Scientific Computing: Molecular dynamics

Problemsheet 1

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Outline

Mac Setup

Using docker to remotelz build the project

Problem: xerces is not available on MacOS and code will be evaluated on a Linux system

Solution: Clion offers remote toolchains to build, run, and debug project

- Similar to WSL described on problem sheet for Windows
- Create Docker container with Ubuntu base image and all necessary files and libraries
- Create a new toolchain in Clion
- Configure Clion's Cmake profile and configuration to use the created docker image
- Use the IDE as you normally would
- Even connect to the container via terminal to do intensive debugging

Be aware that this approach will have its limits

Particle container

Realization of the particle container using vectors

Task: Create a class to encapsulate the particles for convenient iteration

Solution: class ParticleContainer

- Storing particles as a std::vector
- Iterator functions for convenient particle iteration
- Pairwise iterator with only unique pairs

$\Rightarrow$ Operators for range-based loop conditions (e.g. for (**begin**; **end**; ++;))

Design pattern

Refactoring with the strategy pattern

Problem: Methods for I/O and calculations will change frequently

Solution: Strategy as the implemented design pattern

- Define a family of algorithms and encapsulate them
- **Structure:**
  - Simulation as the highest layer for choosing strategy
  - Compartmentalizing I/O, model and physics
  - Enabling Combinations of physics functions through strategy
- **Benefits:**
  - Simple Swapping algorithms
  - Isolation of implementation details
  - Open/Closed Principle: Introduction of new strategies without context change

Force calculation

Task: Implement Force calculation with the pairwise iterator

Solution: Skip repeating calculations due to $F_{ij} = -F_{ji}$

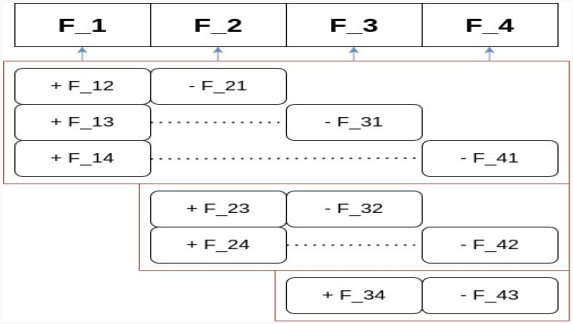

Figure 1: Pattern of pairwise Force calculation

References

https://refactoring.guru/design-patterns/strategy