Finanziato dall'Unione europea NextGenerationEU | Ministero dell'Università e della Ricerca | Italiadomani PIANO NAZIONALE DI RIPRESA E RESILIENZA | ICSC Centro Nazionale di Ricerca in HPC, Big Data and Quantum Computing

NP Transition Matrix code

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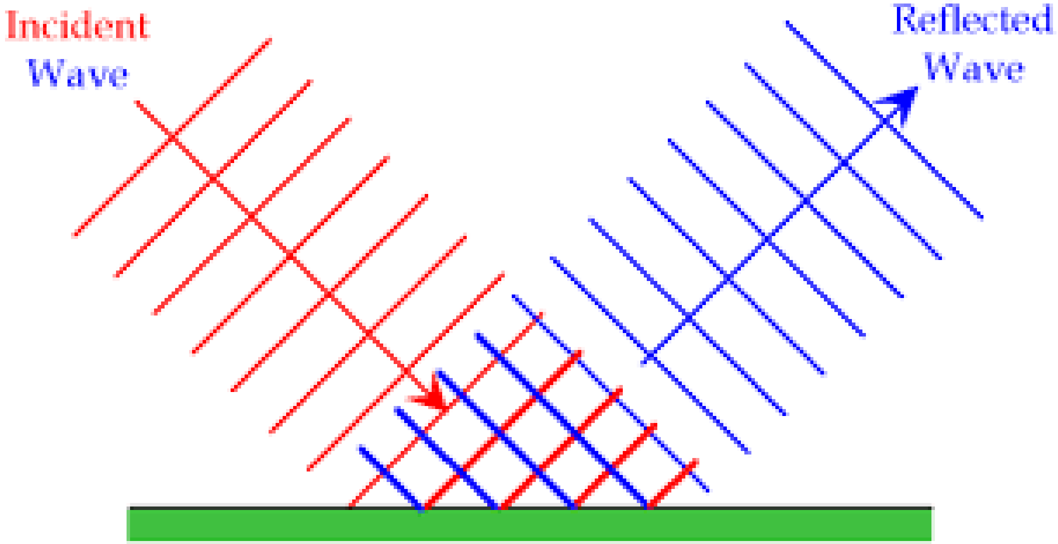
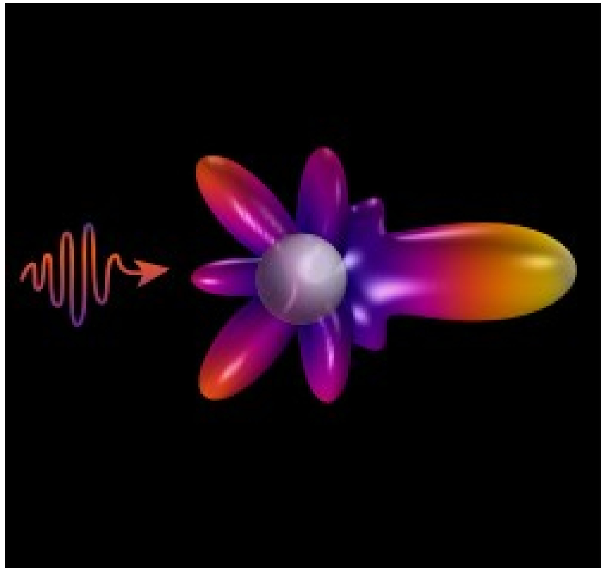
Scientific Rationale





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.

Technical Objectives, Methodologies and Solutions

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

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)

Target speed-up factor: > 100x (with respect to original code) Approach: hierarchical parallelism + GPU offload

Timescale, Milestones and KPIs

The project has been structured in three stages:

- **Profiling (serial part completed)**
  - Identification of bottle-necks
  - Evaluation of resource requirements
  - Transition of core functions to C++

  KPIs:
  - Legacy result reproducibility

- **Parallelization (estimated time: ≥ 5 months)**
  - Representation of data structures
  - Definition of parallel architecture for calculation steps
  - Migration of data structures to parallel architecture

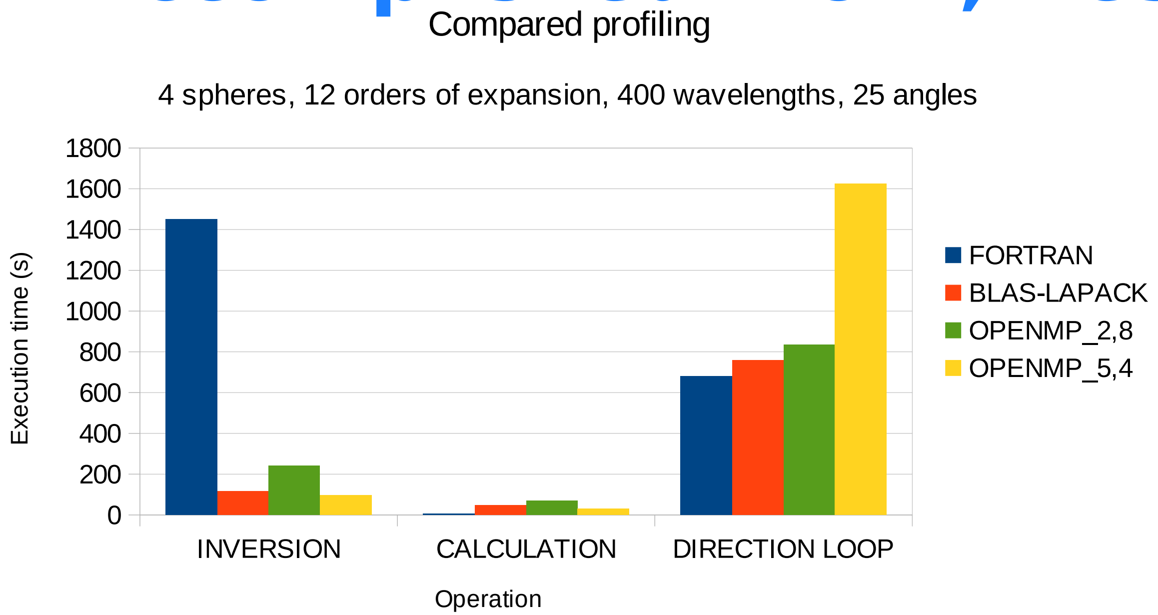
  KPIs:
  - Computing time reduction
  - Resource optimization

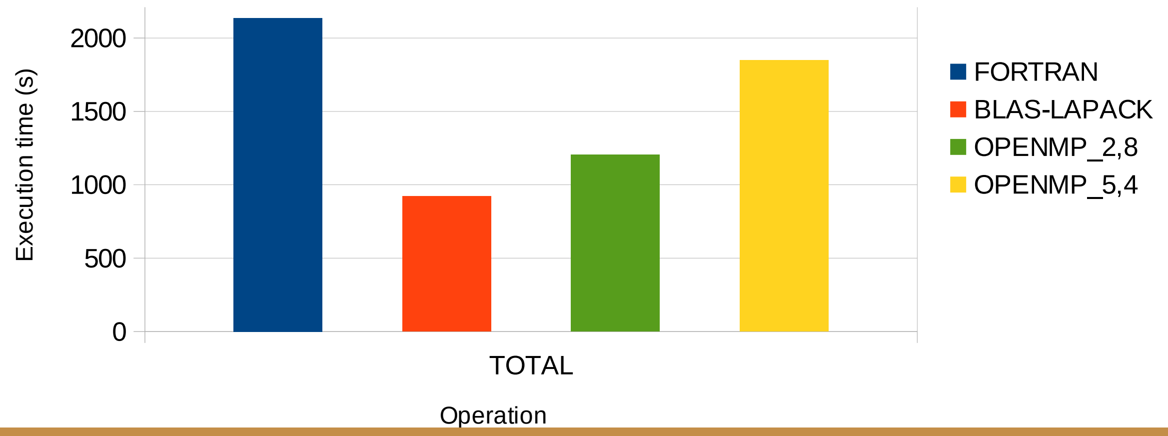
- **Practical application (estimated time: 6+ months)**
  - Customizable configuration system
  - Interstellar dust properties from extinction models
  - Optical tweeners control

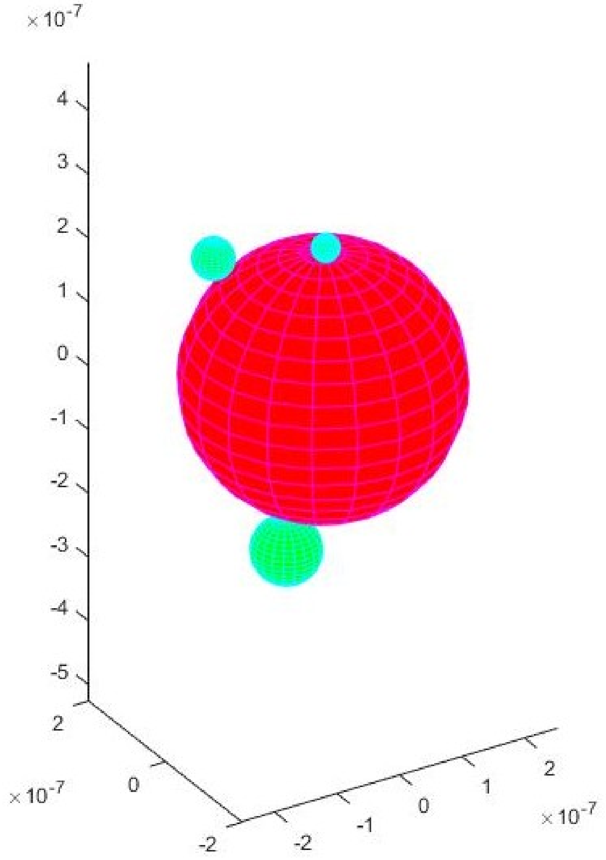
  KPIs:
  - Scatterer complexity
  - System requirements

Accomplished Work, Results

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







1344 x 1344 matrix, 27.56Mb per scale

Next Steps and Expected Results

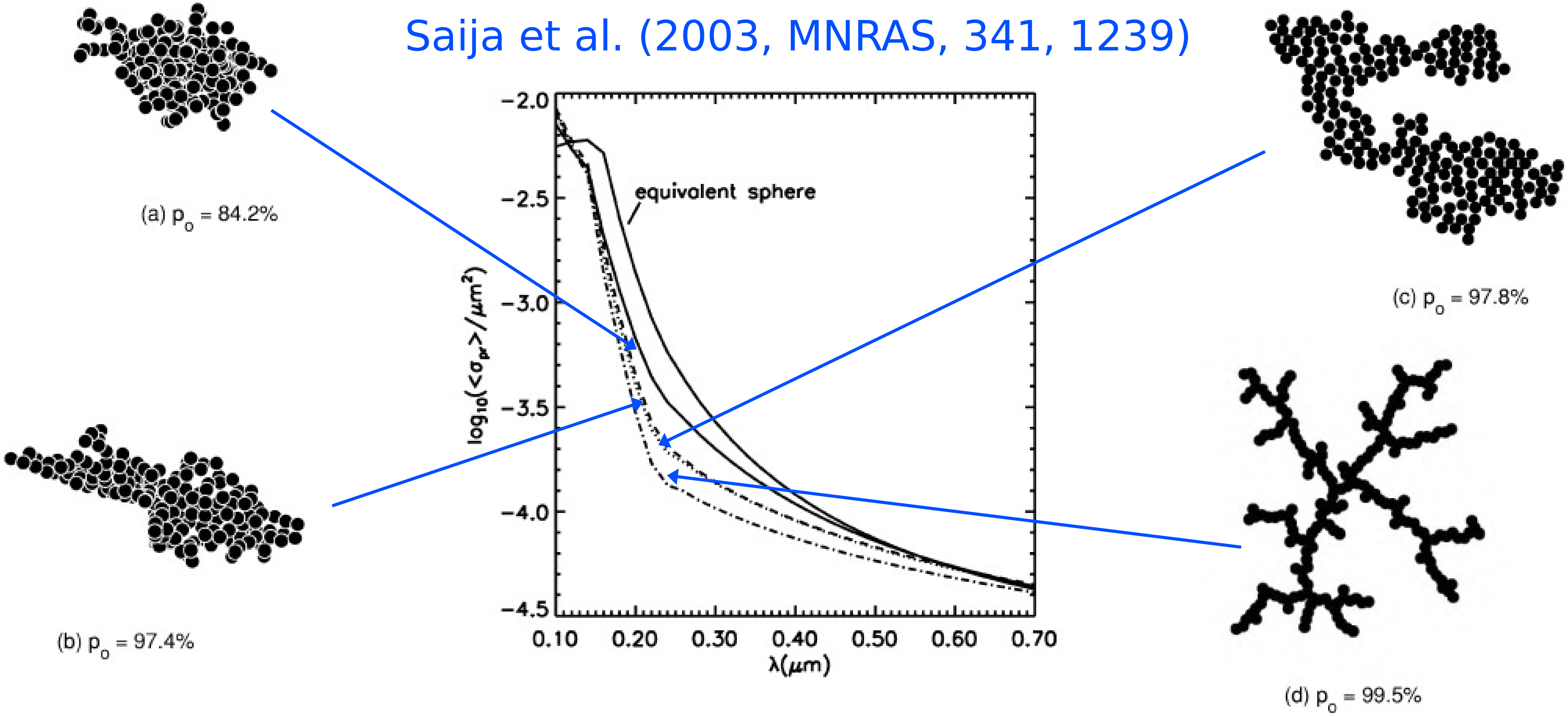
- **STATUS OF THE CODE:**
  - Implemented C++ version of the FORTRAN application suite (M7 KPI)
  - Improved code interface with configurable input/output (M7 KPI)
  - Added I/O capabilities towards HDF5 binary format (M7 KPI)
  - Created inline documentation (M8 KPI)

- **STATUS OF THE PROJECT:**
  - Performed profiling of NP_SPHERE, NP_CLUSTER and NP_TRAPPING (M7 KPI)
  - Achieved 8x speed-up factor on matrix inversion (M8 KPI)
  - Identified second intensive calculation on scattering directions
  - Current activity: parallelisation of scattering direction calculation

- **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)

Back up – Mie theory (limitations)

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



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

Back-up slides: result consistency

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:

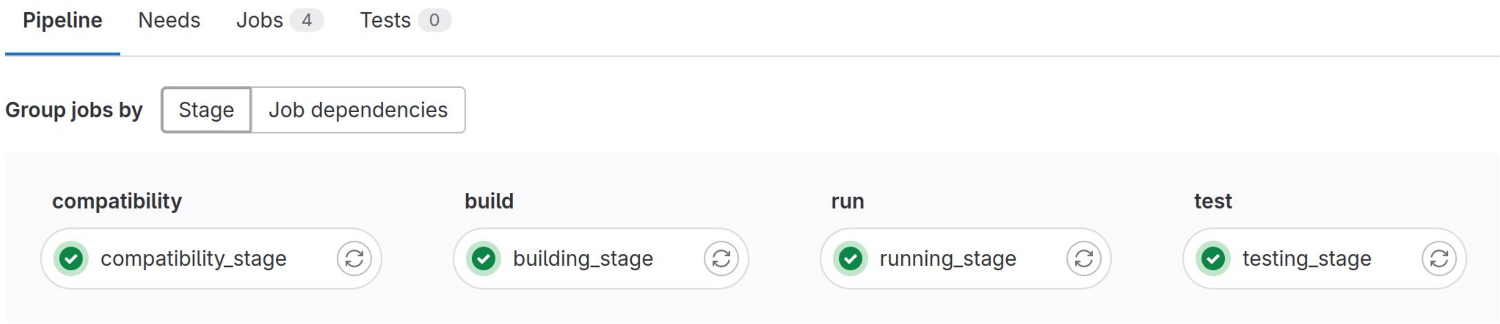
- Development of result parsing scripts

Back-up slides: continuous integration

```
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.

GitLab



Back up - 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_CLUSTER

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

Challenging case.

NP_TRAPPING

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

Computationally intensive.

Target of the first parallel implementation.

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