

An Accelerated Raytracing Method for Radiative Transfer Simulations

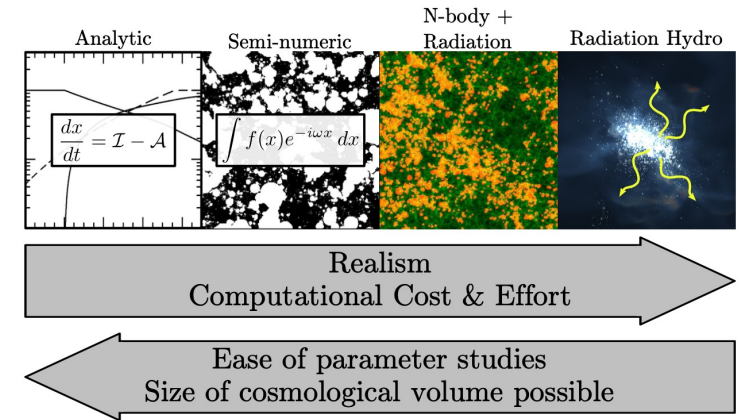
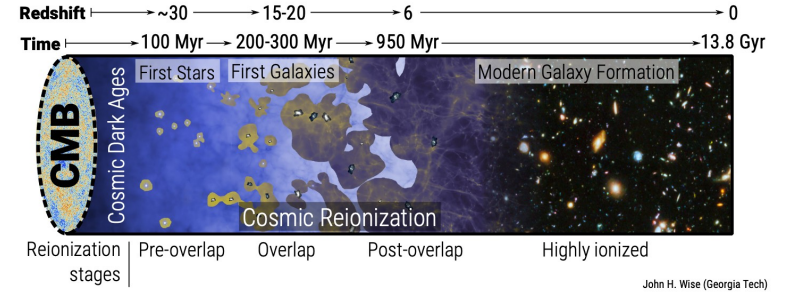
Patrick Hirling (EPFL)

SKACH Spring Meeting

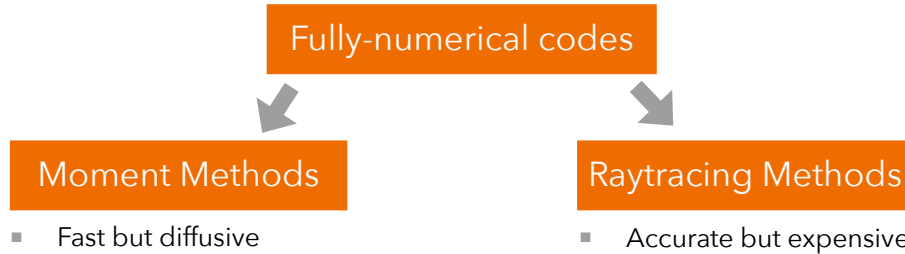
June 1, 2023

Context

- ◆ Epoch of Reionization (EoR, $5 < z < 25$): formation of the first luminous sources whose radiation transitioned the Universe from a cold neutral state to a hot, ionized one
- ◆ Appearance and properties of the primordial sources can be probed by observing the 21-cm signal (HI) with radio interferometric telescopes (e.g. SKA-Low, LOFAR)
- ◆ Modeling the EoR accurately enough for these future observations requires realistic radiative transfer (RT) simulations on scales > 100 Mpc with high resolution and hydrodynamic feedback



J. Wise (2019) arXiv:1907.06653

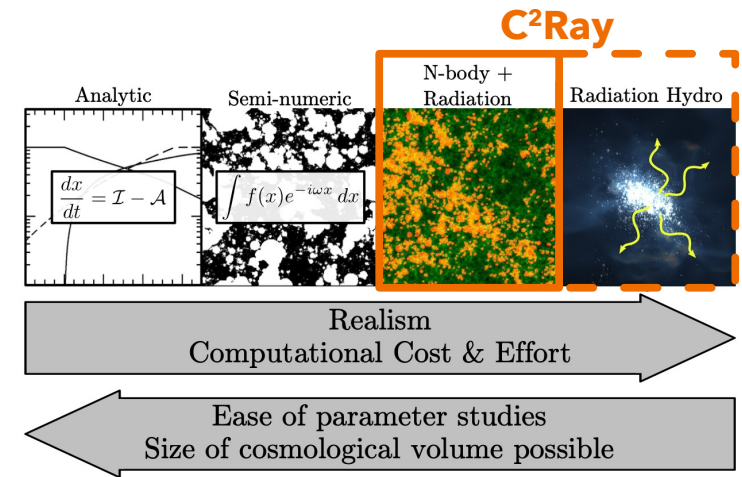


C²Ray

C²Ray (Mellema et al. 2005) is a **fully-numerical raytracing code** extensively used for large-scale EoR simulations

- ♦ **CPU-parallelized** using OpenMP with domain-decomposition & MPI-parallel treatment of sources
- ♦ Designed to be eventually coupled to hydrodynamics
- ♦ Even without this, a typical EoR simulation takes up to **millions of core hours** on several thousand nodes

Can it be made faster using GPU-parallelization ?



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Reionization Simulations

Goal: Time evolution of ionized fraction of hydrogen x in a physical volume due to photoionization and recombination effects

$$\frac{dx}{dt} = (1 - x) \left(\underbrace{\Gamma}_{\text{Photo-ionization}} + \underbrace{n_e C_H}_{\text{Collisional ionization}} \right) - \underbrace{x n_e \alpha_H}_{\text{Recombination}}$$

Γ : Photoionization Rate

Γ is due to ionizing flux from primordial sources:

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

Optical depth:
 $\tau_{\nu} = \sigma_{\nu} N_{HI}$

**continuous form, will vary for a discrete grid but retains similar structure*

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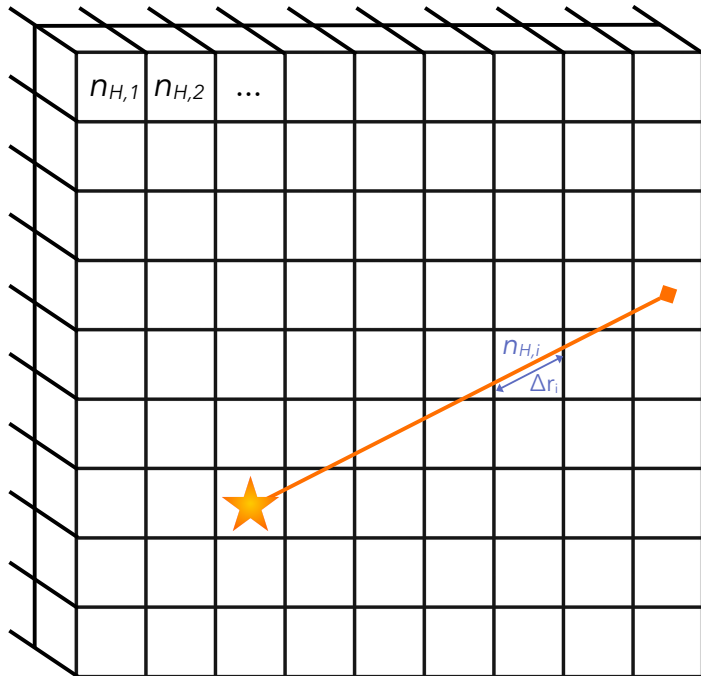
Key Quantity: column density of neutral hydrogen N_{HI}

**continuous form, will vary for a discrete grid but retains similar structure*

Raytracing on a grid

- ◆ Need the column density of hydrogen between source and all grid points, for possibly many sources

$$N_H = \int_{\text{Ray}} n_H(s) ds = \sum_{\text{Crossed Cells}} n_{H,i} \Delta r_i$$



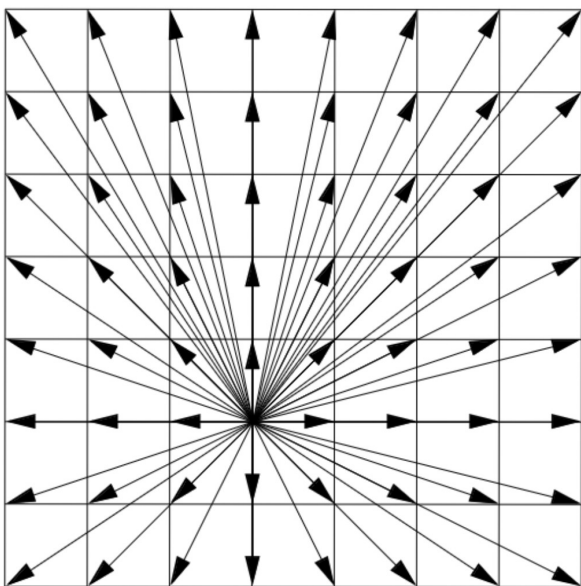
Treating all points (cells) by direct computation is **accurate** but **very expensive**. Several types of raytracing methods exist:

- Long characteristics (e.g. Feautrier 1964)
- Short characteristics (e.g. Kunasz & Auer 1988)
- Adaptive Raytracing (e.g. Abel & Wandelt 2002)
- Cones (e.g. Petkova & Springel 2011)
- Hybrid Methods (e.g. Rijkshorst et al. 2006)

Short vs Long Characteristics

Idea: Compute N_{HI} up to a cell by interpolation with n neighbours closer to the source, add part *within* the cell by direct computation

Long Characteristics



Direct Computation

Accurate

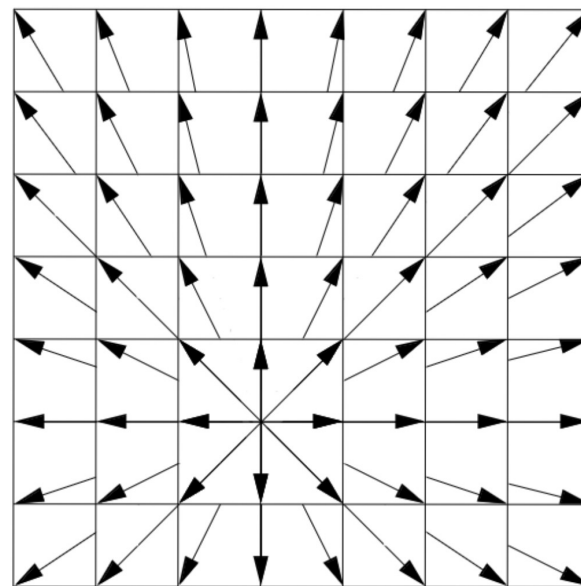
$O(N^4)$

Interpolative

More Diffusive

$O(N^3)$

Short Characteristics

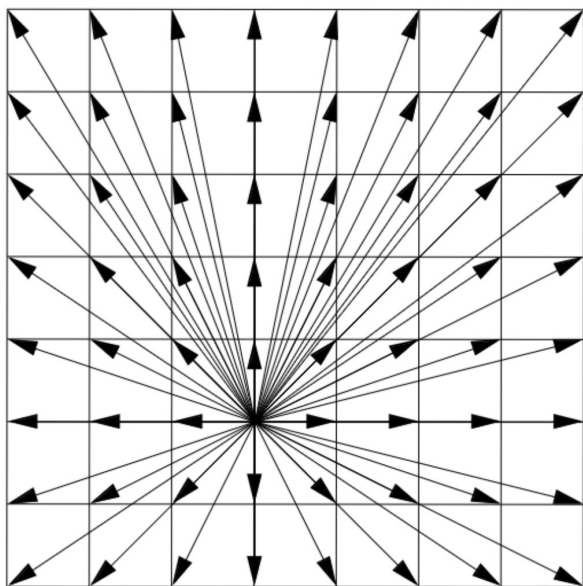


Adapted from Rijkhorst et al. (2006)

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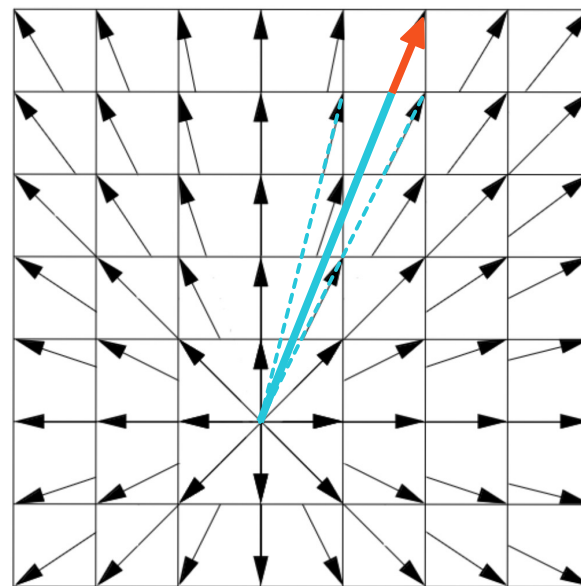
Long Characteristics



Direct Computation
Accurate
 $O(N^4)$

Interpolative
More Diffusive
 $O(N^3)$

Short Characteristics



Adapted from Rijkhorst et al. (2006)

Short vs Long Characteristics

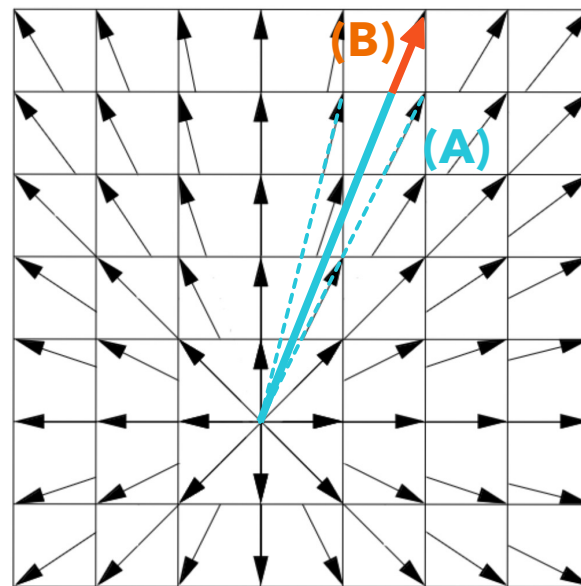
Idea: Compute N_{HI} up to a cell by interpolation with n neighbours closer to the source, add part *within* the cell by direct computation

Interpolative nature of SC methods imposes a causal order in which the grid cells must be treated (need to know (A) before doing (B))

This makes parallelization more challenging

Interpolative
More Diffusive
 $O(N^3)$

Short Characteristics



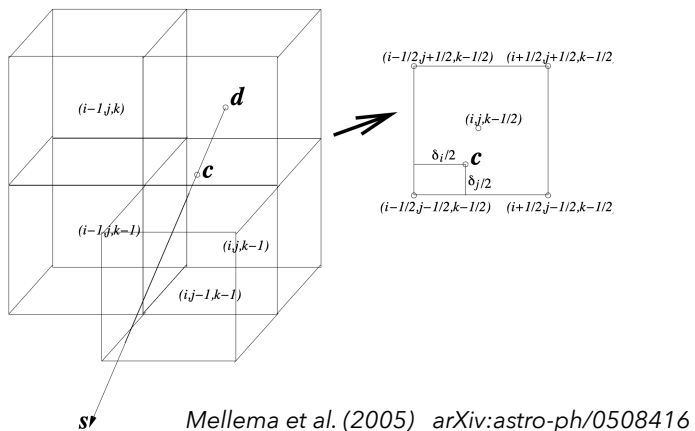
Adapted from Rijkhorst et al. (2006)

Short Characteristics in C²Ray

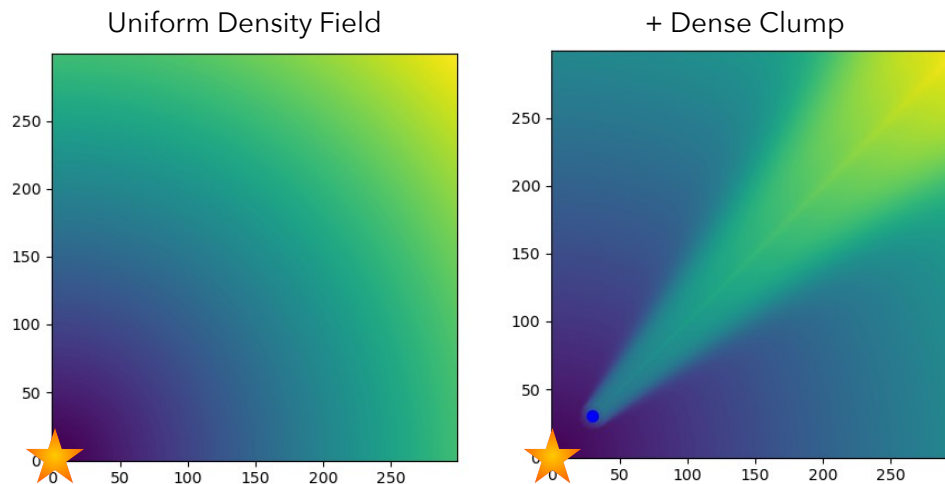
C²Ray uses a version with 4 neighbours (Raga et al. 1999):

$$\begin{aligned} e_1 &= (i, j, k - \sigma_k) \\ e_2 &= (i, j - \sigma_j, k) \quad (+ \text{ special weighting}) \\ e_3 &= (i - \sigma_i, j, k) \\ e_4 &= (i - \sigma_i, j - \sigma_j, k - \sigma_k) \\ \sigma_k &= \text{sign}(k - k_{src}) \end{aligned}$$

- ◆ Currently, grid is treated **in serial** in cubic ($x \rightarrow y \rightarrow z$) order *outward from the source*
- ◆ How to do it in parallel?



Examples of column density obtained using the 4-point SC method

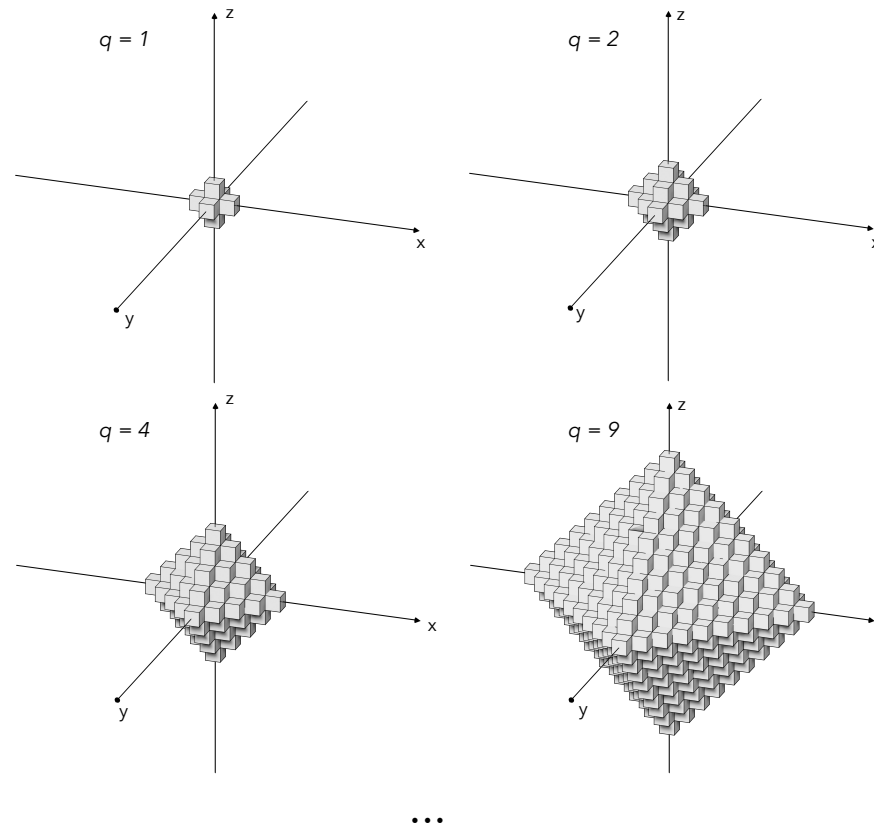


Our Method: OCTA

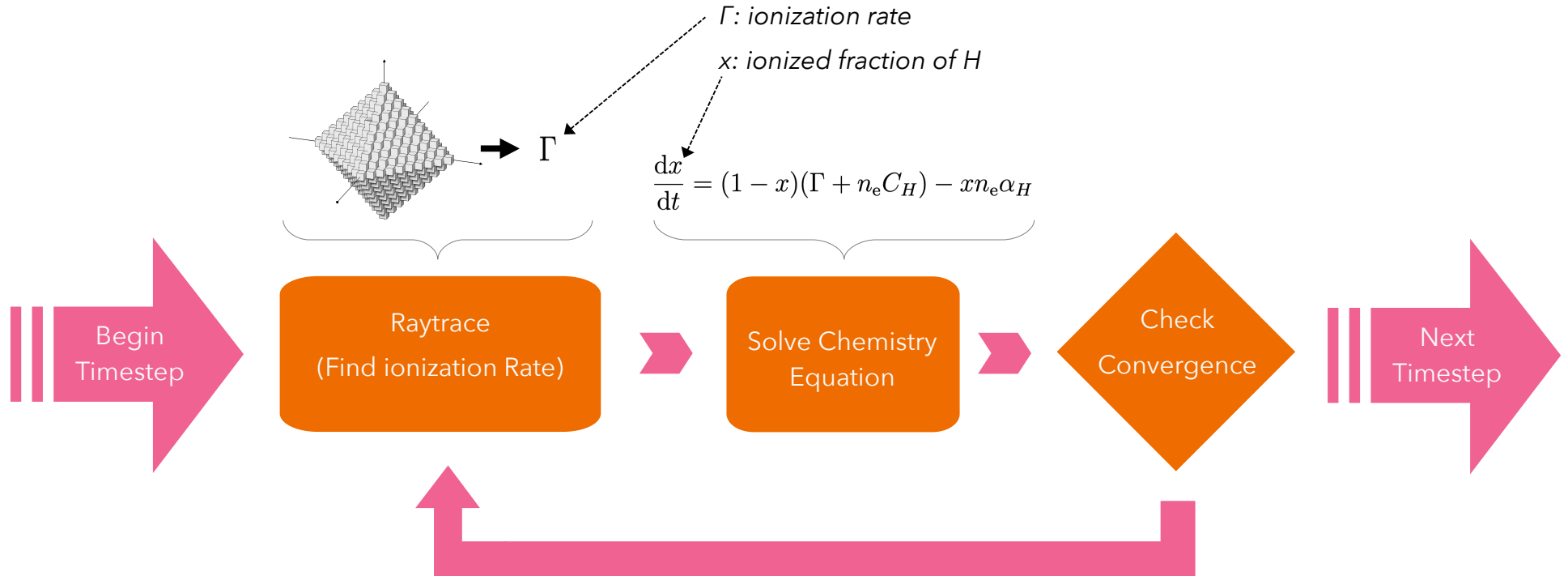
Shape that best follows the geometry of the 4-point method: **octahedral shells**:

- ◆ On a shell, all cells are **independent**
- ◆ All 4 interpolants are “below” the current shell (i.e. already calculated)
- ◆ At each iteration $\sim q^2$ cells can be treated **in parallel** on a GPU

(Source is at the origin)



Integration Into C2Ray



Can be easily adapted for other codes that require raytracing

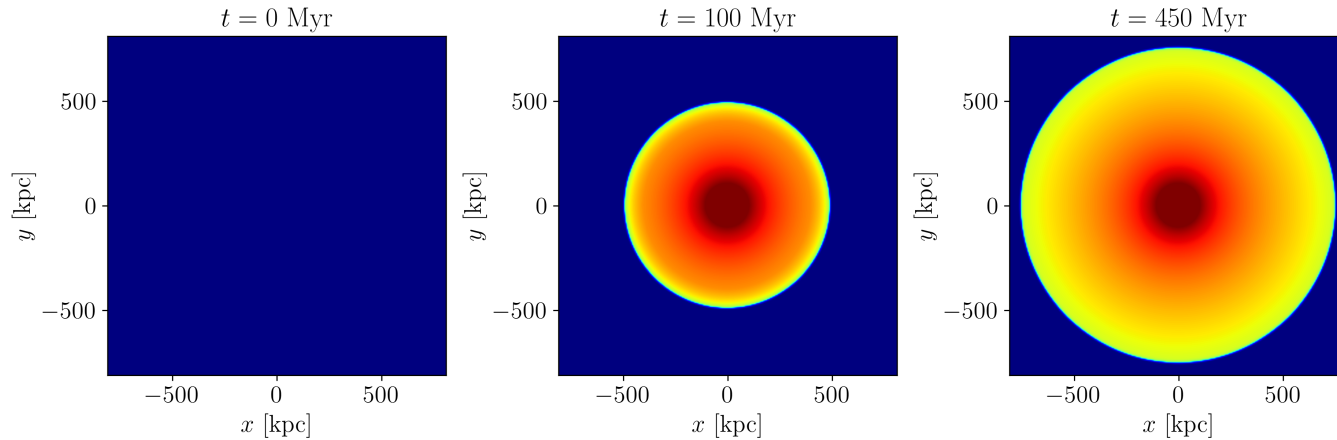
Accuracy-Testing C2Ray + OCTA

Strömgren Sphere (HII region expansion around single monochromatic source in uniform density field)

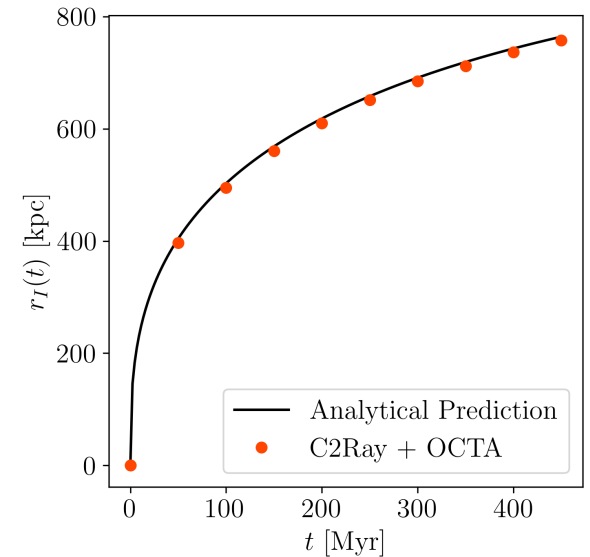
$$r_S = \left[\frac{3\dot{N}_\gamma}{4\pi\alpha_B(T)Cn_H^2} \right]^{1/3} \quad r_I = r_S [1 - \exp(-t/t_{\text{rec}})]^{1/3}$$

$$t_{\text{rec}} = [C\alpha_B(T)n_H]^{-1}$$

(Ionized fraction of Hydrogen shown)



+ Direct comparison with original C2Ray in multi-source cases

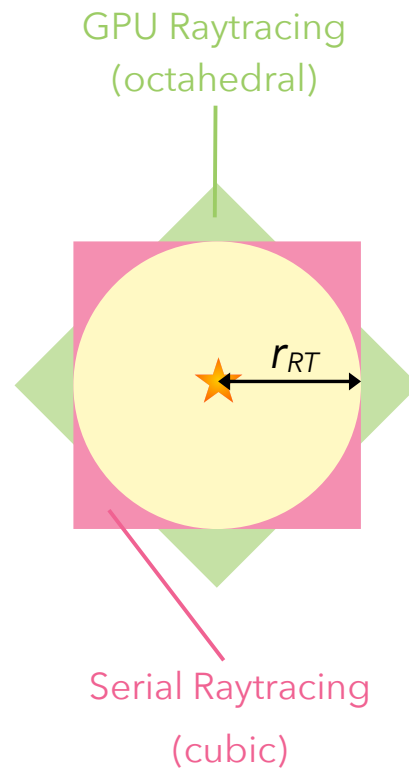
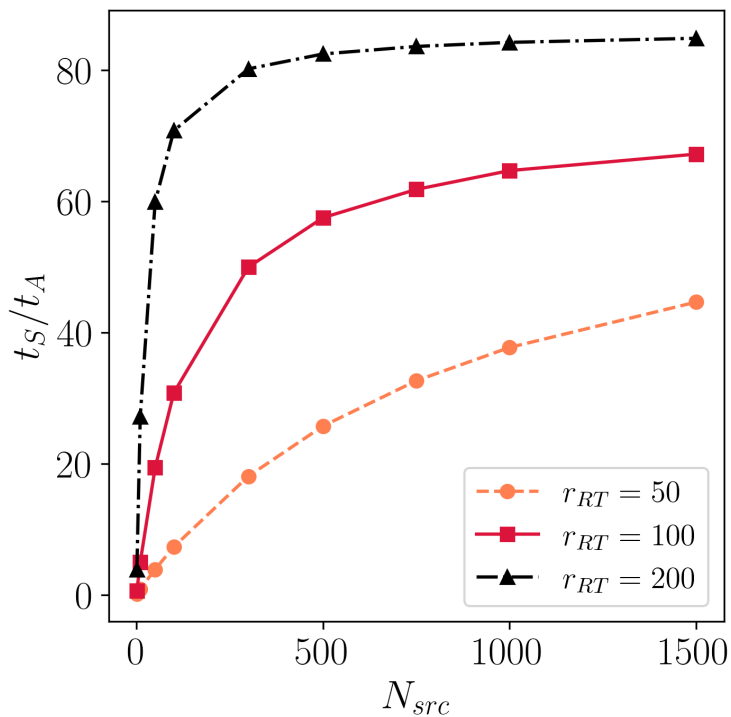
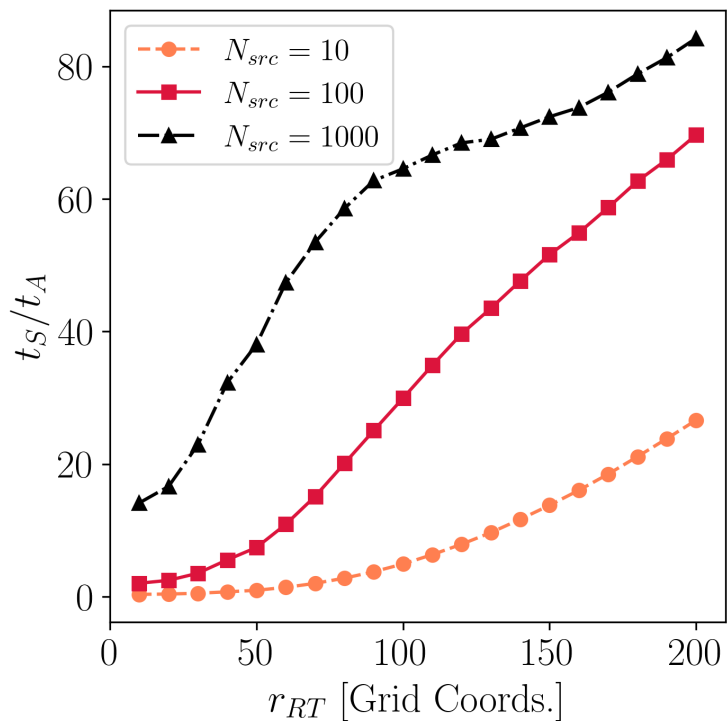


Performance Tests

N_{src} : Number of sources randomly distributed in the volume

t_S : Serial execution time using original method

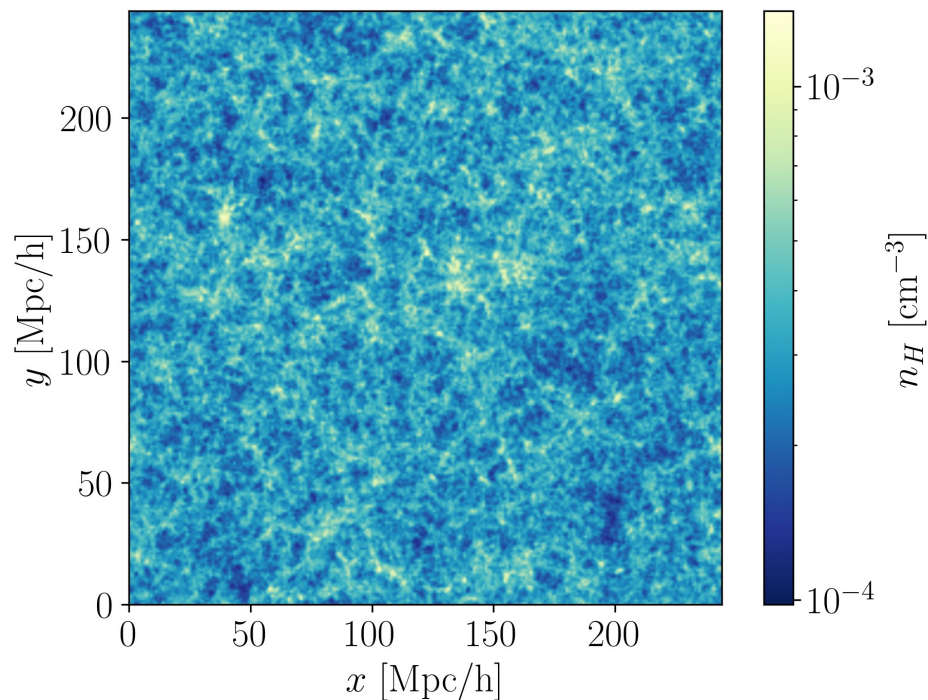
t_A : Accelerated (GPU) execution time using OCTA method



Platform: Piz Daint (1x Intel Haswell + 1x NVIDIA Tesla P100)

Illustrative Application

Fixed Density Field from $(244 \text{ Mpc/h})^3$ hydro simulation at $z = 9$



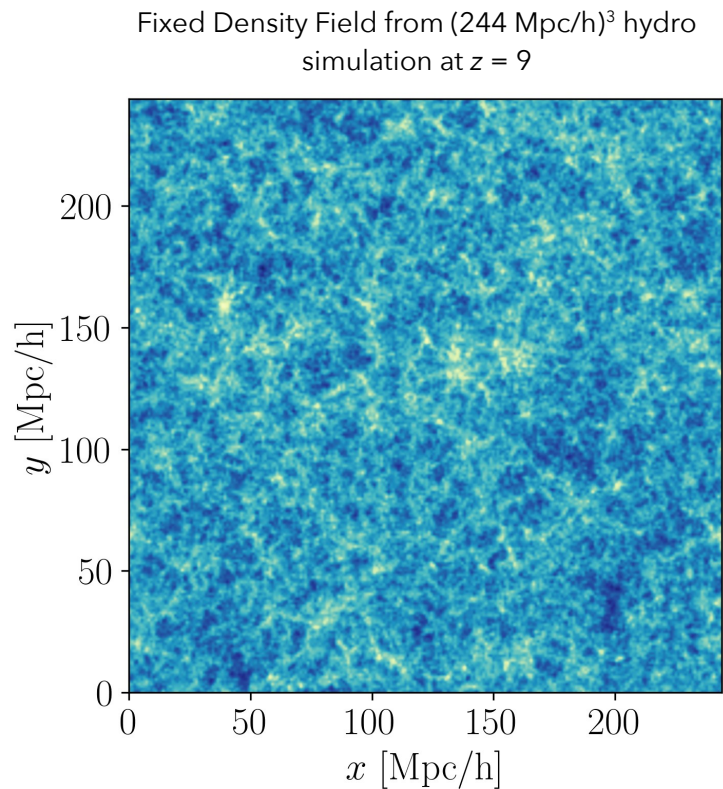
Find 10^5 most massive halos

- ◆ Source model:

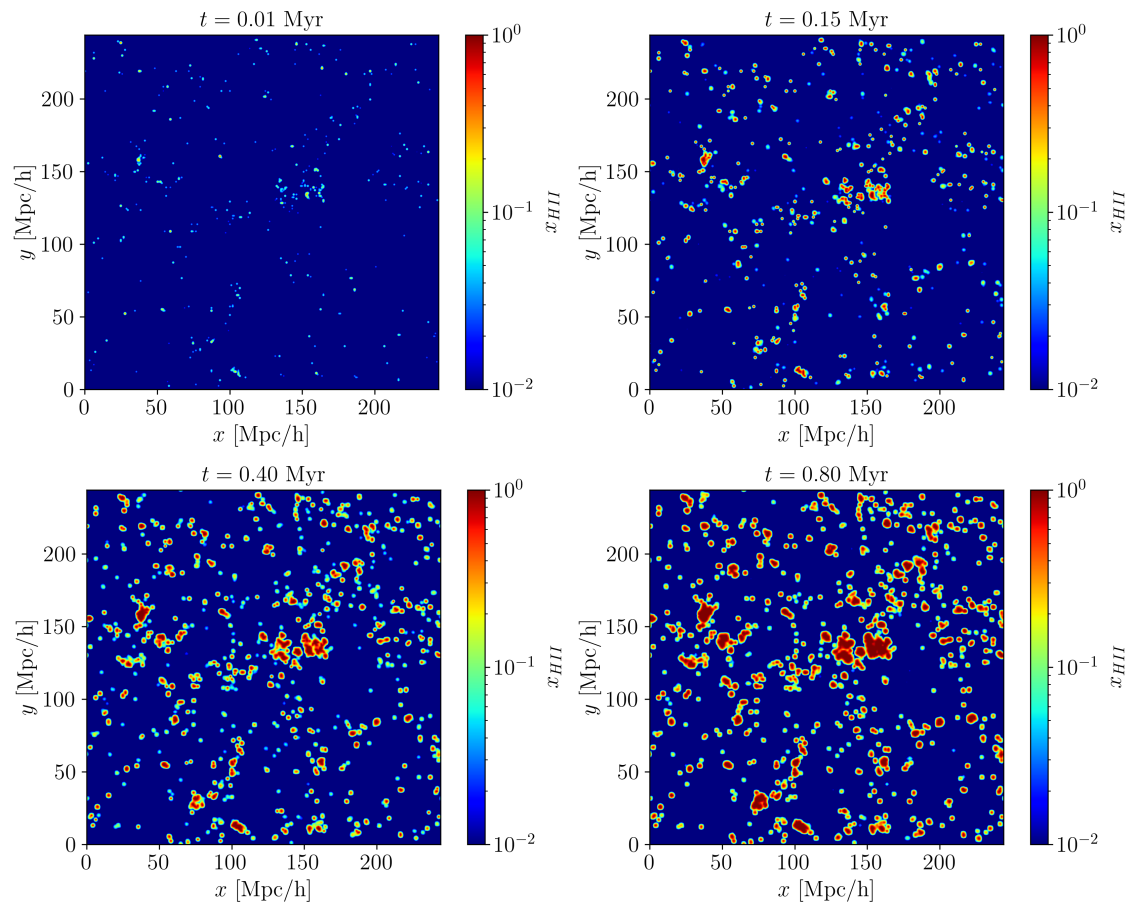
$$\dot{N}_\gamma = f_\gamma \frac{M \Omega_b}{\Omega_0 m_p t_s}$$

- ◆ **$N_{grid} = 250, r_{RT} = 50$**
- ◆ Use a black-body spectrum with $T = 10^5 \text{ K}$
- ◆ Evolve for 0.8 Myr with $\Delta t = 0.1 \text{ Myr}$

Illustrative Application



Computation Time: 25h on a **single node** on Piz Daint



Implementation & Future Development

| 17

- ◆ **OCTA is implemented as a C++/CUDA library with python bindings**
- ◆ Developed for C2Ray but can easily be adapted for other codes and simulations (e.g. SWIFT, FIRE2)
- ◆ Future improvement ideas:
 - Treat multiple sources at once on one GPU
 - Ability to run on GPU clusters (multiple nodes)
 - Adaptive raytracing size (photon statistics)
 - Planning to apply for participation at Eurohack23 at CSCS to develop these ideas
- ◆ **Current goal:** do an actual cosmological EoR simulation and compare with existing result from C²Ray (part of a SKACH Long HPC allocation at CSCS)

Thank you for your attention!