GPU acceleration in Lagrangian Particle Tracking using CUDA for Python and Fortran 2025-01-23

Thisal Mandula Sugathapala

Background

Project Overview

- Lagrangian biophysical particle tracking (LPT) code for microplastics in the ocean.
- Port the LPT code to GPU architecture using CUDA Python and CUDA Fortran.
- Perform a comprehensive comparison of the LPT model's performance across each programming language (Python and Fortran) on CPU and GPU platforms.
    - Performance evaluations on workstation with Nvidia Geforce RTX 3070.
    - Performance evaluations on Vera cluster GPUs (A100, V100, A40, T4).
    - Impact of thread block structure on model performance.
    - MPI vs CUDA.
    - Limitations of running CFD codes on GPU.

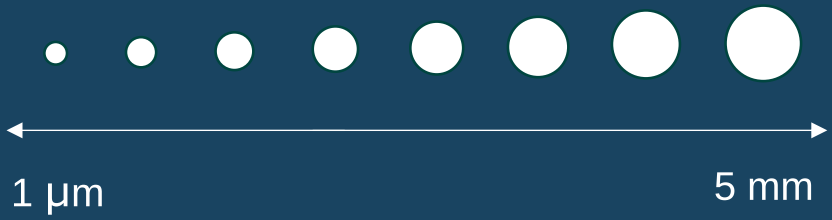
Background

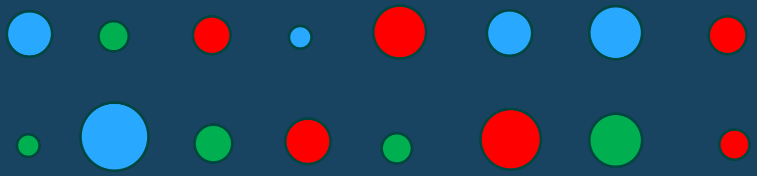
Particle distribution on GPU

Polypropene

Low Density Polyethylene

High Density Polyethylene





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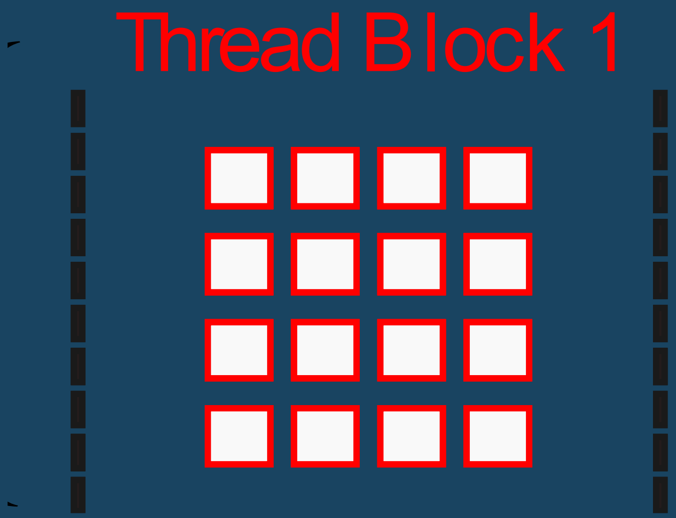

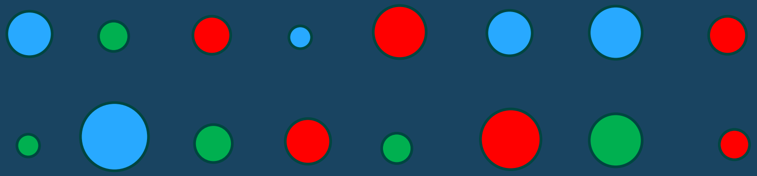

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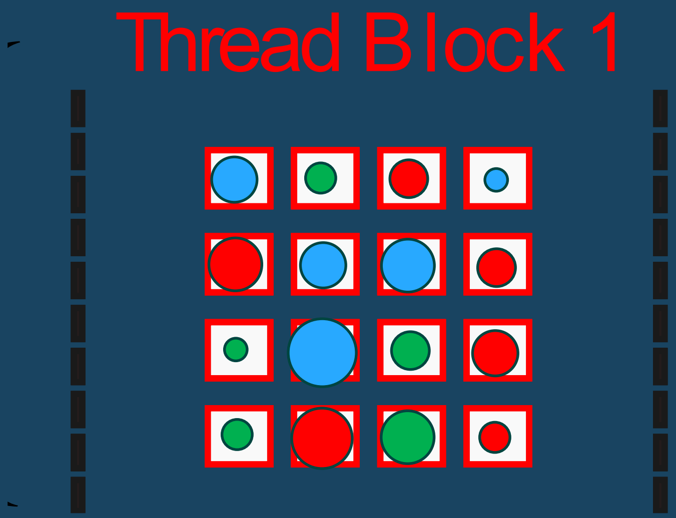
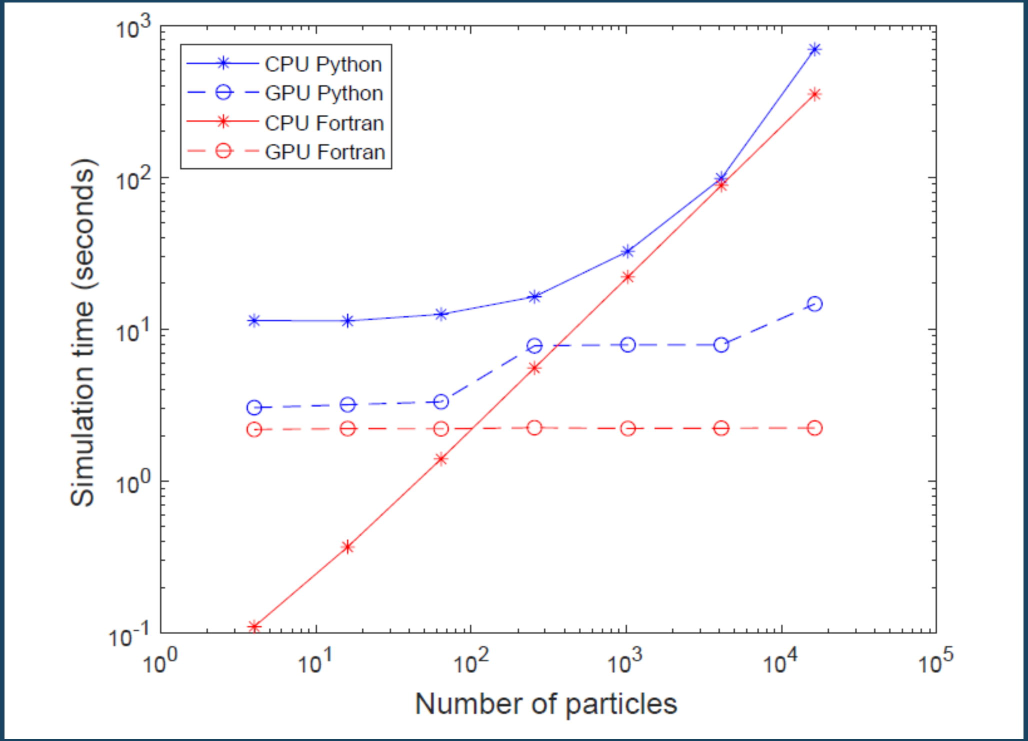


- For 128*128 particles tracked for 100 days at a time step of 100 seconds.
- Python
  - CPU – 696 seconds
  - RTX 3070 GPU – 14 seconds
  - A100 GPU – 1.8 seconds

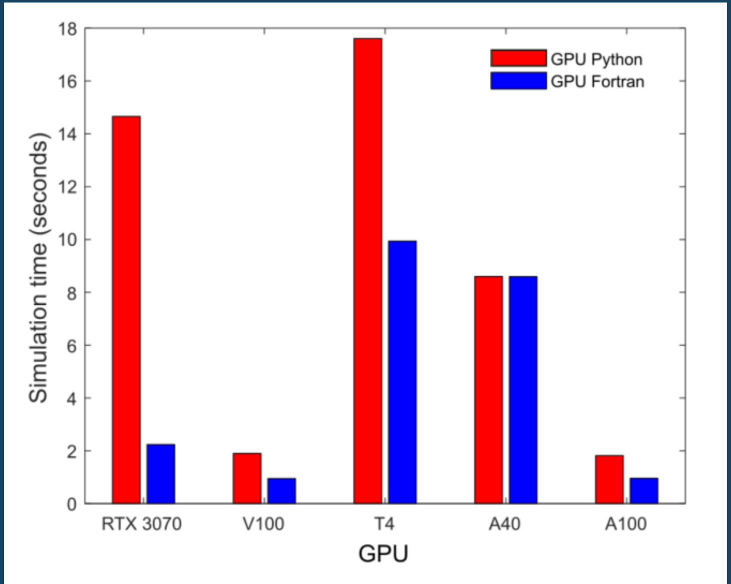
Results

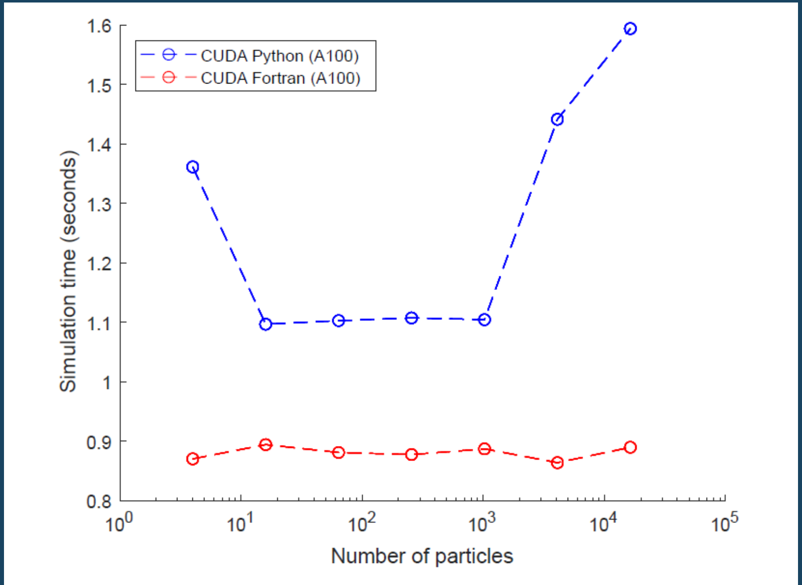
Simulation Time on Nvidia RTX 3070 General Purpose GPU



Results

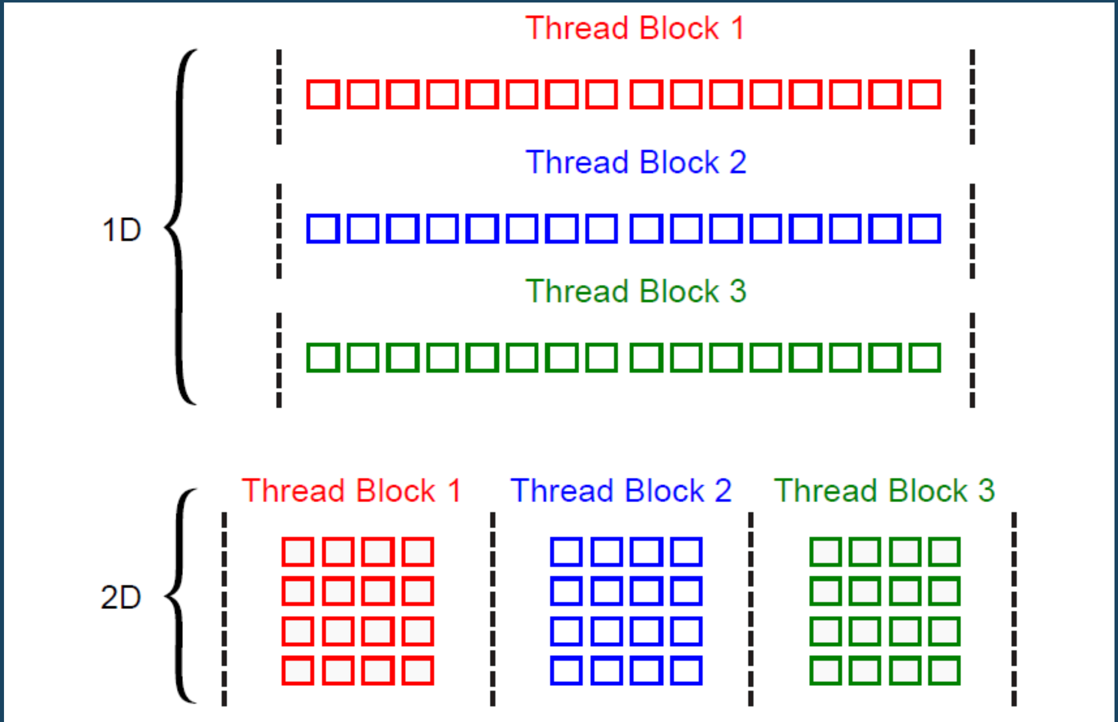
CLUSTER GPU PERFORMANCE COMPARISON (16,384 particles for 100 days)





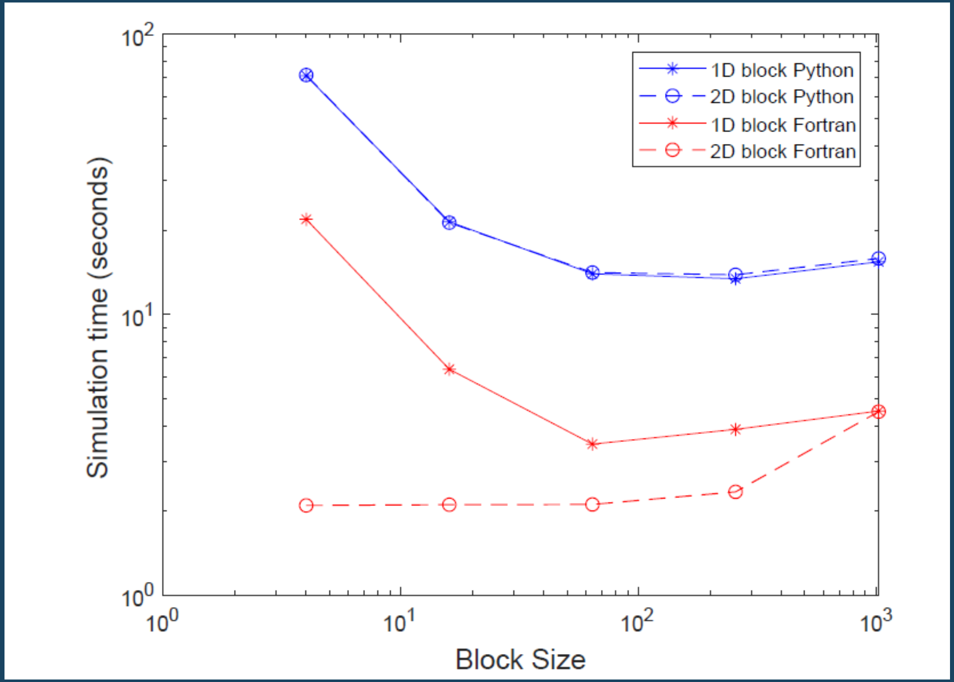
Results

Block size (1D vs 2D)



Results

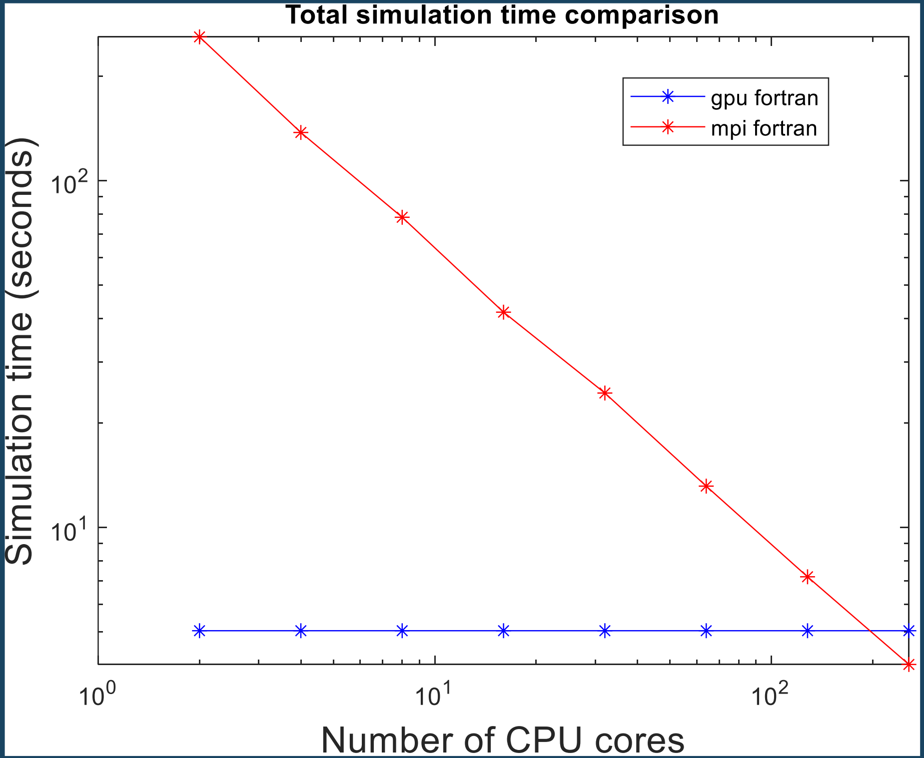
IMPACT OF BLOCK SIZE (256*256 particles for 10000 days without saving results)



A100

Results

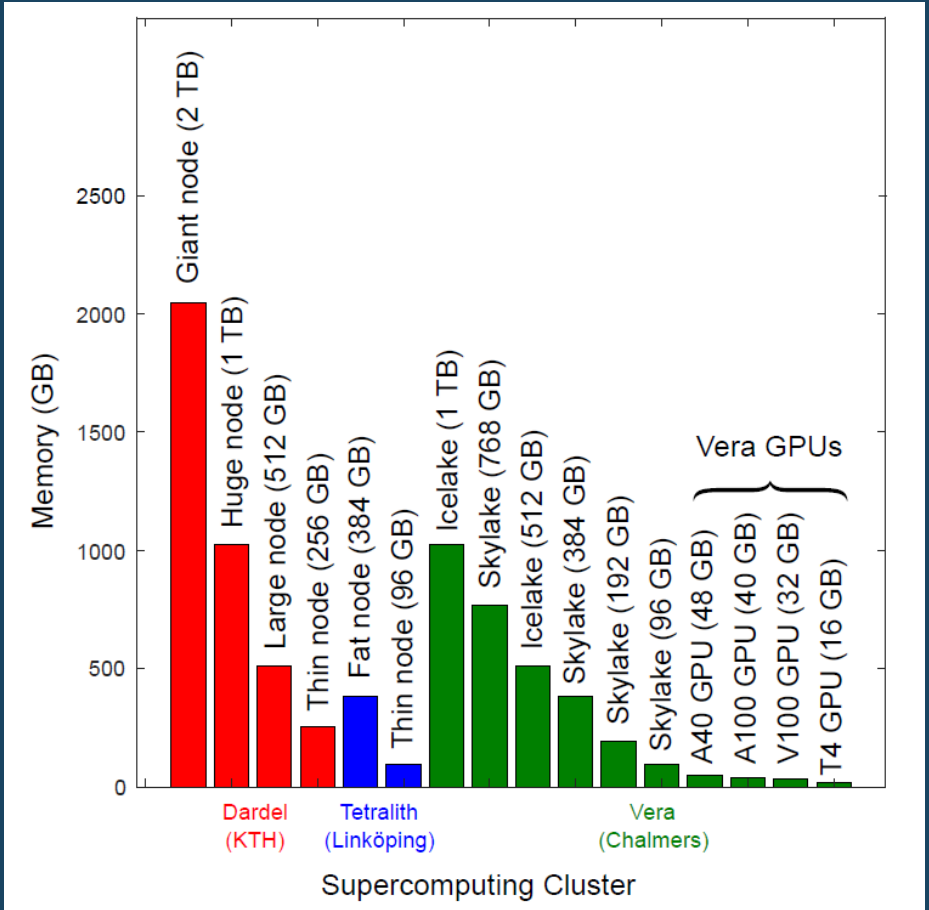
MPI vs CUDA (128*128 particles for 100 days)



- Cross-over point is around 200 CPU cores to match GPU performance.
- On Vera, a V100 GPU costs 80 core hours, and A100 GPU cost 52 core-hours.
- That means there is, at most, potential savings of 120 core hours per hour on V100 and 148 core hours per hour on A100 when running the code on GPU compared to CPU.

Limitations

Limited memory capacity

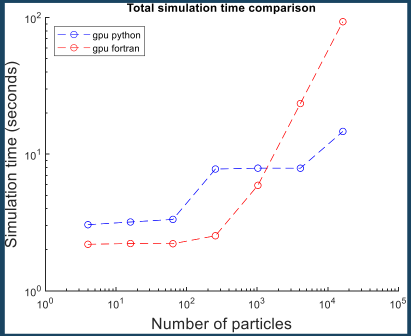


Limitations

Data Transfer Overheads

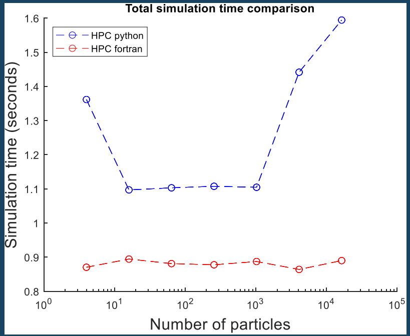
NVIDIA RTX 3070

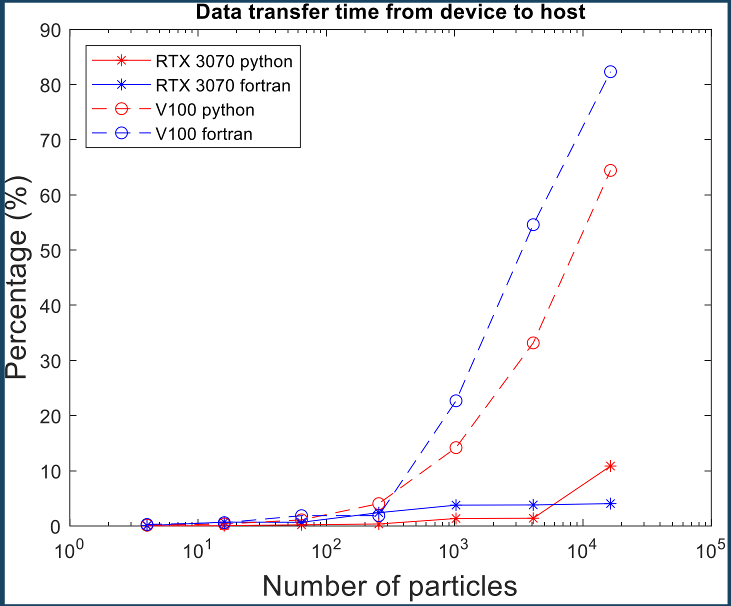
(Math Compute Time)



NVIDIA A100

(Math Compute Time)



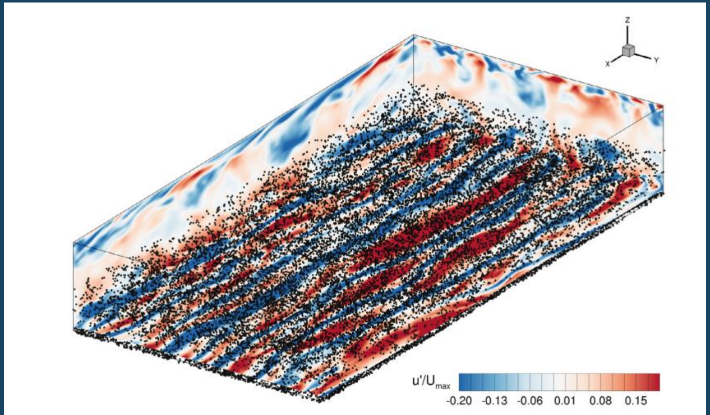


Memory transfer speed affects overall performance?

Limitations

Data Transfer Overheads

GPU acceleration of Eulerian-Lagrangian particle laden flows (Sweet et al.)



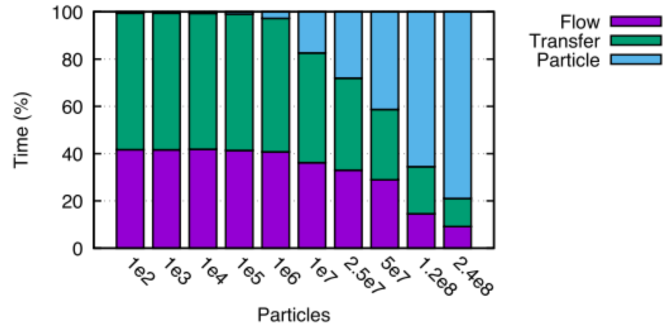


Fig. 5. Percentage breakdown of a single time step for the flow solver (CPU), particle solver (GPU), and transfer time, as a function of particle number.

- Large Scale GPU codes are parallelized across many GPUs.
- Computations are carried out on both CPU and GPU.
- GPU codes developed with NVIDIA's CUDA framework is incompatible with AMD GPUs, which restricts their portability and requires separate implementations for different hardware platforms.

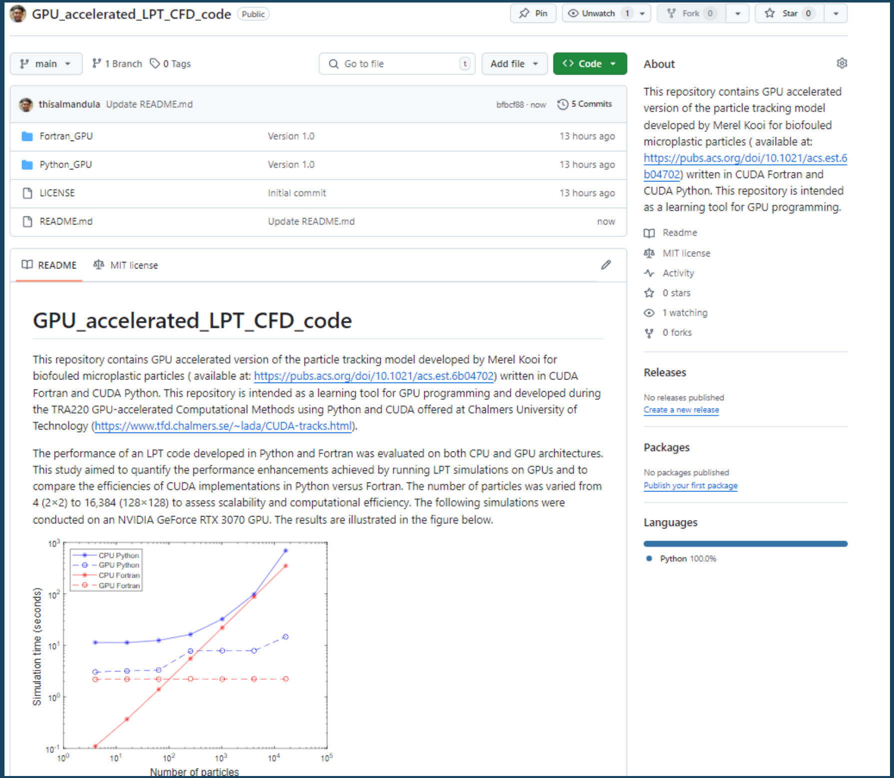
Conclusion

Final Remarks

- Achieved Significant Performance Enhancements by Porting LPT Code to GPU.
  - **CUDA Python:** Attained speedups of up to **350 times.**
  - **CUDA Fortran:** Realized speedups of up to **391 times**.
- Best threads per block structure is 16x16 (256 threads).
- CUDA Fortran is very sensitive to threading structure.
- At the moment, several challenges still hinder GPUs from completely overhauling the CFD Sector.
- Nonetheless, porting CFD codes to GPUs remains a well-funded and actively pursued area of research.

Developed Codes Open Sourced on Gitub

Final Remarks



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