Special Topics in Modeling & Simulation: Proposal 1

Simplified Nuclear Fusion Reactions in A Thermal Box

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Fusion processes are important nuclear processes to understand because scientists around the world are working with national governments to build nuclear fusion reactors in effort to generate consumable energy at the highest efficiency ever known. It is well understood in the fusion community that a desirable fusion power station must achieve 10^{18} fusion interactions per second per m^3 while running constantly [1]. Today, fusion physicists are chiefly concerned with achieving this interaction rate-density. Tremendous and complex super-computing simulations involving the magneto-hydrodynamics of fusion reactors predict that a sustained core temperature of around 110 million degrees Kelvin is necessary to achieve the desired reaction rate-density [2]. The goal of this project is to build a small, trivial, classical fusion reactor and numerically find its optimal temperature for a given rate-density, and study how the principle of detailed balance manifests itself in the simulation (i.e. check that the reaction rates obey the principle).

This project will simulate hard-sphere classical particle collisions in a box, with rules encoded for when particles fuse. Although generously simplified, this simulation will therefore be analogous to the behavior of the plasma inside of a nuclear reactor. The nuclear fusion reaction used in this project will be the Deuterium-Tritium reaction:

$$ {}^{2}_{1}\mathrm{D} + {}^{3}_{1}\mathrm{T} \rightarrow {}^{4}_{2}\mathrm{He}\ (3.5\ \mathrm{MeV}) + {}^{1}_{0}\mathrm{n}\ (14.1\ \mathrm{MeV}), $$

which produces a fused Helium molecule and plenty of thermal energy in the form of fast-moving neutrons. Deuterium has as its electric charge the proton charge, since it is composed of one neutron and one proton; the Tritium molecule has the same positive charge since it is composed of one proton and two neutrons. Therefore the particles repel according to the Coulomb potential

$$ F_C = \sum_{j \in \mathcal{N}} \frac{e^2}{4\pi\epsilon_0} \frac{1}{r_{ij}^2} \boldsymbol{e}_r, $$

where e is the fundamental charge in Coulombs, $\mathcal{N}$ is the set of particles in the neighborhood of particle i, r_{ij} is the radius between particles i and j, and $\boldsymbol{e}_r$ is the unit vector pointing between the two particles. The particles are also attracted to one another by the strong nuclear force. In this project, I will approximate the strong nuclear force as the force due to the Yukawa potential:

$$ V(r) = -\frac{1}{4\pi} \frac{e^{-r}}{r} \Rightarrow \frac{dV}{dr} = F_N = -\frac{e^{-r}}{4\pi r} \left(\frac{2}{r} + 1 \right) \boldsymbol{e}_r. $$

The total force experienced between two Deuterium and Tritium molecules is then $\sum F = F_C + F_N$.

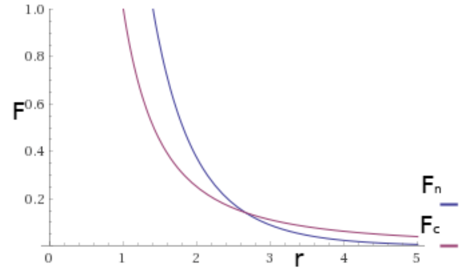

Figure 1: Superimposed plot of the Coulomb force (purple) and the semi-classical nuclear force (blue).

Stripping all constants and from the formula, the total force between any two particles can be written

$$\Sigma F = \sum_{j \in \mathcal{N}} \frac{1}{r_{ij}} \left(\frac{1}{r_{ij}} - e^{-r_{ij}} \left(\frac{1}{r_{ij}} + 1 \right) \right).$$

This is the force equation that will be used in the simulation for this project. It exhibits the property that at long distances, the Coulomb force dominates; but after a crucial inflection point, the nuclear force dominants, as can be seen in Fig. 1. Since a force equation is known, the Euler method can be used to find the numerical equations of motion of the particles. The general approach to modeling fusion processes will be the following programmatic steps:

1. Allow particles to move freely in a box under Brownian motion
2. Thermally excite the box by injecting a stream of high-energy neutrons at time t
3. D-T pairs which are under the inflection radius are *deleted*, replaced with a heavier particle (Helium), and shed a burst of fast-moving neutrons which excite more reactions

Optimistically, I would like this project to numerically predict an ideal temperature for this mock nuclear reactor, given a preferred reaction rate-density (i.e. if the user asks what temperature is needed for a rate of 5 processes per second in the reactor, the program will return an answer). Since this reaction is self-driving and cyclic (neutrons excite more fusion processes which produce more neutrons), I would also like to examine the principle of detailed balance by discerning a maximum reaction rate and/or an equilibrium drive temperature (i.e. a temperature where the fusion reactor does not run-away or die off).

References

[1] Thomas Klinger, *The Superconducting Stellarator Wendelstein 7-X*, Max Planck Institute for Plasma Physics, Lecture, 2016

[2] Jeffrey Freidberg, *Plasma Physics and Fusion Energy*, Cambridge University Press, 2010