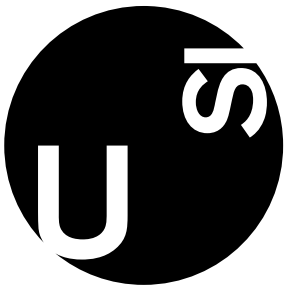

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Implementing Fluid Dynamic Simulation using DPD Method

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Abstract

Digital simulations are useful tools to visualize results, extract information and simulate physical phenomena. There are many methods that can be used to create simulations and each have their own advantages and flaws. One main characteristic to differentiate these types is the length-scale: atomistic models can be used to represent materials and physical objects at the atomic level, leading to precise but computationally expensive simulations; macroscopic models are focused instead on bigger systems, with the advantage of being less computationally demanding. DPD (Dissipative Particle Dynamics) is a method that stands in between the aforementioned scales. By considering groups of atoms as particles we can simulate a fluid in a real time simulation (which would usually be done only in static environments with fixed objects). The aim of this project is to extend an existing physics simulation tool by implementing the DPD method. Simulations of this type are used in a number of different fields, such as the medical one (simulating blood flow in vessels). In our case the purpose of this tool is to mainly be used for didactic means, to show the power and possibilities of informatics.

Advisor
Prof. Antonio Carzaniga

Advisor's approval (Prof. Antonio Carzaniga): Date:

Contents

1 Introduction

Simulating consists in the process of imitating a system or real-world phenomena. This can be done in many different ways but requires in general one or multiple models that represent the behaviour of the target in the simulation. The choice of such model and its definition are key to create an environment which provides valid and reliable results.

There are a number of fields that make extensive use of simulations for different reasons. In some cases, such as for engineering, the system of interest may be dangerous to test, or it may still not have been built. Using simulations allows to test a system before it goes in production, decreasing time and cost in the development stage by applying the trial and error method in a controlled and flexible environment. There is in general an interest in modeling natural systems (a physic system in the case of this project), as well as human systems (commonly economics). This need brought forward an increasing necessity of bigger and more complex simulations, leading us to the role of informatics and computer simulations.

1.1 Computer Simulations

The power of informatics in the context of simulating is the prime example of why it is important for workers and researchers in different fields to learn the basics of computer science and programming. Depending on the complexity and suitability of the model it is possible to simulate virtually any system (accepting in some cases higher degrees of approximation). Another advantage of digital simulations is the possibility of visualizing the results using computer graphics techniques.

Most simulations of natural systems are based on physical laws, thus reducing the problem to the definition of a physics engine. While in general simple physical laws can be reproduced in software, there are cases in which it is only possible (or advised) to use approximations and simplifications in order obtain better performance. The cost of the simulation and the computational power available act as a limit in the way certain phenomena can be modeled. Real-time simulations are based on models that can execute at the same time as the real-world system, allowing to observe very realistic simulations. The problem with this approach is the computational strain that is forced onto the machine running the program, which means that for certain complex simulations either a really powerful machine or a very efficient model and code are required.

1.2 Approaches

Simulations can vary in kind vastly depending on the system they are based on. One big distinction can be made when talking about imitating natural systems and that is length-scale. A simulation of a chemical compund to the atomic level will be very different from one representing the effect of gravity on rigid bodies. This difference can be categorized in three main classes:

Atomistic scale Simulations of this length-scale aim to study the composition of matter itself, resulting in usually computationally expensive processes. The main fields implementing such models are biology, chemistry and physics, especially when the three disciplines intertwine.

Macroscopic scale When describing the global state of a system we don't focus on the single elements but rather on generalizing the dynamics of the phenomena. The model usually consists of sets of equation describing the system (such as equations of motion for Mechanics and Kinematics).

Middleground between scales There are cases in which we would want to describe matter in fine detail without incurring in excessive execution cost. One solution to this problem is to consider particles instead of atoms. These particles are agglomerates of atoms which allow for reasonably precise control of interaction between the elements of the system as well as a good overall representation of the global state. Using a method built on such a length-scale allows for example to simulate hydrodynamic behaviour at a much lower cost.

Fluid Dynamics being a focal point of this project it is important to talk about the difference between CFD (computational fluid dynamics) simulations and real-time simulations. In CFD the objective is to imitate the behaviour of a fluid usually around static objects. This is done to study the characteristics of both elements in the simulation. If we want to consider instead the fluid as an environmental effect, we would want to be able to simulate foreign bodies moving in such fluid. This is not possible with the standard CFD approach since the cost of emulating the fluid is too high to be incorporated in a real-time simulation. The method used for this project allows for such a simulation without compromising excessively on the behaviour of the fluid.

1.3 Goal of the project

The goal of this project was to extend an existing tool consisting of a simple physics engine capable of modeling the effect of gravity on 2D spheres and the collision between those bodies. The choice of direction for the extension was influenced by my interest in the topic of fluid dynamics and by being introduced to the method used by Professor Pivkin. The purpose of the tool also played a major role in the design process, since as a didactic tool to showcase the possibilities of computer programs it was most important to aim for a visually interesting and pleasing result. This fact didn't diminish nontheless the interest in also applying and validating the particular method used for modeling.

2 Fluid Dynamics Simulations

Fluid mechanics is a branch of physics concerned with the behaviour of fluids (such as liquids or gases) when forces are applied to them. Given our objective and the nature of simulations we will mainly focus on the dynamics of fluids. The study of the motion of a fluid involves the correlation of many of its properties such as velocity, density, pressure and temperature. The results of such models are used in a number of different disciplines like (most commonly) aerodynamics and hydrodynamics.

2.1 CFD Simulations

The most common way to model a fluid is through Computational Fluid Dynamics (or CFD) simulations, which, as introduced in 1.2, allow to reproduce the bahaviour of a fluid in an extremely detailed way. The cost of modeling systems using this method is usually expensive, hence making CFD not suitable for real-time applications such as the one developed in this project. The theory and application of this method still makes it worthwhile to study since it gives better insight on why other approaches may or may not work and why they may work better in certain scenarios.

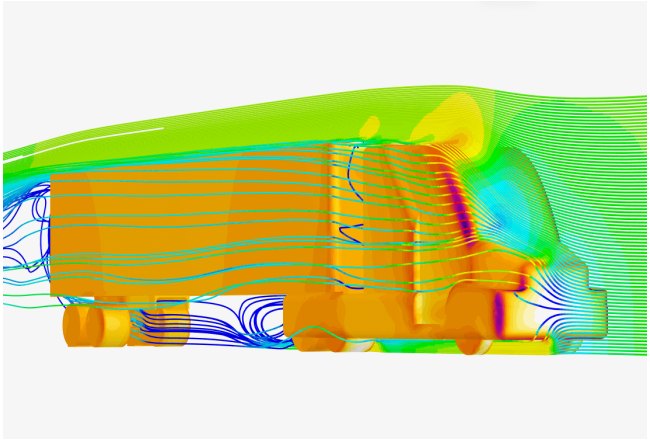

Figure 1. CFD simulation of fluid (Taken from SimScale)

As the name would suggest CFD is a technique based on mathematical computation and numerical analysis, which explains why powerful computers are necessary to create and handle the simulations. The complexity of the system to be modeled is directly correlated to the computing power required to simulate it.

In the following section a theoretical backgorund on the implementation of this method is given in order to accustom the reader to the crucial recurring elements of fluid dynamics.

2.1.1 Navier-Stokes Equations

The Navier-Stokes equations are differential equations used to describe the behaviour of a fluid at a specific point and time. The solution of the equations is effectively a vector field for the velocity of the fluid in each point of interest. Given the velocity field the equations can also relate the other important elements characterizing fluids, namely

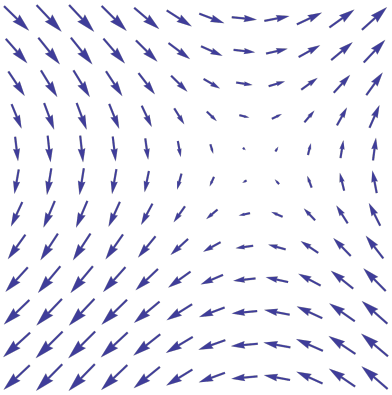

Figure 2. Vector Field to represent for example velocity in each point (Taken from Wikipedia)

pressure, temperature and density. The Navier-Stokes equations for an incompressible fluid with velocity field $\vec{u}$ are

$$\frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla)\vec{u} = -\frac{1}{\rho}\nabla p + \nu \nabla^2 \vec{u}$$

where

- t is the time;
- ∇ is the divergence (which operates on a vector field to give a scalar field);
- ρ is the density;
- p is the pressure;
- ν is the kinematic viscosity (which correlates the dynamic viscosity to the density of the fluid).

Depending on which fluid we are trying to model the Navier-Stokes equations change following the properties of the fluid, but for most cases they remain eqautions for which the solution can only be found with the help of computers.

2.2 DPD Method

Dissipative particle dynamics (or DPD) is a simulation method first introduced by Hoogerbrugge and Koelman [1] used to model hydrodynamic behaviour. The implementation process applied in this project takes inspiration from a paper by Robert D. Groot and Patrick B. Warren [2] which uses the formulation of DPD by Español and Warren as a starting point [3]. The premise of the method is to consider particles as agglomerates of atoms that interact with each other. This formulation leads to a simulation at a length-scale larger than the atomistic scale, but smaller than the macroscopic scale. This intermediate length-scale allows the method to model the properties of the fluid with sufficient detail while avoiding the cost of simulating each atom individually.

The usual set of equations (Navier-Stokes) used to model the behaviour of the fluid is hence replaced by a new formulation of the forces between particles.

3 Implementation

3.1 Extending the existing tool

3.2 Implementing the DPD method

3.3 Choice of parameters

4 Optimizing the Simulation

4.1 Computational cost

4.2 Cell list

5 Conclusion

6 Appendix

References

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