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Centro Nazionale di Ricerca in HPC, Big Data and Quantum Computing

Nano-particle Transition Matrix code

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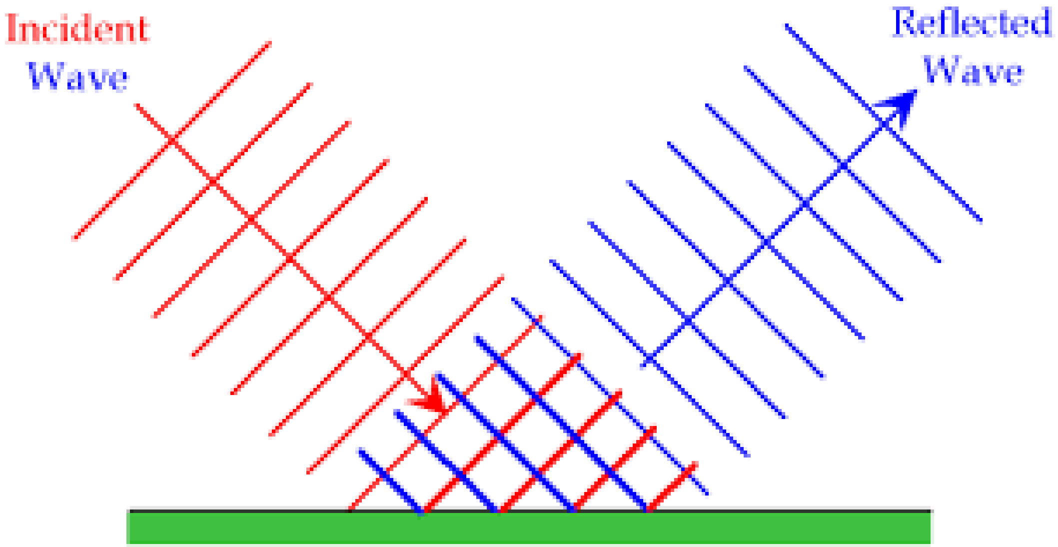
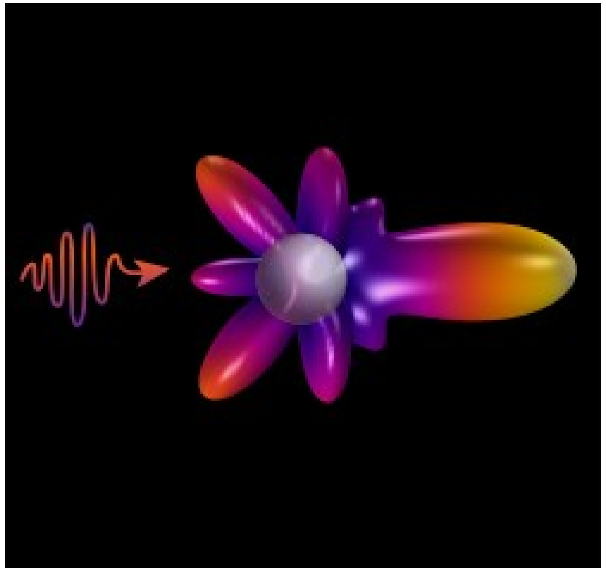
Spoke 3 II Technical Workshop, Bologna Dec 17 -19, 2024

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

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

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

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

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

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

Field expansion truncated at convenient order L_{max} (see Wiscombe 1981, Appl. Opt., 19, 1505)

Dimensions: [2 N_p L_{max} (L_{max} + 2) x 2 N_p L_{max} (L_{max} + 2)]

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

Status report

Milestone	Objectives	Actions	Completion time
M7	• 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

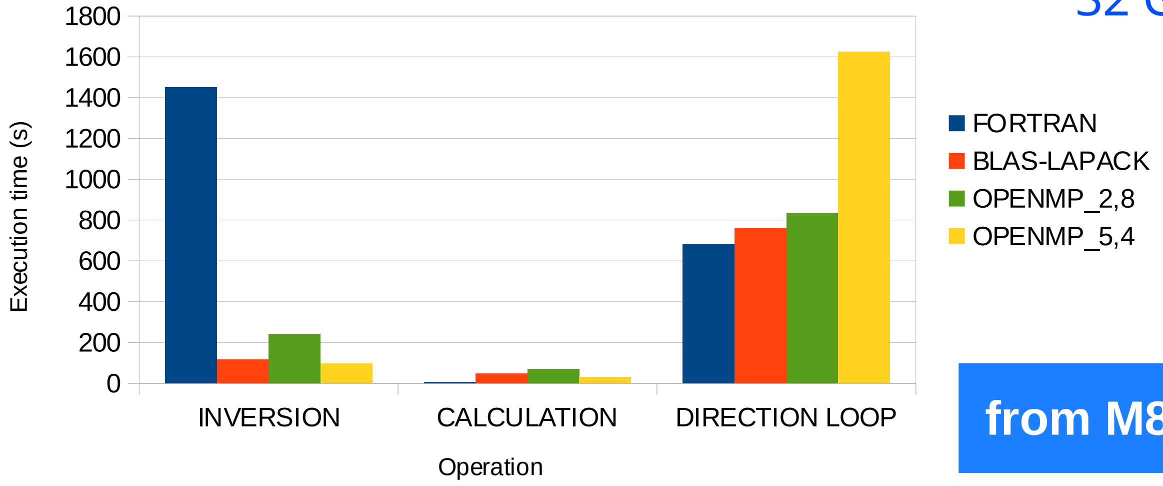
Progress

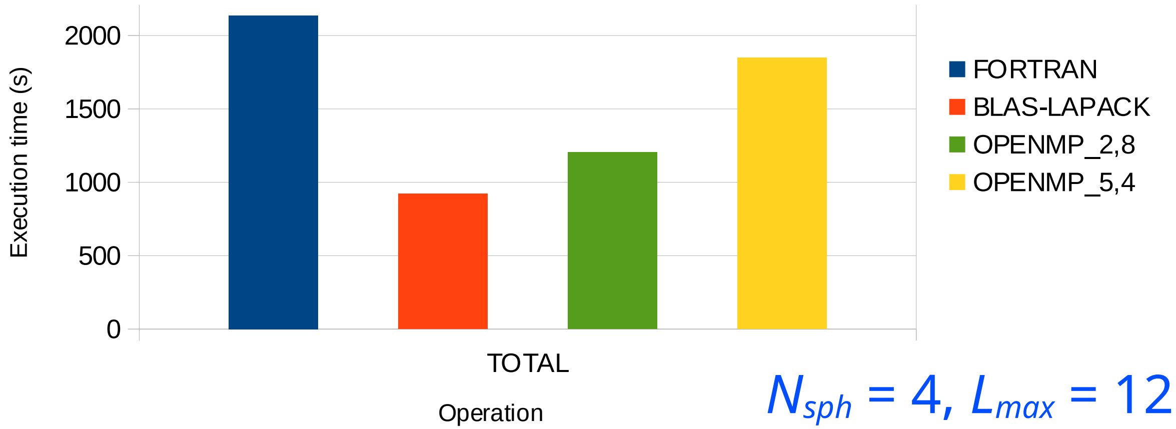
Hardware: ASUS Zenbook

CPU Intel Core i9 (20-core)
8 GB GPU RAM
32 GB RAM

Compared profiling

4 spheres, 12 orders of expansion, 400 wavelengths, 25 angles

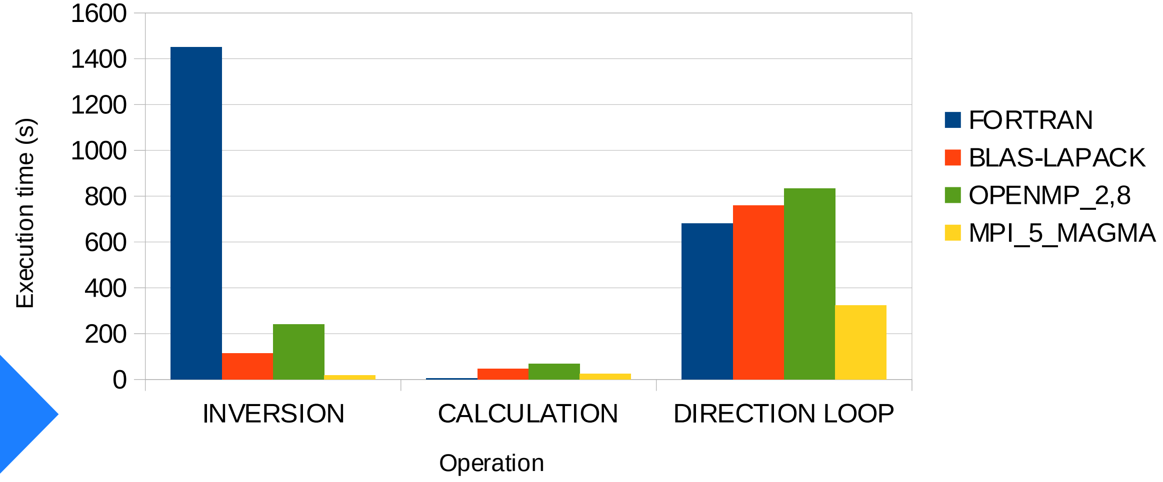


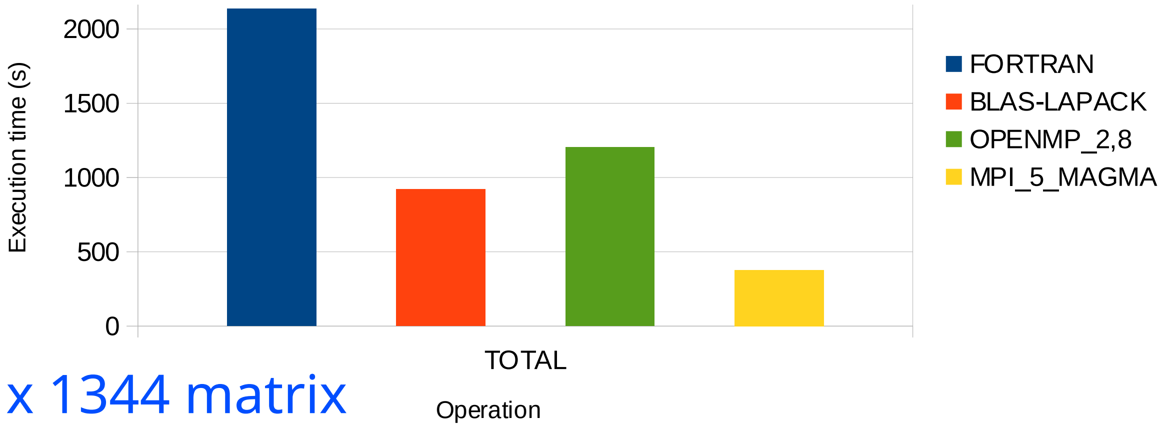


from M8 to M9

Compared profiling

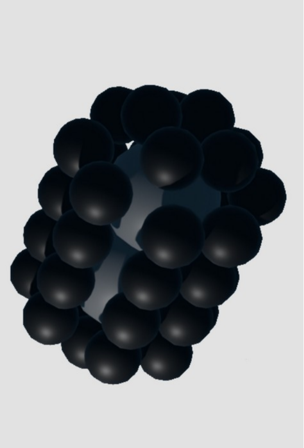
4 spheres, 12 orders of expansion, 400 wavelengths, 25 angles



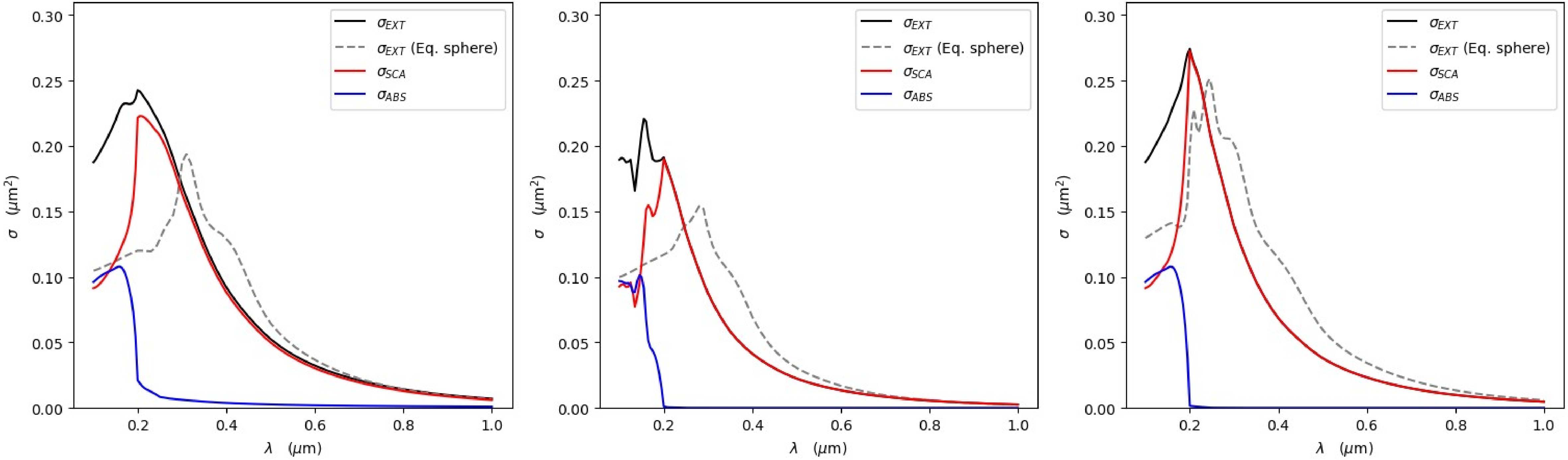


$N_{sph} = 4$, $L_{max} = 12$, 1344 x 1344 matrix

Main Results



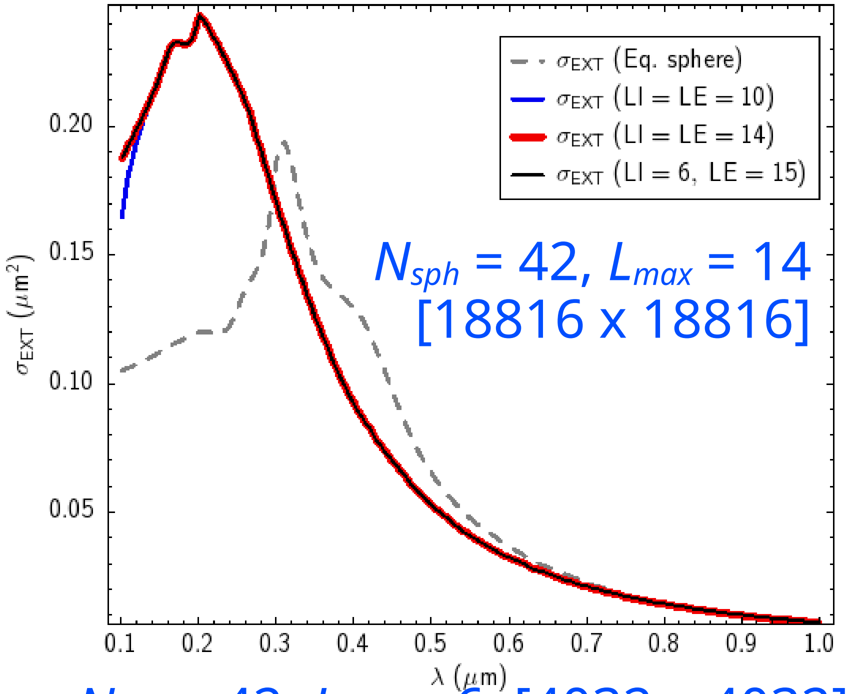
- Parallelisation of main bottleneck through GPU offload (achieved in M8)
- Scalable wavelength MPI parallelisation / secondary bottleneck (achieved in M9)
- Preliminary results in EAS 2024 / SPIG 2024 (achieved throughout M8-M9)
- Participation to training programs (CINECA HACKATHON / ATPESC 2024, in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



Final Steps

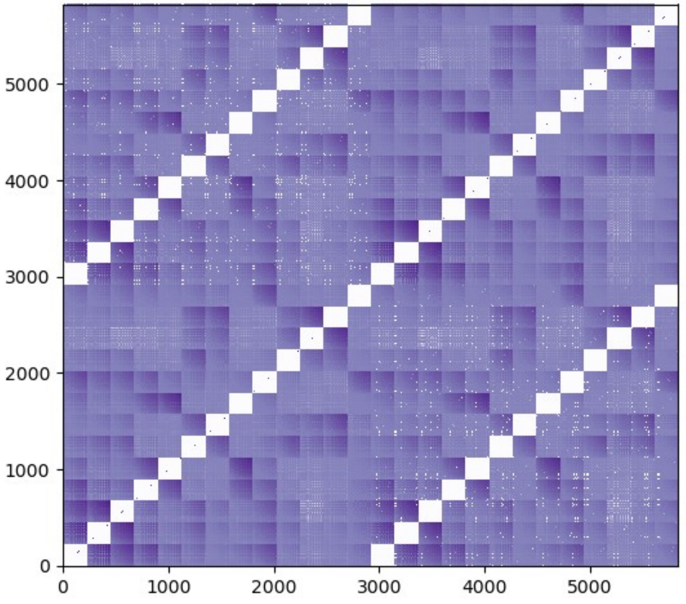
Investigation of numerical stability as function of dynamic range

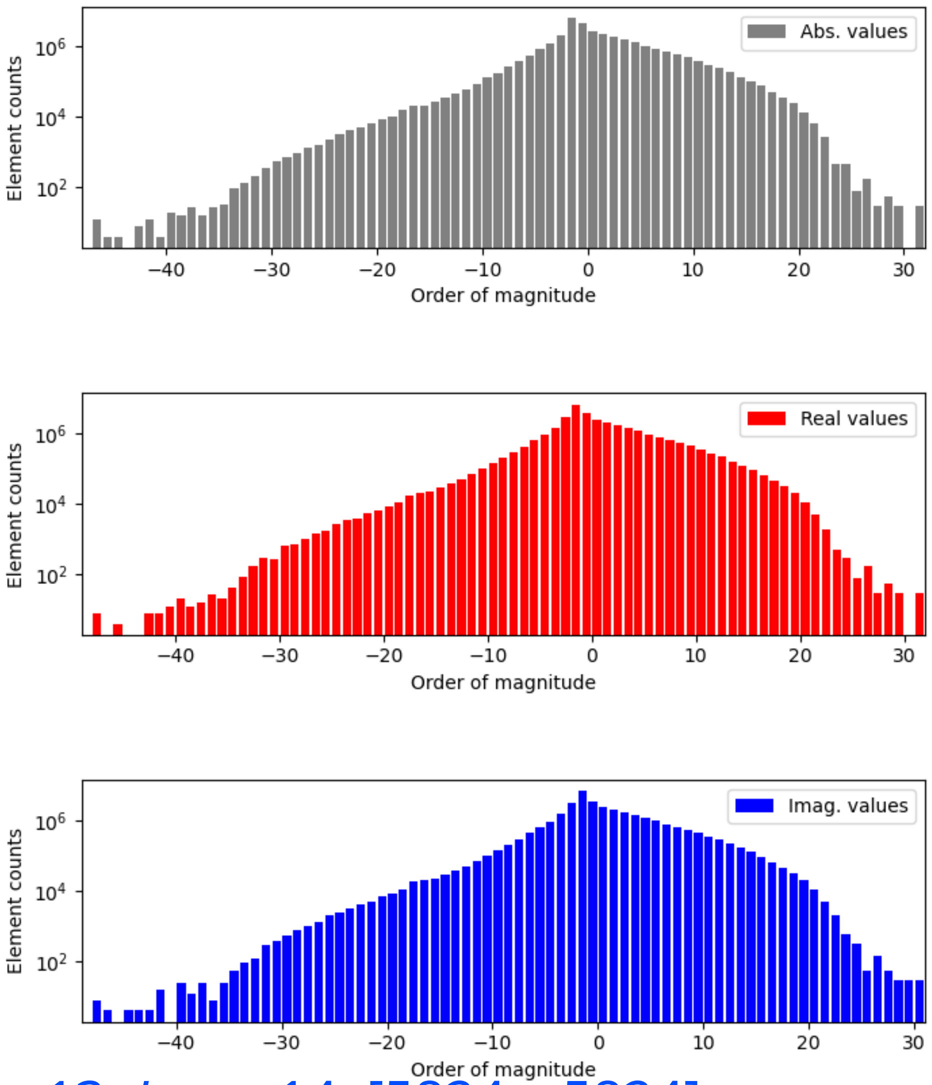
- iterative refinement of matrix inversion / alternative inversion
- expansion order separation / numeric precision configuration



N_{sph} = 42, L_{max} = 14 [18816 x 18816]

N_{sph} = 42, L_{max} = 6, [4032 x 4032]





N_{sph} = 13, L_{max} = 14, [5824 x 5824]

Final Steps

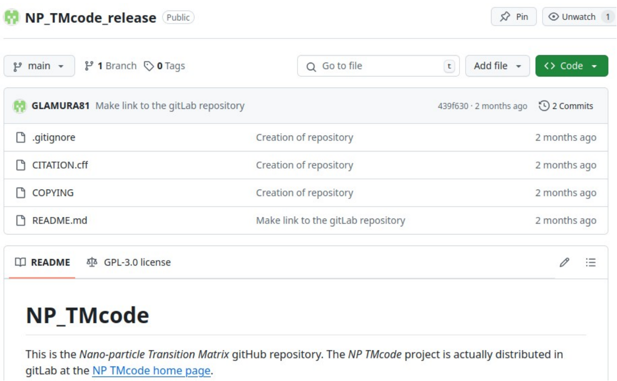
Current activities:

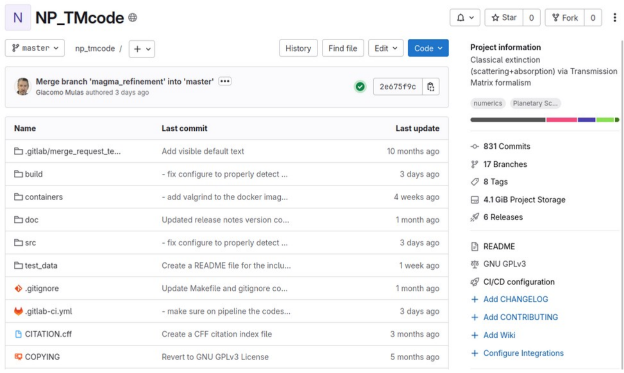
- Implementation of parallel solution of spherical particle with inclusions (expected by Feb. 25)
- Publication of preliminary scientific results for simple models (expected by Jun. 25)
- Improvement of hardware detection and system configuration (expected by Feb. 25)
- Formulation of output in machine 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**





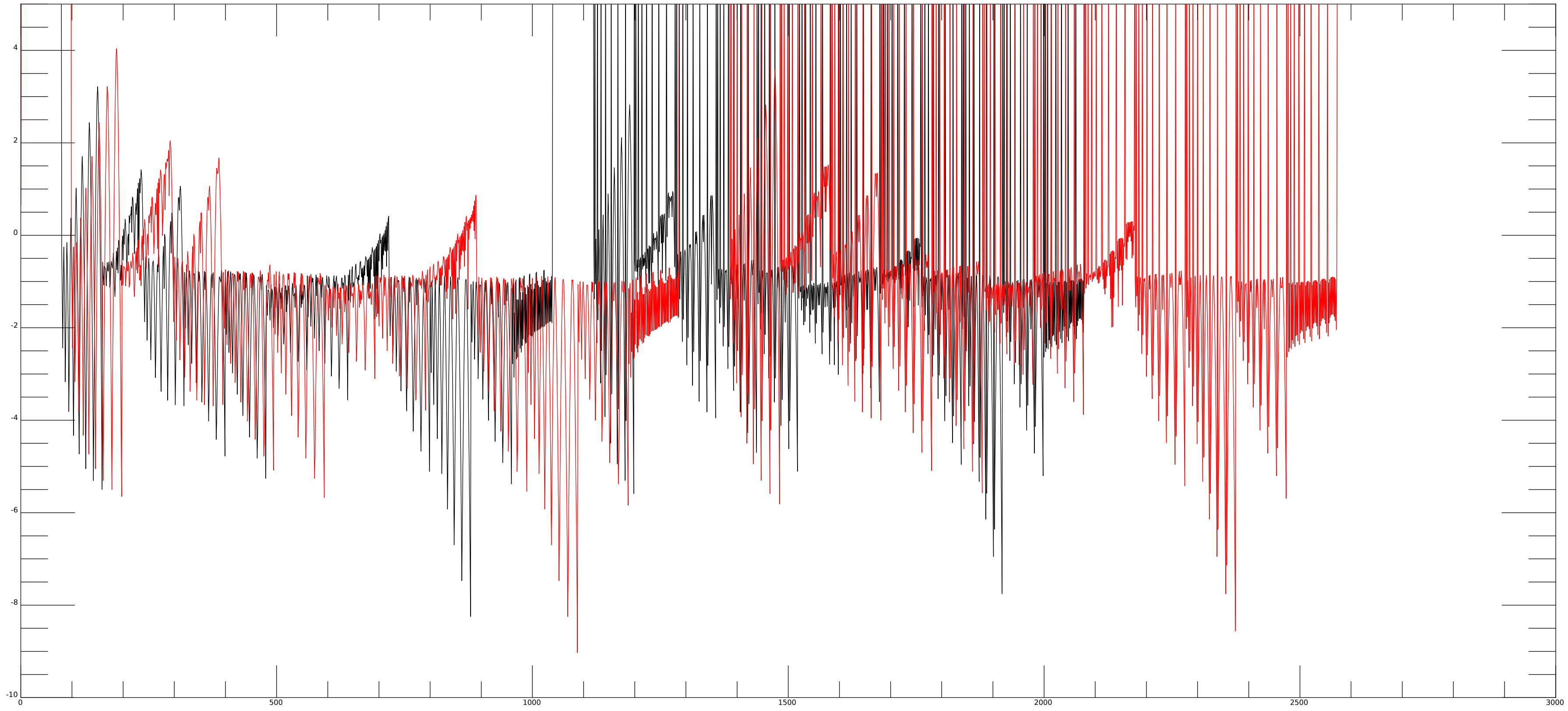
Concluding remarks

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

Enhancement opportunities:

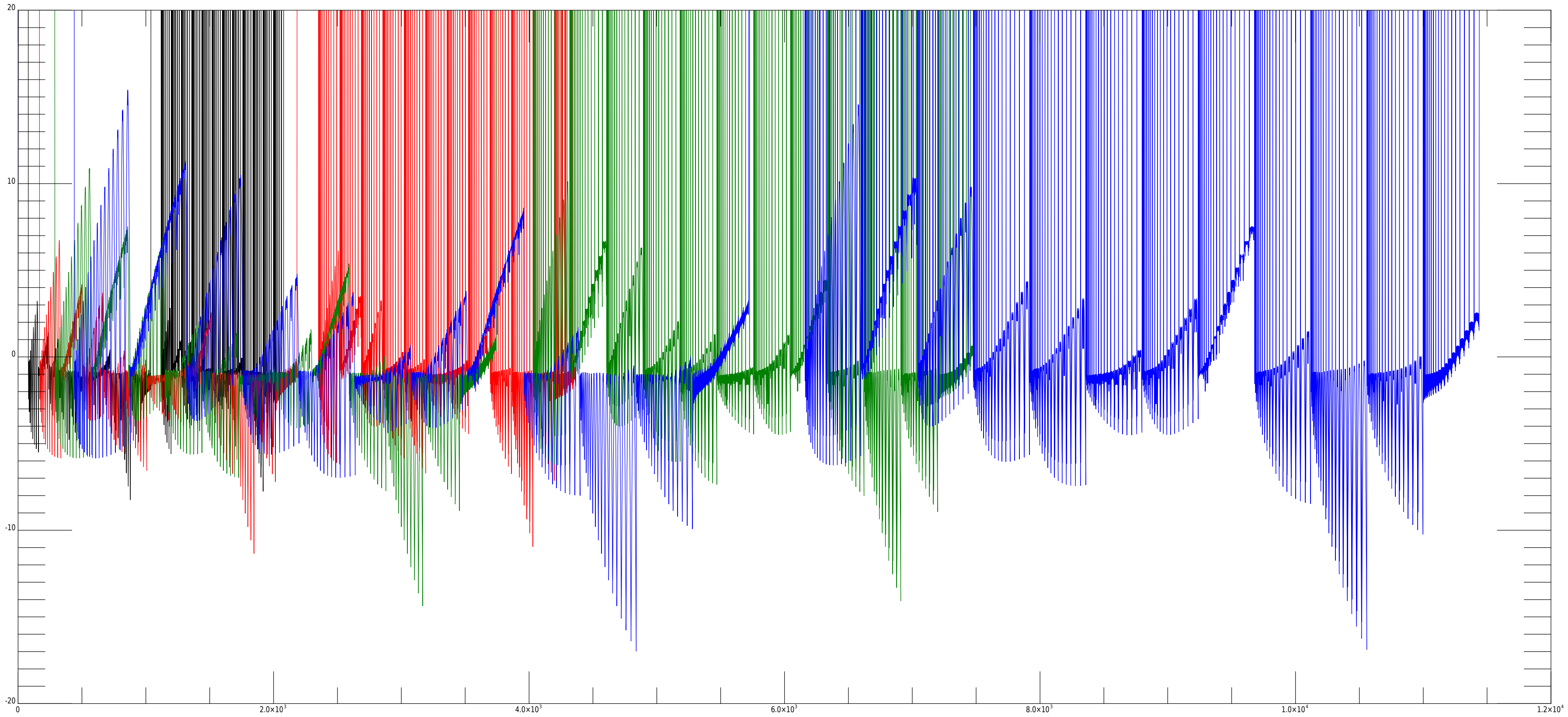
- Explore alternatives to LU factorization matrix inversion
  - System solvers
  - Matrix pre-conditioning (Random Butterfly Transformation)
  - Configurable precision
  - Matrix decomposition according to element magnitude
- Interaction with library developers
  - Started discussion with MAGMA team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

Back-up: distribution of expansion orders



N_{sph} = 13, ROW 0, $\boldsymbol{L_{max}}$ **= 8** vs. $\boldsymbol{L_{max}}$ **= 9**

Back-up: distribution of expansion orders



N_{sph} = 13, ROW 0, L_{max} = 8, L_{max} = 12, L_{max} = 16, L_{max} = 20