Platform for Advanced Scientific Computing

Accelerated Radiative Transfer Simulations for the Square Kilometre Array Observatory

PASC Program 2025–2028

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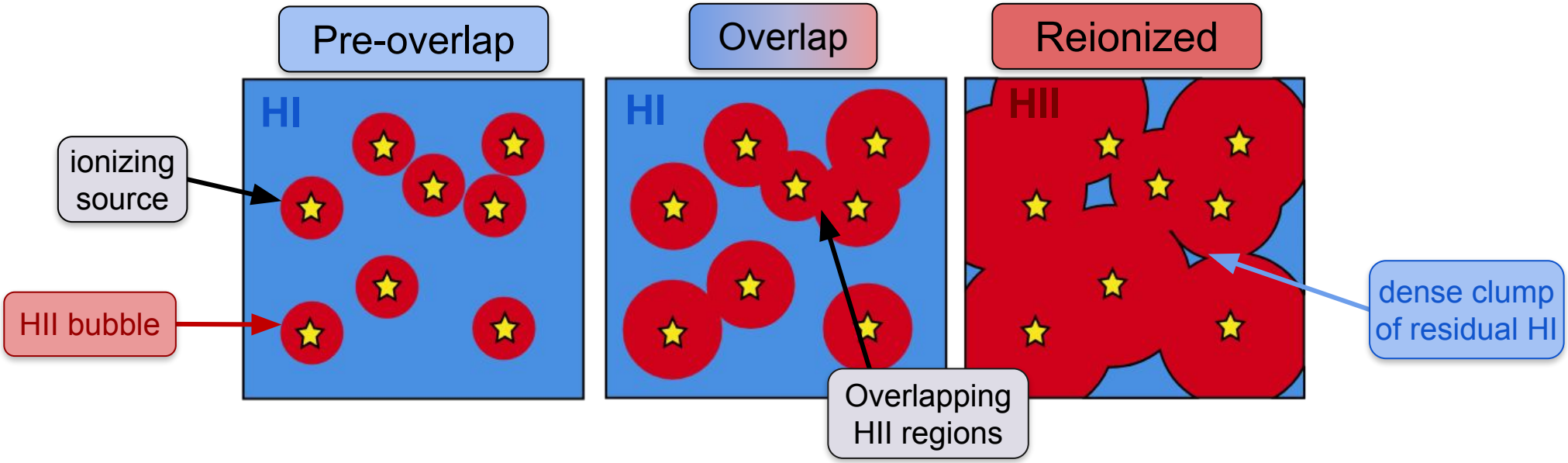
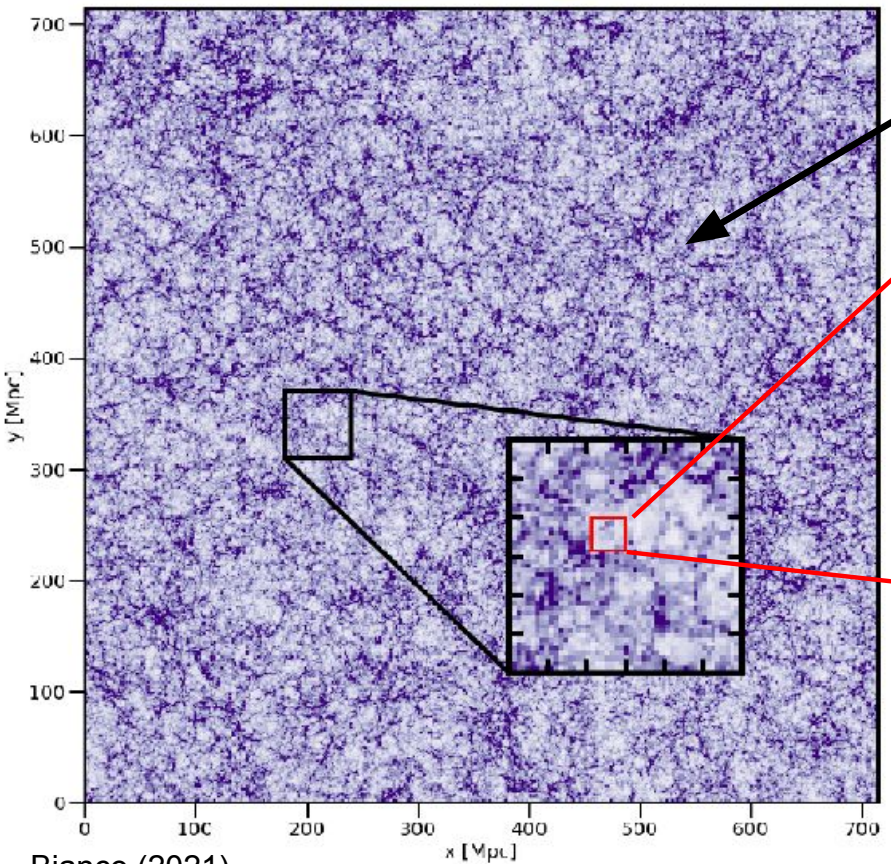
The Epoch of Reionization (EoR)



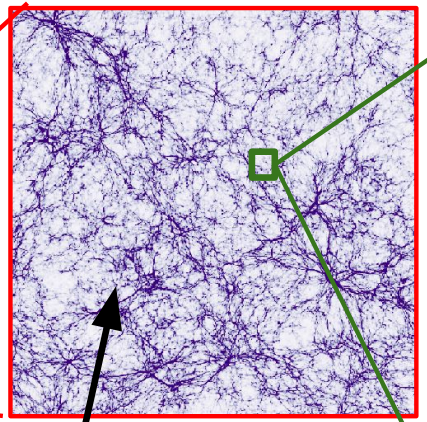
- Appearance of the **first luminous sources** (UV and X-Ray radiation).
- Sources start to **ionize and heat** the Intergalactic Medium (IGM):
  - Formation of ionized regions (HII bubble) around collapse structures.
- Universe transition from a **neutral/cold** state to a **hot/ionized**:
  - Pre-overlap (neutral)→Overlap (partially ionized)→Reionized

An inherently multi-scale problem...



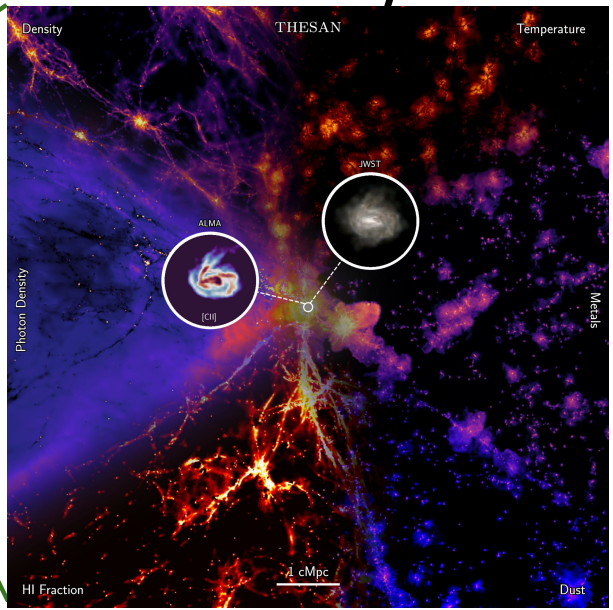
Bianco (2021)

Large-scale simulation
~700 Mpc



Intermediate scale
~ 100 Mpc

Galactic scale
< 1 Mpc

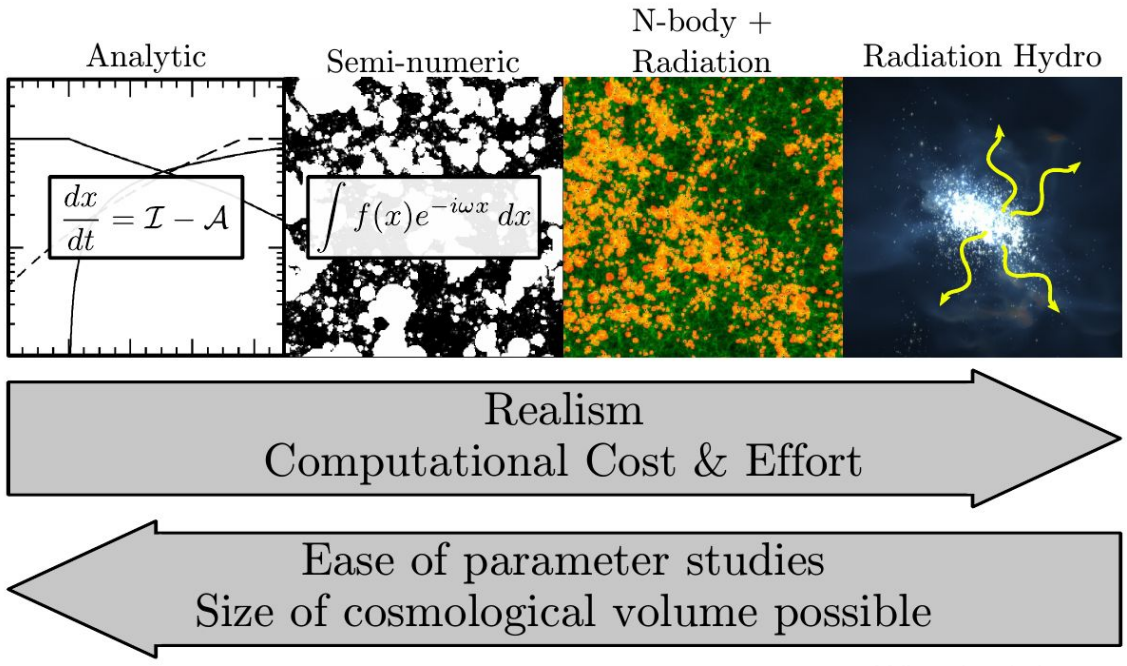


Thesan Collaboration

Cosmological EoR simulations

General **Radiative Transfer** algorithm:

1. Photons emitted from ionizing sources are **propagated in IGM**
2. **Ionization & heating rates** are calculated for HI, HeI and HeII
3. Multi-frequency **chemistry ODE** is solved to determine ionized matter density
4. Simulate a wide range of the cosmic time, but **radiative & hydrodynamic feedback** act on small time step for **convergence**



Wise (2019)

Typical EoR simulation takes up to **millions of core–hours** on several thousand nodes, run in parallel on high performance computers.

Simulating reionization with Radiative Transfer

Solve the differential equation of the **evolution of neutral hydrogen** (HI) during EoR

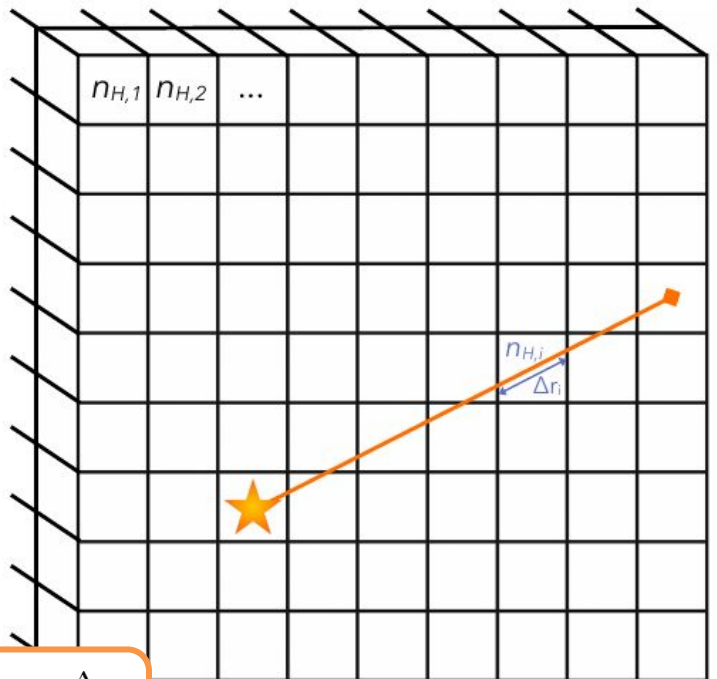
$$\frac{dx_{\mathrm{HI}}}{dt} = \underbrace{-x_{\mathrm{HI}}\Gamma_{\mathrm{ion}}}_{\text{Ionization Rate}} + \underbrace{(1-x_{\mathrm{HI}})n_{\mathrm{e}}\alpha_{\mathrm{H}}}_{\text{Recombination Rate}}$$

Short-characteristic ray-tracing algorithm: propagate photons and determine **column density** along the radiation line of sight.

$$\Gamma_{\mathrm{ion}}(r) = \frac{1}{4\pi r^2}\int_{\nu_{\mathrm{th}}}^{\infty}\frac{L_\nu}{h\nu}\sigma(\nu)e^{-\tau_\nu(r)}d\nu$$

$$\tau_\nu = \sigma_\nu N_{HI}$$

$$N_{HI} = \sum_{i\,\in\,\mathrm{L.o.S}} n_{\mathrm{HI},i}\Delta r_i$$

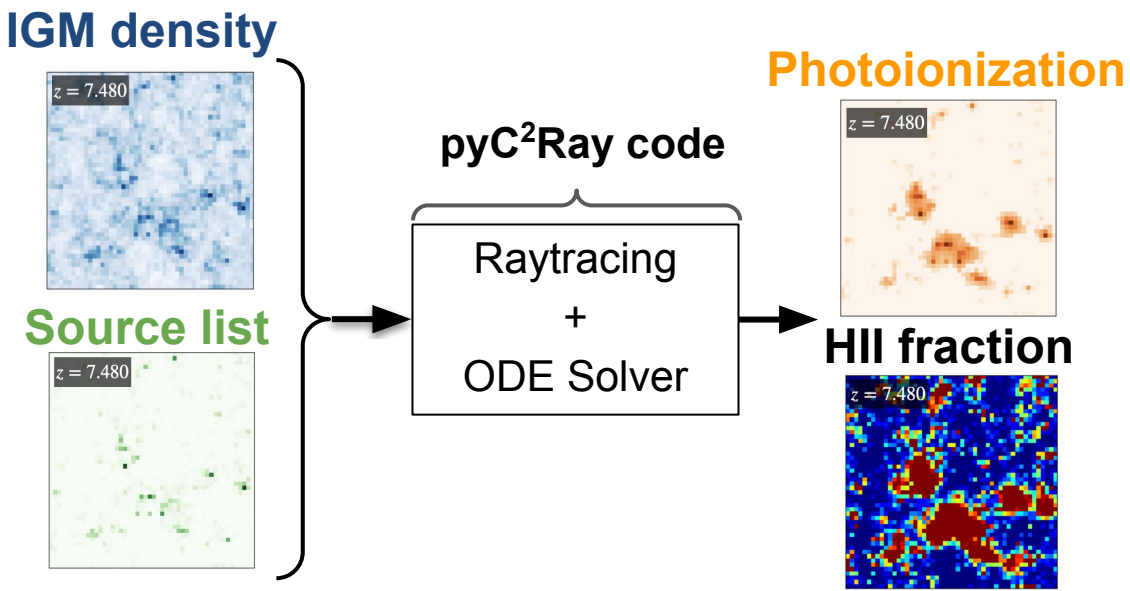


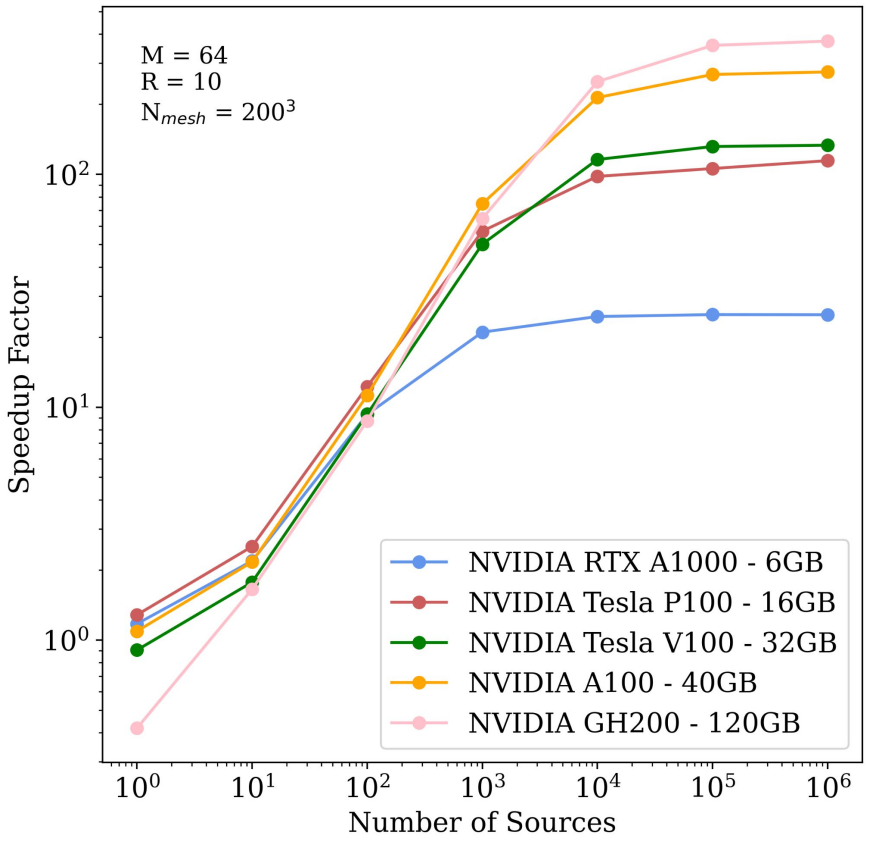
Similar equations can be defined for helium **HeI** and **HeII**

EoR simulations with pyC²Ray

pyC²Ray [2311.01492] is an update of the fully-numerical, Fortran90 *C²-Ray* code [Mellema+06]

- ➔ User-friendly Python interface
- ➔ **ASORA**: new ray-tracing algorithm in CUDA
- ➔ **MPI** parallelisation enabled
- ➔ ~400 speed-up factor on Alps (GH200) vs CPU





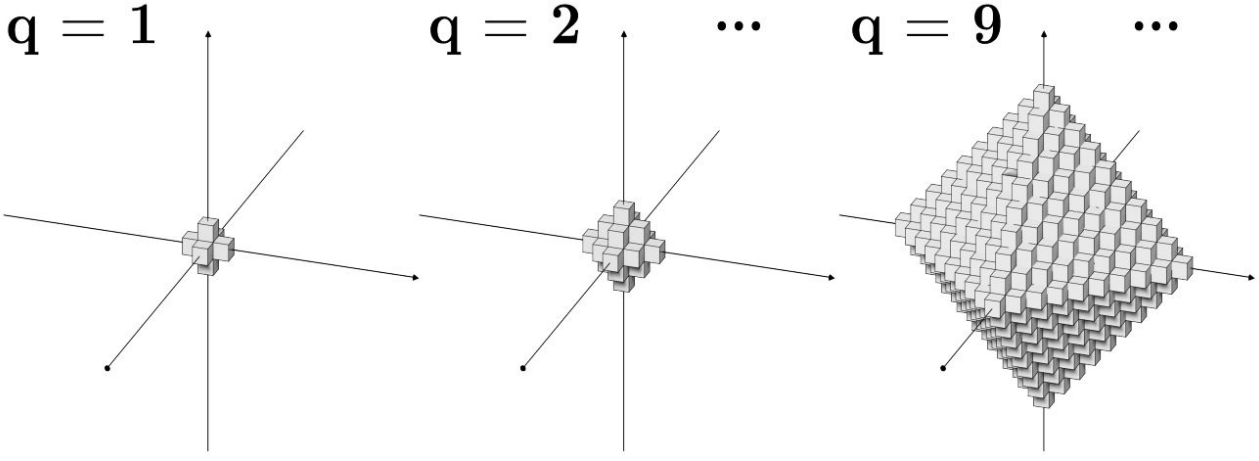
ASORA parallelization details

Accelerated Short-Characteristics Octahedral RAy-tracing

Levels of parallelization across a GPU cluster (e.g. **Daint** on Alps):

1. **Thread-block:** photons propagating from 1 ionizing source, expand in 6-cell octahedral neighborhood, **pixels at each q-shell are independent**

   a. (q, s) → (i, j, k) map
      s ≡ thread index, **q-shell** depends only on pixels from **previous** shell
   b. High occupancy of threads when q ≳ 6

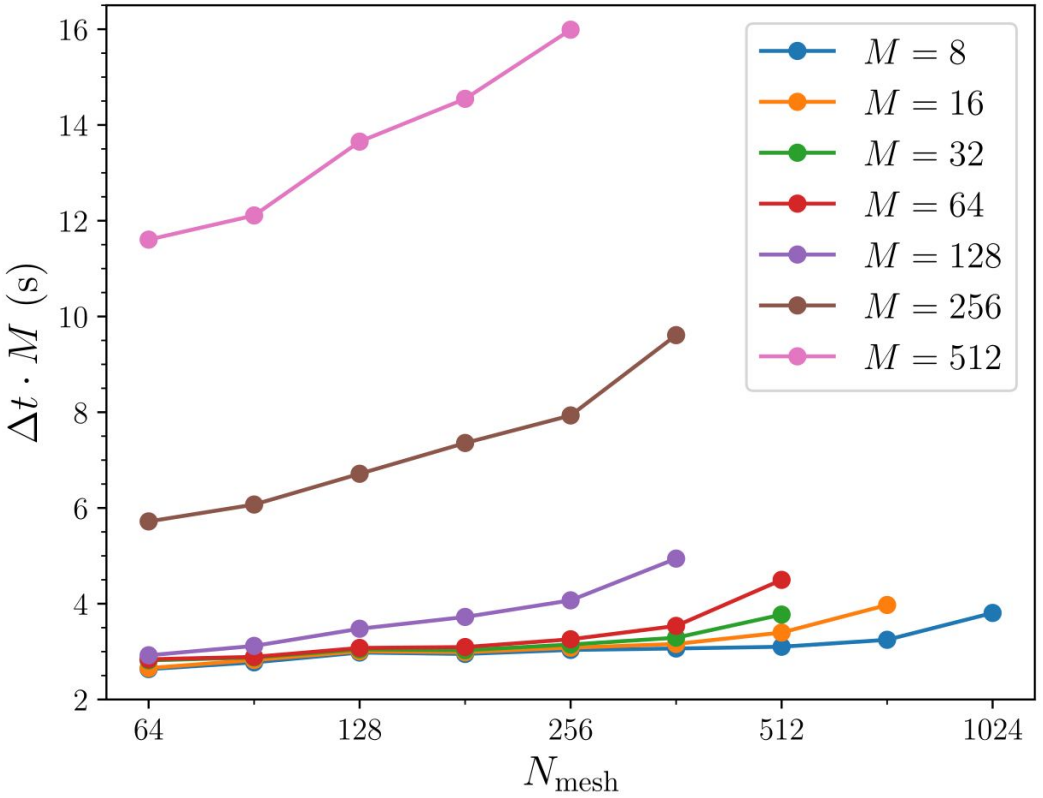


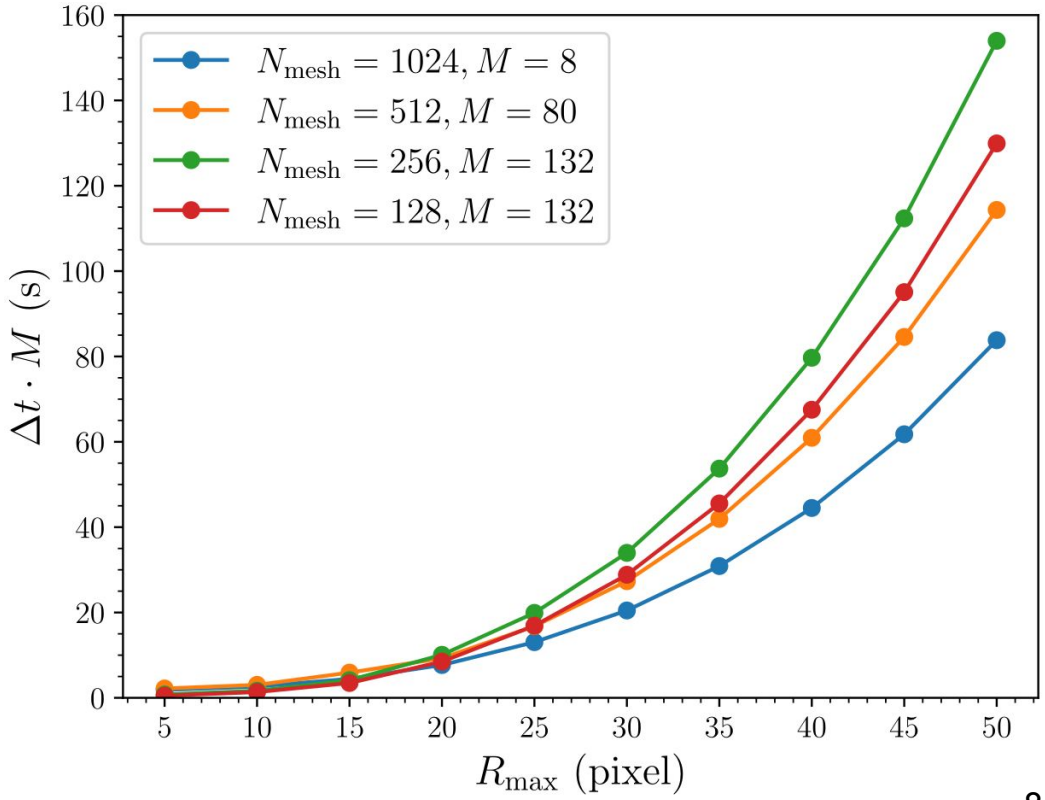
2. **GPU unit:** multiple sources in **batch**, as many as can fit in **global memory**
3. **HPC nodes:** batches are distributed on the cluster using **MPI**

ASORA profiling on Alps with GH200

Performance depends

- directly on: R_{max} maximum propagation distance for γs, K thread-block size
- indirectly on: N_{mesh} grid size of the Universe, M batch size, N_s number of sources





ASORA improvements – memory footprint

Before: column density used 3D mesh grid for storage and calculations

$$\text{Pixels} = N_{\text{mesh}}^3$$

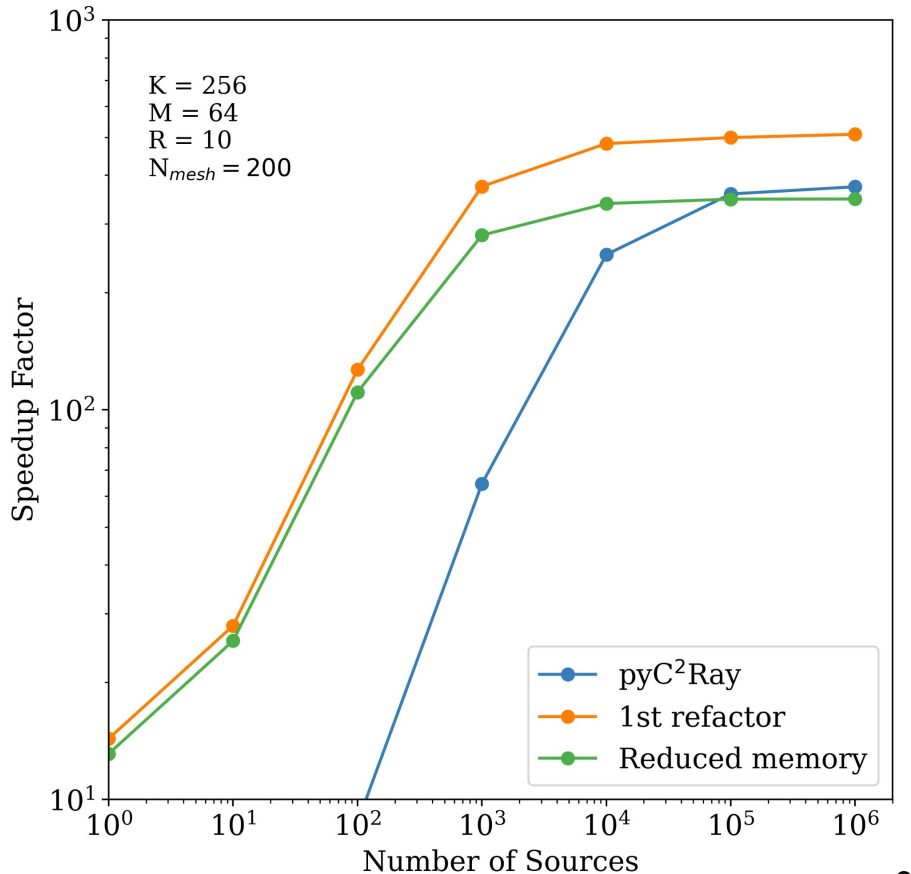
After: memory array that contains exactly the octahedron at a R_{max} distance

$$q_{\text{max}} = \lceil \sqrt{3} R_{\text{max}} \rceil$$

$$\text{Pixels} = 1 + \sum_{1}^{q_{\text{max}}} (4q^2 + 2)$$

Example: with N_{mesh} = 200, R_{max} = 10 column density memory storage reduced to 0.1%

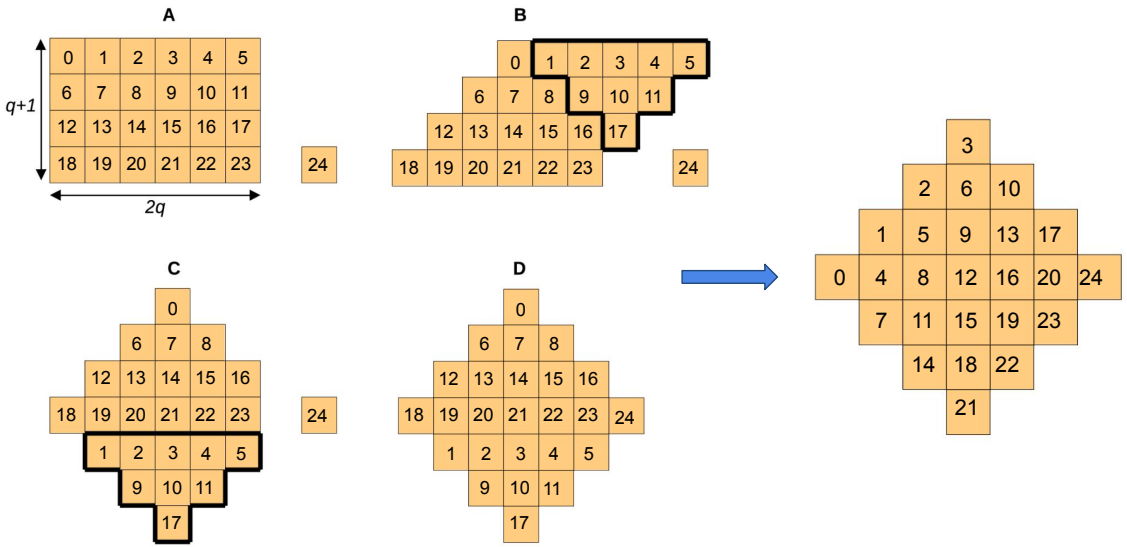
This requires **inverse mapping** (q, s) ↔ (i, j, k) to calculate short-characteristic weights.

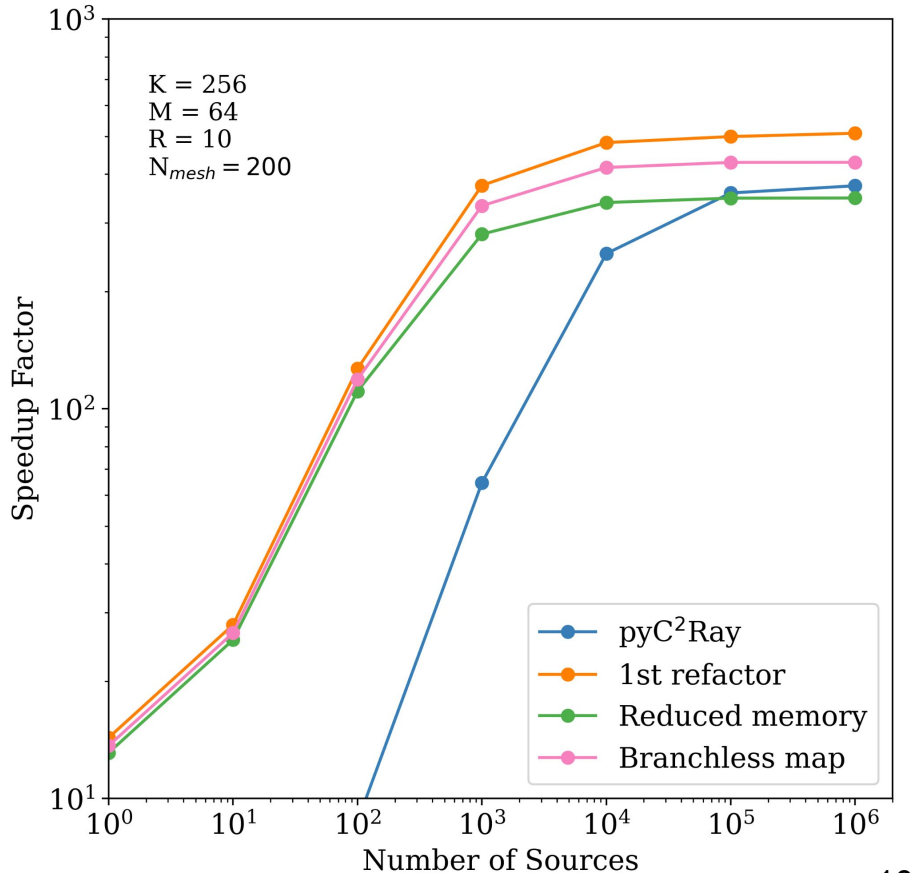


ASORA improvements – branchless mapping

Before: forward and backward mappings have at least 2 branches and 1 integer division

After: branchless forward mapping with 3 integer divisions and linear backward mapping



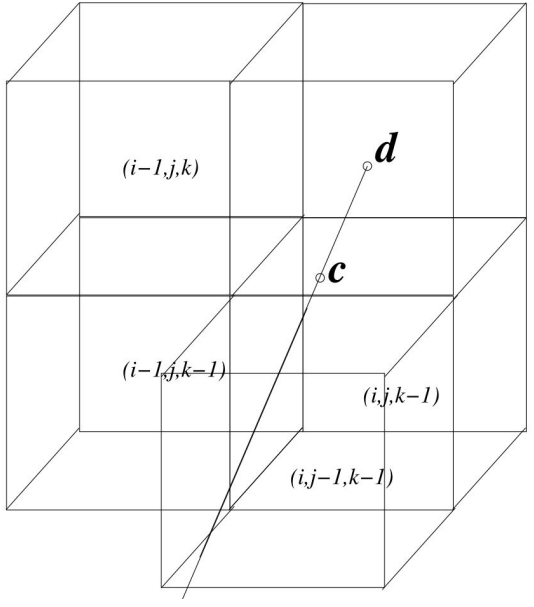


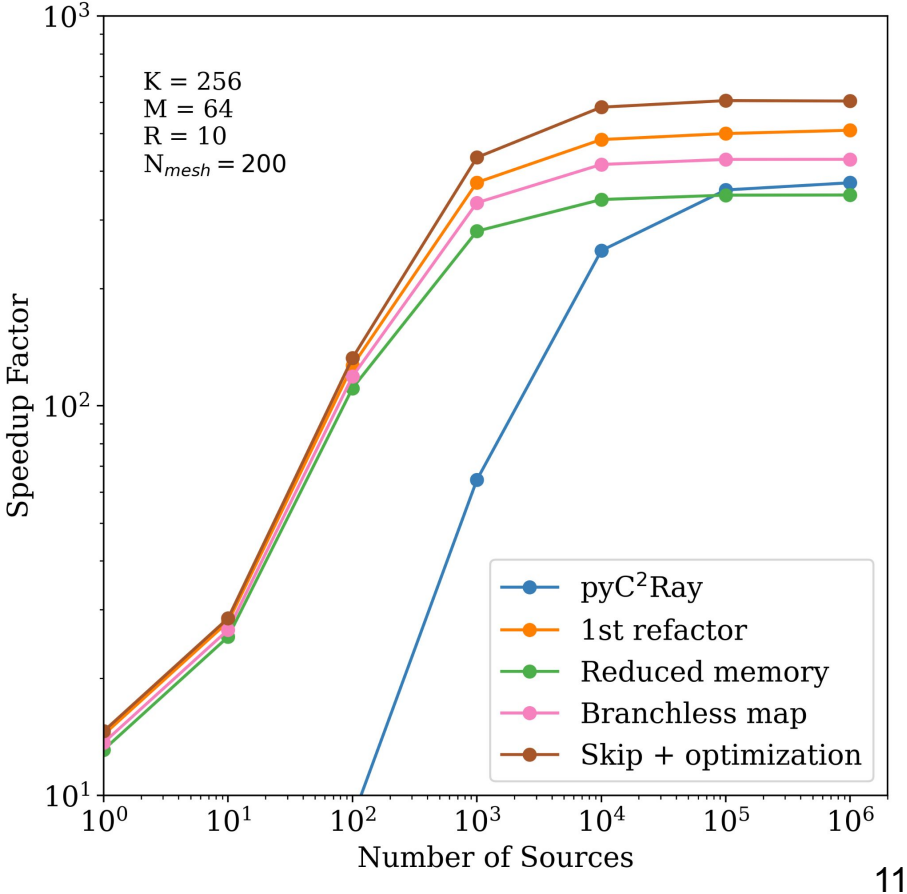
ASORA improvements – skip null pixels

With short-characteristic, a pixel gets **contributions from neighboring 4 pixels** in the direction of the source, for example:
(i, j, k-1), (i, j-1, k-1), (i-1, j, k-1), (i-1, j-1,k-1)

Some pixels have null contribution → **skip expensive memory reads**

These changes led to more optimization possibilities...





pyC^{2}Ray: today and tomorrow

- Hydrogen implementation of ASORA achieves a **~600 speed up factor** (+50% than first iteration) and internal **memory usage down to 0.1%**
- Important code refactors and optimizations for future extensions (see below)

1. **Multi-frequency extension for helium**
   a. Helium can be ionized twice: HeII and HeIII species
   b. Recombination is temperature dependent → compute photo-heating rate
   c. Absorption cross-section is frequency dependent
2. **Particle to mesh framework**
   a. Smoothing kernel to integrate particle-based hydrodynamics simulation
   b. Algorithm to convert to homogeneous or inhomogeneous/adaptive grids
3. **ODE porting to CUDA**
   a. Pixels are treated independently → high throughput application
   b. Reduce memory transfers from/to host when used with ASORA

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Thank you for your attention