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NP Transition Matrix code

G. La Mura, G. Mulas, R. Saija, M. A. Iatì, C. Cecchi-Pestellini

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Scientific Rationale

- The *NP Transition Matrix* code envisages the problem of modelling the scattering of radiation by a distribution of particles with complex geometric and optical properties.

- The code is well suited to investigate scattering processes in **aerosols** (e. g. Sindoni et al. 2006), in the **interstellar medium** (Cecchi-Pestellini et al. 2010) and in all conditions where the shape of particles (and its deviation from spherical geometry) has a large impact.

- The calculation includes **dynamical** and **thermal effects** of the radiation – particle interaction (Borghese, Denti, Saija 2007), for proper evaluation of the scatterers' physical state.

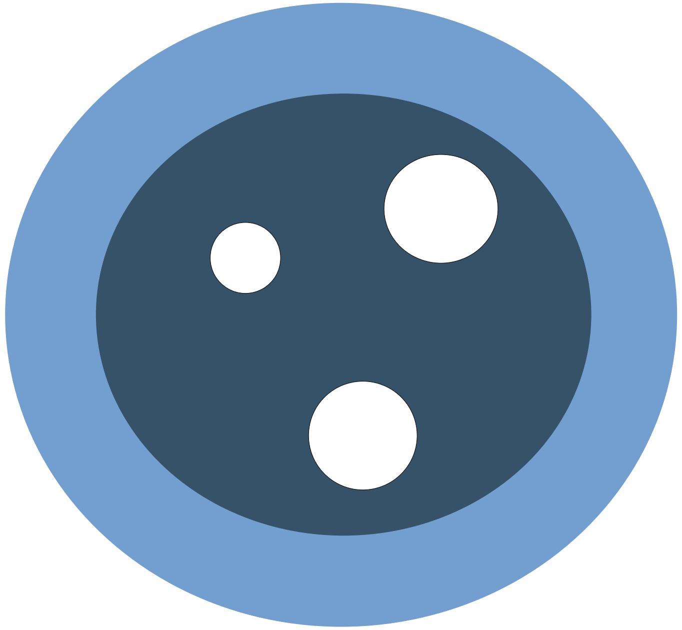
- The presence of non-trivial geometry has important implications on the derivation of differential **interaction cross-sections** and in their result as integrated effects (Saija et al., 2003).

- Detailed modelling of absorption and scattering (extinction), as well as polarization properties are possible (Borghese, Denti, Saija 2007).

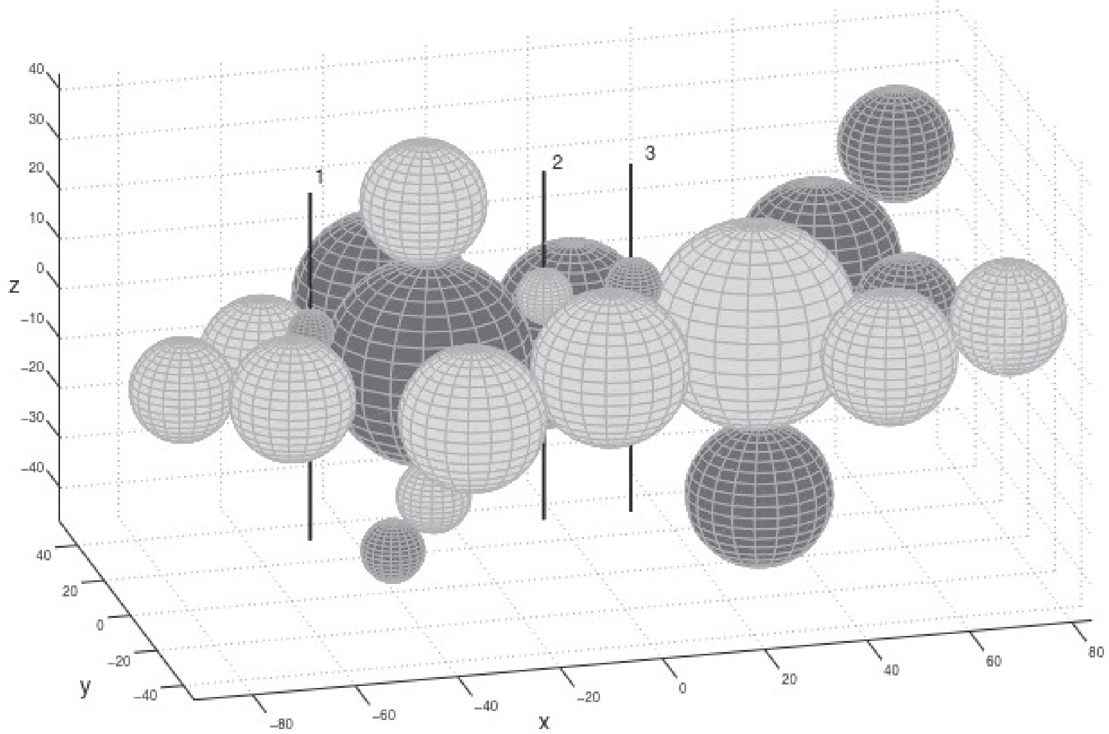
Technical Objectives, Methodologies and Solutions

- **GOAL:**
  - model radiation scattering / absorption by particles with arbitrary shape and optical properties
  - solve the analytical problems arising in absence of spherical symmetry
  - account for thermal and mechanical effects of the radiation – particle interaction
- **APPROACH:**
  - field expansion in **polar spherical harmonics**
  - construction of the **Transition Matrix** from boundary conditions
- **PECULIARITIES:**
  - model complex particles through an arbitrary number of spherical components
  - allow stratification of materials for more realistic grain simulation
- **RESULT:**
  - connect analitically incident and scattered field for every interaction angle (as opposed to numerical solutions based on *Discrete Dipole Approximation*)
  - compute extinction and polarization for both near- and far-field cases (addressing problems such as chirality and chemistry in dust cavities)
  - model forces, torques, dust acceleration, centrifugal stress, evaporation

Technical Objectives, Methodologies and Solutions



Example 1: Spherical particle with layered coating and internal cavities. Different color shades represent changes of material and refractive index



Example 2: representation of a dust particle as aggregate of spherical components. Different color shades represent different coating / material

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Timescale, Milestones and KPIs

The project structure can be narrowed down to three main stages:

- **Profiling (estimated completion: 3 months)**
  - Identification of bottle-necks
  - Evaluation of resource requirements
  - Representation of data structures

KPIs:
- Legacy result reproducibility

- **Parallelization (estimated time: ≥ 5 months)**
  - Transition of core functions to C++
  - Definition of parallel architecture for calculation steps
  - Migration of data structures to parallel architecture

KPIs:
- Computing time reduction
- Resource optimization

- **Practical application (estimated time: 3 months)**
  - Customizable configuration system
  - Interstellar dust properties from extinction models
  - Optical tweeners control

KPIs:
- Scatterer complexity
- System requirements

Accomplished Work, Results

- **ORGANIZATION OF LEGACY CODE:**
  - Existing implementation in (old-fashioned) FORTRAN
  - Scattering solution for a single spherical unit (with internal stratification)
  - Scattering solution for clusters of units
  - Radiation trapping (optical tweeners)

Communication among units handled through physical files

- **SET UP OF DEVELOPMENT ENVIRONMENT:**
  - Source code management in *gitLab*
  - Migration to C++
  - Addition of inline documentation (*doxygen*)

GitLab

- **TEST CASE COLLECTION:**
  - Choice of pre-computed models for profiling activity and consistency checks

Next Steps and Expected Results (by next checkpoint: April 2024)

- **Profiling activity**
  - Definition of the model test suite (published reproducible results)
  - Identification of bottle-necks and parallelisation strategies
  - Choice of parallel architecture (e.g. MPI for wavelength parallelism, OpenMP for T-matrix, porting to GPUs)

- **Code porting**
  - Refactoring of data structures and core functions (using FITS or netCDF instead of binary I/O)
  - Optional integration with algebraic libraries (LAPACK, ScaLAPACK, MAGMA – upon convenience, but with fall-back portable internal routines)
  - Consistency checks between state-of-the-art and ported results

- **Interface development**
  - Improvement of configuration files (human readable formats)
  - Implementation of GUI-oriented setup (depending on time requirements)
  - Introduction of diagnostic tools (for inspection of binary data)

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