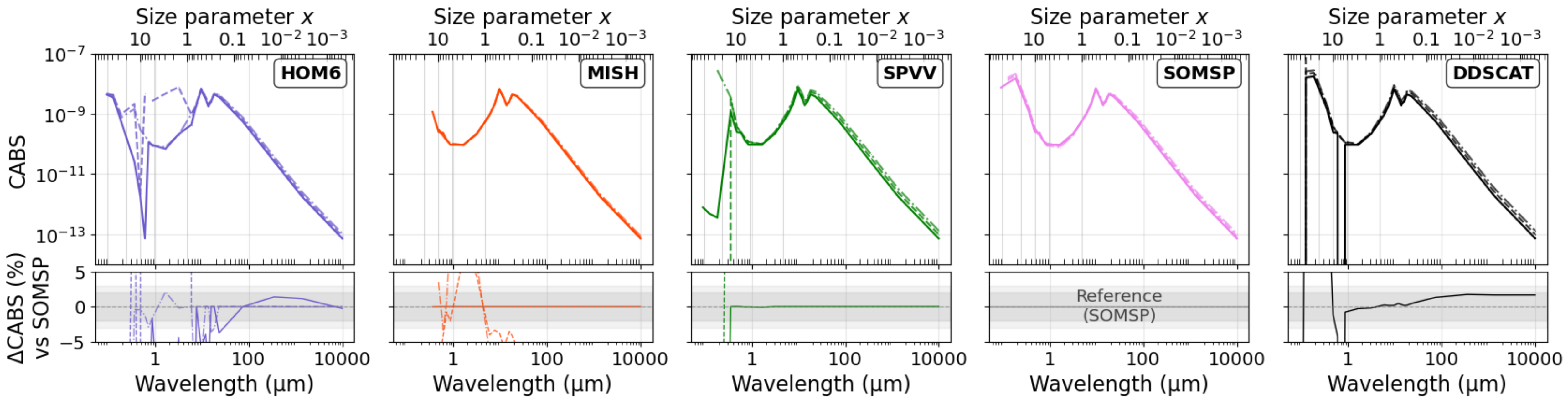

Figure 1: Absorption cross section (CABS) of spheroids for each code for different aspect ratios *a/b=1.0, 1.5, 2.0* (solid, dashed, dashed-dotted) as a function of wavelength λ. Fixed parameters: inclination angle *α = 90°*, grain size *a = 7.5142e-01 μm*. Optical constants (silicate) by Demyk et. al.

POMELO – Polarimetric Optical Matrices for Extinction and Light Scattering Optimization

Framework Architecture

- ***POMELO framework:*** ~21,000 lines Python computational infrastructure
- ***Universal I/O* between** incompatible code formats and coordinate systems
- ***Parallel orchestration:*** Multi-code execution with intelligent load balancing
- ***Data products***: Cross-sections, full Müller matrices, validation metrics, error logs
- ***Benchmarking***: Code performance comparison and reliability assessment
- ***Quality control:*** Systematic error detection and numerical stability tracking
- ***Community ready:*** Modular architecture designed for open-source adoption

Practical Access & Usage

- ***Output formats:*** (polarized) Cross-section files (*_C.bin*) and full Müller matrices (*_Z.bin*) ready for radiative transfer codes
- ***Adaptable formats:*** Universal I/O enables conversion to RADMC-3D, tMCpol, and other RT code requirements
- ***Current access:*** Contact *thomas.vannieuwenhuyse@eso.org*
  Future availability: Web-based access portal and community repository planned

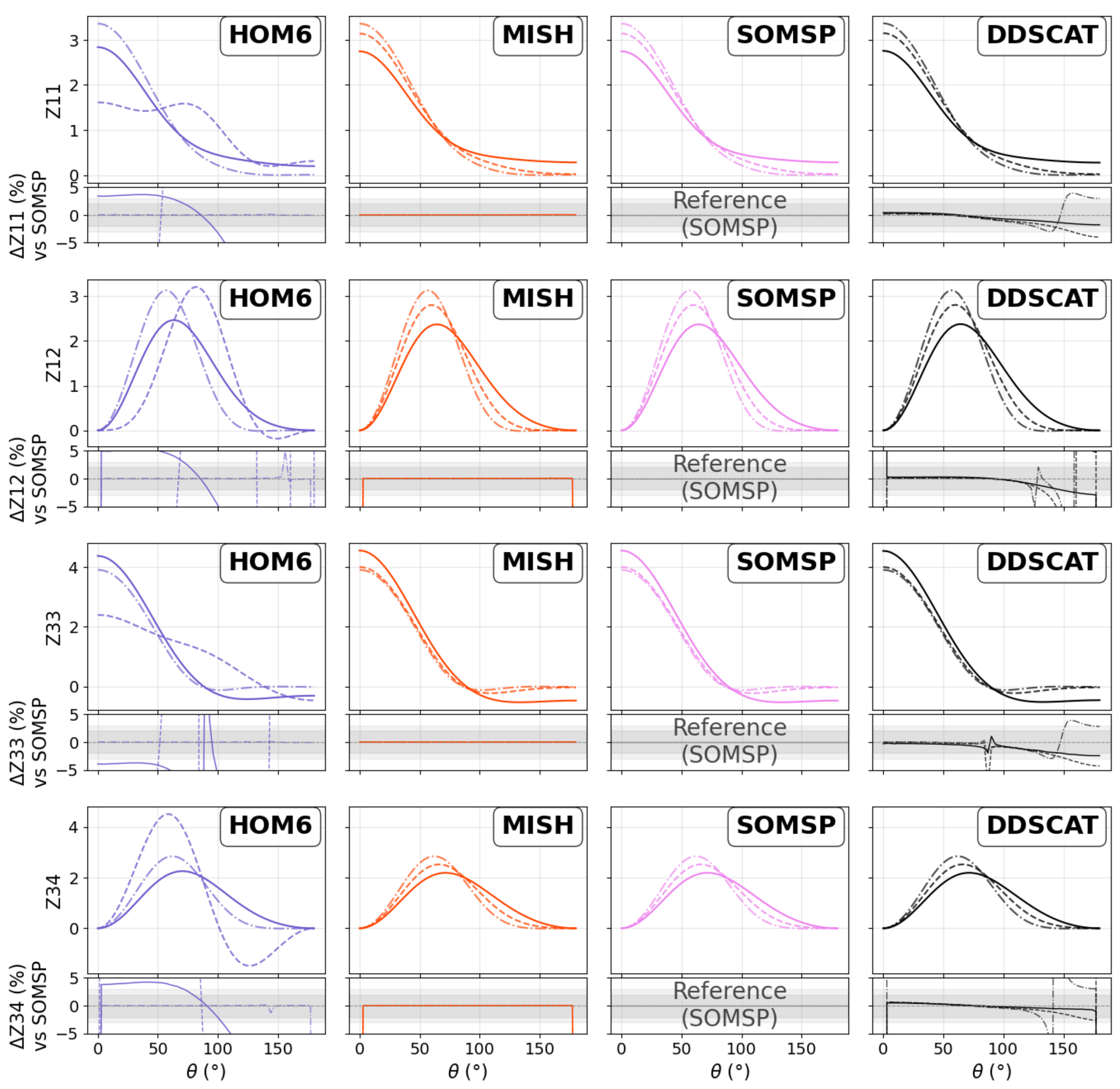

Figure 2: Selected scattering matrix elements (Z11, Z12, Z33, Z34 – rows) for each code (columns) for different aspect ratios *a/b = 1.0, 1.5, 2.0* (solid, dashed, dashed-dotted) as a function of one scattering angle *θ*. Fixed parameters: inclination angle *α = 0°*, primary exit angle *ϕ = 0°*, grain size *a = 1.935e-02 μm*, wavelength *λ = 9.080e-02 μm* (size parameter *x* = 1.339). Optical constants (silicate) by Demyk et. al.

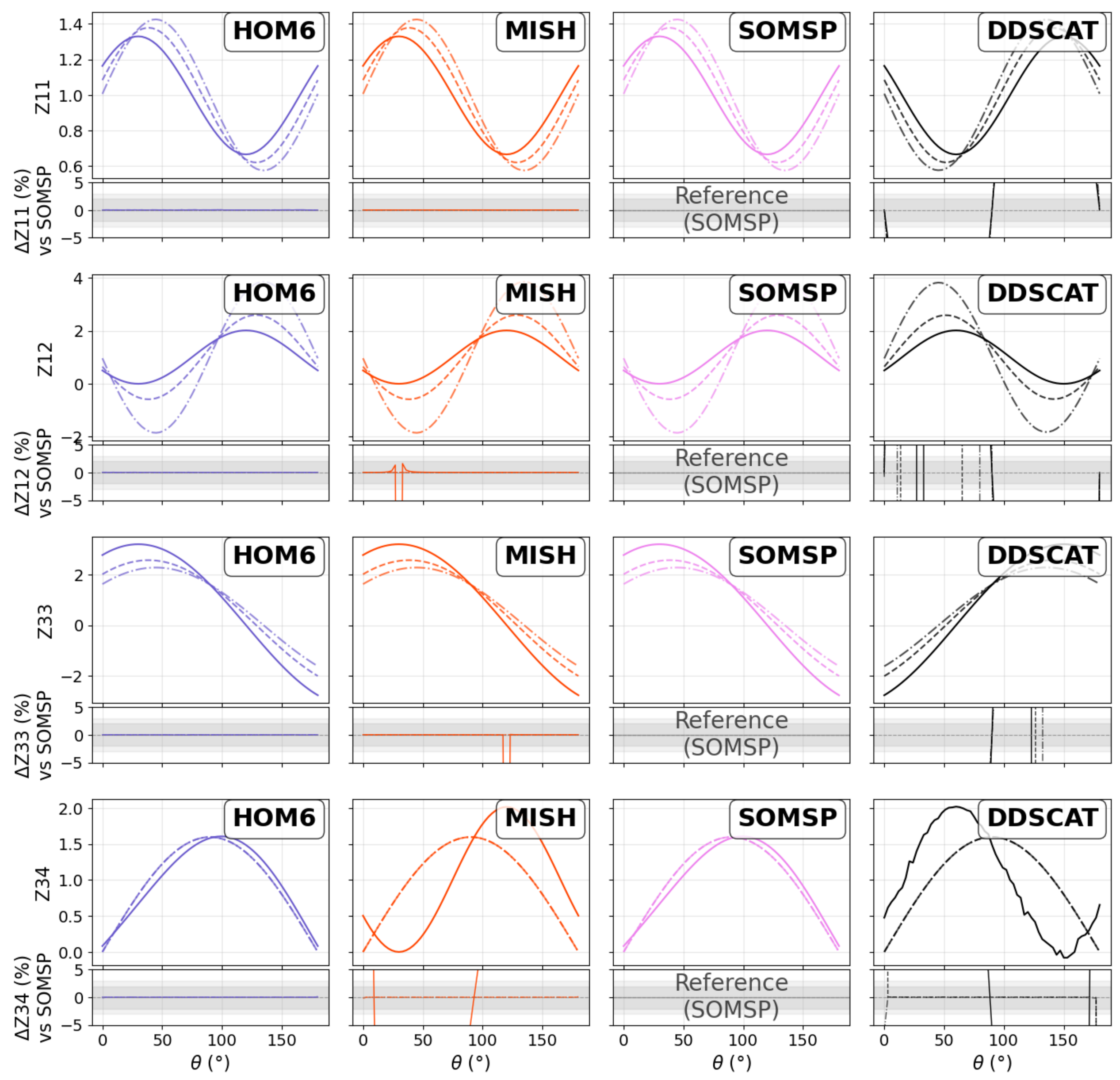

Figure 3: Selected scattering matrix elements (Z11, Z12, Z33, Z34 – rows) for each code (columns) for different aspect ratios *a/b = 1.0, 1.5, 2.0* (solid, dashed, dashed-dotted) as a function of one scattering angle *θ*. Fixed parameters: inclination angle *α = 30°*, primary exit angle *ϕ = 0°*, grain size *a = 2.2190e-01 μm*, wavelength *λ = 350 μm* (size parameter *x* = 0.004). Optical constants (silicate) by Demyk et. al.

Methodology

- **Universal integration framework:** POMELO enables systematic validation across 5 dust scattering codes with incompatible formats
- **Automated execution pipeline:** Parallel processing with error recovery across comprehensive parameter space
- **Statistical validation protocol:** Cross-correlation analysis and systematic difference quantification
- **Benchmark validation:** Kirchschlager et al. (2020) reproduction across multiple computational methods

Community Impact

- Any published dust scattering result can now be systematically validated
- Method selection guidance based on evidence, not tradition
- Quality assurance standard for computational dust research
- Systematic error detection prevents propagation of numerical artifacts
- Community standard for dust code benchmarking

Future Work

- **Radiative transfer integration:** Using scattering/extinction matrix output in tMCpol simulations to predict SEDs and images of dust polarization
- **Observational applications:** Validated extinction, scattering and polarization cross-sections for direct use in RT codes
- **Framework expansion:** Additional dust codes easily integrated through modular interface design

Results

- First comprehensive **cross-method comparison infrastructure** established
- **Systematic validation** achieves 72.3% mean cross-code agreement between the 5 codes with strong correlations (r > 0.99)
- **Quality assurance**
  Detected HOM6 numerical instabilities at aspect ratio a/b = 1.5 *(Fig. 1,2)*
- **Method size parameter x = 2πa/λ validity ranges quantified**
  HOM6 reliable for x < 5 *(dep. on a/b)*,
  MISH reliable for x < 10,
  SPVV reliable for x < 20
- **DDSCAT scattering divergence**
  Matrix elements differ for very small x *(Fig. 3)*
- **Evidence-based recommendation**
  SoMSP optimal for most applications (robust, fast, accurate)

Performance Metrics

- **Parameter Space**
  3 aspect ratios ×
  5 codes ×
  22 wavelengths ×
  5 grain sizes ×
  7 inclination angles ×
  11 × 61 scattering angles
- **Execution Time:**
  2 hours (previously 125+ days manual effort)

Success Rate: 97.3% with automatic failure recovery

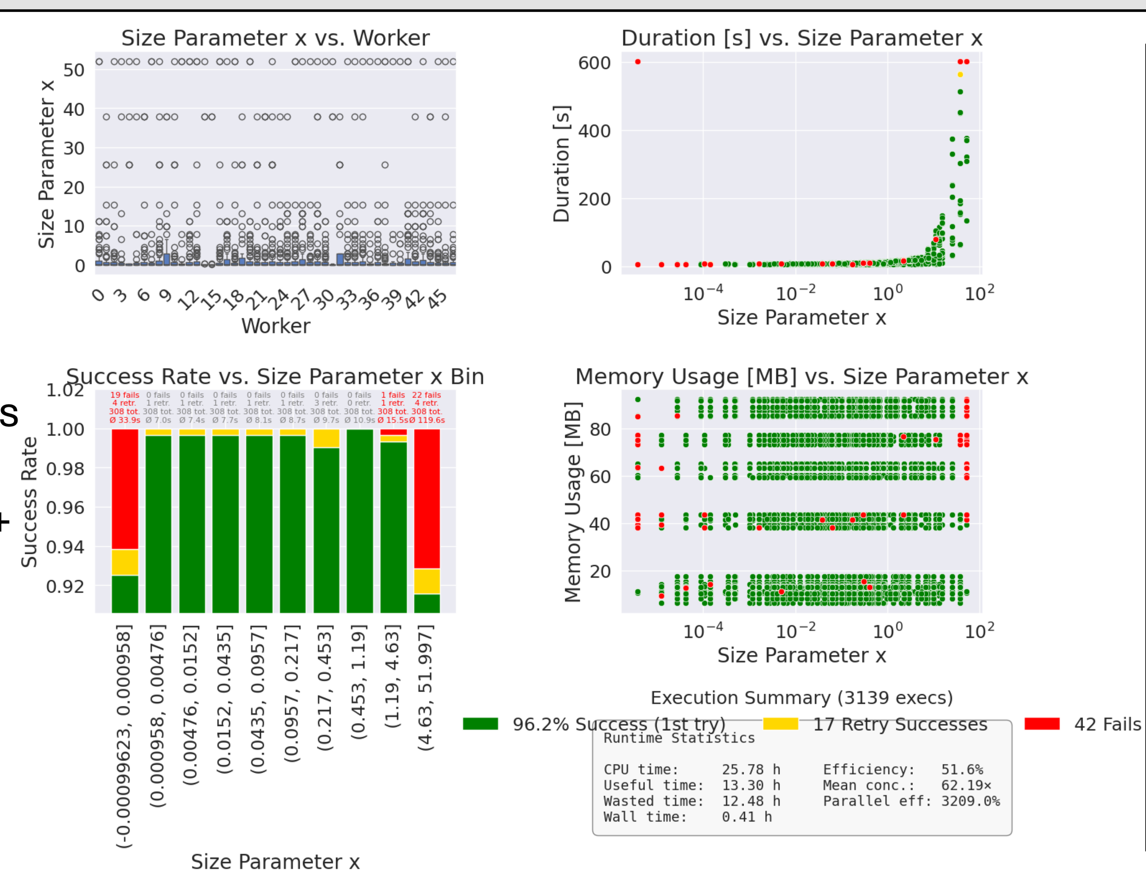

Figure 4: POMELO job diagnostics for the exemplary benchmark run of SoMSP on 48 threads (workers). Displayed are size parameter workload balance between the threads (top left), success rate per size parameter bin (lower left), duration and memory usage per individual calculation (right panels), and timing metrics (bottom right)

References
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MISH: Mishchenko, M. I., Travis, L. D., & Mackowski, D. W. 1996, JQSRT, 55, 535
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