Prof. Dr. O. Rheinbach
Dipl.-Math. F. Röver
Institut für Numerische Mathematik und Optimierung
TU Bergakademie Freiberg

HPC Project WS18/19

We want to simulate the motion of n particles, which interact through a force, e.g., gravitity.

The movement of each particle results from the gravitational forces of all others particles.

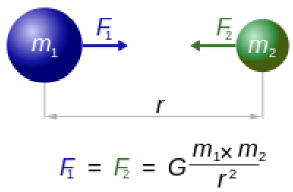
The acceleration a is related to the force F through the well-known relation $F = ma$, where m is the mass of the particle. Each particle's position and velocity are advanced forward in time, here using a very simple numerical scheme. Repeating the process, we simulate the motion of the particles over time.

A sequential pseudo-code can be found in Algorithm 1. The complexity of the algorithm is $O(n^2)$.

Write a parallel programm to perform the simulation using MPI and perform (and document) weak and strong parallel scalability tests on the TUBAF cluster. Choose a reasonable time step size dt, a reasonable number of particles (large enough), and number of time steps.

What are your observations concerning the parallel scalability?

For debugging it is advisable to create output for the movement of the particles which can be visualized using an external tool, e.g., Matlab, Gnuplot, or Paraview. For the scalability tests the output should be switched off.



Source:`https://de.wikipedia.org/wiki/Newtonsches_Gravitationsgesetz`

```
n = Number of particles in simulation;
for i = 0...n do
    ax = 0.0;
    ay = 0.0;
    az = 0.0;
    for j=0...n do
        Δx = x[j]-x[i];
        Δy = y[j]-y[i];
        Δz = z[j]-z[i];
        invr = 1.0/√(Δx² + Δy² + Δz² + eps);
        invr3 = invr³;
        f=m[j]*invr3;
        ax += f*Δx;
        ay += f*Δy;
        az += f*Δx;
    end
    xnew[i] = x[i] + dt*vx[i] + 0.5*dt*dt*ax;
    ynew[i] = y[i] + dt*vy[i] + 0.5*dt*dt*ay;
    znew[i] = z[i] + dt*vz[i] + 0.5*dt*dt*az;
    vx[i] += dt*ax;
    vy[i] += dt*ay;
    vz[i] += dt*az;
end
for i = 0...n do
    x[i] = xnew[i];
    y[i] = ynew[i];
    z[i] = znew[i];
end
```

Algorithm 1: Particle Simulation