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NP Transition Matrix code

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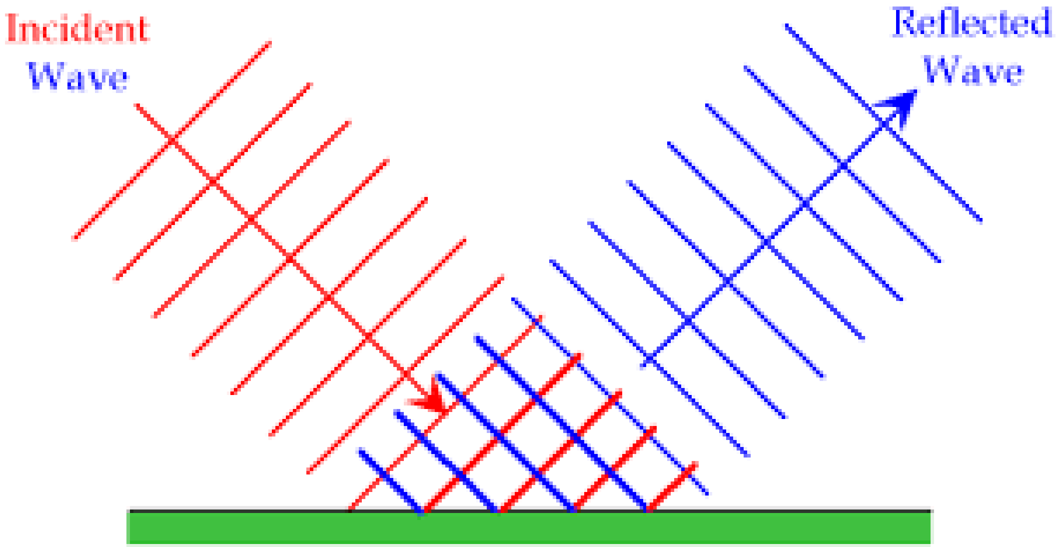
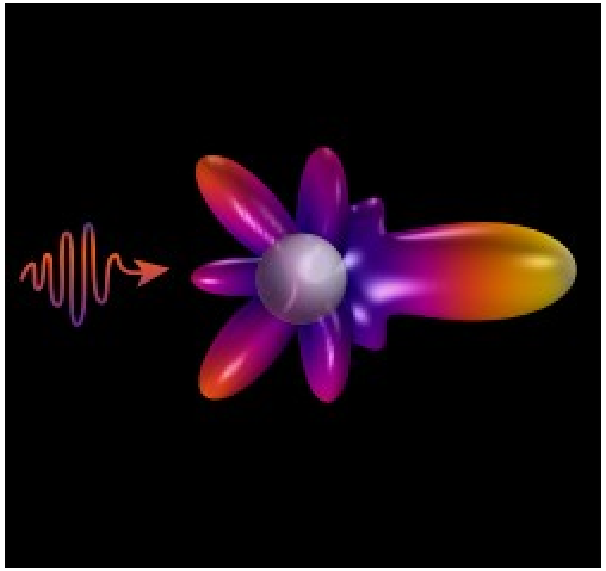
Scientific Rationale



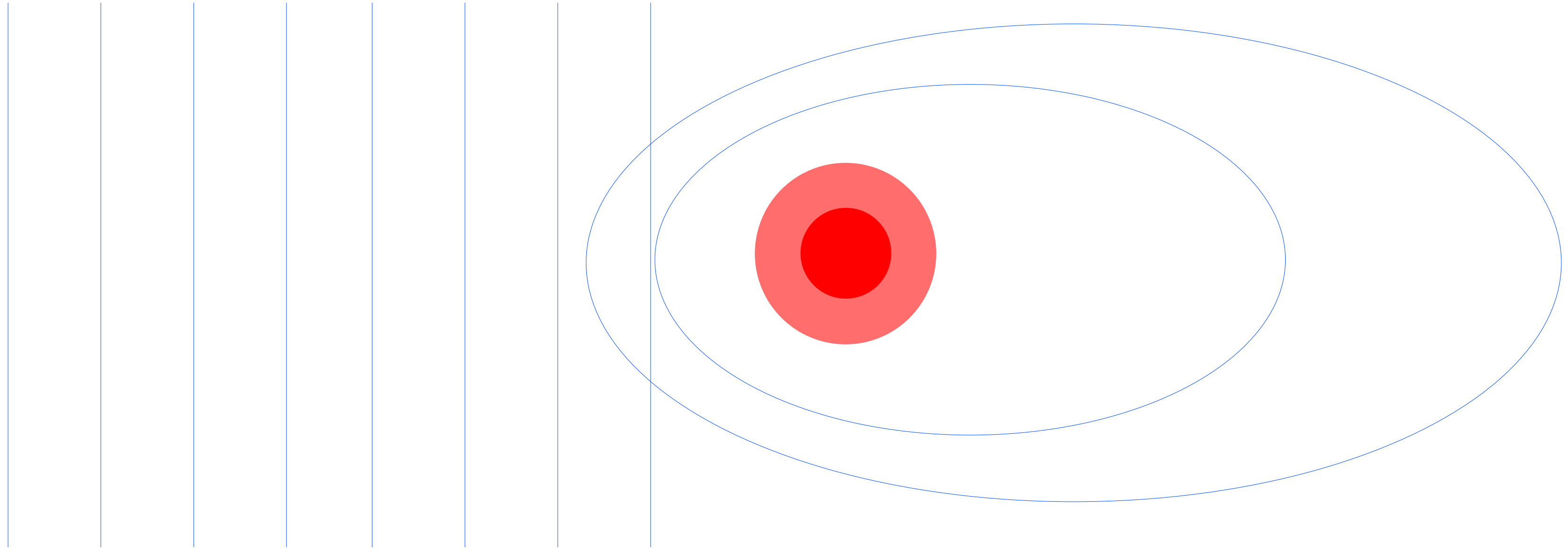


Radiation scattering on particles embedded in a transmissive medium has many applications:

- physics of aerosols (atmospheric physics)
- material investigation
- radiation transfer
- interstellar medium and extinction

Exact solution possible only in simple cases.

Scientific Rationale – Mie theory



Ideal case

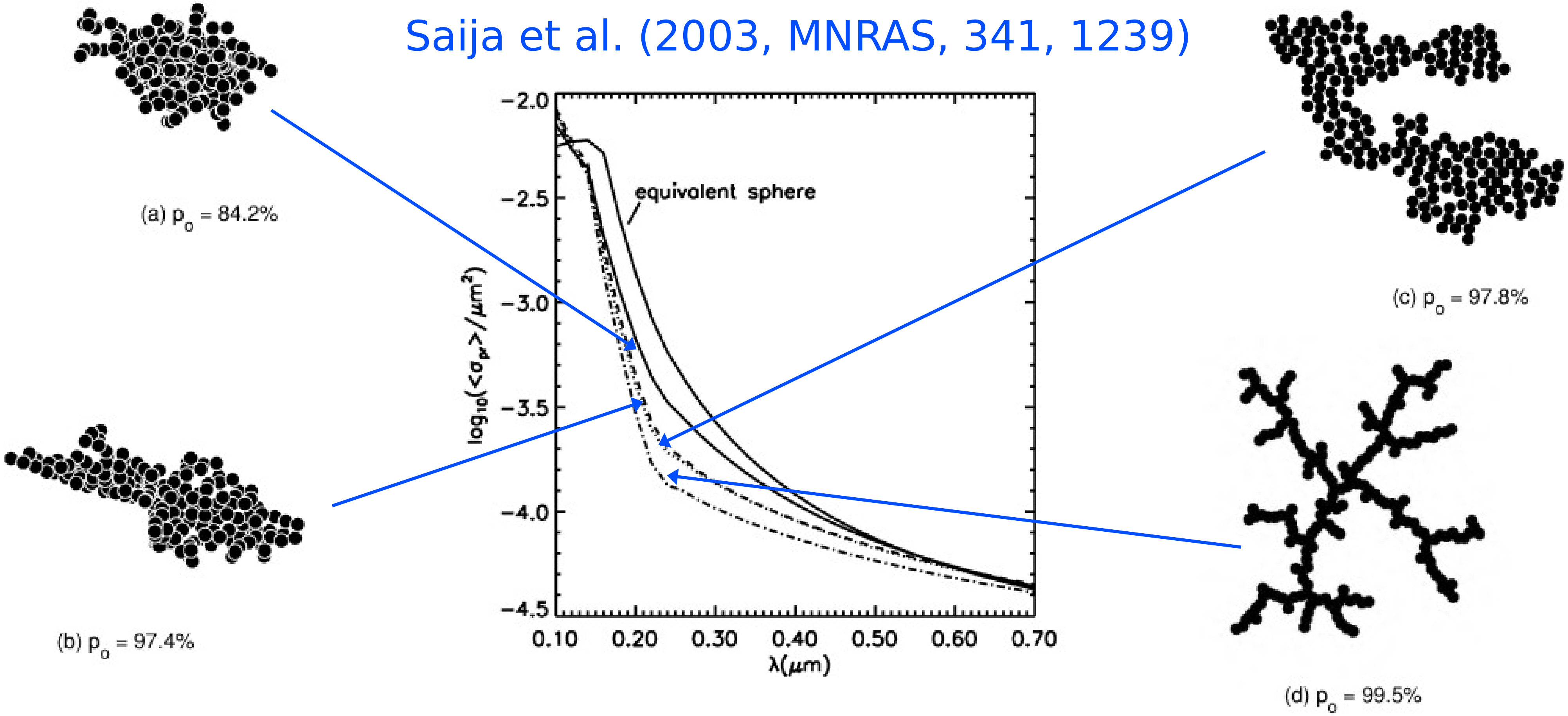
Limited practical use

Deviates substantially from realistic situations

Mie theory offers an **exact** treatment of the problem:
- based on solution of the Maxwell field equations
- valid for vector fields impinging a spherically symmetric system
- intermediate between Rayleigh regime and geometric optics

Scientific Rationale – Mie theory (limitations)

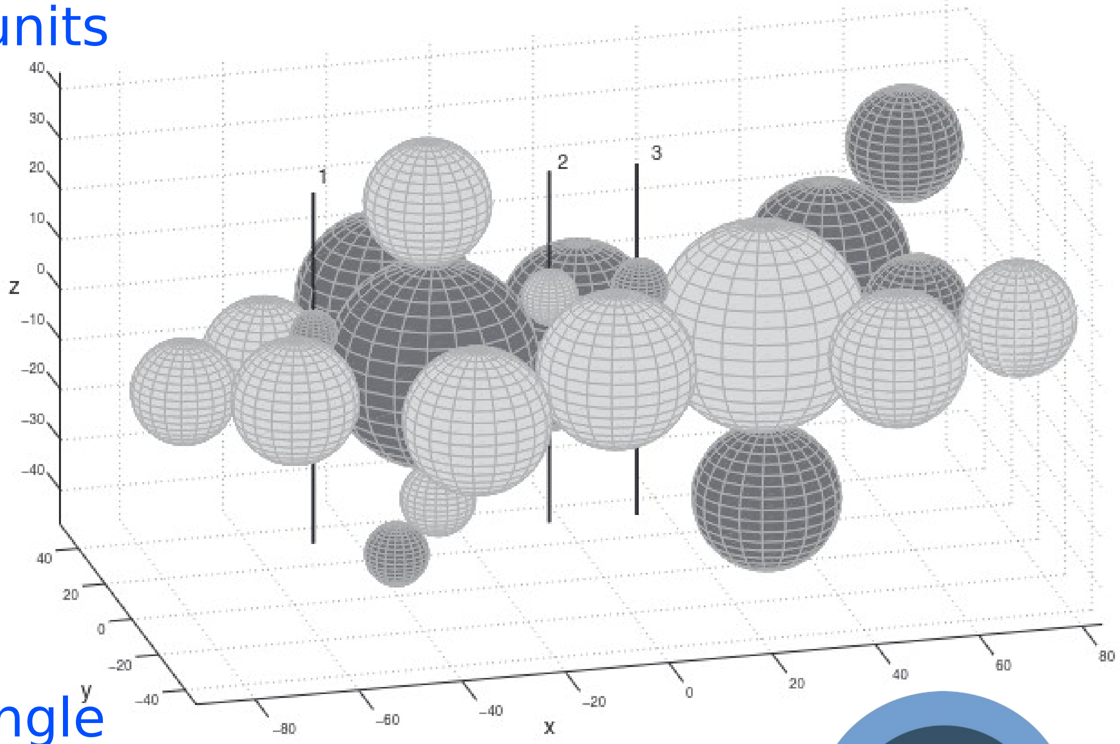
Saija et al. (2003, MNRAS, 341, 1239)



Cannot handle asymmetry, multiple scattering, porosity (expected in realistic particles)

Scientific Rationale – Transition Matrix approach

Method:
- Model particles as combinations of spherical units
- Account for material optical properties
- Expand fields in spherical vector harmonics
- Set boundary conditions on transition layers
- Connect incident and scattered fields



Advantages:
- Leverage field equation linearity
- Construct a linear matrix operator
- Derive differential and integrated properties

Results:
- Radiation intensity as function of scattering angle
- Radiative forces and torques exerted on the particle
- Thermodynamic effects due to absorption
- Polarization properties

Transition Matrix – Analytical definition

Vector fields: $\begin{cases} \boldsymbol{E} = E_0 \hat{\boldsymbol{e}} \exp(i\boldsymbol{k}\cdot\boldsymbol{r}) \\ i\boldsymbol{B} = in E_0 (\hat{\boldsymbol{k}} \times \hat{\boldsymbol{e}}) \exp(i\boldsymbol{k}\cdot\boldsymbol{r}) \end{cases}$

Multipolar exp.: $\begin{cases} \boldsymbol{E} = E_0 \sum_{plm} \boldsymbol{J}_{lm}^{(p)}(\boldsymbol{r}, k) W_{lm}^{(p)}(\hat{\boldsymbol{e}}, \hat{\boldsymbol{k}}) \\ i\boldsymbol{B} = in E_0 \sum_{plm} \boldsymbol{J}_{lm}^{(p)}(\boldsymbol{r}, k) W_{lm}^{(p')}(\hat{\boldsymbol{e}}, \hat{\boldsymbol{k}}) \end{cases}$

Incident field: $\boldsymbol{E}_I = E_0 \sum_{plm} \boldsymbol{J}_{lm}^{(p)}(\boldsymbol{r}, k) W_{lm}^{(p)}(\hat{\boldsymbol{e}}_I, \hat{\boldsymbol{k}}_I)$ Scattered field: $\boldsymbol{E}_S = E_0 \sum_{plm} \boldsymbol{H}_{lm}^{(p)}(\boldsymbol{r}, k) A_{lm}^{(p)}(\hat{\boldsymbol{e}}_I, \hat{\boldsymbol{k}}_I)$

The *Transition Matrix* is the linear operator defined by: $\boldsymbol{E}_S = S\,\boldsymbol{E}_I$

its elements being the complex quantities $S_{lml'm'}^{(pp')}$ that verify:

$$A_{lm}^{(p)}(\hat{\boldsymbol{e}}_I, \hat{\boldsymbol{k}}_I) = \sum_{p'l'm'} S_{lml'm'}^{(pp')} W_{l'm'}^{(p')}(\hat{\boldsymbol{e}}_I, \hat{\boldsymbol{k}}_I)$$

Dimensions: $[2\,N_p\,L_{max}\,(L_{max} + 2) \times 2\,N_p\,L_{max}\,(L_{max} + 2)]$

Borghese, Denti & Saija (2007, DOI:10.1007/978-3-540-37413-8)

Transition Matrix – Application domain

A critical parameter of the scattering problem is the scale factor:

$$\chi = \frac{2\pi\sqrt{\varepsilon_M}}{\lambda} r$$

expressing the ratio between the radius of the particle's envelope *r* and the radiation wavelength. The scattering process needs an **analytical solution** whenever $0.1 \leq \chi \leq 10$. For $\chi << 0.1$, the problem falls into **Rayleigh approximation**, while for $\chi >> 10$ it approaches the domain of **geometric optics**.

The condition to achieve convergence (non-absorbing materials, non resonant frequencies), is given by Wiscombe's expansion limit criterium (Wiscombe 1980, Appl. Opt., 19, 1505):

$$\begin{cases} L_{max} \simeq \chi + 4.05\,\chi^{1/3} + 2 & \text{for a single sphere or a cluster of spheres in far field regime} \\ L_{max} \simeq \chi + 11\,\chi^{1/3} + 1 & \text{for a cluster of spheres in near field regime} \end{cases}$$

NPTMcode overview

The application suite is divided in 3 main programs.

Needs input from the other codes

NP_SPHERE

Light-weight code to solve radiation scattering by a single particle in spherical symmetry.

Trivial case.

NP_TRAPPING

Evaluation of the radiative forces exerted on the structure of the particle.

Computationally intensive.

NP_CLUSTER

Version handling multiple scattering ba an asymmetric particle made of many spheres.

Challenging case.

Target of the first parallel implementation.

Auxiliary software to parse input and output (interface to popular plotting packages)

Project layout

The project has been structured in three stages:

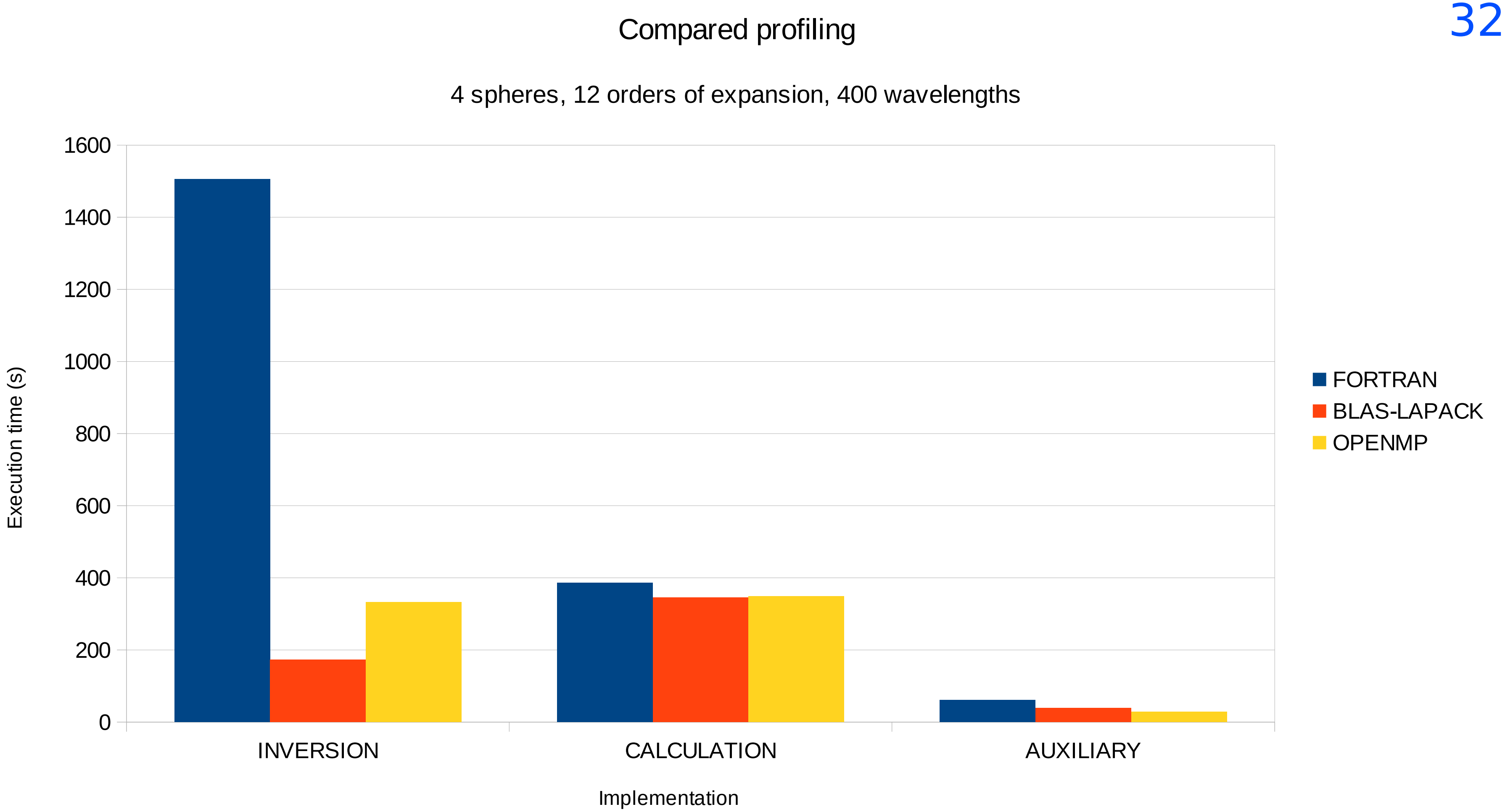
- **Profiling (serial part completed)**
  - Identification of bottle-necks
  - Evaluation of resource requirements
  - Representation of data structures
- **Parallelization (estimated time: ≥ 5 months)**
  - Transition of core functions to C++
  - Definition of parallel architecture for calculation steps
  - Migration of data structures to parallel architecture
- **Practical application (estimated time: 6+ months)**
  - Customizable configuration system
  - Interstellar dust properties from extinction models
  - Optical tweeners control

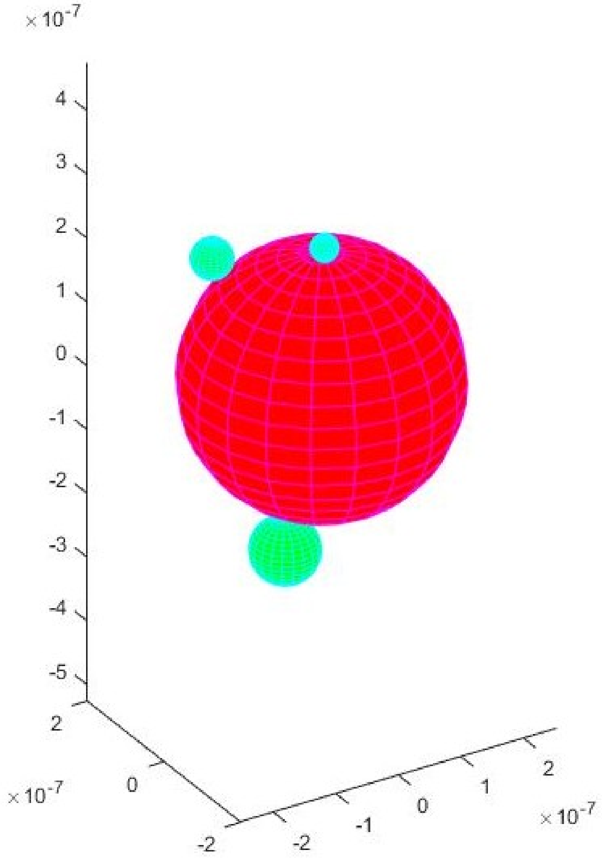
KPIs

- Profiling:
  - Legacy result reproducibility
- Parallelization:
  - Computing time reduction
  - Resource optimization
- Practical application:
  - Scatterer complexity
  - System requirements

Profiling of NP_cluster

Hardware: ASUS Zenbook
CPU Intel Core i9 (20-core)
32 GB RAM





1344 x 1344 matrix, 27.56Mb per scale

Not only performance...

Comparison between ../RESULT_FORTRAN/OCLU and c_OCLU

Numeric noise is marked **GREEN**, warnings are marked **BLUE** and errors are marked **RED**.
Comparison yielded 0 errors, 46146 warnings and 19113 noisy values.

```
00079:  FSAC(1,1)=  7.1991343E-21  4.2610087E-21   FSAC(2,1)=  6.0525559E-27  1.6310944E-27
ORIG :  FSAC(1,1)=  7.1991343E-21  4.2610087E-21   FSAC(2,1)=  6.0511318E-27  1.6313331E-27
00091:  FSAC(2,2)=  7.1991343E-21  4.2610087E-21   FSAC(1,2)= -6.0525559E-27 -1.6310944E-27
ORIG :  FSAC(2,2)=  7.1991343E-21  4.2610087E-21   FSAC(1,2)= -6.0511318E-27 -1.6313331E-27
00107:  SAS(1,1)=  7.4715138E-21  2.8655015E-21, SAS(2,1)=  0.0000000E+00 -0.0000000E+00
ORIG :  SAS(1,1)=  7.4715138E-21  2.8655015E-21, SAS(2,1)= -2.1537682E-38  8.6150727E-38
00108:  SAS(1,2)=  0.0000000E+00 -0.0000000E+00, SAS(2,2)=  7.4715138E-21  2.8655015E-21
ORIG :  SAS(1,2)=  2.1537682E-38 -8.6150727E-38, SAS(2,2)=  7.4715138E-21  2.8655015E-21
00110:           9.8749429E-14  0.0000000E+00 -0.0000000E+00  0.0000000E+00
ORIG :           9.8749429E-14  0.0000000E+00  0.0000000E+00 -2.1756081E-30
00111:           0.0000000E+00  9.8749429E-14  0.0000000E+00 -0.0000000E+00
ORIG :           0.0000000E+00  9.8749429E-14  2.6507892E-31  0.0000000E+00
00112:          -0.0000000E+00  0.0000000E+00  9.8749429E-14  0.0000000E+00
ORIG :           0.0000000E+00 -2.6507892E-31  9.8749429E-14  0.0000000E+00
00113:           0.0000000E+00  0.0000000E+00  0.0000000E+00  9.8749429E-14
ORIG :          -2.1756081E-30  0.0000000E+00  0.0000000E+00  9.8749429E-14
00115:           9.8749429E-14  0.0000000E+00 -0.0000000E+00 -0.0000000E+00
ORIG :           9.8749429E-14  1.2160925E-47  1.3253946E-31 -1.0878041E-30
00116:           0.0000000E+00  9.8749429E-14 -0.0000000E+00  0.0000000E+00
ORIG :           1.2160925E-47  9.8749429E-14 -1.3253946E-31 -1.0878041E-30
00117:          -0.0000000E+00 -0.0000000E+00  9.8749429E-14  0.0000000E+00
ORIG :          -2.6507892E-31  2.6507892E-31  9.8749429E-14  0.0000000E+00
00118:           0.0000000E+00 -0.0000000E+00  0.0000000E+00  9.8749429E-14
ORIG :          -2.1756081E-30 -2.1756081E-30  0.0000000E+00  9.8749429E-14
```

Result stability and consistence are clearly fundamental requirements, but:

- Approximated solutions computed with different hardware will have different values
- Plotting all possible results is not practical
- Negligible values are subject to noise

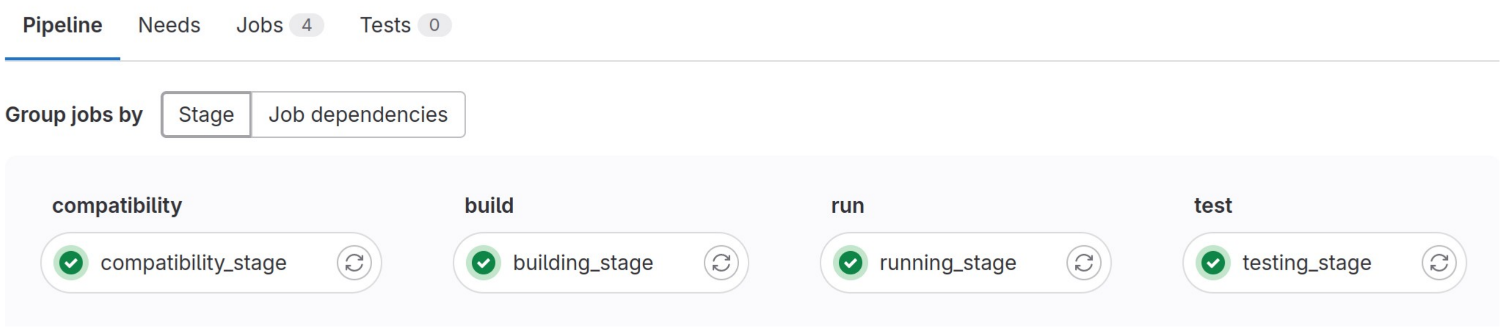
Solution:

- Development of result parsing scripts

Safety checks

```
00168:   FSAC(1,1)=  6.4636561E-21  4.6221195E-21   FSAC(2,1)=  2.7761176E-23 -6.2673970E-24
ORIG :   FSAC(1,1)=  6.4636560E-21  4.6221195E-21   FSAC(2,1)=  2.7761170E-23 -6.2674066E-24
00169:    SAC(1,1)=  6.4636561E-21  4.6221195E-21    SAC(2,1)=  2.7761176E-23 -6.2673970E-24
ORIG :    SAC(1,1)=  6.4636560E-21  4.6221195E-21    SAC(2,1)=  2.7761170E-23 -6.2674066E-24
00170:   RE(FSAC(1,1))/RE(TFSAS)=  8.4061596E-01, IM(FSAC(1,1))/IM(TFSAS)=  1.0751162E+00
ORIG :   RE(FSAC(1,1))/RE(TFSAS)=  8.4061595E-01, IM(FSAC(1,1))/IM(TFSAS)=  1.0751162E+00
00175:    TQEl=  3.5159140E-01,  TQEr=  3.1212508E+01,  TQEk= -2.8620626E-01
ORIG :    TQEl=  3.5159157E-01,  TQEr=  3.1212508E+01,  TQEk= -2.8620620E-01
00176:    TQSl= -4.3640865E+00,  TQSr=  7.6938290E+00,  TQSk= -6.3629176E-01
ORIG :    TQSl= -4.3640864E+00,  TQSr=  7.6938287E+00,  TQSk= -6.3629180E-01
00177:    TQEx=  3.5159140E-01,  TQEy=  3.1212508E+01,  TQEz= -2.8620626E-01
ORIG :    TQEx=  3.5159157E-01,  TQEy=  3.1212508E+01,  TQEz= -2.8620620E-01
00178:    TQSx= -4.3640865E+00,  TQSy=  7.6938290E+00,  TQSz= -6.3629176E-01
ORIG :    TQSx= -4.3640864E+00,  TQSy=  7.6938287E+00,  TQSz= -6.3629180E-01
00181:   8.1310425E-14  2.6427161E-14  1.0773759E-13  7.5470807E-01
ORIG :   8.1310426E-14  2.6427161E-14  1.0773759E-13  7.5470807E-01
00186:   FSAC(2,2)=  6.4824372E-21  4.5610939E-21   FSAC(1,2)=  3.1293951E-23 -1.0408036E-23
ORIG :   FSAC(2,2)=  6.4824372E-21  4.5610939E-21   FSAC(1,2)=  3.1293952E-23 -1.0408034E-23
00187:    SAC(2,2)=  6.4824372E-21  4.5610939E-21    SAC(1,2)=  3.1293951E-23 -1.0408036E-23
ORIG :    SAC(2,2)=  6.4824372E-21  4.5610939E-21    SAC(1,2)=  3.1293952E-23 -1.0408034E-23
00188:   RE(FSAC(2,2))/RE(TFSAS)=  8.4305849E-01, IM(FSAC(2,2))/IM(TFSAS)=  1.0609215E+00
ORIG :   RE(FSAC(2,2))/RE(TFSAS)=  8.4305850E-01, IM(FSAC(2,2))/IM(TFSAS)=  1.0609215E+00
00191:   Fl=  3.0552305E-15, Fr= -7.1362650E-16, Fk=  4.2319282E-14
ORIG :   Fl=  3.0552305E-15, Fr= -7.1362653E-16, Fk=  4.2319282E-14
00192:   Fx=  3.0552305E-15, Fy= -7.1362650E-16, Fz=  4.2319282E-14
ORIG :   Fx=  3.0552305E-15, Fy= -7.1362653E-16, Fz=  4.2319282E-14
00193:    TQEl=  6.7079923E-01,  TQEr=  3.3885619E+01,  TQEk=  3.2262771E-01
ORIG :    TQEl=  6.7079936E-01,  TQEr=  3.3885619E+01,  TQEk=  3.2262772E-01
```

- Tests designed to distinguish **warnings** (values that are different, but consistent within tolerance threshold) from **errors** (inconsistent values) and **noise** (negligible values)
- Tolerance can be adjusted upon request
- New features are only implemented after the succesful execution of a standard test suite.



Project roadmap

- **STATUS OF THE CODE:**
  - Implemented C++ version of the FORTRAN application suite (M7 KPI)
  - Improved code interface with configurable input/output (M7 KPI)
  - Added I/O capabilities towards HDF5 binary format (M7 KPI)
  - Created inline documentation (M8 KPI)

- **STATUS OF THE PROJECT:**
  - Performed profiling of NP_SPHERE, NP_CLUSTER and NP_TRAPPING (M7 KPI)
  - Identified matrix-inversion computationally intensive task (M7 KPI)
  - Obtained 8x speed-up factor on the same hardware with link to specialized libraries (M8 KPI)
  - Next bottle-neck: resource management

- **DEVELOPMENT PLAN:**
  - Implement hierarchical parallelism (foreseen speed-up factor between 100x and 200x)
  - Introduce GPU offload (directly for L.A. functions + dedicated development, M8 KPI)
  - Investigate interstellar extinction through realistic scattering models (M9 KPI)