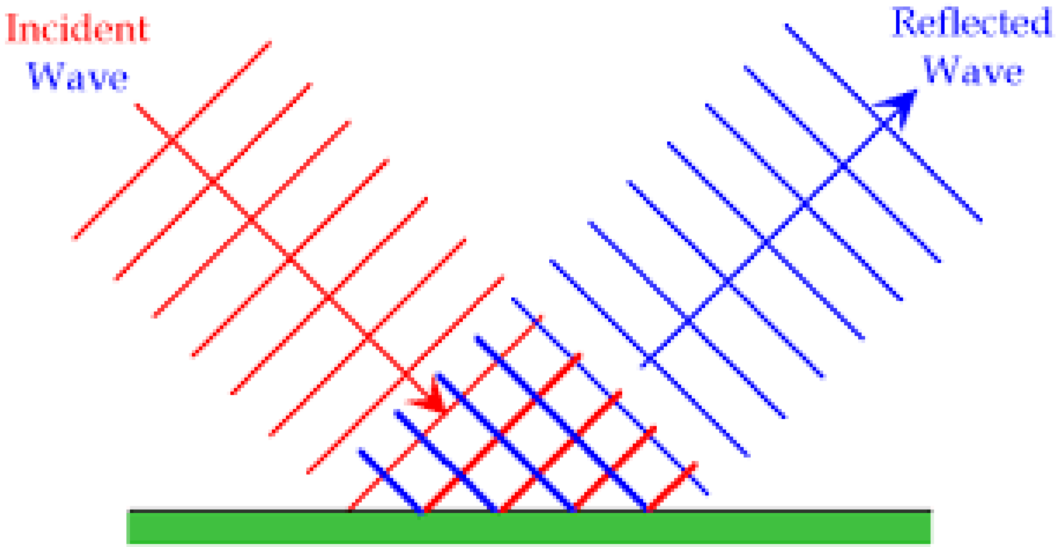
Finanziato dall'Unione europea NextGenerationEU | Ministero dell'Università e della Ricerca | Italiadomani PIANO NAZIONALE DI RIPRESA E RESILIENZA | ICSC Centro Nazionale di Ricerca in HPC, Big Data and Quantum Computing

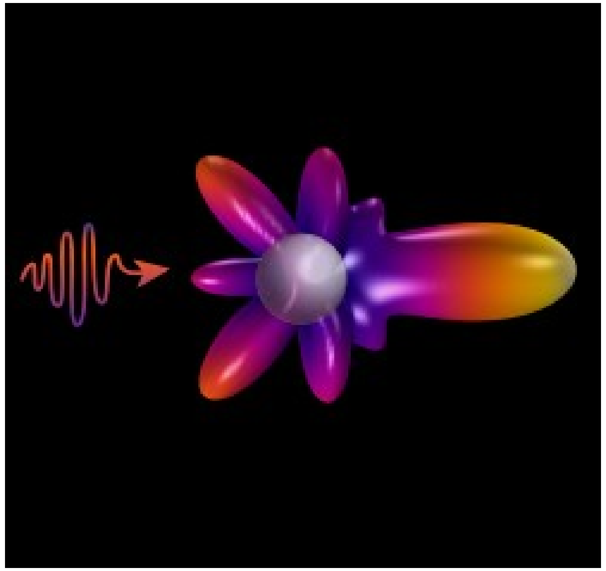
Nano-Particle Transition Matrix code

G. La Mura, G. Mulas, M. A. Iatì, C. Cecchi Pestellini,
G. Aresu, S. Rezaei, R. Saija

Spoke 3 III Technical Workshop, Perugia 26-29 Maggio, 2025

Scientific Rationale





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

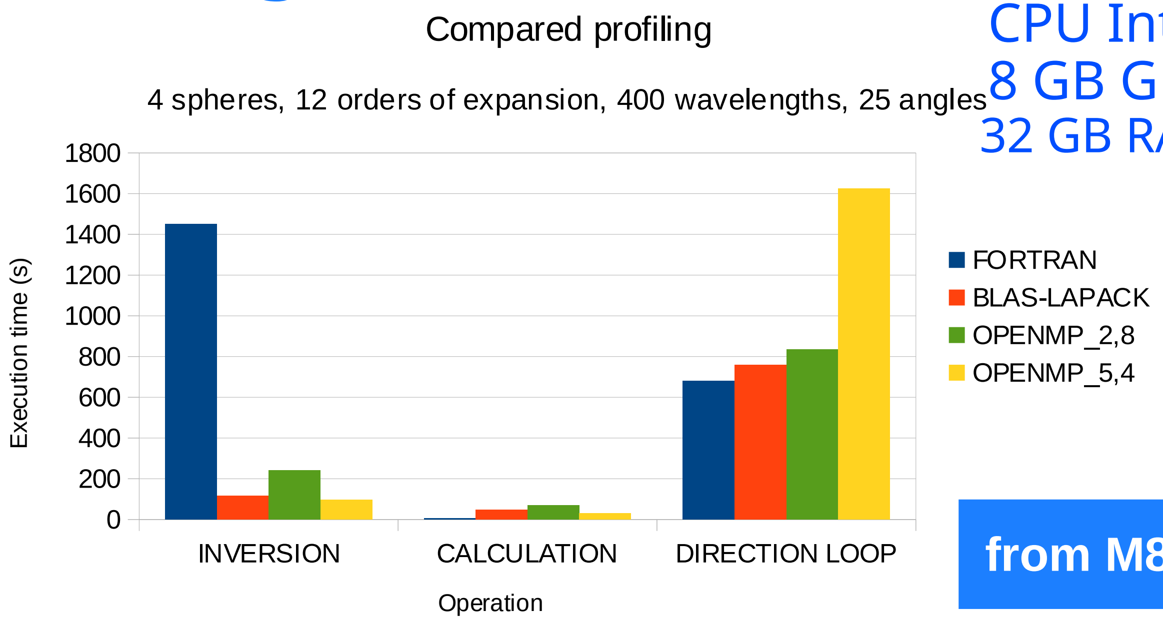
- physics of aerosols (atmospheric physics)
- material investigation
- radiation transfer
- interstellar medium and extinction

Exact solution possible only in simple cases.
For realistic cases, numerical approaches are needed → T-matrix

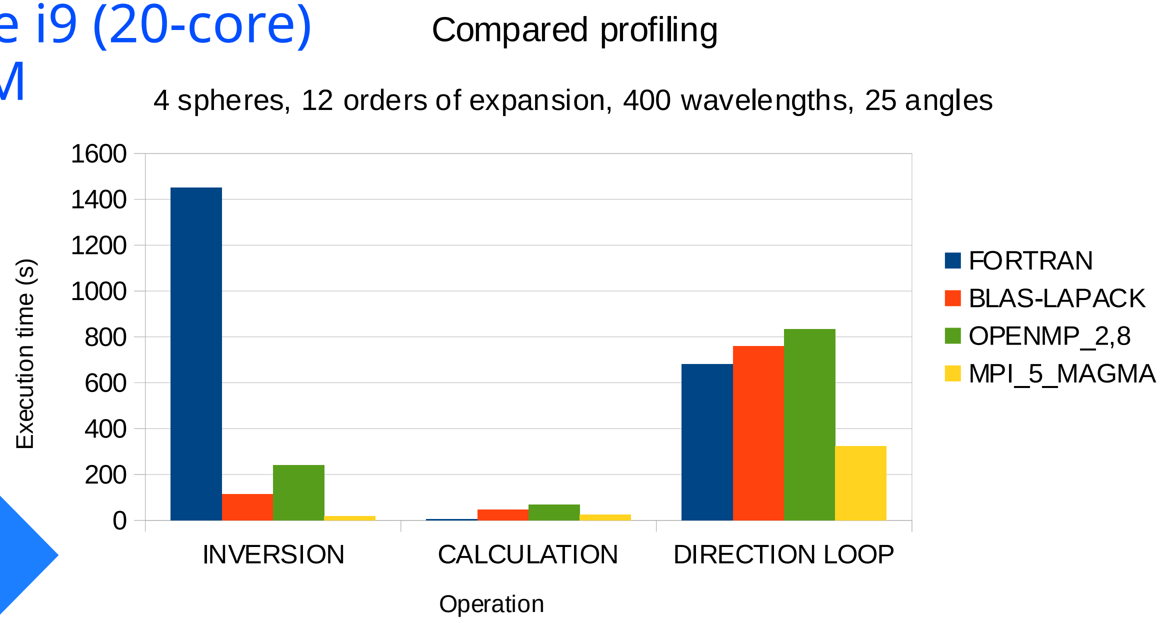
Finanziato dall'Unione europea NextGenerationEU
Ministero dell'Università e della Ricerca
Italiadomani PIANO NAZIONALE DI RIPRESA E RESILIENZA
ICSC Centro Nazionale di Ricerca in HPC, Big Data and Quantum Computing

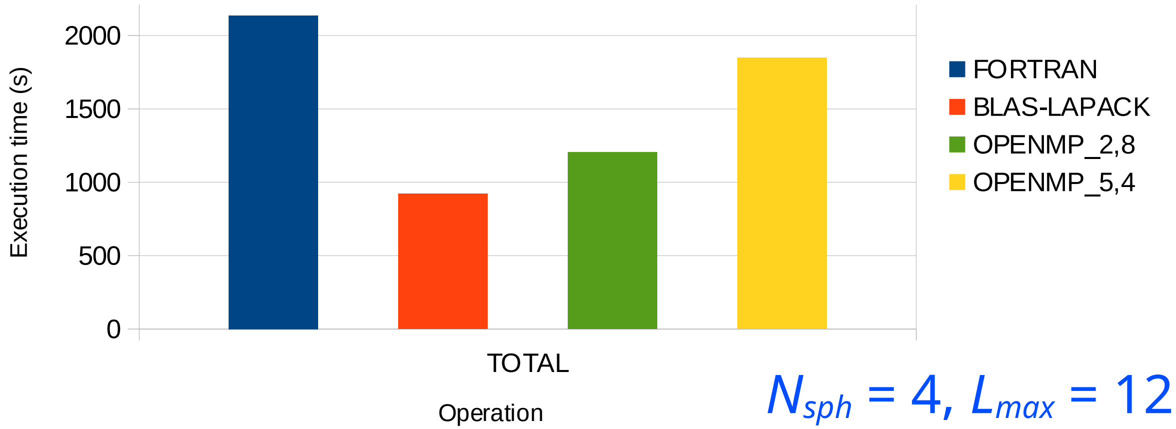
Progress (1 of 2)

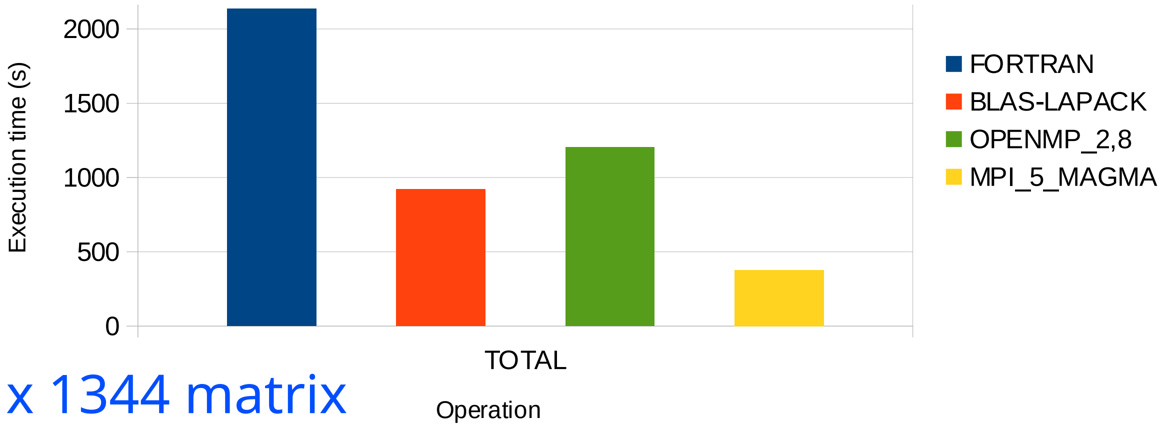
Hardware: ASUS Zenbook
CPU Intel Core i9 (20-core)
8 GB GPU RAM
32 GB RAM



from M8 to M9





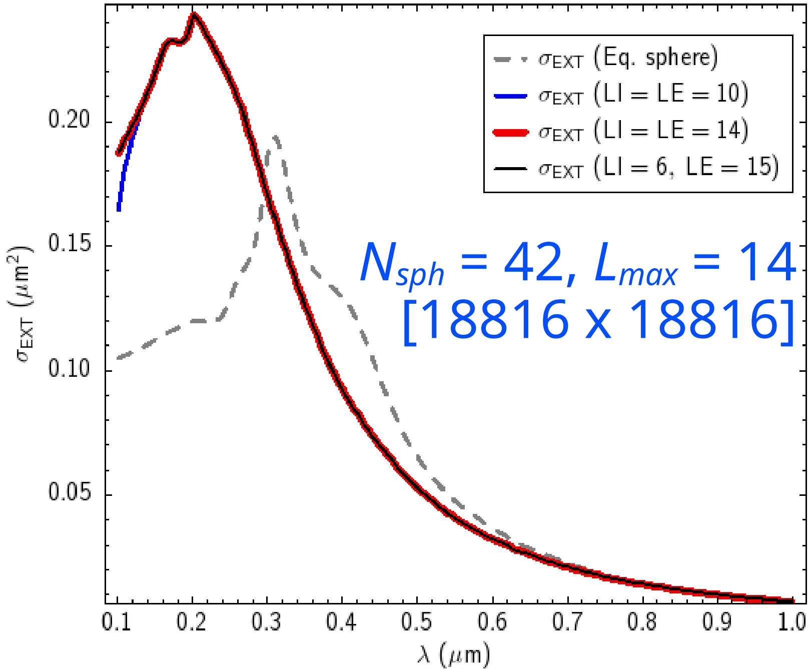


N_{sph} = 4, L_{max} = 12, 1344 x 1344 matrix

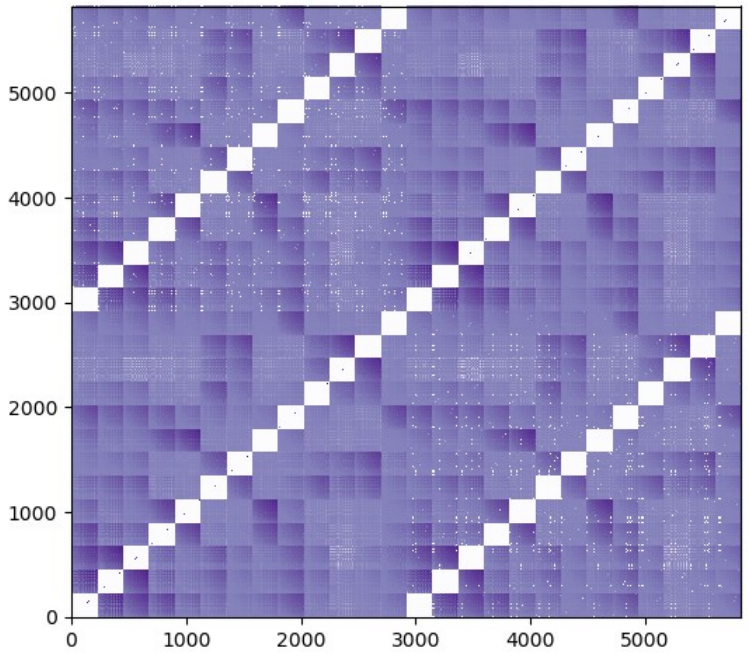
Technical Objectives, Methodologies and Solutions

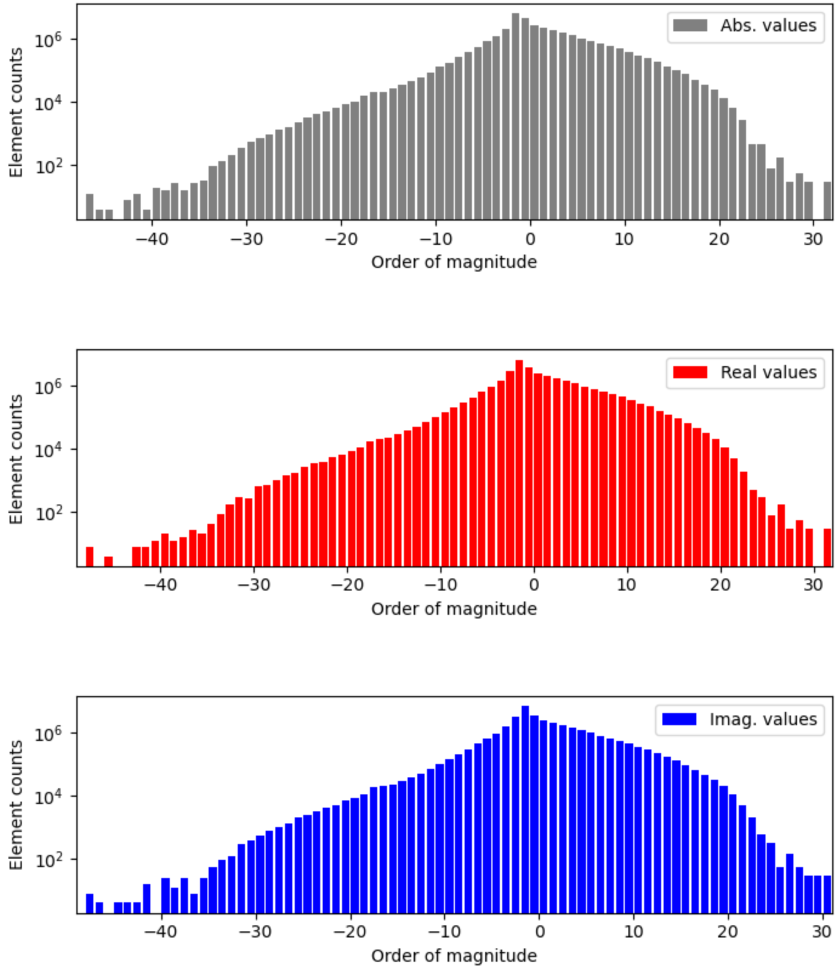
Make complex models accessible to scalable hardware:

- port linear algebra operation to optimized libraries & GPUs
- use MPI / OpenMP to parallelize independent scales



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





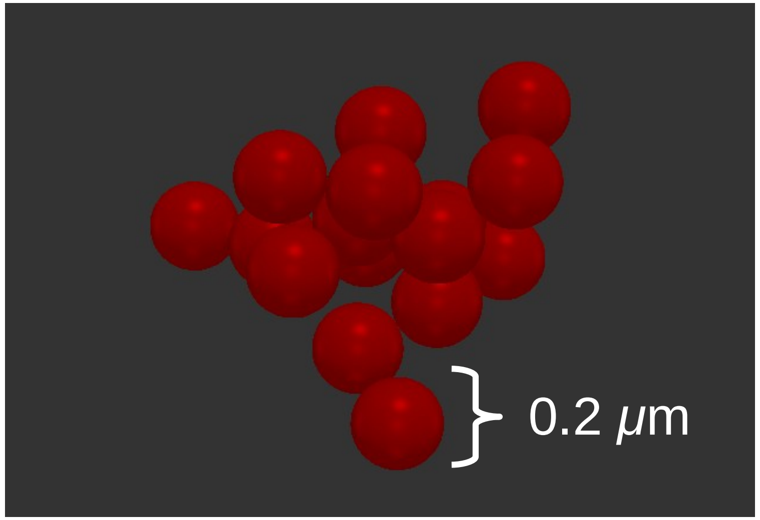
N_{sph} = 42, L_{max} = 6, [4032 x 4032]

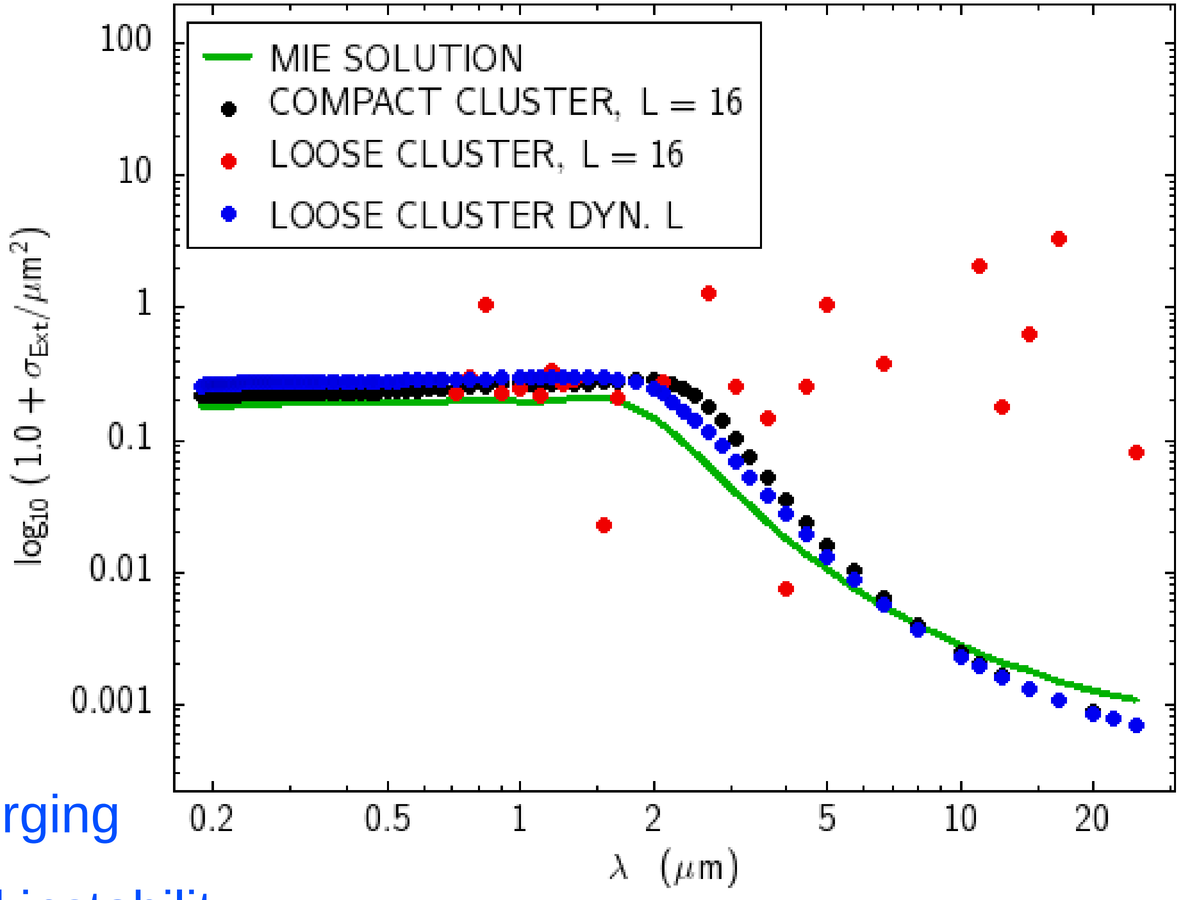
N_{sph} = 13, L_{max} = 14, [5824 x 5824]

Technical Objectives, Methodologies and Solutions

Increase the range of accessible parameter space:

- auto-detect / adjust calculation order
- iterative matrix inversion refinement
- new model definition in YAML format
- implementation of full scalability



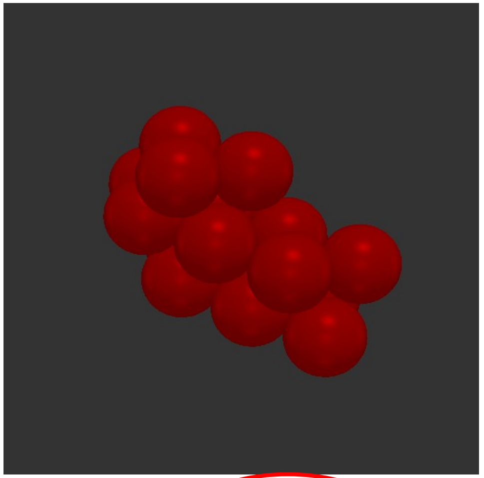


Dynamic L → OK

Small L → not converging

Large L → numerical instability

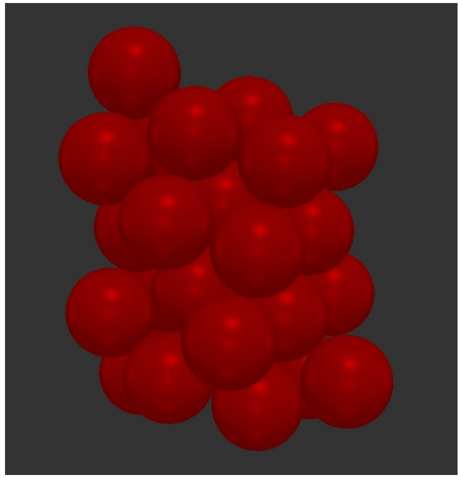
Main Results



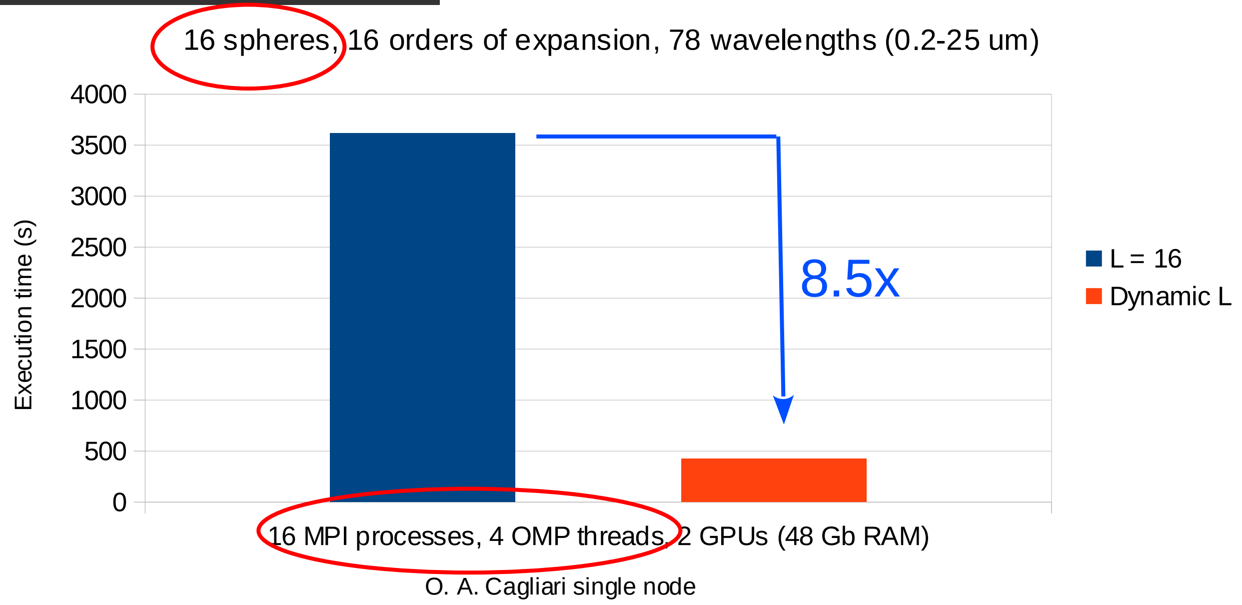
Dynamic order configuration led to further 8x speed up.

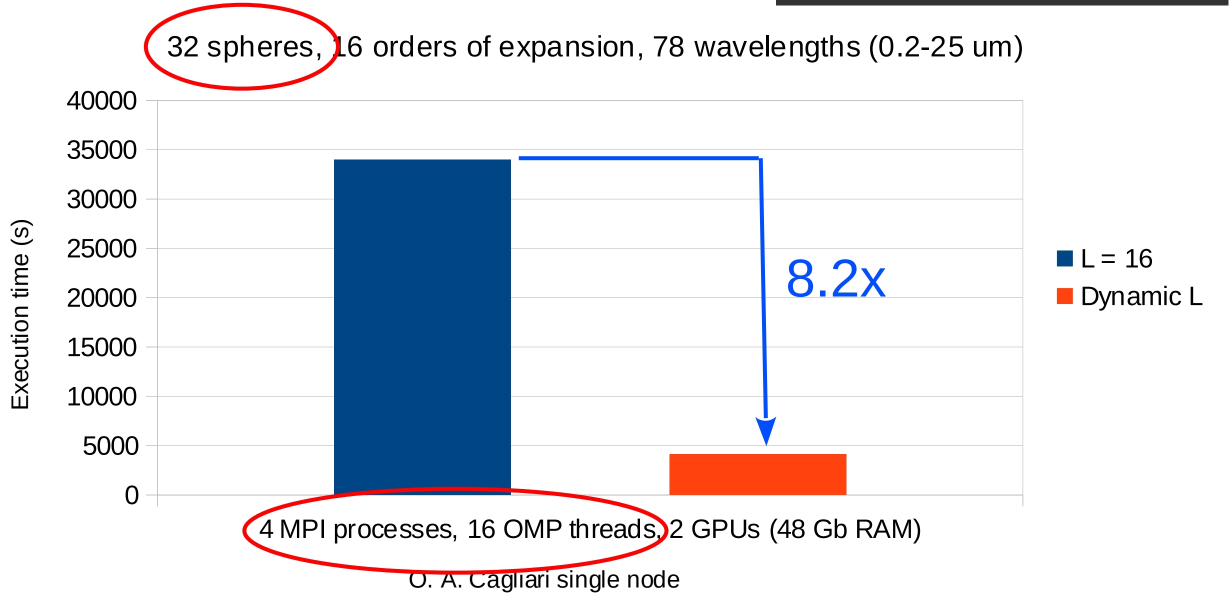
- Improvement not strongly dependent on matrix size
- Largely affected by wavelength range
- Tested with best configuration for different particles

2.5 um radius particle



3.0 um radius particle

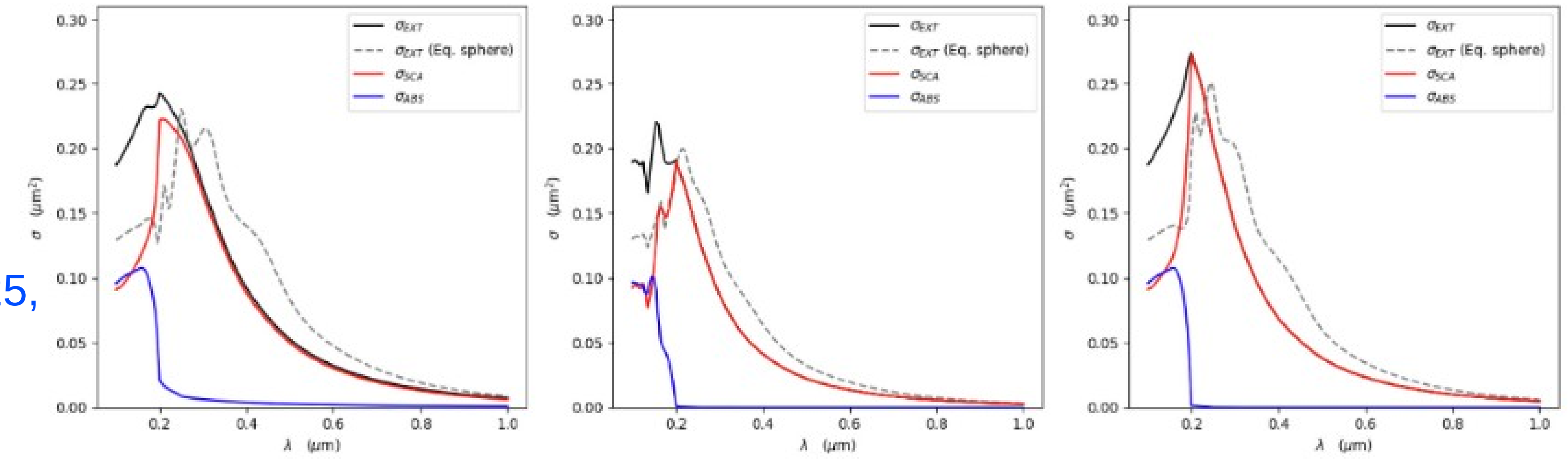




Main Results

Publication I (KPI):

Interstellar dust as a dynamic environment (Adv. in Sp. Res., 2025, DOI:10.1016/j.asr.2025.05.002)



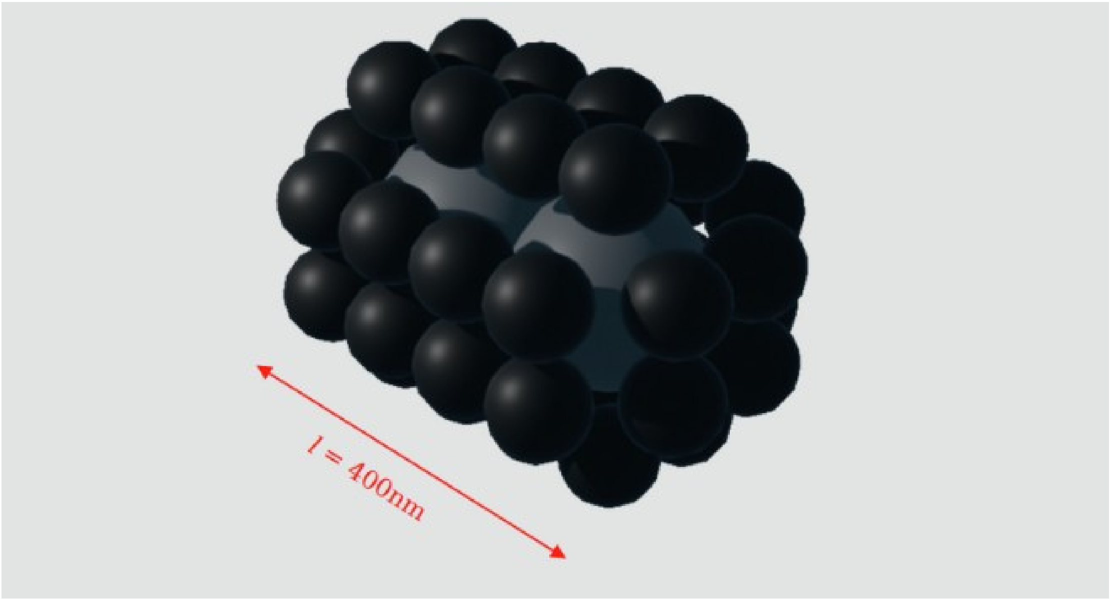
Available online at www.sciencedirect.com
ScienceDirect
Advances in Space Research xxx (xxxx) xxx
ADVANCES IN SPACE RESEARCH (a COSPAR publication)
www.elsevier.com/locate/asr

Interstellar dust as a dynamic environment ☆

Giovanni La Mura [a,*], Giacomo Mulas [a], Maria Antonia Iatì [b], Cesare Cecchi-Pestellini [c], Shadi Rezaei [d,b,e], Rosalba Saija [d,b]

[a] INAF - Osservatorio Astronomico di Cagliari, Via della Scienza 5, Selargius 09047, Italy
[b] CNR - Istituto per i Processi Chimico-Fisici, Viale F. Stagno d'Alcontres 37, Messina 98158, Italy
[c] INAF - Osservatorio Astronomico di Palermo, Piazza del Parlamento 1, Palermo 90134, Italy
[d] Università di Messina - Dip. di Scienze Matematiche e Informatiche, Scienze Fisiche e Scienze della Terra, Viale F. Stagno D'Alcontres 31, Messina 98166, Italy
[e] University of Kurdistan, Dept. of Physics, Faculty of Science, Pasdaran Street, Sanandaj416l6613566176, Iran

Received 14 January 2025; received in revised form 28 April 2025; accepted 1 May 2025



Progress (2 of 2)

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
M10a	• Configurable implementation • Output optimization • Advanced models	• autoconf → proprietary config • Binary I/O refactoring • Inclusion kernel ported	April 2025
M10b (end)	• Technical paper / Science res.	• Improved input & documents	exp. Dec. 2025

Final Steps

Current activities:

- Calculation of models for exo-planetary atmospheres
- Profiling & parallelization of TRAPPING code
- Production of code description technical paper
- Documentation and interface development

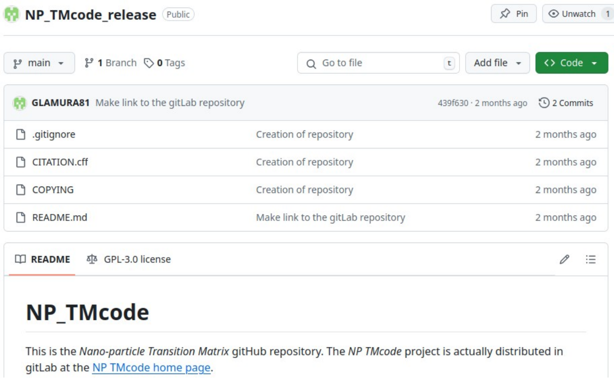
Project status and goals:

- Overall progress ~80% completed
- Development of advanced particle models
- Publication of code technical description (Dec. 25)

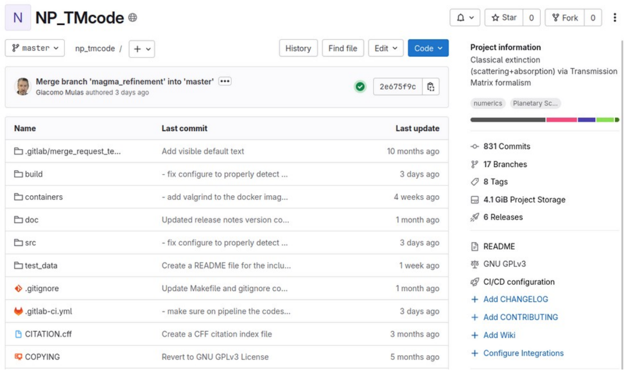
Achievable by December 2025? **Yes**

Activity	Relevant milestone	Official release	Release date	Activity progress
Code porting	M7	NP_TMcode-M7.00	January 19, 2024	100%
Sequential code profiling	M7	NP_TMcode-M7.00	January 19, 2024	100%
Parallel implementation	M8	NP_TMcode-M8.03	June 27, 2024	80%
Scalable parallelism	M9	NP_TMcode-M9.01	October 25, 2024	90%
Parallel profiling	M10a	NP_TMcode-M10a.03	April 7, 2025	80%
Documentation	M10b	TBD	exp. December 31, 2025	60%
Scientific application	M10b	TBD	exp. December 31, 2025	50%
Overall progress:			**exp. December 31, 2025**	80%

GitHub repository



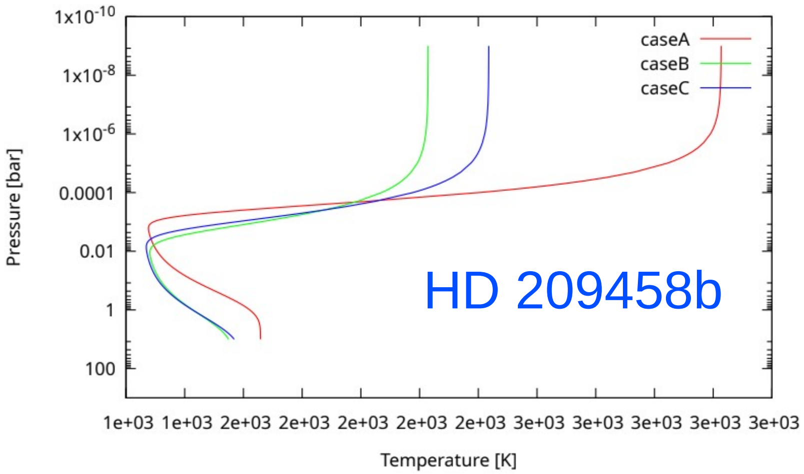
GitLab homepage

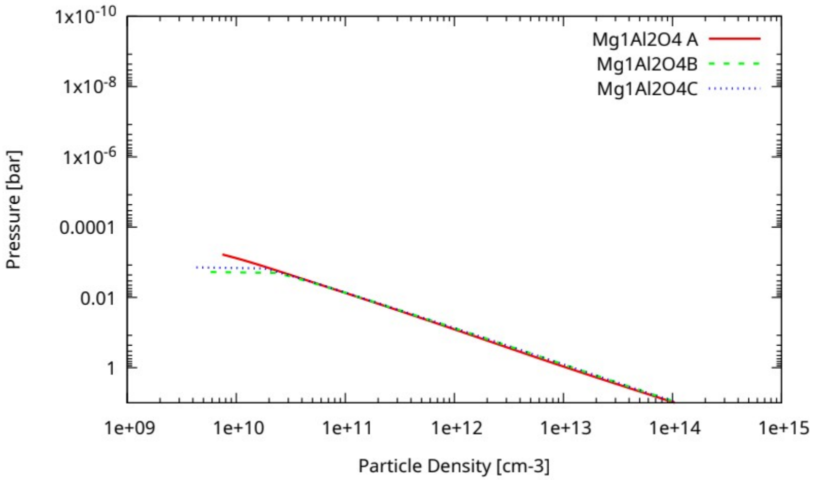


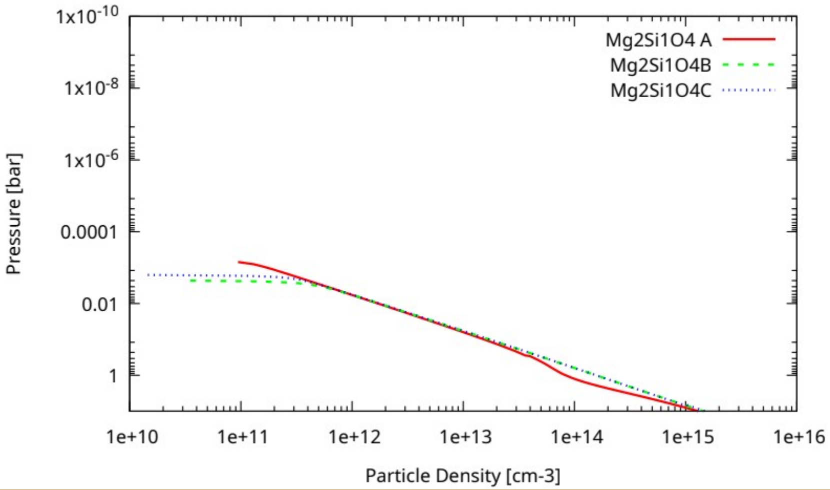
Final Steps

Exo-planetary atmospheres important for:

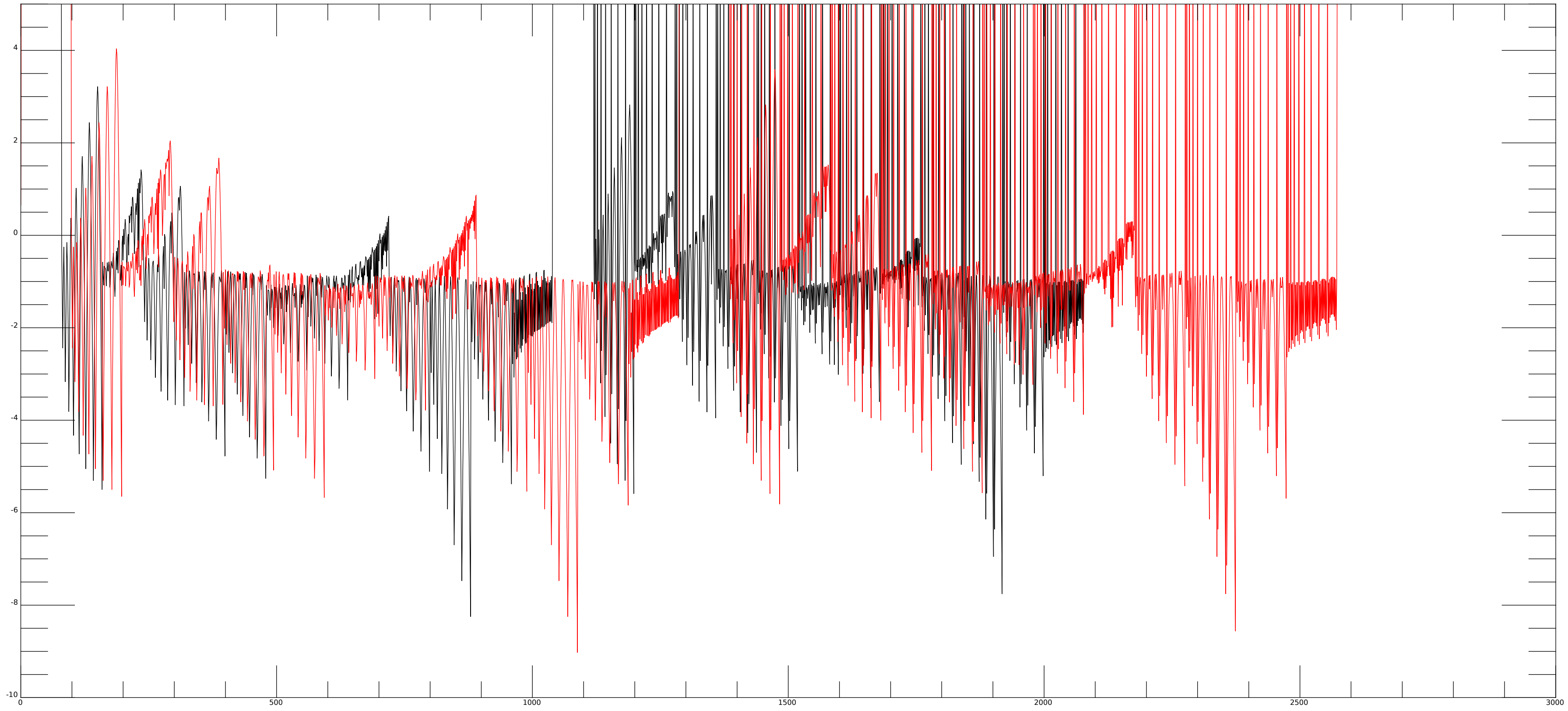
- Upcoming detailed datasets from major astronomical facilities (JWST, SKA, E-ELT)
- Lack of quantitative constraints from current models
- Large particle sizes (benchmark for code possibilities)
- Stability of involved chemical compounds





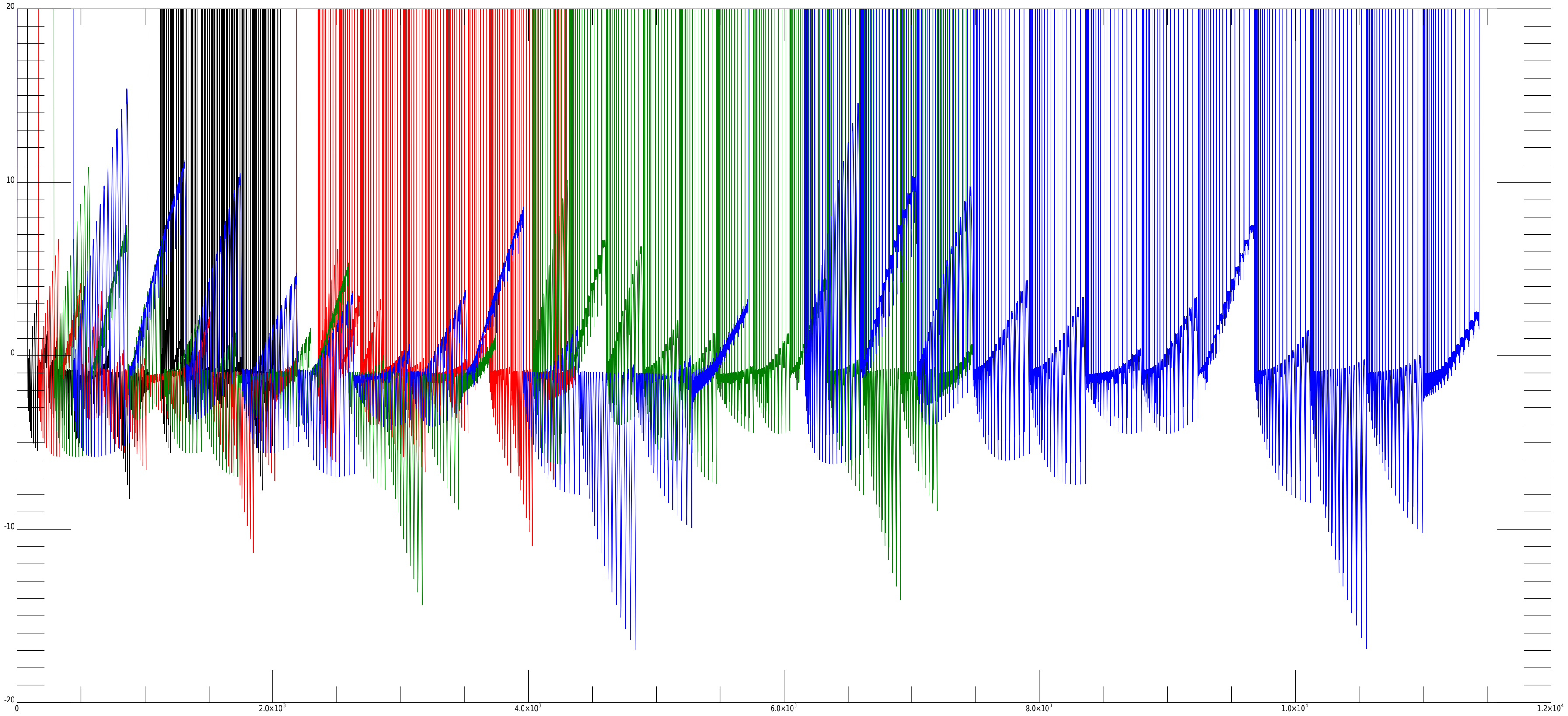


Back-up: distribution of expansion orders



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

Back-up: T-Matrix definition

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)