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Nano-particle Transition Matrix code G. La Mura, G. Mulas, M. A. Iatì, C. Cecchi-Pestellini, S. Rezaei, R. Saija

Spoke 3 II Technical Workshop, Bologna Dec 17 -19, 2024

ICSC Italian Research Center on High-Performance Computing, Big Data and Quantum Computing

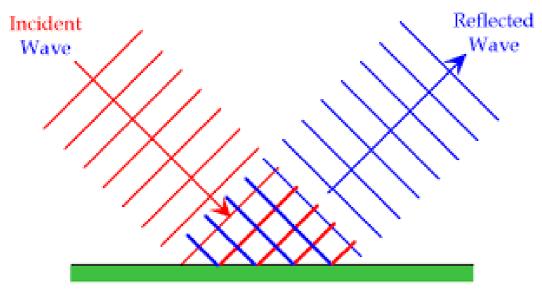


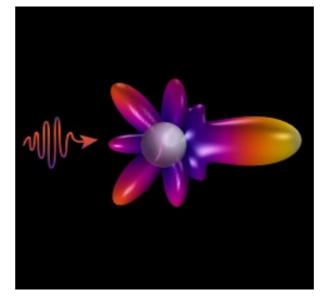






Scientific Rationale



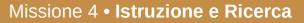




Radiation scattering on particles embedded in a transmissive medium has many applications:

- 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: $\begin{cases} \boldsymbol{E} = E_0 \boldsymbol{\hat{e}} \exp(i \boldsymbol{k} \cdot \boldsymbol{r}) \\ i \boldsymbol{B} = i n E_0 (\boldsymbol{\hat{k}} \times \boldsymbol{\hat{e}}) \exp(i \boldsymbol{k} \cdot \boldsymbol{r}) \end{cases}$ Multipolar exp.:

$$\begin{cases} i \mathbf{B} = i n E_0 \sum_{plm} J_{lm}^{(p)}(\mathbf{r}, k) W_{lm}^{(p')}(\mathbf{\hat{e}}, \mathbf{\hat{k}}) \end{cases}$$

 $(\boldsymbol{E} = \boldsymbol{E}_0 \sum \boldsymbol{J}_{lm}^{(p)}(\boldsymbol{r}, \boldsymbol{k}) W_{lm}^{(p)}(\boldsymbol{\hat{e}}, \boldsymbol{\hat{k}})$

Incident field

d:
$$\boldsymbol{E}_{I} = E_{0} \sum_{p lm} \boldsymbol{J}_{lm}^{(p)}(\boldsymbol{r}, \boldsymbol{k}) W_{lm}^{(p)}(\boldsymbol{\hat{e}}_{I}, \boldsymbol{\hat{k}}_{I})$$
 so

cattered field:

$$\boldsymbol{E}_{\boldsymbol{S}} = \boldsymbol{E}_{0} \sum_{plm} \boldsymbol{H}_{lm}^{(p)}(\boldsymbol{r}, \boldsymbol{k}) \boldsymbol{A}_{lm}^{(p)}(\boldsymbol{\hat{e}}_{I}, \boldsymbol{\hat{k}}_{I})$$

The *Transition Matrix* is the linear operator defined by: $E_{s} = S E_{I}$

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

 $A_{lm}^{(p)}(\boldsymbol{\hat{e}}_{I}, \boldsymbol{\hat{k}}_{I}) = \sum_{p'l'm'} S_{lml'm'}^{(pp')} W_{l'm'}^{(p')}(\boldsymbol{\hat{e}}_{I}, \boldsymbol{\hat{k}}_{I})$ **Dimensions:** $[2 N_p L_{max} (L_{max} + 2) \times 2 N_p L_{max} (L_{max} + 2)]$

Field expansion truncated at convenient order

L_{max} (see Wiscombe 1981, Appl. Opt., 19, 1505)

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









Status report

| Milestone | Objectives | Actions | Completion time | |
|------------|---|--|-----------------|--|
| Μ7 | Porting of original code to C++ Code profiling Bottle-neck identification | Program kernels ported Development cases profiled Heaviest step: inversion | February 2024 | |
| M8 | Parallelization of bottleneck First GPU offload (library driven) Profiling of advanced models | Implemented MAGMA Configured OpenMP & MPI Developed advanced models Attended CINECA HACKATHON | June 2024 | |
| M9 | Scalable implementation Hierarchical parallelism Preliminary science results | Attended ATPESC 2024 Added OpenMP offload Poster in EAS 2024 Invited talk in SPIG 2024 | October 2024 | |
| M10 | Configurable implementation Output optimization Advanced models | autoconf → proprietary config Binary I/O refactoring Inclusion kernel ported | exp. March 2025 | |
| CONCLUSION | • Technical paper / Science res. | Improved input & documents | exp. Dec. 2025 | |

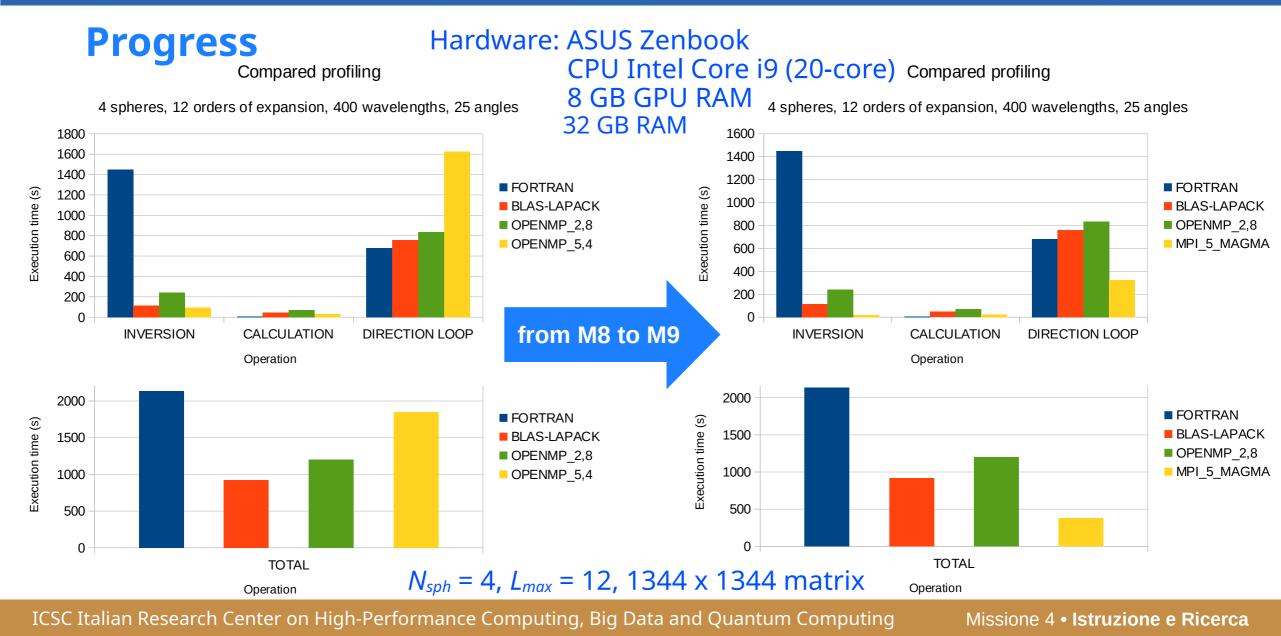
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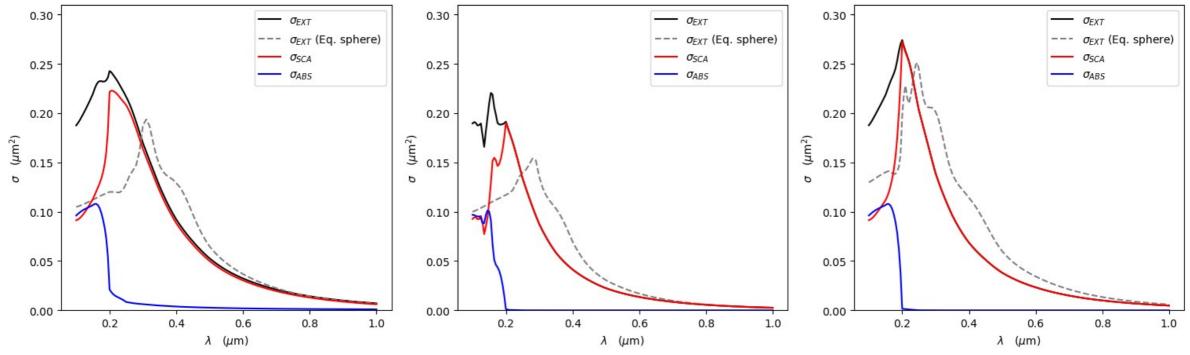






Main Results

- Parallelisation of main bottleneck through GPU offload (achieved in M8)
- Scalable wavelength MPI parallelisation / secondary bottleneck (achieved in M9)
- Preliminary results in EAS 2024 / SPIG 2024 (achieved throughout M8-M9)
- Participation to training programs (CINECA HACKATHON / ATPESC 2024, in M9)



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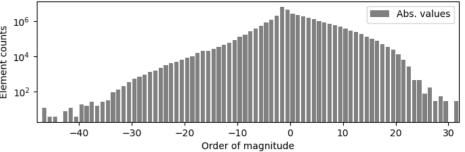


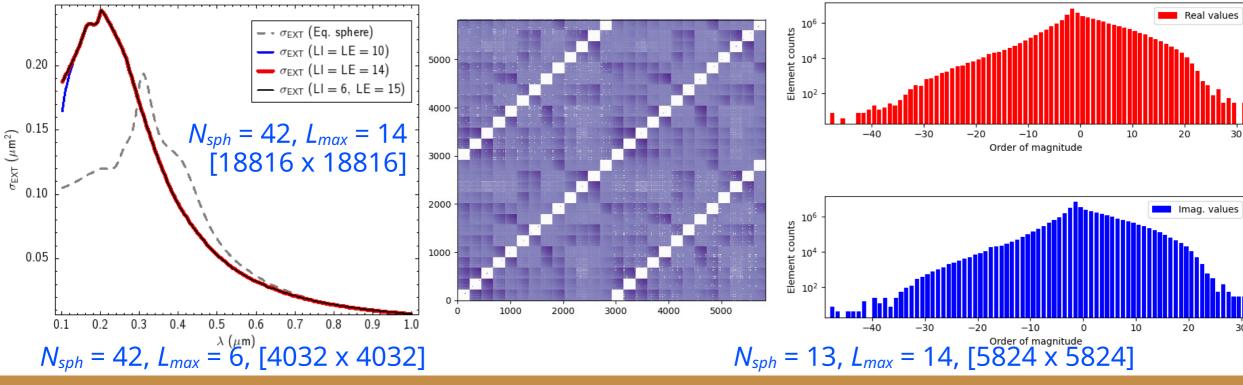


Final Steps

Investigation of numerical stability as function of dynamic range

- iterative refinement of matrix inversion / alternative inversion
- expansion order separation / numeric precision configuration















Final Steps

Current activities:

- Implementation of parallel solution of spherical particle with inclusions (expected by Feb. 25)
- Publication of preliminary scientific results for simple models (expected by Jun. 25)
- Improvement of hardware detection and system configuration (expected by Feb. 25)
- Formulation of output in machine format, with better human readable visualization (Jun. 25) Goals yet to be fulfilled:
- Improvement of model building / input definition
- Development of advanced particle models
- Publication of code technical description (Dec. 25)
 Achievable by December 2025? Yes

| NP_TMcode_release Public | | 🖈 Pin | O Unwatch 1 | N NP_TMcode | | | △ ~ ☆ Star 0 ♥ Fork 0 |
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| This is the Nano-particle Transition Matrix gitHub repository. The NP TMcode project is gitLab at the NP TMcode home page. | | ject is actually distrib | uted in | COPYING | Revert to GNU GPLv3 License | 5 months ago | + Configure Integrations |

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Concluding remarks

Numerical stability is an anticipated issue, yet never actually met by sequential code.

Enhancement opportunities:

- Explore alternatives to LU factorization matrix inversion
 - System solvers
 - Matrix pre-conditioning (Random Butterfly Transformation)
 - Configurable precision
 - Matrix decomposition according to element magnitude
- Interaction with library developers
 - Started discussion with MAGMA team
 - Investigate arbitrary precision solovers with GPU offload capabilities (GMP, XMP)

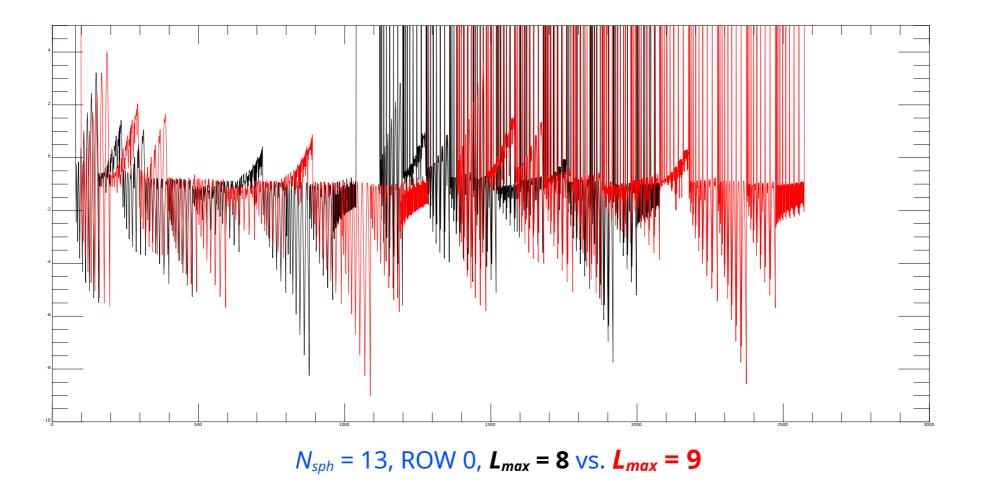








Back-up: distribution of expansion orders











Back-up: distribution of expansion orders

