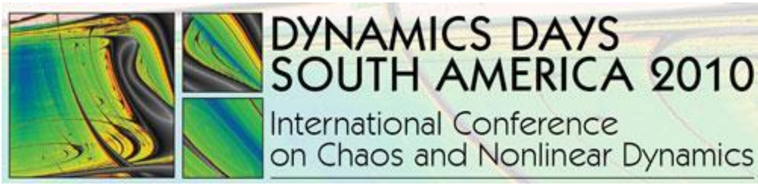

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Phase transition liquid-gas simulation in a bi-dimensional net

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Abstract

Using a bi-dimensional net we simulate the behavior of particles of a fluid, along an isotherm. Number of collisions against the walls of the system is analyzed as a function of the number of particles, showing a phase transition which resembles the one from liquid to gas, showing some features of the Virial expansion. Although the model seems to be so simply, many characteristics of phase transitions can be analyzed from these results.

Keywords: Applications of Nonlinear Sciences, phase transition.

Introduction

Modeling the phase transition from liquid to gas is not always easy to manage when all the features are taking in count, a real model would have to manage all the freedom degrees using a lot of memory and running time in a computer. By the way, many models have been proposed [1], in order to simulate these phenomena, which have a lot of application in nonlinear sciences, due the characteristics of it.

In this work we propose a two dimensional model in a square net, using some of the features of cellular automata in order to simulate the interaction between particles in a fluid. As a first step, we use this model to simulate an ideal gas with interaction of particles only with the walls of the system, as a next step, we let the particles interact between them. This interaction resembles collisions without any potential of attraction or repulsion, only like hard spheres.

We use a square net with a fixed size which can be fulfilled with what we are calling our particles, so we can play with the number of particles in a fixed volume, what finally will represent our control parameter for the phase transition. Our particles are also square and for the real gas we let them interact with their nearest neighbors and the next nearest neighbors. At each step of our simulation, we let the particles to move only one position due their velocity direction, if the chosen site is not empty, this represents a collision and the direction of the velocity of both particles is changed. This way, we keep the temperature of the system constant and the distribution of velocities is peaked in one square for step of simulation.

Results

In our simulations we obtain the number of collisions with the walls of the system, as a function of the number of particles. Using this number of collision we can easily obtain the pressure of the system, using some values of velocity, mass and time of the simulation. This way we can follow some given isotherm of the system. For the ideal gas we obtain a linear behavior of the pressure as a function of the number of particles, with no signal of phase transition.

When interaction between particles is allowed, the linear behavior is observed only for a small number of particles. When the number of particles is great, we observe a different behavior which can only be fitted with the first terms of the Virial expansion [2], as we can see in figure 1. This way we can simulate the principal characteristics of the phase transition liquid – gas.

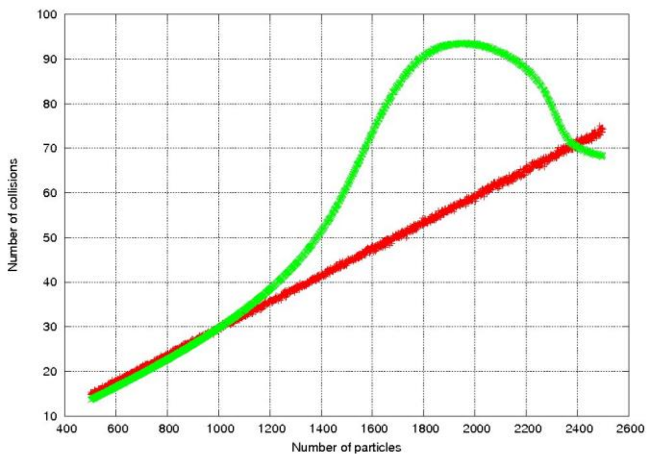

Figure 1. Behavior of the number of collision as a function of the number of particles. For the ideal model we can see a linear behavior of the isotherm (red line). The real model fits a Virial expansion function of a higher order (green line).

We also are in the possibility to calculate the behavior of the Gibbs free energy as a function of the pressure, where the phase transition is also observed resembling some way the shape of the spinodal.

We can also use percolation tools in order to calculate the size of the biggest cluster in the system and also the number of the cluster as a function of the number of particles, denoting also the principal change of behavior of the system when the phase transition happens.

Conclusion

We can simulate in a very simple way the phase transition from liquid to gas, using a discrete model in a bi dimensional square net. Our results let us study some special characteristics of this phase transition.

We can resemble phase transition with this simply model which is a characteristic of many nonlinear systems so we can apply some other systems.

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