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- **Bachelors:** Computer Science
- **Key Area Mathematics**
 - Seminary Computational Mathematics (K. Sturm)
 - Sci. Comp. for FEM (J. Schöberl)
 - Computational Finance (A. Jüngel)
- **Key Area Informatics**
 - Algorithmics (G. Raidl)
 - Heuristic Optimization Techniques (G. Raidl)
 - Machine Learning (R. Mayer)
- **Current Occupation:** Project Assistant at TUW Institute of Photonic Technologies
- **Favorite Lectures:** Computational Science on Many-Core Architectures (K. Rupp)

Introduction

This thesis aims to enhance a CUDA-based particle engine [1] for simulating laser beam propagation in material processing. This approach outperforms field-based methods, which cannot accurately model reflections and refractions. Each photonic parcel is computed independently for speed, and missing features plus performance improvements for handling over 10^5 particles were developed in this work.

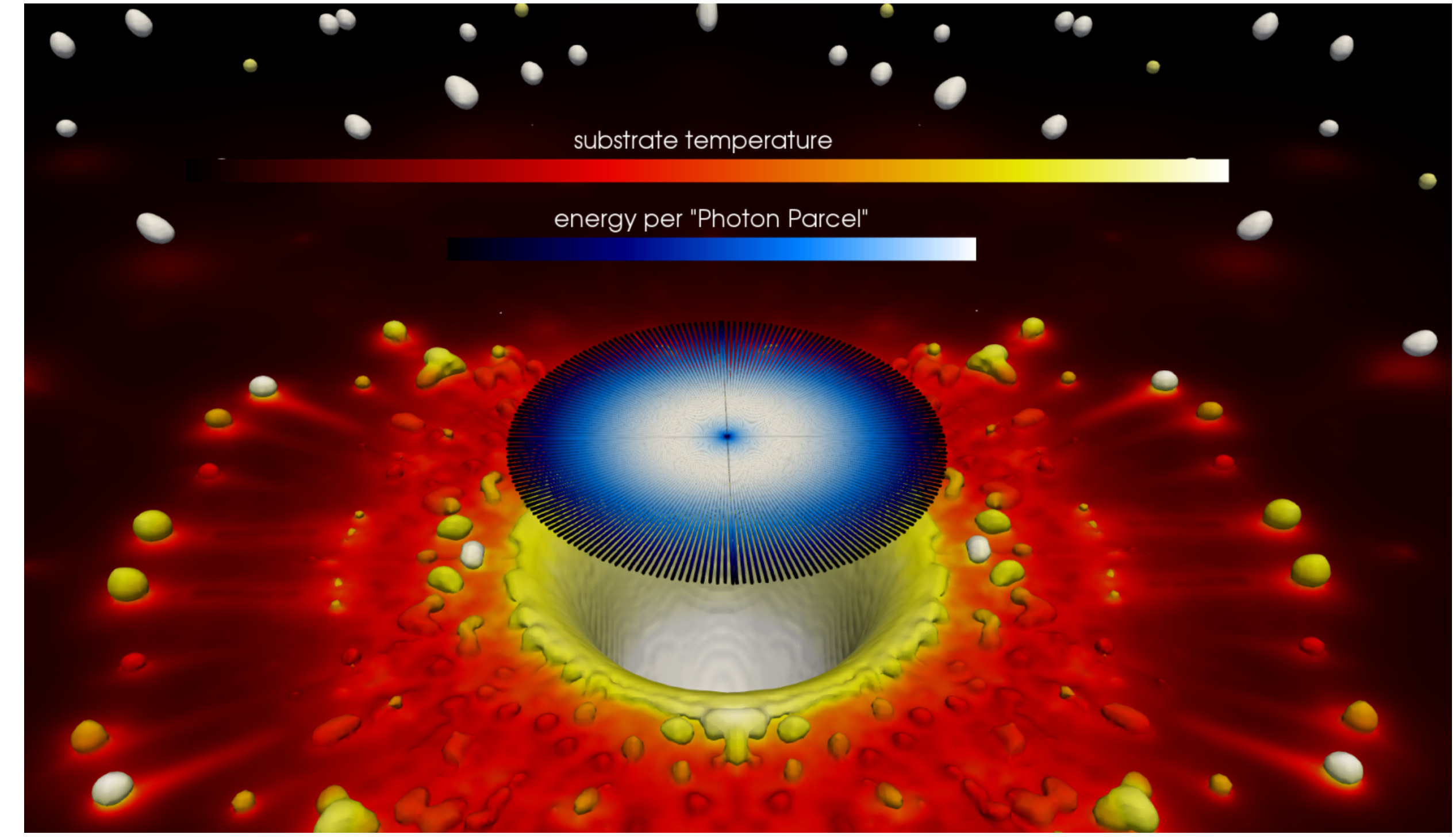


Figure: Particles in a simulation drilling SiO2

Method & Implementation

The entire solver is built on OpenFoam[®]. In sequence, it solves phase and energy advection, beam propagation, heat conduction, phase changes, and then pressure-velocity calculations [2]. The particle engine only modifies beam propagation, now using parallelized particles. The CPU collects mesh and particle data and transfers them to the GPU, where particles traverse the mesh, compute their trajectories, and calculate absorbed energy. After computation finishes on the GPU, the absorbed energy field is returned to the CPU.

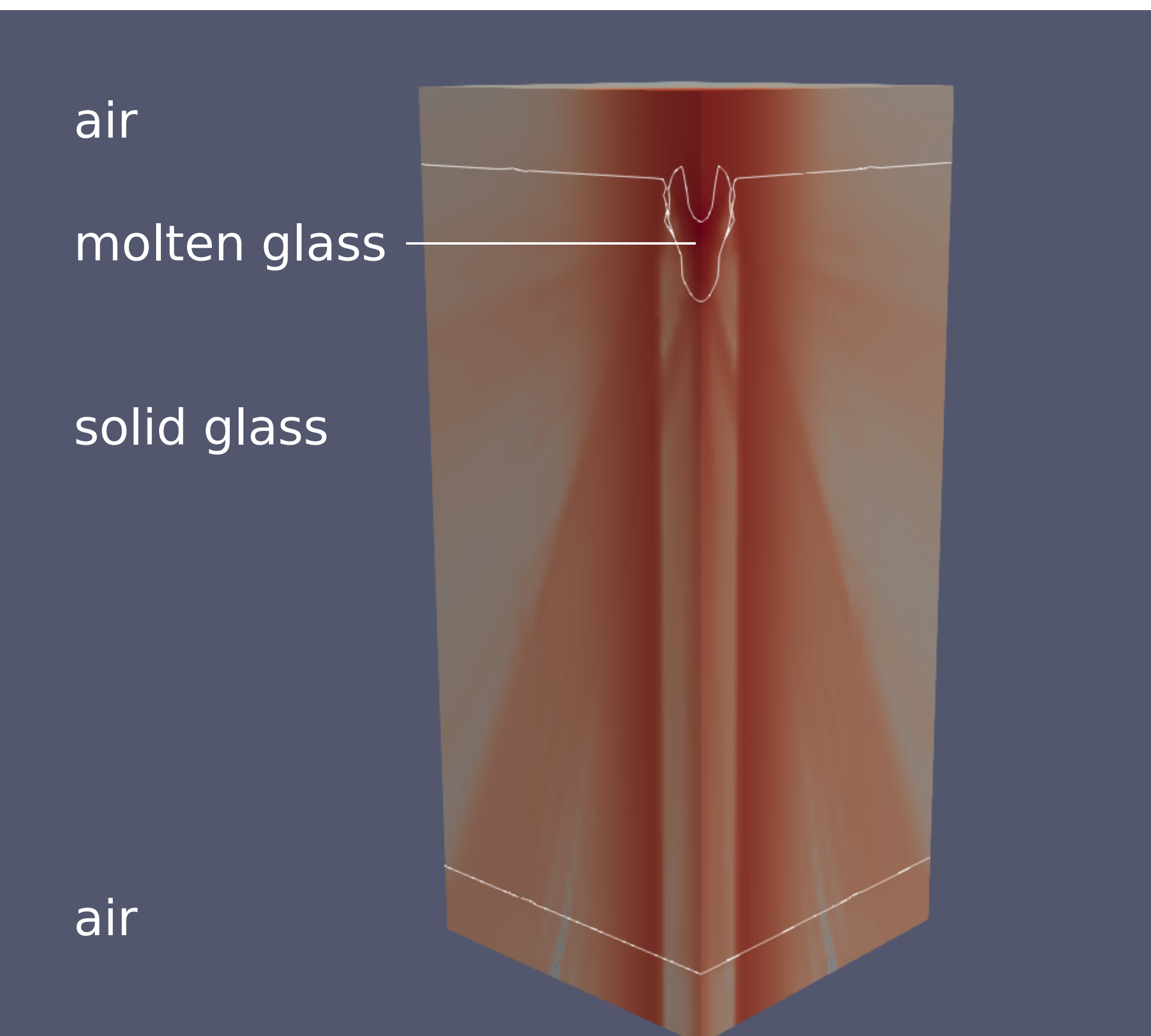


Figure: Transmitted intensity in a glass drilling simulation

Parallelization

The FVM solver can already be parallelized by splitting the mesh into multiple parts, each computed by an individual processor. MPI handles data exchange across processor boundaries. Various approaches were possible, but ultimately, all mesh and particle data are collected by a single processor, transferred to the GPU, and then the results are distributed back to the CPU cores.

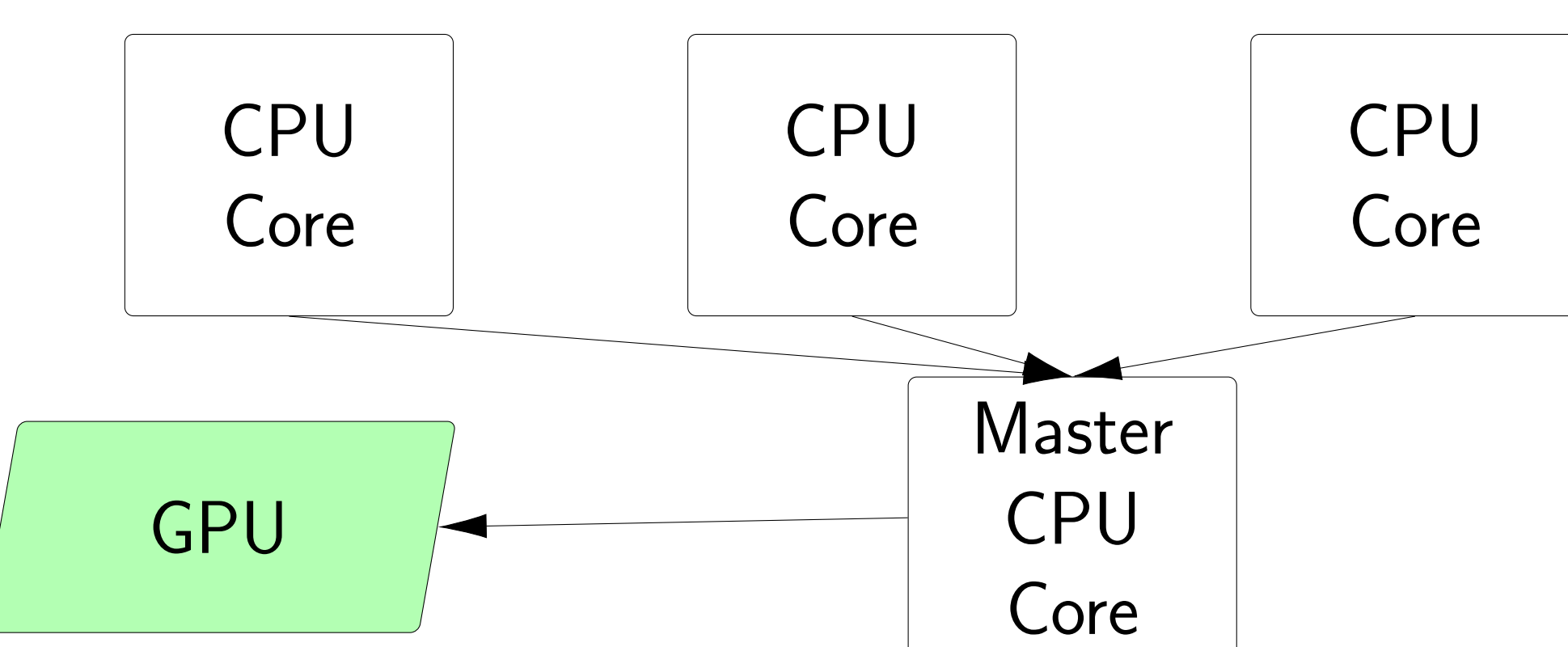


Figure: Data is gathered on the master core, from where it is transferred to the GPU

Dynamic Mesh

Dynamic mesh refinement is critical in mesh-based simulations to ensure high resolution in areas of interest (e.g., high velocities, liquid phase). This capability should also apply to the particle engine, which required an adjusted particle-tracking algorithm. Because of the dynamic mesh, crossing a face may require a particle to choose among four possible adjacent cells.

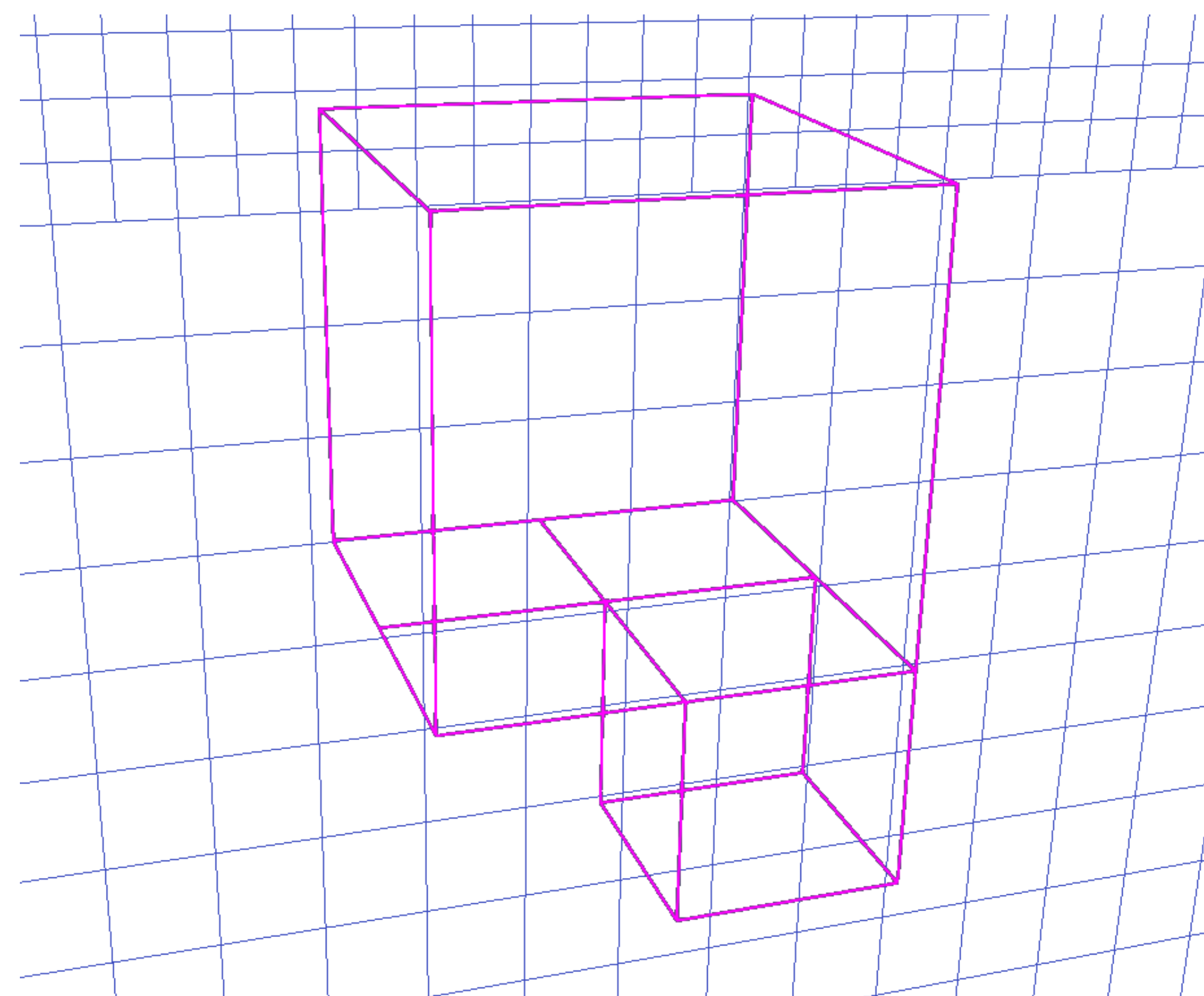


Figure: Refinement interface in a dynamic mesh

Laser Polarization

An additional polarization vector was introduced per photonic parcel to more accurately model light behavior. This modifies calculations at phase boundaries, building on Fresnel equations. At Brewster's angle, the reflected beam is s-polarized (perpendicular to the plane of incidence).

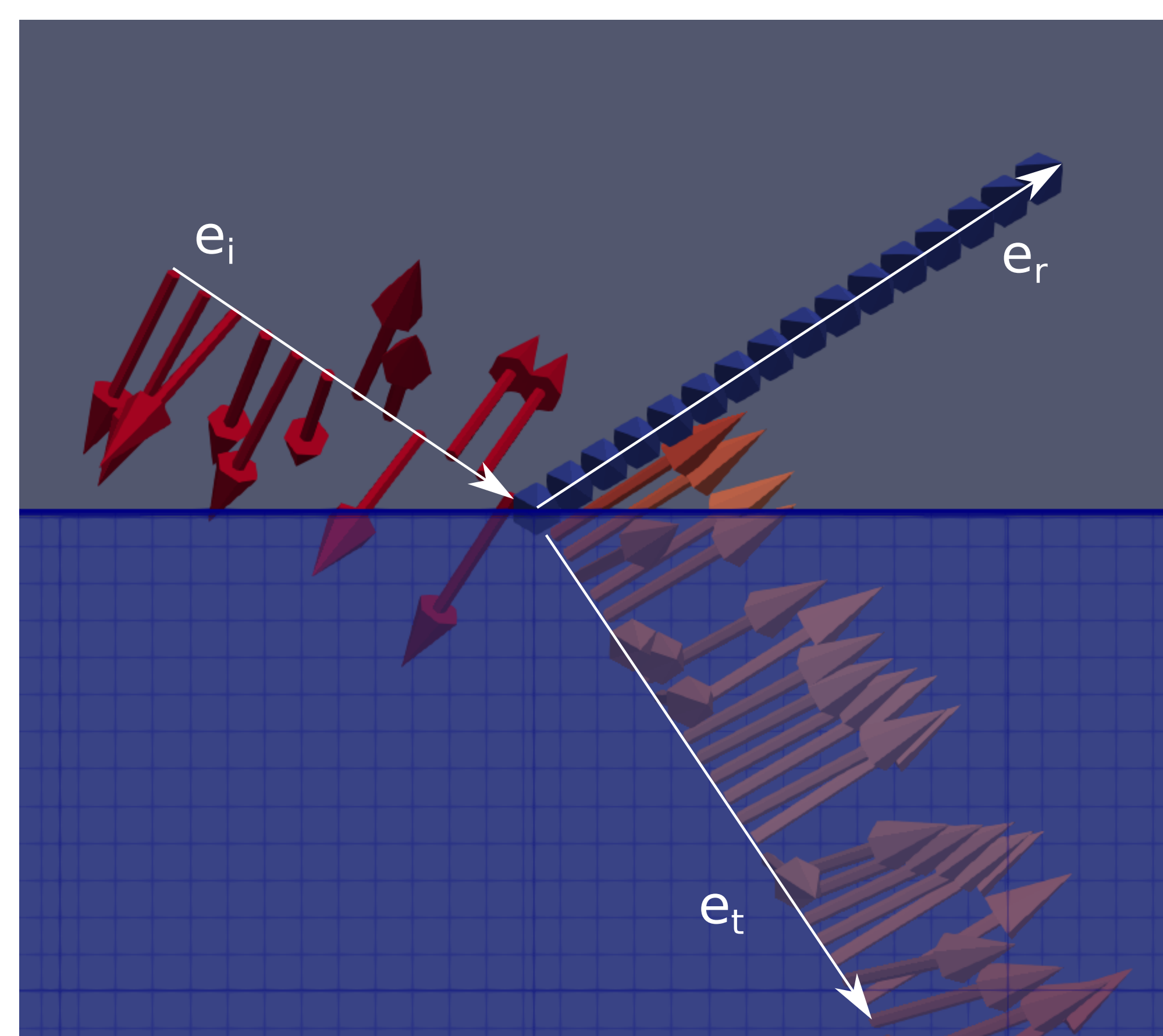


Figure: Randomly polarized particles reflecting and refracting at Brewster's angle

Speedup

Various parts of the code, including particle creation and attribute calculations, were optimized for speed. Additional logic minimizes data transfers between the CPU and GPU, and other algorithmic refinements further reduce runtime. As a result, the particle engine becomes usable for some simulations, though future improvements remain possible.

Inteference

Another goal was to capture the wave-like characteristics of photons, enabling interference. This is achieved by assigning each particle a phase attribute, requiring a new absorption model to compute interference-based absorption.

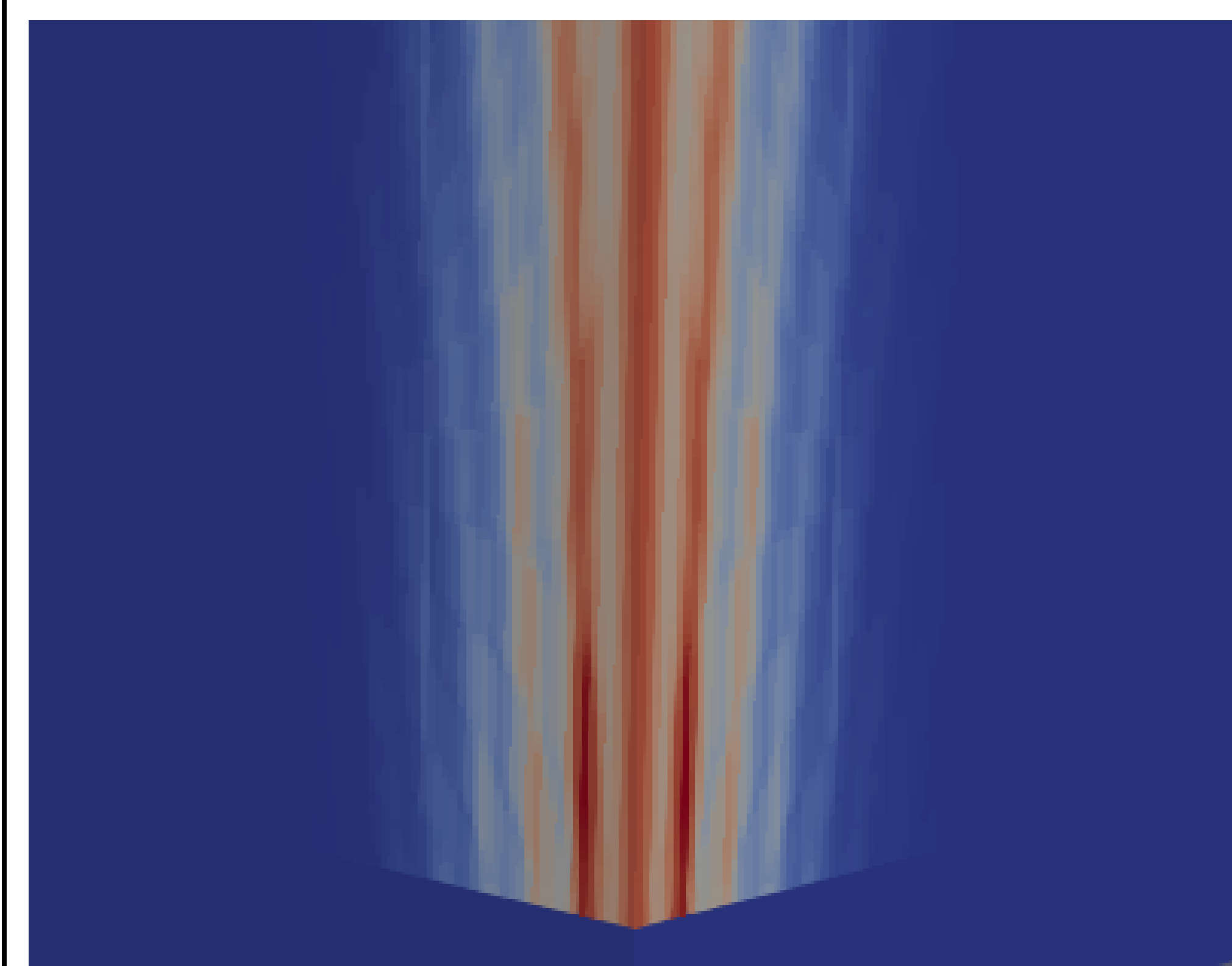


Figure: Interference patterns in absorbed energy

Laguerre-Gaussian Beam

For a project of a client, we needed to model a Laguerre-Gaussian beam. This changes the initial attributes of the photons, namely the energy and phase, which leads to different absorption patterns.

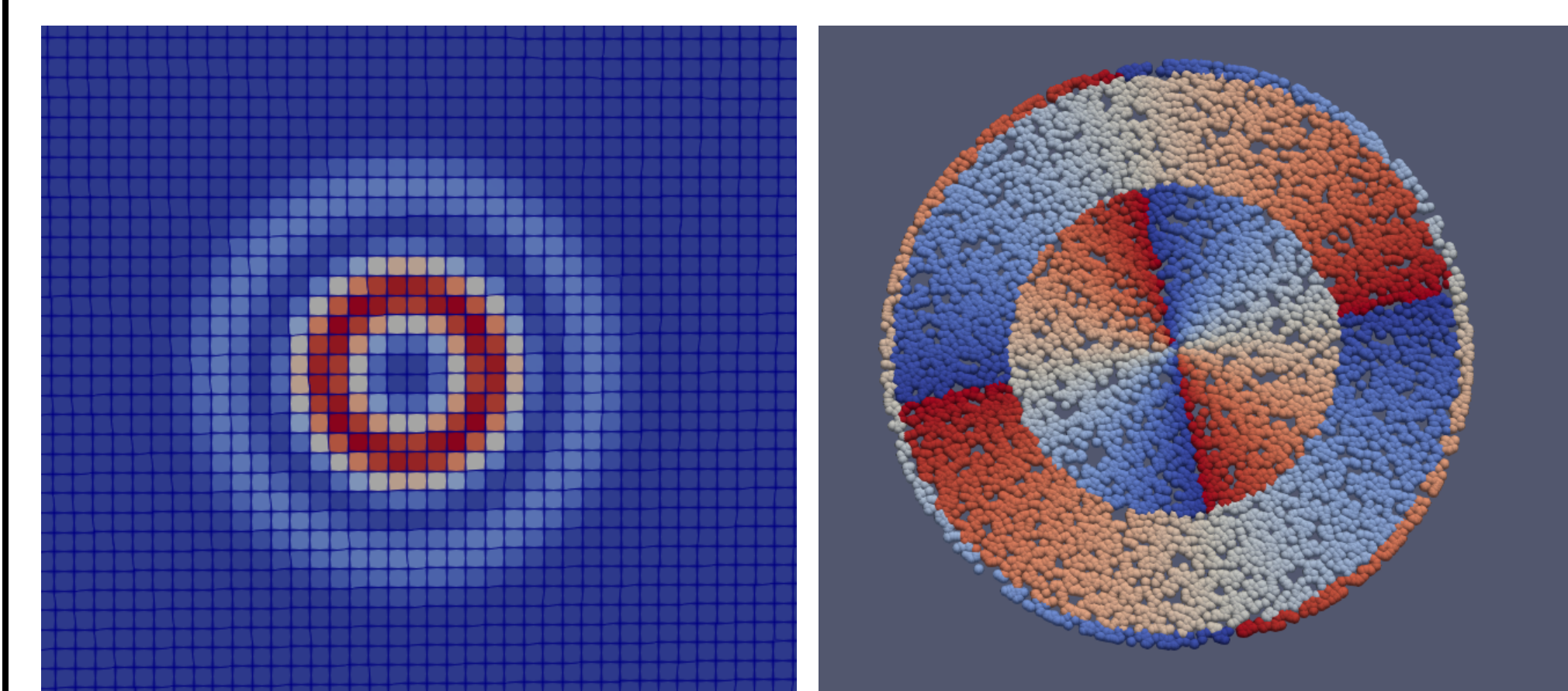


Figure: Absorption pattern and particle phase of a Laguerre-Gaussian Beam, radial index = 2 and topological charge = 2

References

- [1] Lukas Heisler. "GPU Accelerated FVM-DEM Simulation of Laser Based Manufacturing in OpenFOAM[®]". Available at <https://doi.org/10.34726/hss.2023.107360>. Master's thesis. TU Wien, 2023.
- [2] Constantin Zenz et al. "A compressible multiphase Mass-of-Fluid model for the simulation of laser-based manufacturing processes". In: *Computers & Fluids* 268 (2024), p. 106109. ISSN: 0045-7930. DOI: <https://doi.org/10.1016/j.compfluid.2023.106109>.