

SPH – A COMPARISON OF NEIGHBOR SEARCH METHODS BASED ON CONSTANT NUMBER OF NEIGHBORS AND CONSTANT CUT-OFF RADIUS

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Abstract: Two methods of neighbor search for the SPH algorithm are presented, based on a constant number of neighbors and a constant cut-off radius. First, feasible methods of comparison were analyzed. Then, the two selected methods were compared visually and computationally. Considering the use of the SPH algorithm for simulating incompressible fluids, the obtained results suggest that the method with a constant cut-off radius is better than that with a constant number of neighbors. The simulation results of both methods are practically indistinguishable, while the computational costs favor one of them.

Keywords: SPH, simulations, incompressible fluids, constant cut-off radius method, constant number of neighbors method, breaking dam, side gap, time effectiveness

1. The goal of comparison

Two methods used in the SPH algorithm for creating a list of neighbors for each particle have been analyzed. A variable range of interactions was used in the original SPH method in order to create a list of neighbors of approximately the same size for each particle [1]. As a result, a mechanism was obtained automatically adjusting the range of interactions. The greater the number of neighboring particles and their density, the lower the range of inter-particle interactions; the more rarely the particles are distributed, the larger the distance of interactions. This manner of neighbor search was devised and adopted for cosmological SPH simulations [2]. In

such simulations density assumes a wide range of values and the application of this method is well justified. However, in simulations of incompressible fluids, this method of neighbor search is not the best solution, since particle density is nearly constant in such simulations. Therefore, the condition of each particle having the same number of neighbors can be achieved by implementation of the constant cut-off radius method. A comparison of these two methods should determine which is more advantageous when applied to a specific simulation.

2. The algorithms

The algorithms differ in the way neighboring particles are chosen for each particle. Both algorithms use a cubic cell structure comprising the computational box. Neighboring particles are chosen only from the current cell and the cells surrounding it, *i.e.* 26 neighboring cells. A list of particles located inside the cell and a list of particles located in the neighborhood of the current cell (in total 27 cells) are created for each time step of the implemented simulation.

Table 1. The description of “constant N ” and “constant r_{cut} ” algorithms

constant N	constant r_{cut}
The evaluation of new particles' positions and velocities.	The evaluation of new particles' positions and velocities.
The list of particles from 27 neighboring cells is sorted with respect to distances from particle i . The closest N particles are assumed to comprise the list of neighbors of particle i .	The neighbor of particle i is any particle j such, that distance between them is smaller than the cut-off radius r_{cut} .
Basing on interparticle interactions new particles' accelerations are evaluated.	Basing on interparticle interactions new particles' accelerations are evaluated.

A short description of a single simulation step for both algorithms is given in Table 1.

In the method with a constant number of neighbors, there is no need to sort the whole list. The list may be split into two parts only, one containing N closest neighboring particles and the other containing the rest [2]. Ordering of neighboring particles in any of these two parts is irrelevant. The cut-off radius of each particle is assumed to be the distance from its farthest neighbor. As the distance may vary for various particles, all particles may have different cut-off radii.

In the method with a constant cut-off radius, each particle may have a different number of neighbors. This is a consequence of the fact that particle density can vary in time and space and so the number of particles inside the sphere of radius r_{cut} and centered on a given particle, *i.e.* the number of neighbors, varies as well.

3. Differences in the algorithms

3.1. Symmetry of neighborhood

In the method with a constant cut-off radius, the neighborhood relation:

$$(i \text{ is neighbor of } j) \Leftrightarrow (j \leftrightarrow i)$$

of two particles is symmetric: $(j \leftrightarrow i) \Rightarrow (i \leftrightarrow j)$. Unfortunately, this is not true in the case of the method with a constant number of neighbors, where there is no fixed, global cut-off radius for all particles. Instead, each particle is assigned its own cut-off radius, $r_{\text{cut},i}$, which can vary in time. Therefore, there can be two particles i and j that $r_{\text{cut},i} < r_{ij} < r_{\text{cut},j}$. This implies $(j \leftrightarrow i) \wedge \neg(i \leftrightarrow j)$, which means that the neighborhood is not symmetric in this case.

This causes some difficulties: since particle i , as a neighbor of particle j , acts with force on this particle, particle j does not react with force on particle i as it is not in the list of neighbors of particle i . This violates Newton's third law and violates the principle of conservation of momentum. When particles i and j are mutually neighbors but have different cut-off radii assigned, Newton's third law will be violated as well. In such a case, forces experienced by particles would have different values. In order to fulfill Newton's third law, the kernel function, W_{ij} , of the SPH algorithm is symmetrized [3]. The implemented symmetrization is given by the following formula:

$$W_{ij} = \frac{1}{2}(W(r_{ij}, h_i) + W(r_{ij}, h_j)). \quad (1)$$

3.2. Particles' behavior close to the surface

When the method with a constant number of neighbors is applied, particles located close to the fluid's surface are assigned greater interaction ranges than those located further from the surface. This is a consequence of the particles tendency to collect the same, fixed number of neighbors, irrespective of their location. As the number of particles inside a sphere of radius equal to the interaction range located close to the surface is smaller than that inside a sphere of the same radius located further from the surface, the radius of the sphere should be enlarged.

3.3. The size of cells

In both methods, distances between pairs of particles should be evaluated when building the list of neighbors. Such evaluation may be very expensive in terms of computation when there are many pairs of particles to process. Therefore, it is essential to adjust the size of cells so that the number of particles processed in the neighbor search procedure is as small as possible.

When using the method with a constant cut-off radius, the size of cells (length of the cube's edge) should be equal to the largest cut-off radius used in the simulation. If the size is larger, there can be additional, expendable particles inside the neighboring 27 cells. The distance to these particles, evaluated in the neighbor search procedure, would certainly be larger than the interaction range. Therefore, evaluation of distances to these particles can be omitted, since the list of neighbors is the same as when the cell size equals the largest cut-off radius.

Adjusting the size of cells in the method with a constant number of particles is not so straightforward. The first guess is a radius given by Equation (2). However, because neighbors of an SPH particle may be arranged in an irregular, non-symmetric way, there are three possible situations:

- there are less than N SPH particles in the surrounding 27 cells;
- there are N or more SPH particles in the surrounding 27 cells, but the list of neighbors is different, when the size of cells is greater;

- there are N or more SPH particles in the surrounding 27 cells, and the list of neighbors remains the same if size of cells is greater.

The latter situation, the most desirable, is not always the case for cell size equal to r_N . Therefore, when comparing neighbor search procedures, a cell size of $1.26r_N$ was used (so that the cell's volume is doubled). Of course, this is a compromise, since the volume of the sphere of N neighbors in the corners of the box containing the fluid should be 4, or even 8 times greater.

4. The method of comparison

In order to compare two methods, the simulations' parameters should be matched. In particular, the number of neighbors, N , in the method with a constant number of neighbors and the cut-off radius (interactions range), r_{cut} , in the method with a constant cut-off radius should be matched. There is no need to compare the methods' computational times when the number of neighbors in one of them does not fit the number of neighbors in the other. The size of input data should be equal when comparing computational time. Therefore, apart from setting the same values of parameters such as viscosity, time step, *etc.*, it is necessary to match the N and r_{cut} parameters in the run simulations.

If the volume of fluid, V_{SPH} , assigned to a single SPH particle is known, the relation of these parameters is given by:

$$\frac{4}{3}\pi r_{\text{cut}}^3 = N \cdot V_{\text{SPH}}. \quad (2)$$

This equation may also be validated by in a simulation. Several simulations were run for the method with a constant number of neighbors, N , and the average cut-off radius, r_{cut} , was evaluated for each of them. Similarly, several simulations were run for the method with a constant cut-off radius, r_{cut} , and the average number of neighbors, N , was evaluated for each. The results are shown in Figure 1.

There are three plots shown in Figure 1:

- $r_{\text{cut}}(N)$ – the graph of cut-off radius, r_{cut} , in a function of N obtained from a series of simulations with the method with a constant number of neighbors;
- $N(r_{\text{cut}})$ – the graph of number of neighbors, N , in a function of r_{cut} obtained from a series of simulations with the method with a constant cut-off radius;
- th – the graph of the formula (2).

Both empirical relations shown in Figure 1 fit together, while the graph of the formula (2) is different, most probably because the formula (2) does not cover all the factors of the simulation. This discrepancy seems to be a result of dependences of r_{cut} and N occurring close to the fluid surface (corners and borders of the box, free surface), where there are less particles inside the sphere with radius r_{cut} than might be evaluated from the above formula.

While comparing the methods' computational times, the empirical relation was used instead of the theoretical one (the formula (2)). The empirical relation, obtained from the simulations' results, is more precise than the theoretical one, as it takes into account also additional factors, not present in the theoretical equation. However, this relation cannot be used in every situation. There is no use to apply it when the

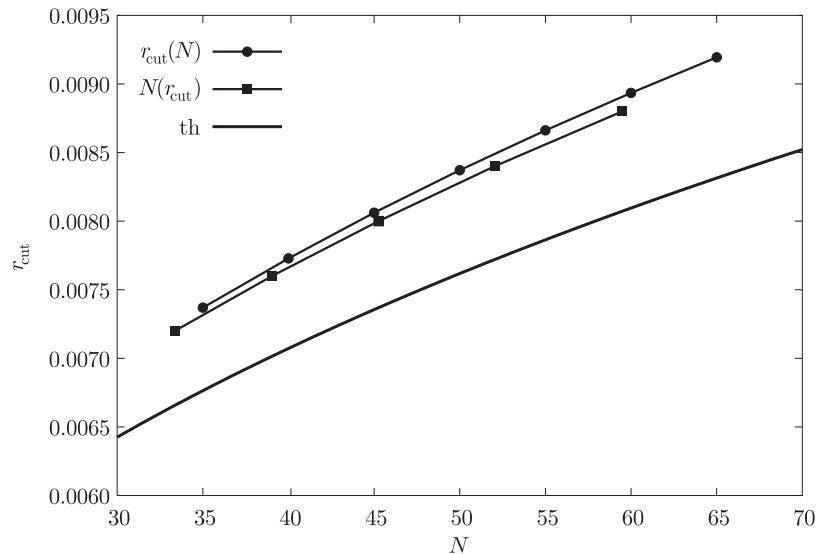


Figure 1. The relation between cut-off radius, r_{cut} , (in program units) and the number of neighbors, N

shape of the box (and fluid) changes so that the surface to volume of fluid ratio is significantly changed.

The results of two series of simulations were used for fitting the curve and finding its coefficients, *i. e.*:

$$N = 1.33 \cdot 10^8 \cdot r_{\text{cut}}^3 - 1.42 \cdot 10^6 \cdot r_{\text{cut}}^2 + 1.3 \cdot 10^4 \cdot r_{\text{cut}} - 37. \quad (3)$$

The above relation was used while comparing two methods.

5. Visual comparison of the methods

Snapshots of two simulations run with the same parameters but different neighbor search methods are shown in Figures 2 and 3 so that the methods' operation when simulating the breaking dam phenomenon and the phenomenon of fluid flowing out of the box through a gap in its side can be compared visually. The minor differences visible in the snapshots are irrelevant for the simulated phenomena.

In Figures 2 and 3 densities of particles are marked in color. Each color from dark-blue to red has a value of density assigned to it: the closer to red, the greater the density.

Density ranges from 995 kg/m^3 to 1005 kg/m^3 . Although the simulated fluid is assumed to be incompressible, densities differ from the assumed 1000 kg/m^3 – dark-blue and red particles are visible. This is a consequence of the nature of the computational method used in the simulation and the applied equation of state, where the hydrodynamic force depends on the particle's to fixed, global density ratio. When these densities are equal, there is no hydrodynamic force.

According to the applied equation of state, the value of pressure (and the value of the hydrodynamic force) depends on the speed of sound. In simulations shown in Figures 2 and 3 the authors purposefully used values much smaller than the actual

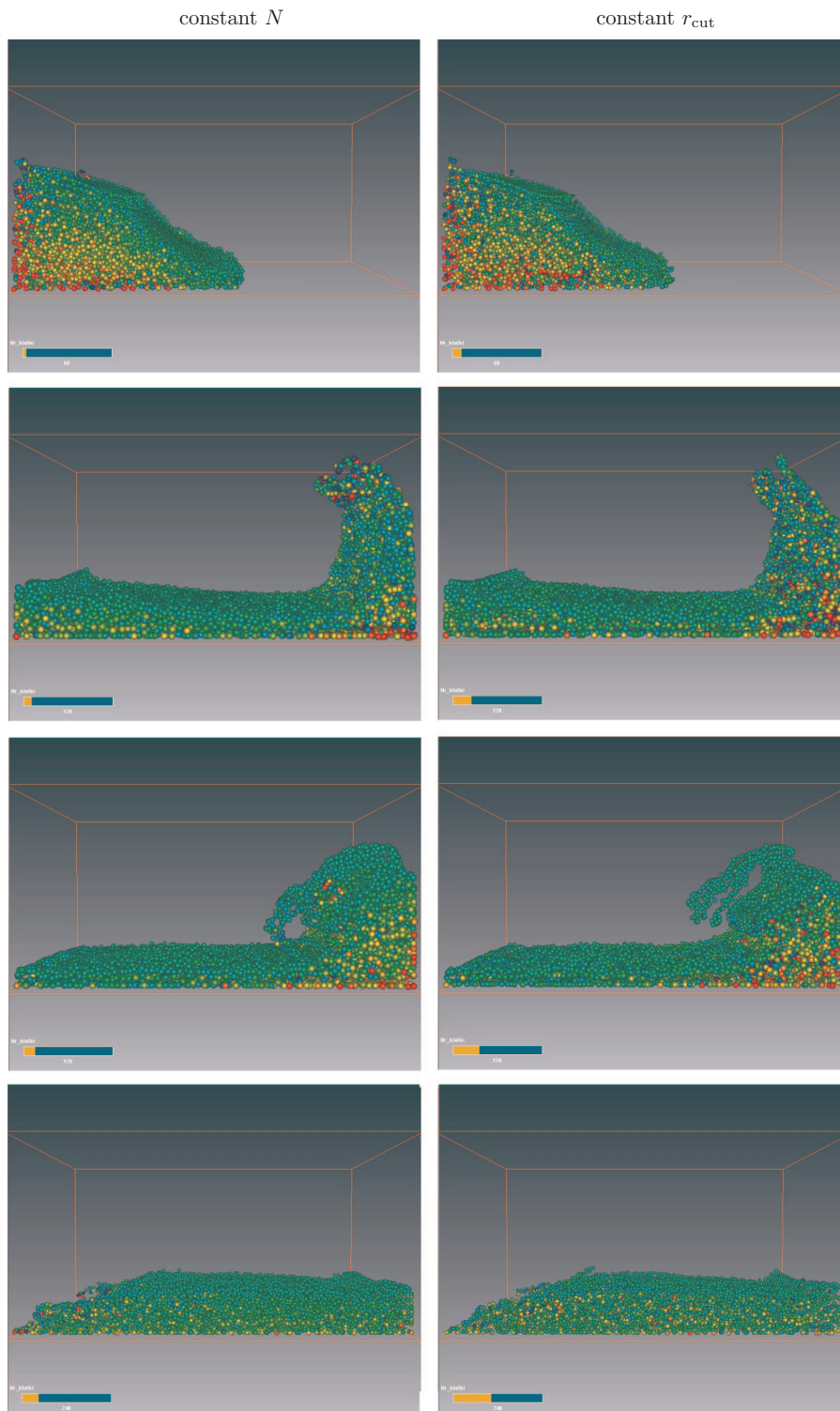


Figure 2. Comparison of two different neighbor search methods: the breaking dam simulation

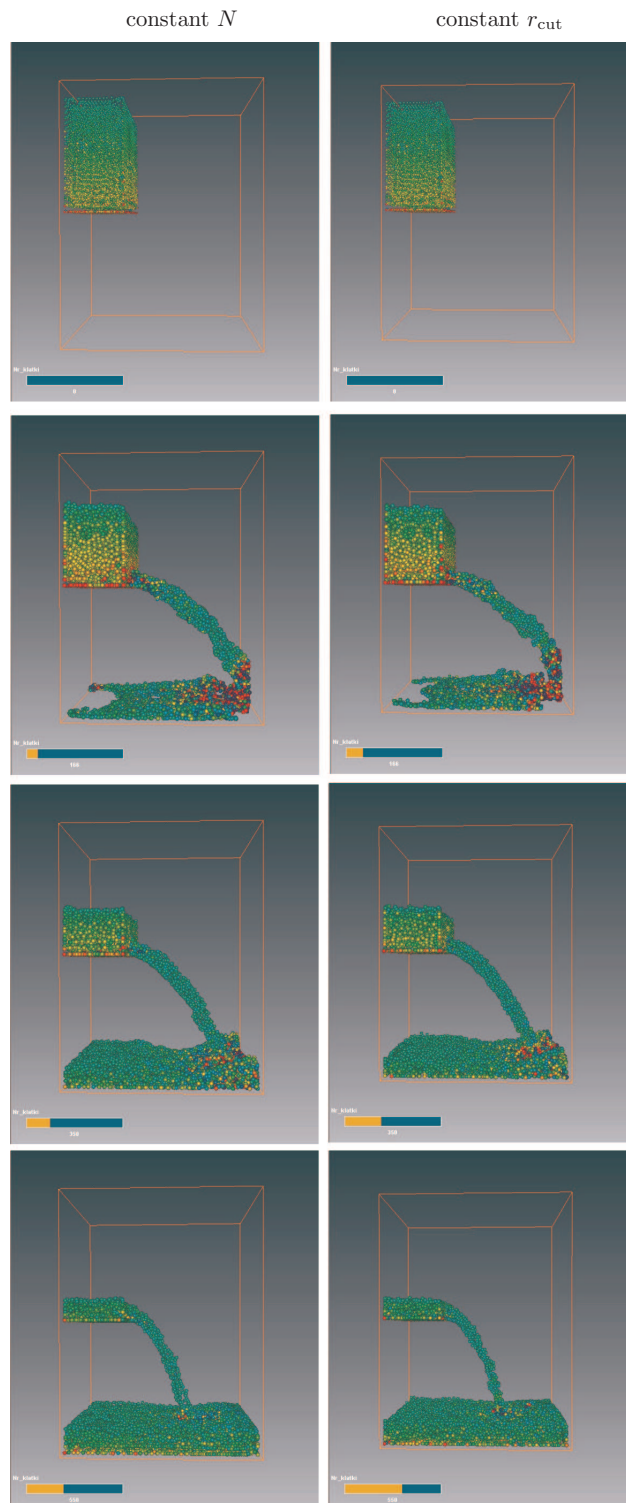


Figure 3. Comparison of two different neighbor search methods: the 'side gap' simulation

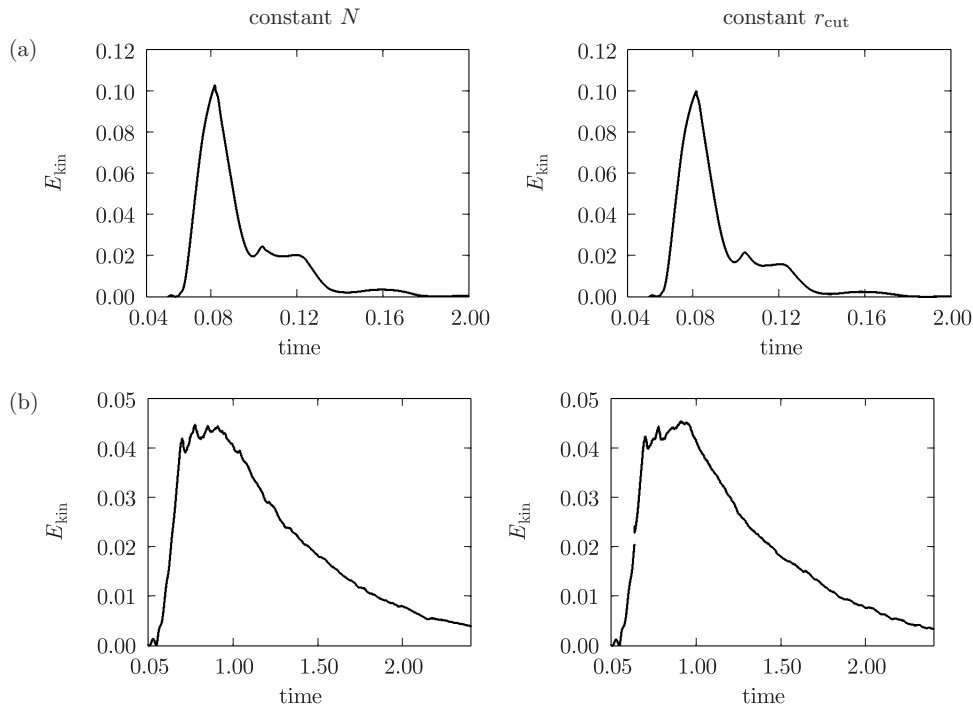


Figure 4. Comparison of kinetic energy of the system (in program units) during a simulation for two different phenomena: (a) breaking dam, (b) a gap in the side

one (15m/s instead of 1500m/s). The actual value of the speed of sound implies such a time step so small that it is completely useless for practical reasons [4].

Plots of the system's kinetic energy for both compared methods and two different phenomena are shown in Figure 4; there is no significant difference in the compared methods' results.

6. Comparison of computational time

In addition to visual comparison, the computational times of both methods were compared. Calls to function `gettimeofday()` were put into the source code of the simulation, which measured the execution time of the main parts of the simulation's loop in every step.

The measured time of the neighbor search procedure during the whole period of simulation is shown in Figure 5. This simulation was run in order to model the breaking dam phenomenon. The computational time of the neighbor search procedure is almost constant during the whole period of simulation: it is independent of the dynamics of the currently modeled fluid. We therefore assumed that computational times of procedures might be measured in any step of the simulation.

Two simulations were run with the same sets of parameters but different neighbor search methods in order to compare their computational time. The number of neighbors and the cut-off radius were fixed by means of the formula (3). The main loop of the simulation was divided into five parts:

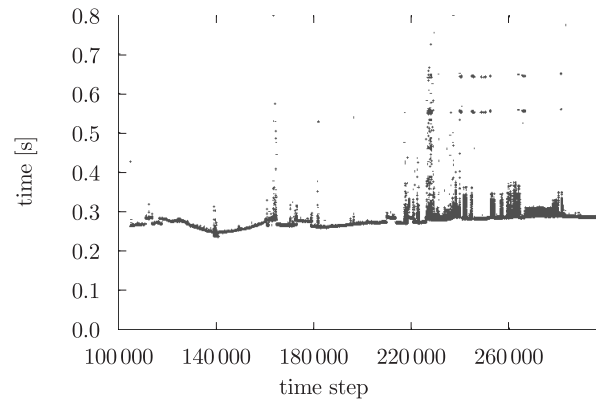


Figure 5. Computational time of the neighbor search procedure during the whole simulation period

- **moving** – new positions and velocities are evaluated,
- **collecting** – auxiliary procedure building lists of neighboring particles,
- **neighbors** – lists of neighbors are created in this procedure,
- **force-density** – new accelerations and densities are evaluated,
- **stats** – auxiliary procedure printing system’s kinetic energy.

For all parts of the main loop the execution time was measured for both types of neighbor search procedures. The results are shown in Figure 6.

There are three types of results for both plots shown in Figure 6: one concerns the method with a constant cut-off radius, another – the method with a constant number of neighbors with cell size equal to the cut-off radius obtained for the assigned number of neighbors, and yet another – the same method with cell size equal to 1.26 times the cut-off radius obtained for the assigned number of neighbors. Only the first and last of these results should be compared, the second is given as a reference only.

It follows from Figure 6 that:

- only the neighbor search procedure’s execution time is significantly affected,
- the neighbor search procedure is much more effective for a constant cut-off radius than for a constant number of neighbors (the constant cut-off radius procedure requires only evaluation of distances and their comparison, the other method additionally requires a sorting procedure).

After summing computational times for all parts of the simulation’s main loop, the execution time of the constant cut-off radius method is 1.5–2.5 times better than that of the method with a constant number of neighbors. The exact relation of this difference to the number of neighbors (for cases with a constant cut-off radius and with a constant number of neighbors where cell size was multiplied by 1.26) is shown in Figure 7.

7. Conclusions

As far as the SPH method is used to simulate incompressible fluids, the neighbor search method based on a constant cut-off radius is superior to the method

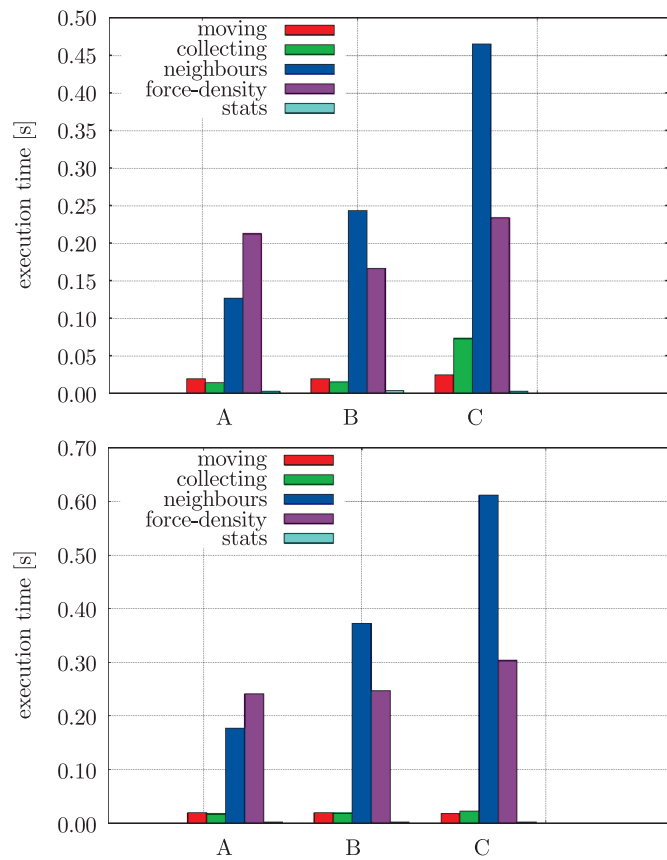


Figure 6. Computational time comparison for $N=35$ (top) and $N=55$ (bottom), $r_N=r(N)$, and for various method types: A – constant r_{cut} ; B – constant N ($L=r_N$); C – constant N ($L=1.26r_N$)

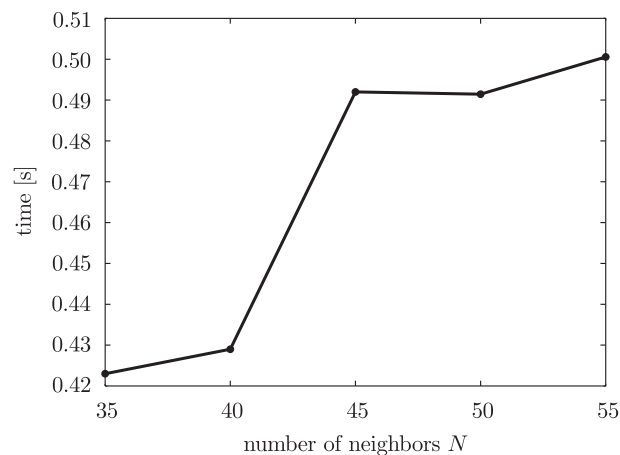


Figure 7. The difference in execution time with regard to the number of neighbors

with a constant number of neighbors. The results of both methods are practically indistinguishable, while computational costs favor the method with a constant cut-off radius. The method with a constant number of neighbors is still preferable

when applied to simulate compressible fluids, for which densities can vary without limitations. A variable cut-off radius is then desirable which can be easily achieved by implementation of the constant number of neighbors method.

Another advantage of the constant cut-off radius method is that no “zero-energy mode” effect has been observed there, in contrast to the method with a constant number of neighbors. This effect, observed as fast oscillations of pressure, disturbs the results and makes fluid behave in a way different than in reality. However, the authors have not analyzed the reasons of the increased vulnerability of the method with a constant number of neighbors to this effect; this remains a potential subject of future work.

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