# Finding A model for Simulating Thermophoresis

## Final Project for Computational Physics

**Shahrzad Zare**

## 1 Introduction

Thermophoresis means the movement of different kinds of particles which have different responses to thermal gradient. One of the systems that shows this kind of movement is the combination of many micro particles and one macro particle located between two walls with different temperatures. Micro particles collide with the macro particle and make it move. While the macro particles which are closer to the warmer wall have higher velocities and push the macro particle stronger, the pressure caused by the micro particles closer to the colder wall pushes the macro particle in the opposite direction. As a matter of fact, different factors such as number of micro particles, kind of interactions, and size of particles can affect the motions. Having a model to simulate this system, can help us to understand the cause and kind of movements better and compare the effect of those factors.

## 2 The Model

### 2.1 Spacial Coordinates

In this project, the system is defined in two dimensional space which is simulated by a box with periodic condition. The particles move in this box.

### 2.2 Producing Temperature Gradient with the Micro Particles

Instead of having two walls, it is possible to assume that the micro particles are in equilibrium with one or several heat baths. In order to simulate this equilibrium, the temperature should be defined for the system. Since temperature could be defined for many particles but not just one particle, the horizontal axis is divided into many regions each in equilibrium with a heat bath. It is equivalent to have a specific fixed temperature.

There are many micro particles in the box which have no radius. This means that the probability of collision between them is zero, so they do not collide. Also, there is no interaction between them. As a matter of fact, they act together like an ideal gas. The definition of temperature for each region in 2D is as follows:

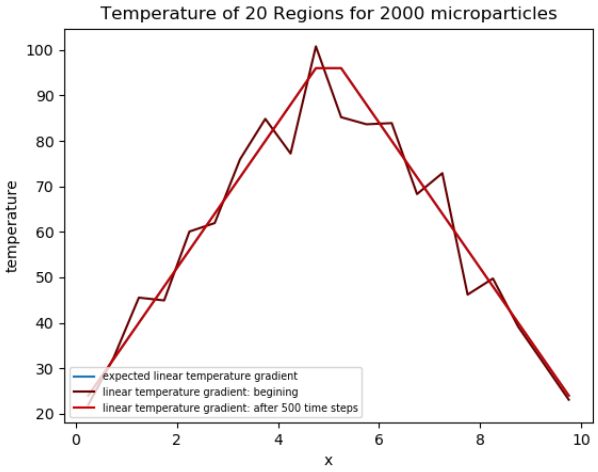
$$Temperature = \frac{E_k}{N \times k} \tag{1}$$

Where $E_k$, $N$ and $k$ represent kinetic energy, number of micro particles and Boltzmann constant.

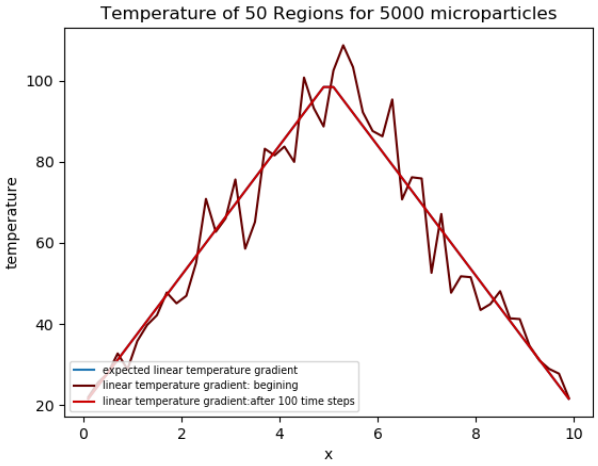
In order to find a canonical ensemble with a specific temperature, people usually use Monte Carlo method based on the Boltzmann distribution as probability function. Since in this project the system has time evolution and the temperature should be fixed during the simulation, using this method in each time step is not time efficient. Instead, a thermostat is applied in each time step. It means that the velocities are multiplied by a correction coefficient defined as follows:

$$Correction\ Coefficient = \sqrt{\frac{N \times k \times T}{E_k}} \tag{2}$$

Time evolution is calculated by Verlet integration which is same as Euler method in case of zero forces. Begins from a uniform random distribution for locations and Boltzmann distribution for velocities [1], the desired temperature will be obtained by this thermostat.
Figure 1 shows that 100 micro particles per region could produce the specific desired temperature. The Boltzmann distribution produces temperature gradient approximately at the beginning of the simulation. After applying thermostat, the desired temperature gradient is obtained more accurate.




(a) In this simulation, the horizontal axis was divided to 20 regions, and the number of micro particles was 2000.



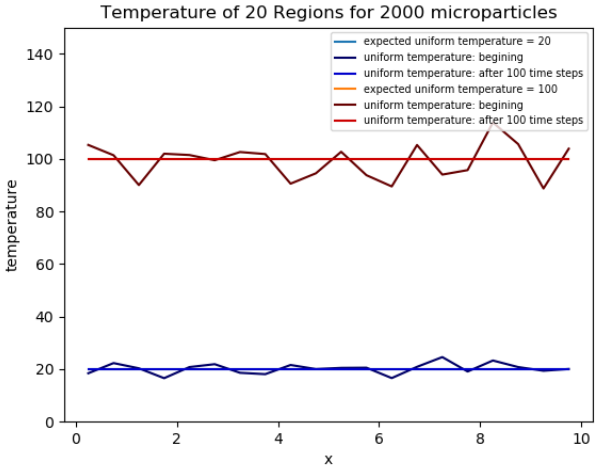

(b) In this simulation, the horizontal axis was divided to 50 regions, and the number of micro particles was 5000.

Figure 1: The result of simulating triangular (linear) temperature gradient

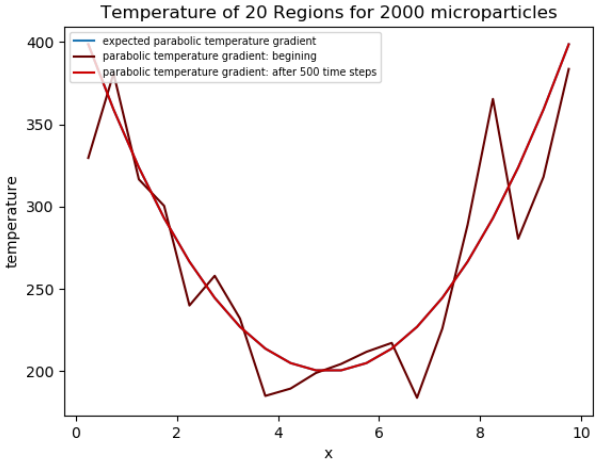
Figure 2 shows the result of two other kinds of temperature gradient.

Figure 3 shows that the system does not need relaxation time for achieving the desired temperature gradient because the variance decries dramatically after applying thermostat for just one time. Although the plot shows zero variance for time steps higher than 1, the variance is not exactly zero, but it is much smaller than the variance at the beginning of the simulation.

[1] $e^{\frac{-E_k}{k \times T}}$




(a) Uniform temperature




(b) Parabolic temperature gradient

Figure 2: The result of simulating two other kinds of temperature gradient

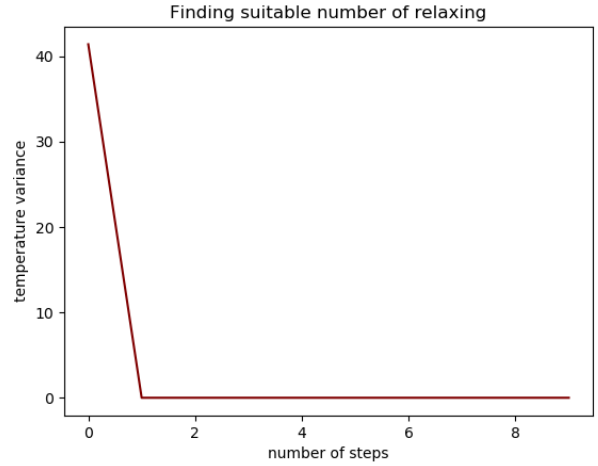
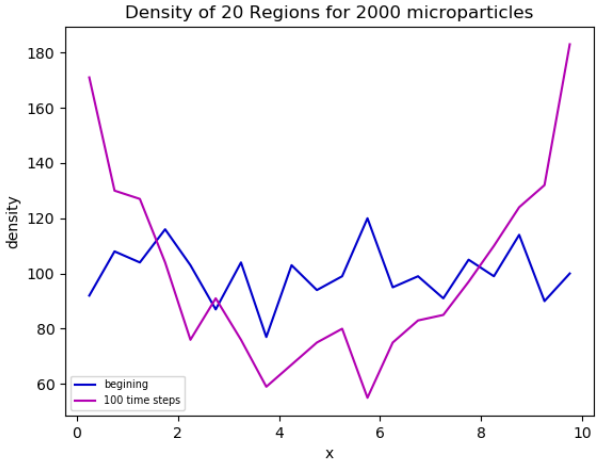


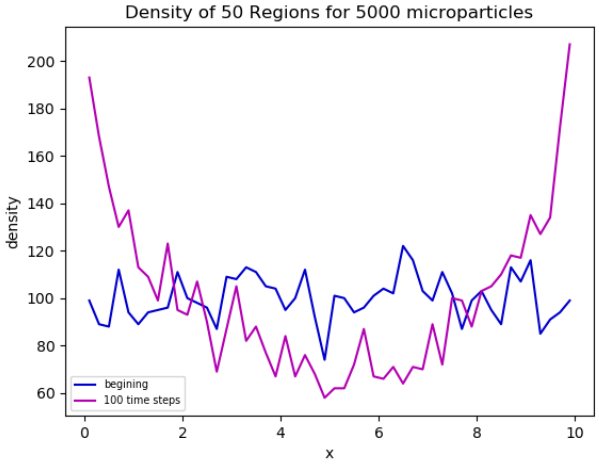

Figure 3: Finding relaxation time for obtaining desired temperate

## 2.3 Density

As figure 4 shows, the system needs some time to achieve the final density based on the temperature gradient because the initial condition for their locations make an almost uniform density at the first step. The relaxation time is almost 100 time steps.




(a) In this simulation, the horizontal axis was divided to 20 regions, and the number of micro particles was 2000




(b) In this simulation, the horizontal axis was divided to 50 regions, and the number of micro particles was 5000

Figure 4: Density for parabolic gradient

## 2.4 The Interaction between Macro Particle and Micro Particles

The micro particles interact with the macro particle just when they collide each other. The collision is assumed to be elastic, so the local energy and momentum are conserved.

# 3 The Results

## 3.1 Producing Temperature Gradient with the Micro Particles

One of the samples of the graphical result of simulating temperature gradient is shown in figure 5. The particles which are located in hottest region are shown by red spots and the particles which are located in coldest region are shown by black spots. The other colors present the temperatures in between. The hotter regions have less density than colder regions.

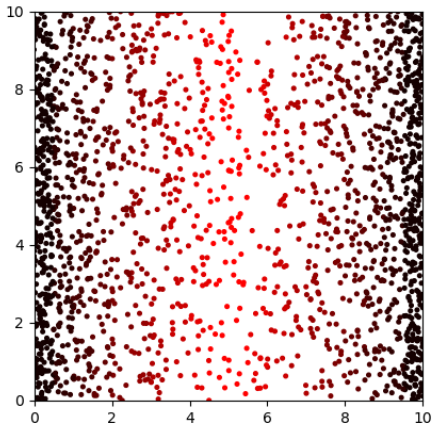
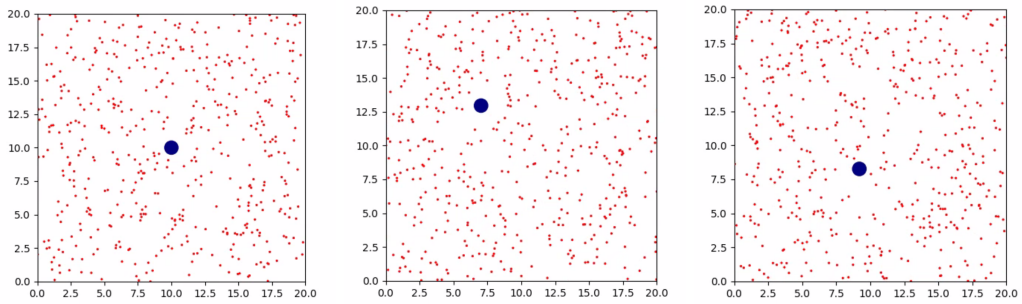



Figure 5: One of the samples of the graphical result of simulating parabolic temperature gradient with the hottest region in the middle of the simulation box

## 3.2 Random Walk

Figure 6 represents some different time steps of the macro particle's motion in the pool of micro particles with uniform temperature. The motion is not along a specific direction. As the path in figure 7 shows, the macro particle has a random walk. The path in figure 7 is according to one of the simulations under uniform temperature other than the simulation which is represented in figure 6.




(a) Beginning of the simulation (b) After about 200 time steps (c) After about 500 time steps

Figure 6: The graphical view of macro particle's motion in the simulation box with uniform temperature

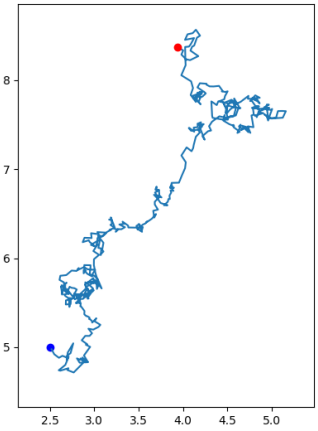



Figure 7: An enlarged view of the simulation box which shows the path of macro particle's random walk under the uniform temperature

### 3.3 Thermal Trap

With this model, it is also possible to make different kinds of thermal traps. Linear temperature gradient is not strong enough to make a good trap, but the parabolic temperature gradient is better for this purpose. Figure 8 shows this trap. The particle has small motions in coldest region.

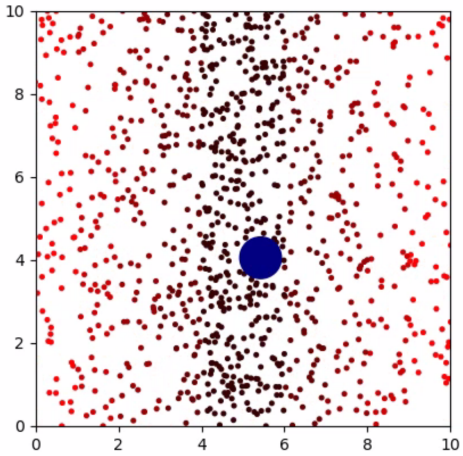
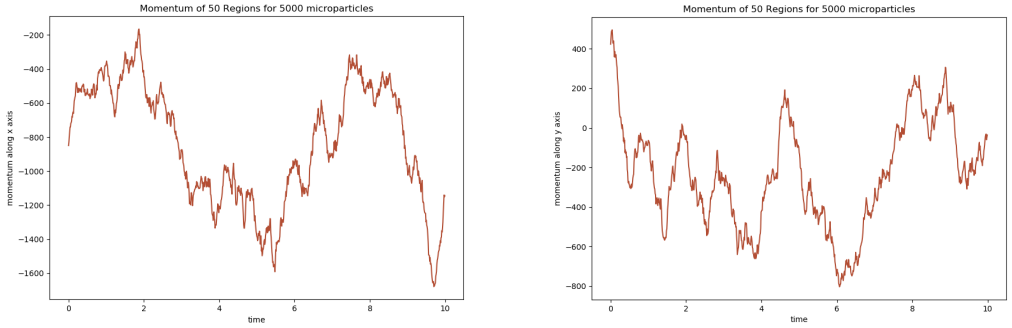



Figure 8: Thermal trap with parabolic temperature gradient

# 4 Verifying the Model

## 4.1 Finding a Sufficient Verification Method

Since the micro particles do not have interaction (do not see each other) and the thermostat corrects the velocities repeatedly, there should not be a total momentum conservation. As a matter of fact, measuring total momentum could not be a sufficient verification method. Figure 9 confirms this.




(a) Total momentum along horizontal axis (b) Total momentum along vertical axis

Figure 9: Total momentum according to time

As the system is in equilibrium with one or several heat baths, energy is not conserved. As a result, measuring total energy is not a sufficient verification method either. Figure 10 confirms this.

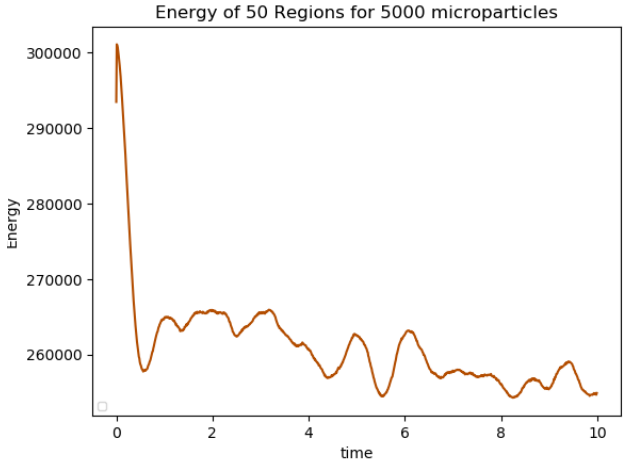



Figure 10: Total energy

Instead of calculating energy and momentum, it could be a sufficient way to study the system in an almost well known condition like uniform temperature gradient. In this condition, the random walk of macro particle should be Brownian. It means that the mean squared displacement must obey the following equation:

$$Mean\ Squared\ Displacement = 2 \times D \times time \tag{3}$$

Where $D$ is mass diffusivity:

$$D = \frac{k \times T}{6 \times \pi \times \eta \times r} \tag{4}$$

Where $k$, $T$, $\eta$ and $r$ represent Boltzmann constant, temperature, viscosity and the radius of macro particle.

## 4.2 Verification Results

Figure 11 shows that the macro particle's random walk is not Brownian unless in the first steps. In this figure, the location variance of two simulations under same circumstances are shown.

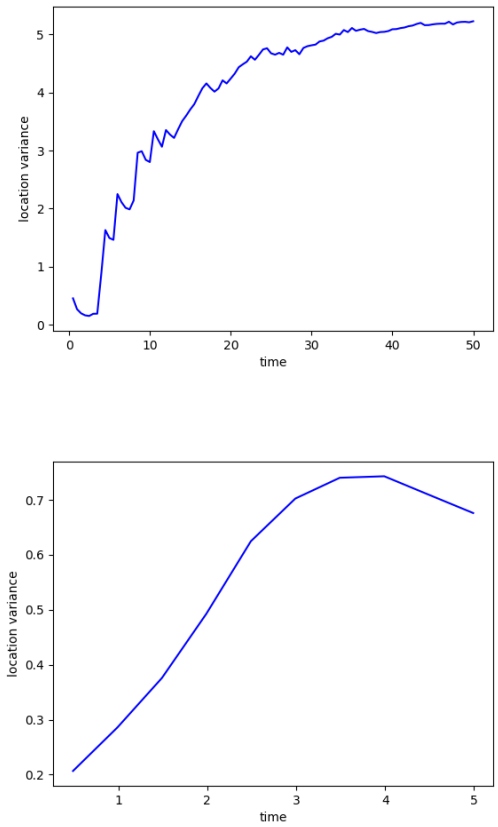
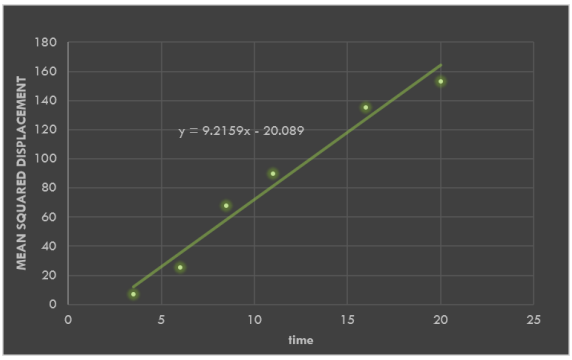


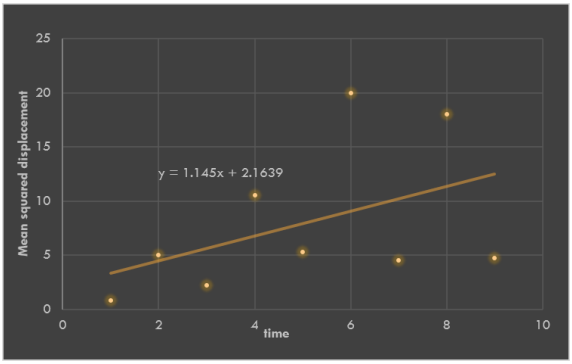

Figure 11: Mean squared displacement according to time

Figure 12 shows the mean squared displacement for two different macro particle's radius in first steps which present almost linear behaviour. The ratio of slopes approximately matches with equation 4.

$$\frac{D_1}{D_2} = \frac{r_1}{r_2} \tag{5}$$




(a) Macro particle's radius equal to 0.5




(b) Macro particle's radius equal to 5

Figure 12: Mean squared displacement according to time

### 4.3 Suggested Corrections for the Model

The probability of each event in Brownian Motion depends only on the state attained in the previous event. The behaviour of mean squared displacement shows that this model has a kind of memory which may caused by the thermostat. This thermostat multiplies both horizontal and vertical components of velocity by a same coefficient which means that each collision carries information from the beginning of the simulation or the micro particle's previous collision. This problem might be solved by applying a velocity's random rotation every some time steps.

## 5 Future Plans

The codes which are prepared for this model are flexible enough to apply different corrections such as velocity's random rotation. They are also flexible enough to apply different circumstances and change initial variables and basic constants such as length of time steps, number of regions and radius of macro particle. There are also some flags to turn on or off the thermostat and choose the temperature gradient.

After modifying the model in a way that satisfies the Brownian motion, the viscosity could be calculated. In addition, the code has an option to define temperature on each side of macro particle. In that case, the micro particles are in equilibrium with one heat bath and probable temperature differences are produces by the collisions between micro and macro particles. Finding a model for this collision could be a future plan in order to simulate self-thermophoresis.

Another future plan could be simulating thermal traps and comparing the results with following article:

Braun Dieter, Libchaber Albert, 2002, "Trapping of DNA by Thermophoretic Depletion and Convection", Physical Review Letters