Density Calculation in the Smoothed-Particle Hydrodynamics Method using Parallel Programming

Supercomputing Modelling Final Exam Project
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1 Introduction

$$\rho_{ij} = \sum_{k=0}^{M} \rho_k e^{-\alpha\sqrt{(x_{ij}-x_k)^2+(y_{ij}-y_k)^2+(z_{ij}-z_k)^2}}$$

ρ_k, x_k, y_k, z_k — input data particles density and coordinates
$M = 65536$ — number of particles in input data.
$x_{ij} = -R + 2R\frac{i}{n_x-1}$
$y_{ij} = 0$
$z_{ij} = -R + 2R\frac{j}{n_z-1}$

2 Density Heat Maps

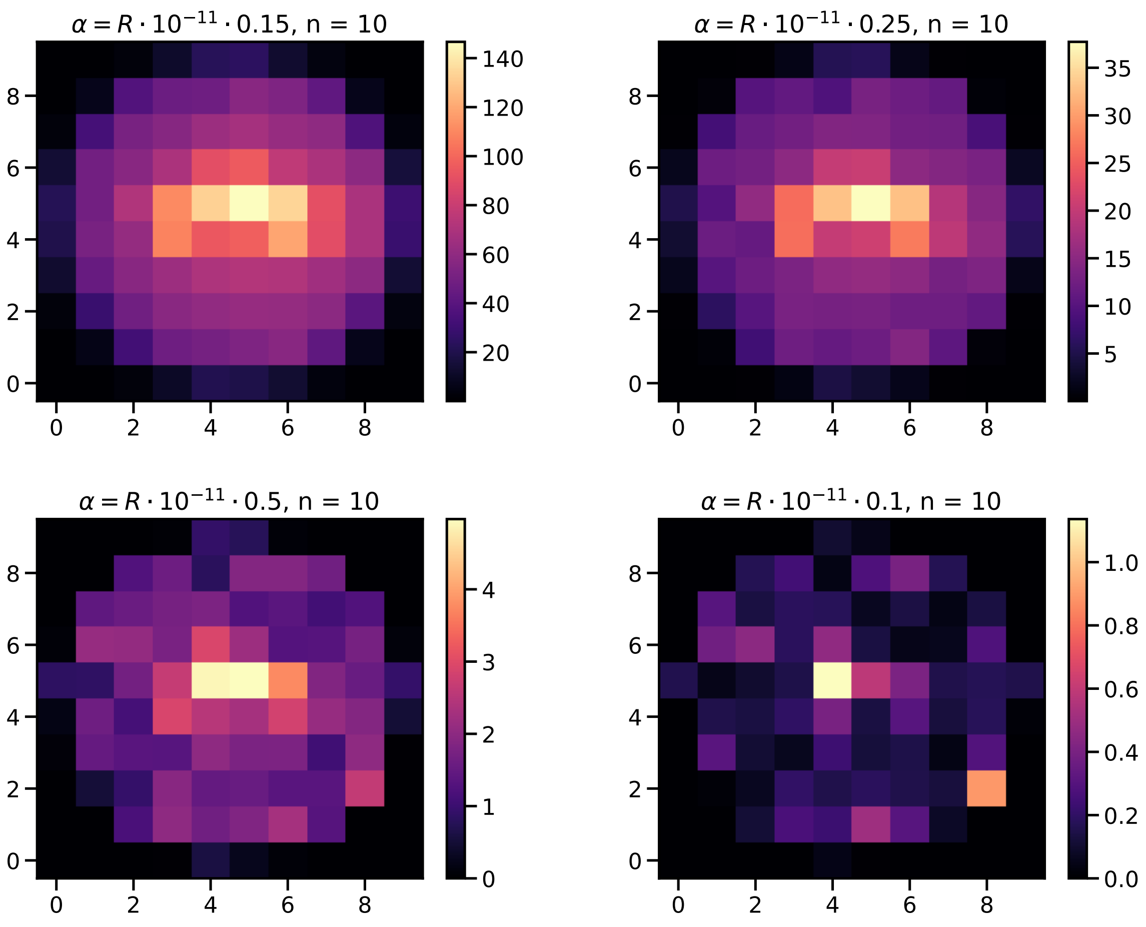


Figure 1: Comparison of the effect of the parameter α for $n_x = n_z = 10$.

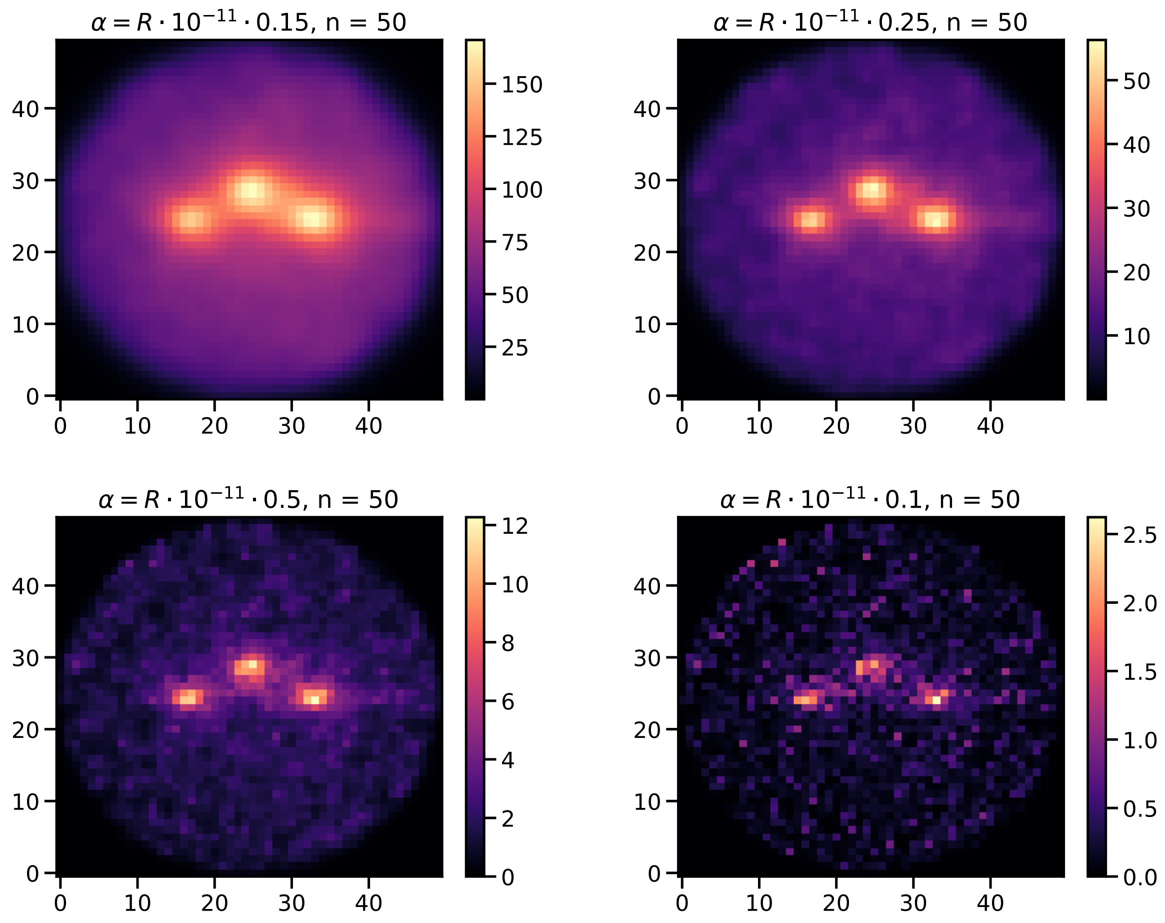


Figure 2: Comparison of the effect of the parameter α for $n_x = n_z = 50$.

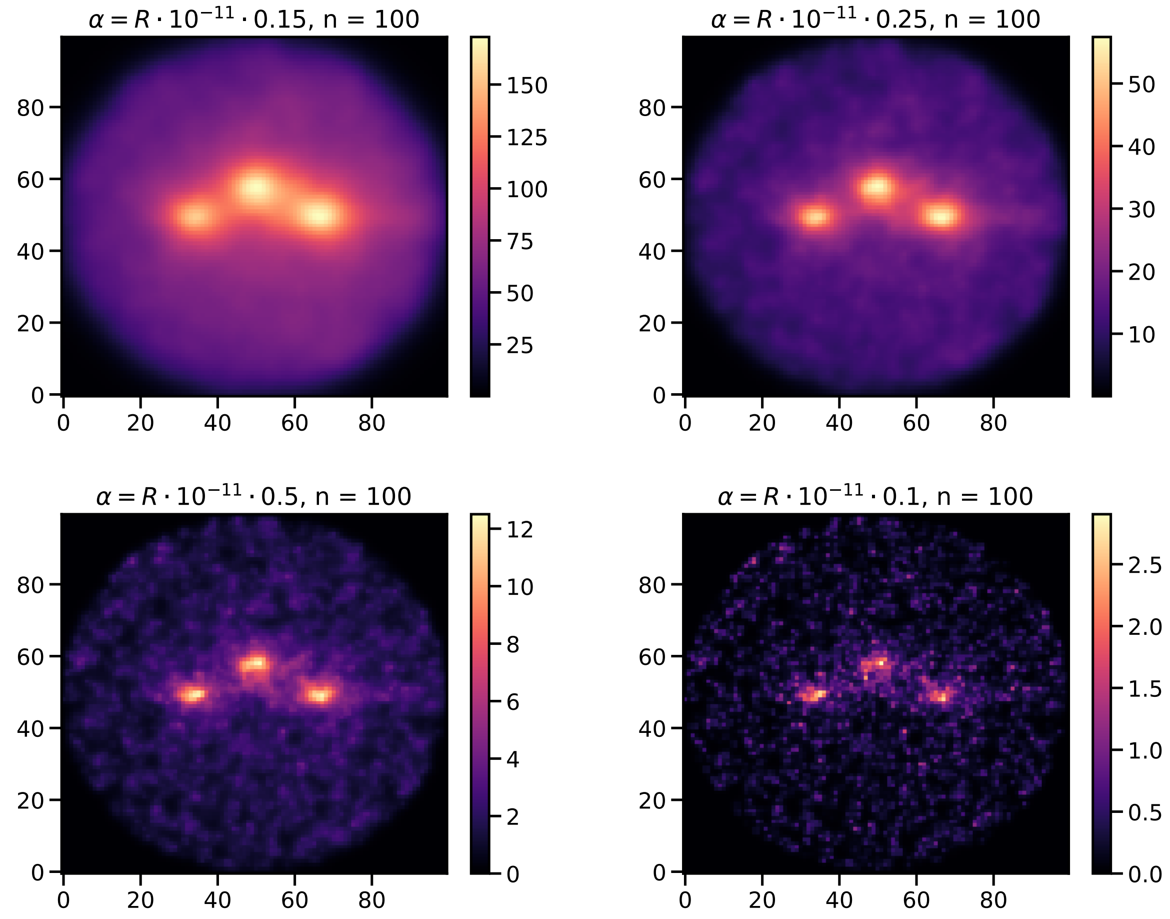


Figure 3: Comparison of the effect of the parameter α for $n_x = n_z = 100$.

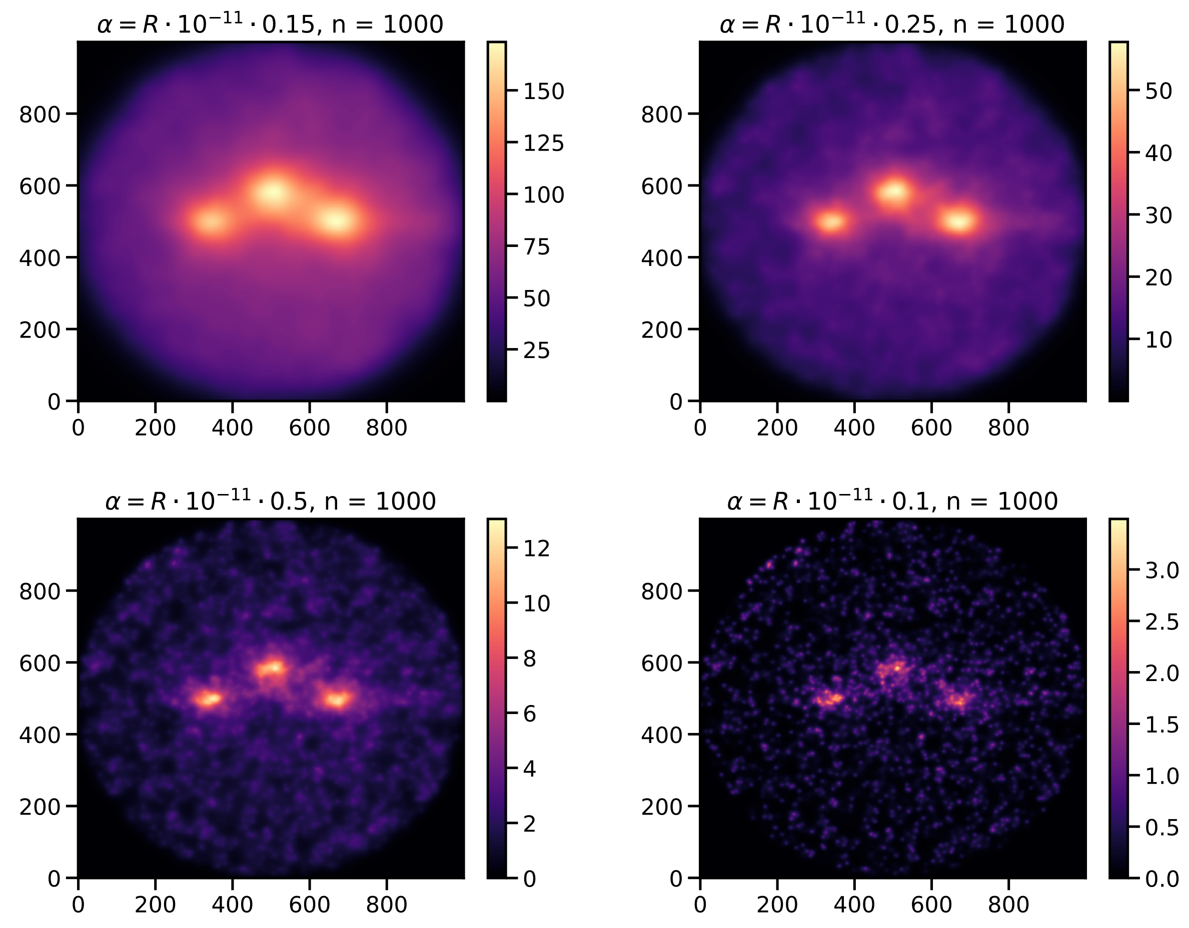


Figure 4: Comparison of the effect of the parameter α for $n_x = n_z = 1000$.

3 MPI Implementation

3.1 Code

Inside main:

```
for (int k = 0; k < 8; k++) {
    // Size of total grid
    int n = n_arr[k];

    // Size of partial grid for each proccess
    int pn = n / size;
    if (n % size != 0)
        pn++;

    double *grid, *partial_grid;

    grid  = new double [pn * size * n];
    partial_grid  = new double [pn * n];

    for (int p = 0; p < 4; p++) {
        double alpha = alpha_arr[p];

        gettimeofday(&t1, 0);
        get_grid(grid, partial_grid, data, pn, n, alpha);
        gettimeofday(&t2, 0);

        if (rank == 0) {
            time = (1.0e6 * (t2.tv_sec - t1.tv_sec) +
                    t2.tv_usec - t1.tv_usec) / 1000.0;
            cout << n << " " << time << endl;
            print_output(grid, n, p);
        }
    }

    delete [] grid;
    delete [] partial_grid;
}
```

Function 'get_grid':

```
void get_grid(double *grid, double *partial_grid, double *data,
    int pn, int n, double alpha) {
    int rank;
    MPI_Comm_rank(MPI_COMM_WORLD, &rank);

    for (int i = 0; i < pn; i++)
        for (int j = 0; j < n; j++)
            partial_grid[i * n + j] = 0;

    for (int i = 0; i < pn; i++) {
        for (int j = 0; j < n; j++) {
            double xij = get_coord((double)(i + rank * pn),
                    (double)n);
            double zij = get_coord((double)j, (double)n);

            for (int k = 0; k < N; k++) {
                double x       = data[k * 4 + 0];
                double y       = data[k * 4 + 1];
                double z       = data[k * 4 + 2];
                double density = data[k * 4 + 3];

                partial_grid[i * n + j] += density * exp(-alpha *
                        sqrt((x - xij) * (x - xij) +
                             (z - zij) * (z - zij) +
                             (y - 0)   * (y - 0)));

            }
        }
    }
    MPI_Gather(partial_grid, pn * n, MPI_DOUBLE, grid, pn * n,
            MPI_DOUBLE, 0, MPI_COMM_WORLD);
}
```

3.2 Time Analysis

$$T_{paral}(P, N) = T_{arithm}(N, P) + T_{comm}(N, P)$$

$$T_{arithm}(N, P) = N \cdot \frac{N}{P} \cdot M \cdot \underbrace{\tau \cdot T}_{\text{cost of arighmetic operations inside loop}}$$

$M = 65536$ — number of particles in input data.
T — number of arithmetic operations.
τ — time for 1 arithmetic operation.

$$T_{comm}(N, P) = \left(\alpha + \frac{1}{\beta} \underbrace{\frac{N^2}{P}}_{\text{message length}} \right) \underbrace{\sqrt{p}}_{\text{torus}}$$

$$S(N, P) = \frac{T_{arithm}(N, P)}{T_{paral}(N, P)}$$

$$E(N, P) = \frac{S(N, P)}{P}$$

Table 1: Constants found through fitting.

Meaning	Notation	Value
Execution time of arithmetic operations within loop	$\tau \cdot T$	$2.32 \cdot 10^{-9}$
Latency	α	$1.18 \cdot 10^{-4}$
Bandwidth	β	$2.06 \cdot 10^{5}$

3.3 Speedup and Efficiency

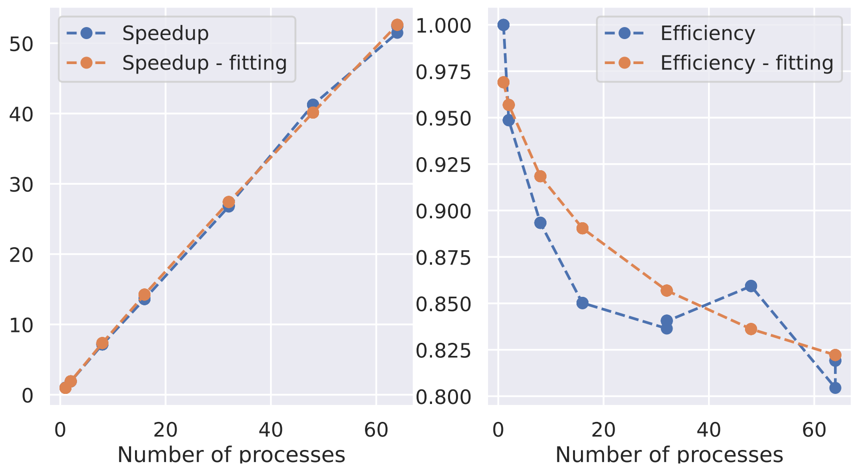


Figure 5: Speedup and efficiency of the MPI implementation

4 OpenACC Implementation

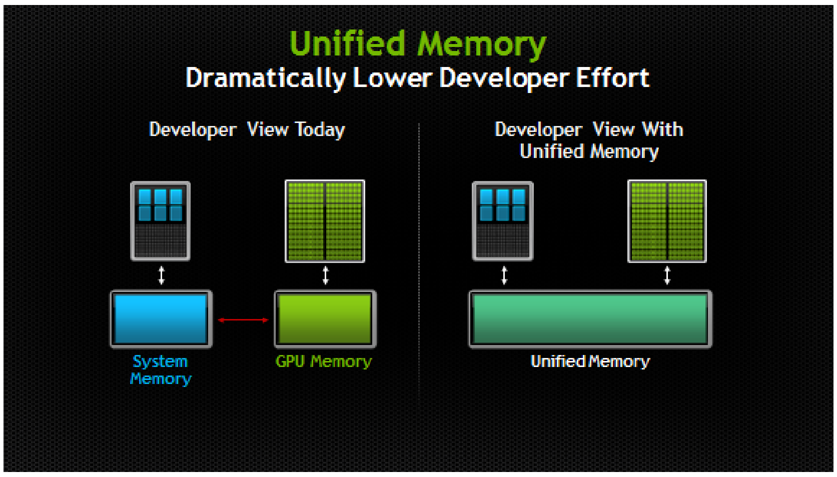
4.1 Code

```
#pragma acc data copyin(data[0:N*4]) copyout(grid[0:n*n])
{
    #pragma acc parallel loop
    for (int i = 0; i < n; i++) {
        #pragma acc loop
        for (int j = 0; j < n; j++) {
            double xij = -R + (double)i / (double)(n - 1) * 2 * R;
            double zij = -R + (double)j / (double)(n - 1) * 2 * R;

            double cell_ij = 0;
```

```
                #pragma acc loop reduction(+:cell_ij)
                for (int k = 0; k < N; k++) {
                    double x       = data[k * 4 + 0];
                    double y       = data[k * 4 + 1];
                    double z       = data[k * 4 + 2];
                    double density = data[k * 4 + 3];
                    cell_ij += density * exp(-alpha *
                        sqrt((x - xij) * (x - xij) +
                             (z - zij) * (z - zij) +
                             (y - 0)   * (y - 0)));
                }
                grid[i * n + j] = cell_ij;
            }
        }
    }
```

4.2 Compiling: Unified Memory



```
pgc++ -lstdc++ -O2 -Wall -std=c++11 -acc -ta=nvidia:managed -Minfo=accel
```

The 'managed' option lets us use Unified Memory.

Unified Memory creates a pool of managed memory that is shared between the CPU and GPU, bridging the CPU-GPU divide. Managed memory is accessible to both the CPU and GPU using a single pointer. The key is that the system automatically migrates data allocated in Unified Memory between host and device so that it looks like CPU memory to code running on the CPU, and like GPU memory to code running on the GPU.

5 Time Metrics and Comparison between MPI and OpenACC Implementations

Table 2: Time Comparison in ms

n	CPU Sequential	GPU - OpenACC Unified Memory	GPU - OpenACC
10	28.32 ± 4.99	6.01 ± 0.33	132.39 ± 15.76
20	42.46 ± 0.17	21.67 ± 0.02	140.18 ± 14.40
50	201.92 ± 0.75	133.44 ± 0.56	186.12 ± 2.37
100	604.44 ± 7.37	530.51 ± 0.54	261.90 ± 10.90
250	2975.23 ± 0.19	3340.00 ± 12.82	1012.77 ± 18.90
500	10938.35 ± 28.79	13524.73 ± 15.61	3655.64 ± 86.08
750	23834.98 ± 35.10	30457.03 ± 13.72	8085.92 ± 145.40
1000	41643.85 ± 1.59	54320.40 ± 19.08	13032.73 ± 70.97

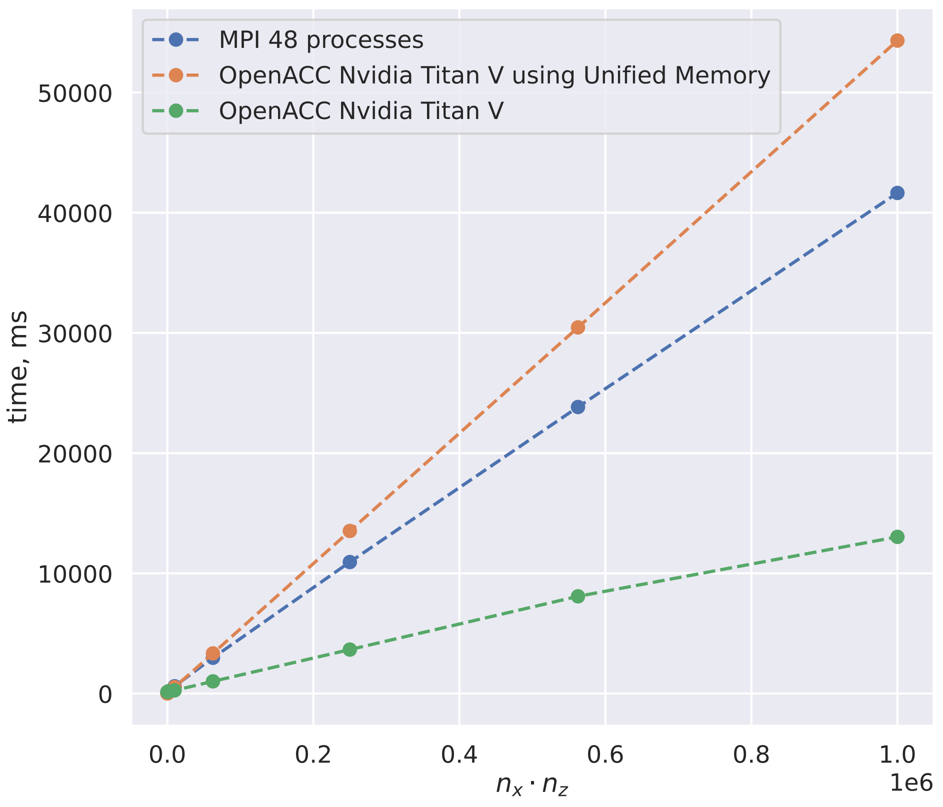


Figure 6: Dependence of the run time at maximum optimization for different values of $n_x \cdot n_z$ for MPI and OpenACC implementation.

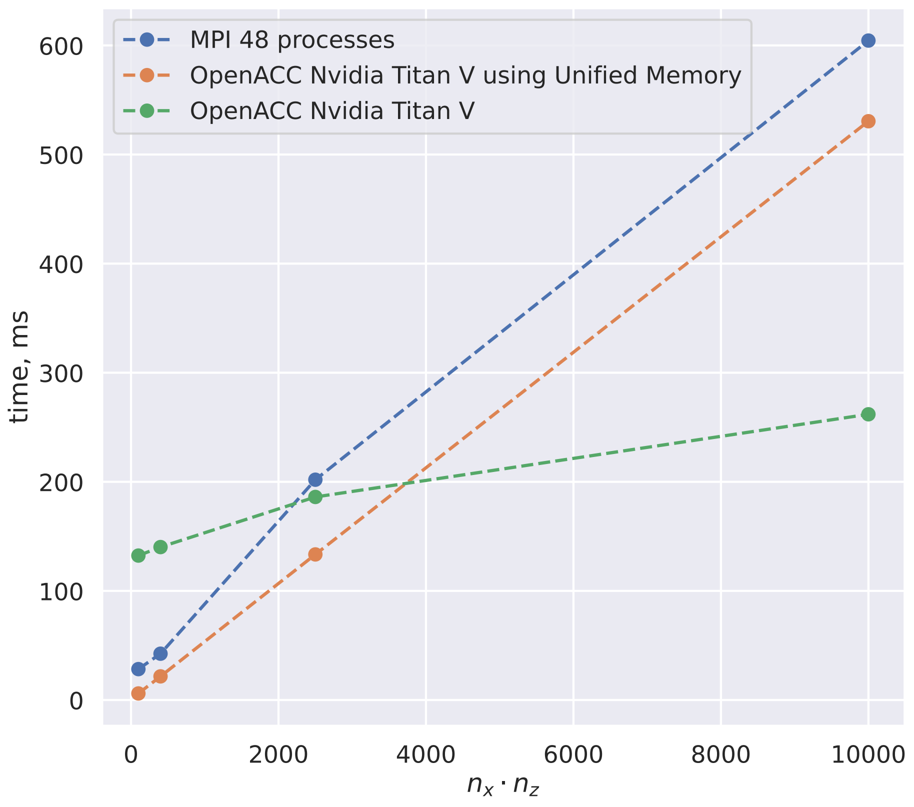


Figure 7: Dependence of the run time at maximum optimization for small values of $n_x \cdot n_z$ for MPI and OpenACC implementation.