SIMULATION OF PARTICLE MOVEMENT IN A TWO-DIMENSIONAL MODEL SYSTEM USING MATLAB

Anna Jadlovská[1], Slávka Jadlovská[1], Peter Rabatin[1], Mária Šviková[2]

[1]Department of Cybernetics and Artificial Intelligence, Faculty of Electrical Engineering and Informatics, Technical University of Košice, Letná 9, 042 00 Košice, Slovakia
[2]High School of St. Thomas Aquinas, Zbrojničná 3, 040 01 Košice, Slovakia

Abstract

Particle interaction in a 2D system is an open research topic whose results advance the miniaturization of electronic devices. We study a mechanical model system of small magnets interacting on an air layer. The aim of this paper is to describe a MATLAB application we developed to facilitate offline processing of video sequences recorded from the model. The obtained results are compared to theoretical assumptions about particle movement to verify the suitability of the model system for simulating phase transitions in a 2D thermodynamic system.

1 Introduction

The study of particle interaction in two-dimensional (2D) systems is an important area of physical research, inspired by the ever-increasing demands upon the miniaturization of electronic devices. Gaining detailed insight into the mechanism of phase transitions improves the understanding of structural and dynamical properties of matter at the molecular level. Research teams worldwide have in particular studied the processes of melting and crystallization in 2D systems using a variety of computer-aided experimental approaches. According to [1], 2D crystals display an interesting property of first melting into a hexatic phase and then into liquid phase via two continuous phase transitions. Other studies of interest have focused on the melting properties of 2D crystal electrons on the surface of liquid helium [2], block copolymer films [3], or colloid systems [4].

At the Department of Cybernetics and Artificial Intelligence (DCAI), we are able to simulate phase transitions using a mechanical model system of small disc magnets moving on an air layer with repulsive dipolar interaction, which resembles the structure of a 2D crystal. The air current blown onto the air table affects the velocities of all magnets and allows us to observe the simulated transition from the organized crystal phase into the random (liquid) phase. The air table is integrated with a camera system which is used to record the movement of magnets at different air current velocities.

The presented paper focuses on the description of the *Magtrack* application, which we developed in MATLAB to facilitate the offline processing and subsequent analysis of recorded video sequences of simulated particle movement [5]. The application implements an algorithm that determines the trajectories of individual magnets by detecting the position of each magnet in consecutive frames of the video sequence and joining them to form a trajectory. The implementation heavily relies on the built-in functions of the *Image Processing Toolbox*. Selected thermodynamic characteristics are evaluated from the obtained trajectories, and the suitability of the mechanical model for particle movement simulation is verified by comparing the experimental results to known theoretical assumptions in areas: velocity distribution, lattice formation and phase transitions. Some ideas for future work are outlined in the conclusion.

2 Two-Dimensional Model System for Particle Movement Simulation

Study of phase transitions in a 2D system requires the design and construction of an optimal model which would meet all requirements for a correct simulation of particle interaction. The idea for using a mechanical model system of interacting magnets to simulate internal structure of matter comes from [6]. At the moment, different configurations of this system are in use at the *High School of St. Thomas Aquinas* and at the *DCAI FEEI TU*, where the research teams respectively focus on the physical and technical aspects of the experiment. While the configuration of the mechanical model system located at the High School is described in detail in [7], this paper deals with the model system located in the *Laboratory of Mechatronic Systems* at the DCAI, which was constructed by *Kybernetika, Ltd* (a commercial business based in Košice) and is depicted in Fig. 1.

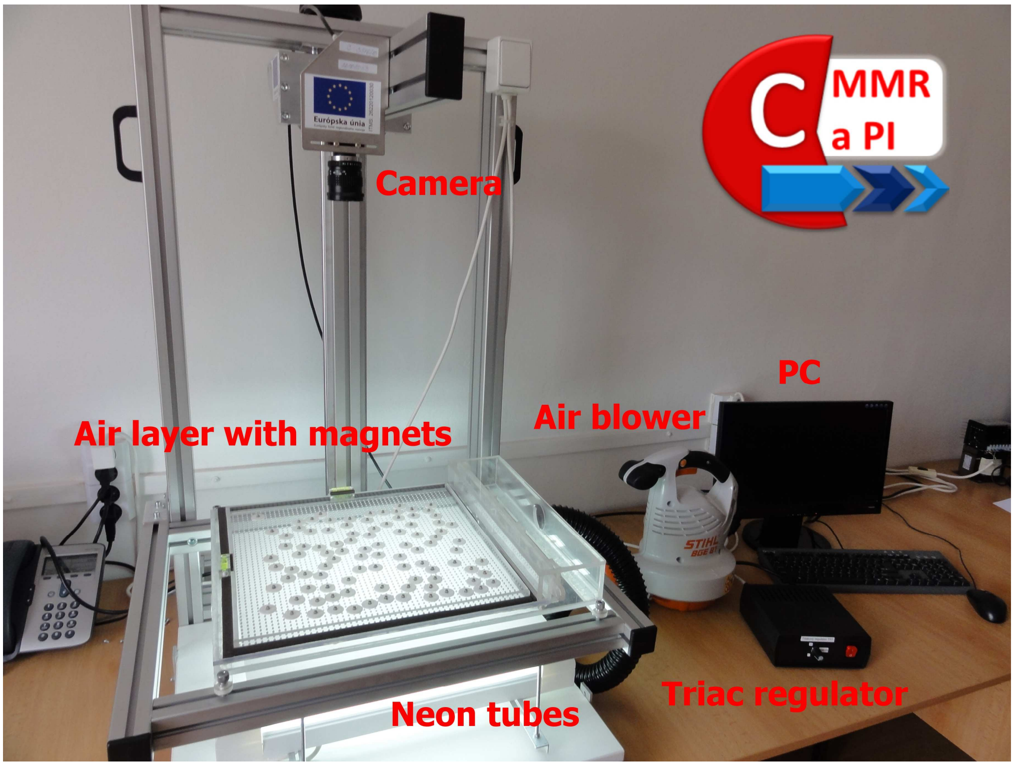

Figure 1: Simulation of particle movement in a two-dimensional system using a mechanical model of small magnets

The main part of the model system is a closed plexiglass block container (8x40x40cm) with small vents (diameter 1 mm, spacing 6 mm) on the top plate. Disc-shaped neodymium magnets (diameter 3 mm) attached to round pads are placed on the plate. By changing the number and shape of magnets, diverse structures of matter can be simulated. An air blower (maximum volume: 570 m^3/h) powered by a 6-position triac controller supplies air inside the container (air table) through a side opening. The air surge coming through the vents forms an air layer which causes the magnets to rise slightly and start interacting with each other and with the magnetic edge of the air table with repulsive magnetic forces. An integrated camera system is used to record the movement of magnets at different air current velocities for subsequent analysis. The communication between the camera (AVT Marlin F-131c, color, frame rate 25 fps, resolution 1280x1024) and the PC takes place through the *FireWire* interface. The air table is lit from below by four 12W neon tubes to improve object recognition against the background during image processing.

Fig. 2 depicts an input-output block scheme of the model system. Based on the above description, it is composed of two main subsystems. The motor voltage [V] is the control input into the air blower, while the volume of air current [m^3/s] is the air blower output, which acts as an input into the 2D model system. The planar coordinates of each magnet are considered the model output. Two possible disturbance forces acting upon the model include an unlevelled air table and neglected pressure changes inside the air table.

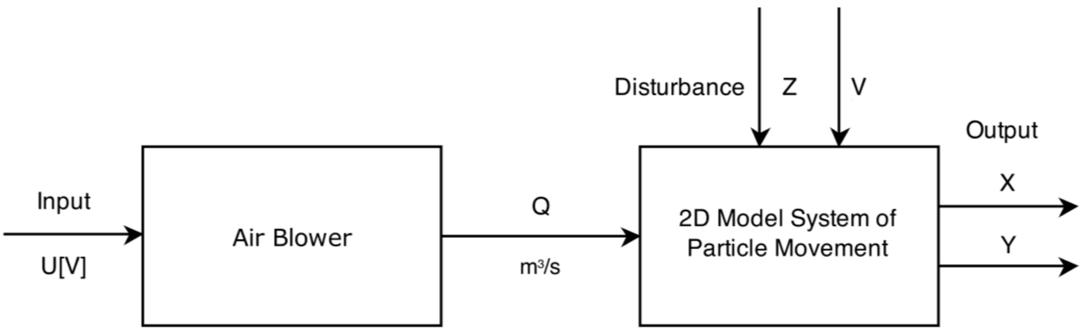

Figure 2: Input-output block scheme of the model system

Since the presented model system has been included into the set of existing models of the *Center of Modern Control Techniques and Industrial Informatics* at the DCAI FEEI TU (http://kyb.fei.tuke.sk/), more useful information about the model, including a photo/video gallery, can be found at http://kyb.fei.tuke.sk/laboratoria/modely/mmsdpc.php (Slovak version), or alternatively at http://kyb.fei.tuke.sk/laben/modely/gnpkyb.php (English version).

3 *Magtrack* Application – Design, Implementation and Use

To be able to use the model system of small magnets for experimental research into 2D systems, we needed to develop an application which would enable us to process and analyze the captured video sequences of magnet movement. As a result, we made use of the vast image processing capabilities of MATLAB to develop the *Magtrack* application [8]. The menu interface of the application is depicted in Fig. 3. Language modifications will be part of the upgraded version.

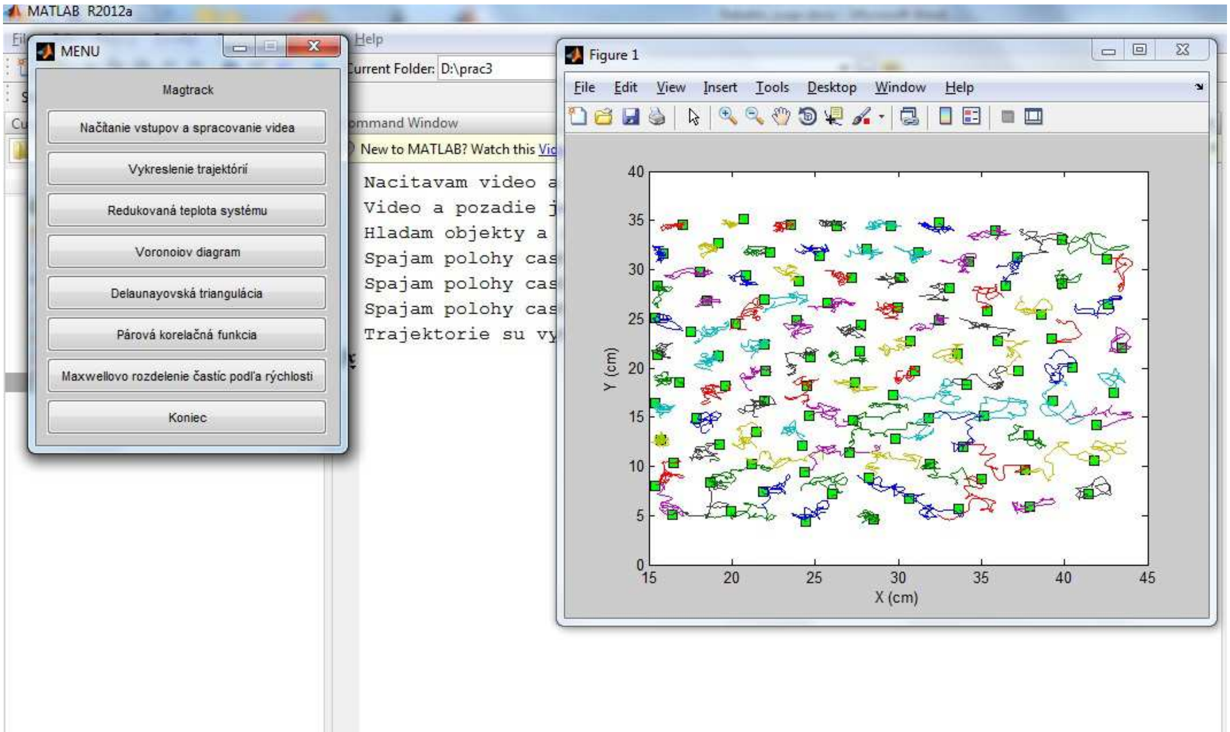

Figure 3: Using the *Magtrack* application for trajectory tracking

Magtrack is logically composed of two modules which need to be run sequentially. The *processing module* processes the recorded video sequences and returns a set of trajectories for each magnet over given time. The *verification module* contains custom functions for computing selected thermodynamical characteristics from the obtained trajectories. The functionality of both modules will be described below.

3.1 Processing Module – Determination of Particle Trajectories

Before a video sequence is recorded, an image of a brightly lit, empty air table needs to be made, since it will be used as the background image during the segmentation stages of image processing. The required number of magnets is then placed on the air table (changing the number leads to the simulation of different phases), and the volume of air current blown into the table is set on the triac controller. Video recording is started and stopped manually. A video sequence in the .avi format is obtained, which is subsequently imported by the processing module of *Magtrack* together with the background image.

The design and implementation of the *processing module* is based on the standard two-step procedure for determining the trajectory of an object from a set of consecutive frames: particle detection and spot linking, as illustrated in Fig. 4.

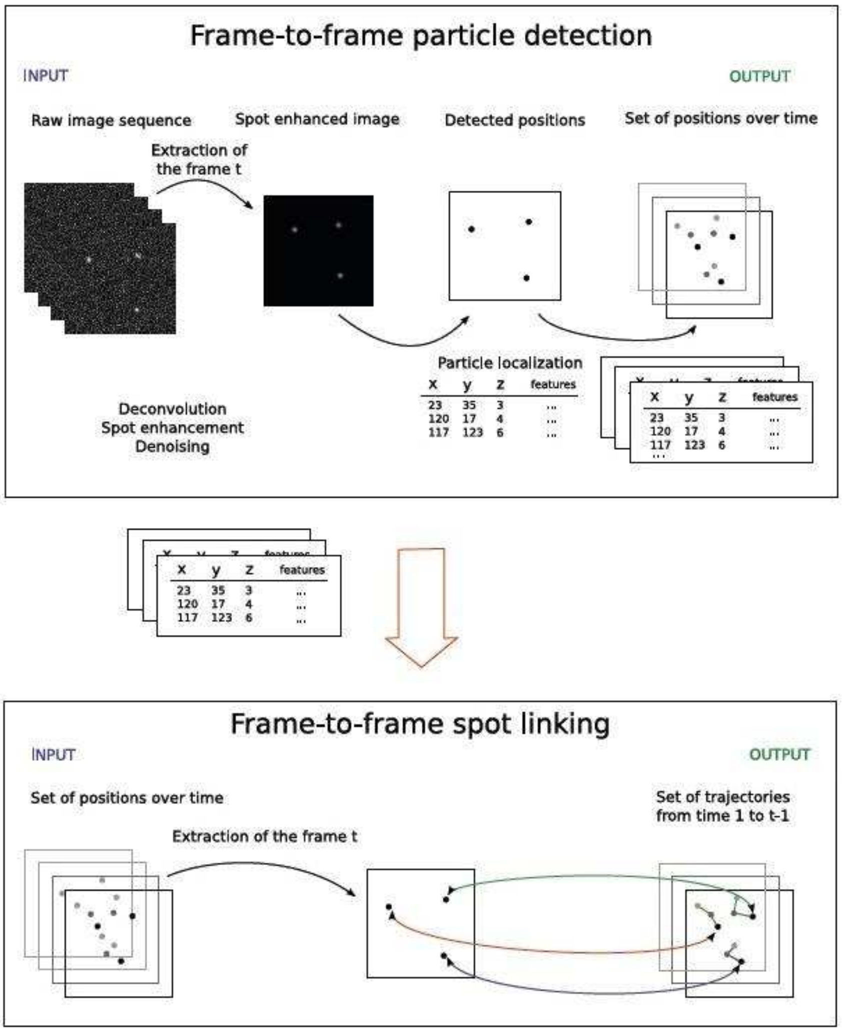

Figure 4: Standard two-step procedure for obtaining trajectories, implemented in *Magtrack* [9]

Each frame in a recorded video sequence contains a number of image distortions, usually as a result of uneven light conditions. As part of preprocessing, minor hue corrections and a RGB-to-grayscale conversion are performed for each frame. The individual frames of the sequence are substracted from the background image and subsequently converted into binary, using an experimentally obtained threshold value. In the resulting images, magnets are represented by white areas and the background is black. The frames are next filtered by morphological dilation and erosion, which remove all distortions whose size is negligible compared to magnet size, hence preventing false particle detections. The denoised binary frame is next segmented into individual objects using an algorithm which searches for inside contours. For every object described by the contours, the area is computed and the coordinates of a centerpoint are located [8].

Recording the trajectories of particles throughout a video sequence is known from literature as *particle tracking*. A *trajectory* is defined as a sequence of position detections of a single particle in time, and we need to assign the set of detections in each frame to the already active trajectories [9].

Let $z_{t_i}^k$ be the trajectory of *i*-th particle, composed of a set of *k* detections from frame 1 to frame *k:*

$$z_{t_i}^k = \{z_{t_i}(1), z_{t_i}(2), ..., z_{t_i}(k)\} \tag{1}$$

Let Z^l be a set of detections in the whole sequence with length l :

$$Z^l = \bigcup_{k=1}^{l} Z(k) \tag{2}$$

where $Z(k)$ is a set of all position detections (i.e. the positions of all particles) in the *k*-th frame.

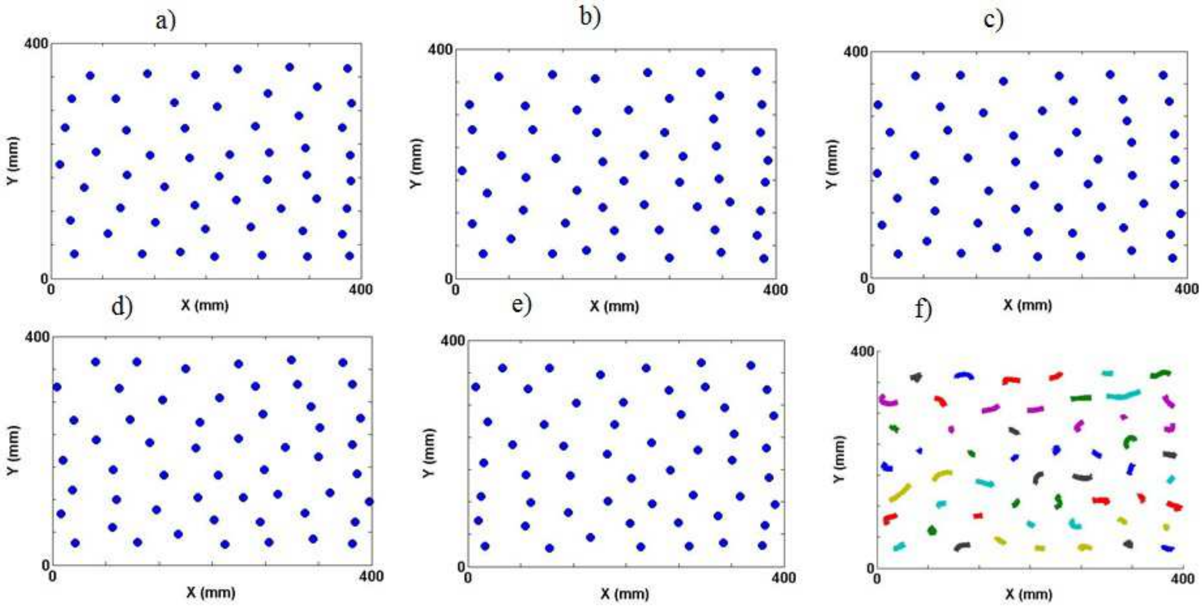

Figure 5: a)-e) particle positions at individual times f) final trajectories

Fig. 5 illustrates how the positions of individual simulated particles in five consequent frames a)-e) are linked into trajectories (f) in *Magtrack*. The implemented algorithm is based on the assumption of *ideal particle detection*, i.e. Z^1 is assumed to contain a detection of every particle in every frame and include no false detections. Moreover, if frame rate significantly exceeds particle dynamics, then the particle moves a short distance between individual frames, i.e. it will be detected very close to its position in a preceding frame. Each trajectory is therefore iteratively extended by the point which is the closest to the previous detection, i.e. in (k+1)-th step, trajectory $z_{t_i}^k$ is extended by the detection of the (presumably i-th) particle from $Z(k+1)$ with a minimum Euclidean distance from the previous detection $z_{t_i}(k)$.

3.2 Verification Module – Evaluation of Thermodynamic Characteristics

Using the custom functions implemented in the *verification module* of Magtrack, we will now try to answer the following questions about the suitability of the model system for simulating phase transitions in a thermodynamic system:

- Does the interaction of magnets meet the requirements for a proper simulation of particle interaction in a 2D system?
- If so, what kinds of lattices are formed and how do they depend on the volume of air current?
- Can different phases and phase transitions be observed?

To simplify the experiments, we define *reduced temperature* τ [m^2s^{-2}] as:

$$\tau = \sum \frac{\left(v_i^2\right)}{N} \tag{3}$$

where v_i is the velocity of i-th particle and N is the number of particles. Particle velocities are calculated from their displacement and the time interval between two consecutive frames.

It can be seen from Fig. 6 that the reduced temperature proportionally depends on the volume of air current blown into the air table, and that it fluctuates around a mean value for the whole length the video sequence, proving that the system of interacting magnets could model a thermodynamic system. The terms „higher/lower reduced temperature“ and „higher/lower air current blown into the air table“ can now be used synonymously with respect to their influence on thermodynamic characteristics.

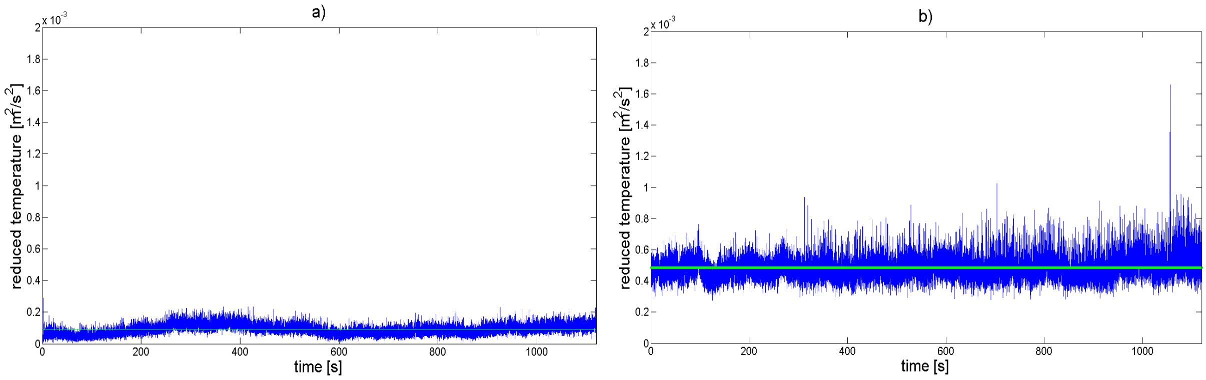

Figure 6: Reduced temperature for the a) lower b) higher volume of air current

The air current increases the kinetic energy of the magnets, which differs from the natural process of heating and rather resembles mechanical shaking [7]. It was therefore necessary to verify whether the velocities in a system of small magnets are of a *Maxwellian distribution* [10]. Fig. 7 depicts the velocity distribution for several values of reduced temperature. The distribution is computed by a function which divides the velocities of all particles at a given time step into a finite number of containers and returns the number of particles in each. An average number of particles in each container is computed for the whole video sequence described by τ . It can be concluded that the experimentally obtained velocity distribution is consistent with theoretical assumptions: a maximum is displayed for every τ ,and as τ increases, the mode value moves towards higher velocities.

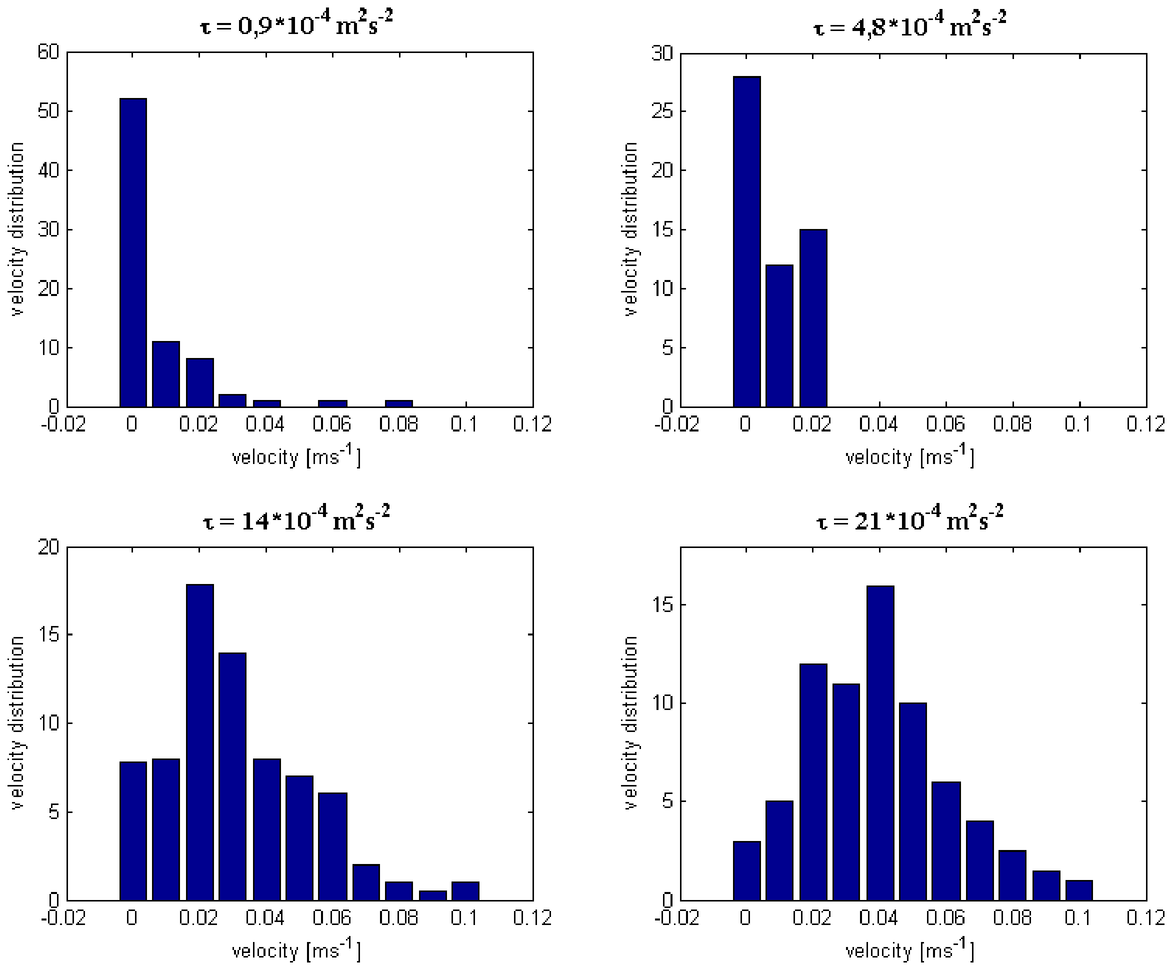

Figure 7: Observation of Maxwellian velocity distribution in an experimental system

Plotting particle trajectories provides important information about the system internal dynamics. Fig. 8a), b) depict the trajectories for the low volume of air current (and consequently, low τ), which models the low value of actual temperature in a thermodynamic system. Particles only move around their equilibria, creating a hexagonal (equilateral triangular) lattice. If the volume of air current is increased, particles quit their equilibria and move freely around the air layer, as in Fig. 8c). However, such movement is obviously not completely random: areas with a greater probability of locating the particle form a square lattice. We can therefore observe a change in the symmetry of the lattice with the increasing reduced temperature.

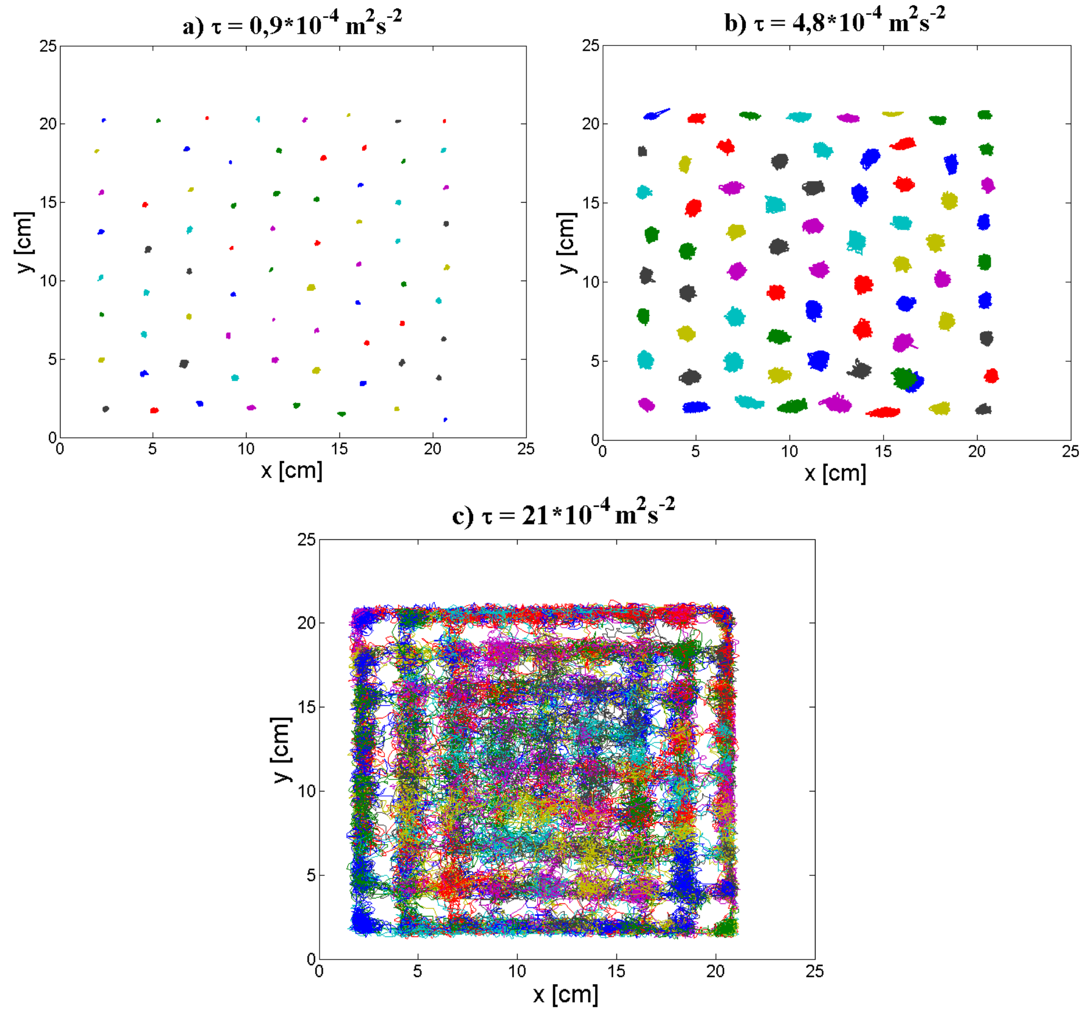

Figure 8: Particle trajectories for different velocities

The *pair correlation function* describes how density varies as a function of distance from a reference particle, and therefore provides information about the phase of the system [11]. In Fig. 9, such functions are computed for two different values of τ. In the *crystal phase*, the correlation function forms a system of repeating maxima. With the increasing reduced temperature, the amplitudes of maxima gradually decrease, and so does the probability of finding the same number of neighbors around a single particle. This process corresponds to melting into a random (liquid) phase, where the first significant maximum corresponds to the short distance order.

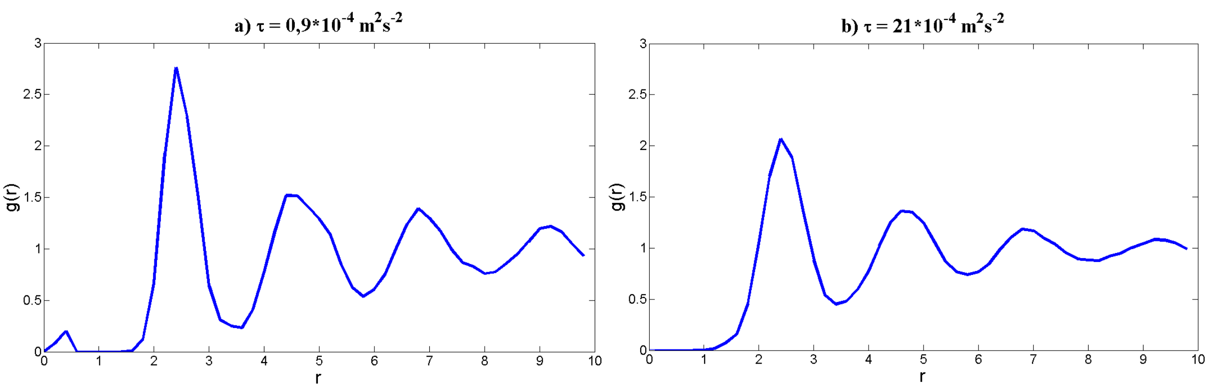

Figure 9: Pair correlation functions for a) a low τ – crystal phase b) a higher τ – random phase

Finally, heat-generated topological dislocations which play an important role in melting of 2D crystals can be identified using *Delaunay triangulation* (connects a particle with its closest neighbors) and a *Voronoi diagram* (creates an elementary cell around the selected particle) [12]. Both methods allow us to find particles with a number of neighbors other than six, i.e. triangular lattice dislocations.

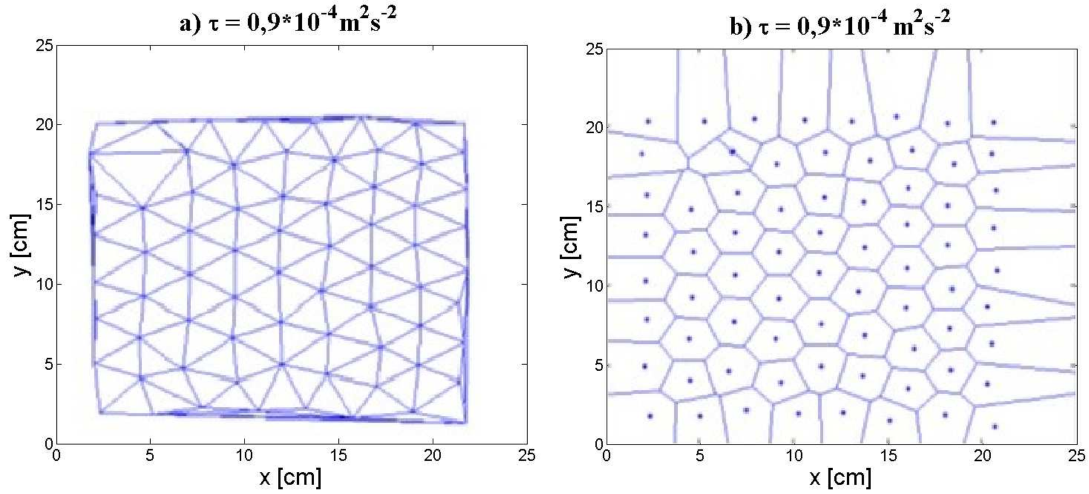

Figure 10: a) Delaunay triangulation b) Voronoi diagram for a low τ – crystal phase

Fig. 10 depicts the *Delaunay triangulation* and a *Voronoi diagram* for a low value of reduced temperature. The regular triangular lattice and regular hexagonal elementary cells prove this is the crystal phase. In Fig. 11, both graphs are generated for the random phase. Dislocations can be identified as particles with a number of neighbors lower or higher than six, which also shows up in the shape of an elementary cell. Comparison of both figures provides an insight into the process of a crystal lattice deformation caused by heating. Dislocations form in the crystal structure and the process of simulated melting in a 2D particle system can be observed.

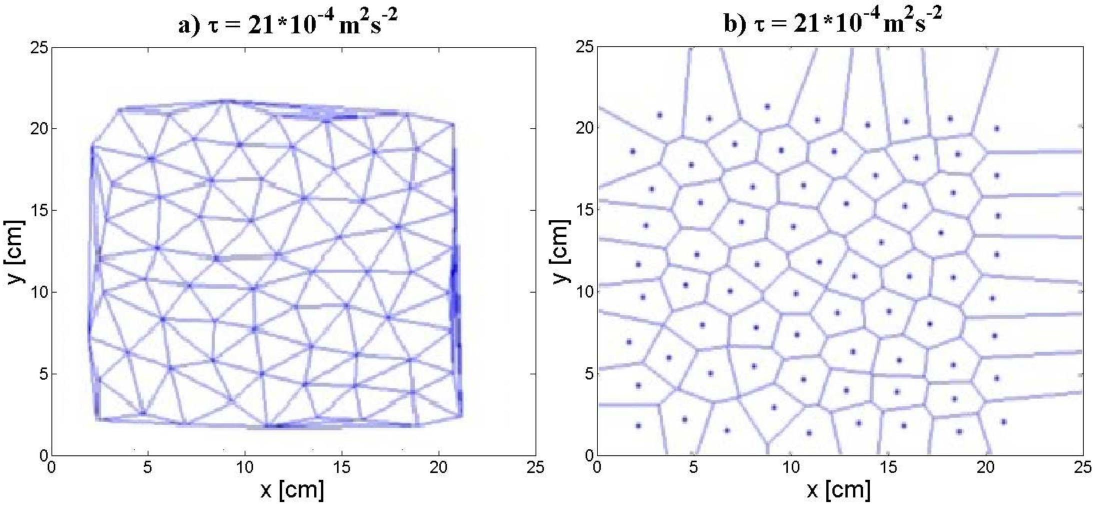

Figure 11: a) Delaunay triangulation b) Voronoi diagram for a higher τ – random phase

It can be concluded from the performed experiments that all questions posed at the beginning of this chapter have been answered successfully. It is therefore possible to use the mechanical model of small magnets for simulating phase transitions in a 2D thermodynamic system.

4 Conclusion

At the Department of Cybernetics and Artificial Intelligence, FEEI TU, a mechanical model system of small disc magnets, moving on an air layer with repulsive dipolar interaction, is used for simulating particle interaction in 2D systems. This paper describes the *Magtrack* application, which we developed in MATLAB to facilitate trajectory tracking of individual magnets from the recorded video sequences of magnet movement. The trajectories were determined by connecting the closest position detections in consecutive frames. *Image Processing Toolbox* was heavily involved in the design and implementation of the tracking algorithm. Afterwards, selected thermodynamic characteristics were evaluated from the trajectories using a set of custom-designed functions. It was shown that the system of small magnets meets the requirements for a proper simulation of particle interaction in a 2D system – it is possible to assign reduced temperature to the volume of input air current, and the velocities of magnets clearly follow the Maxwellian distribution. It was concluded from the analysis of generated trajectories that increasing reduced temperature causes a change in the symmetry of the lattice – a transition between a hexagonal and square lattice was observed. Structural analysis was performed by generating Delaunay triangulation and a Voronoi diagram for low and high reduced temperatures, and the simulated transition from the crystal (organized) into the random phase (i.e. melting) was observed from the increased number of dislocations.

Our future work on the experiment will progress in several directions. From the technical point of view, we plan to implement digital control of the air blower and to graphically determine how the magnet velocities depend on both the air current and motor voltage. The current outline of remote control of the model includes the implementation of a remote server, which will be accessed by ethernet from a secured website displaying a live stream of magnet movement.

At the moment, *Magtrack* is only able to process pre-recorded video sequences. The upgraded version of the application will also support real-time particle tracking. Next, we plan to improve the current particle tracking algorithm because the probability of incorrect connection of particle centerpoints between frames increases with higher velocities. The improved algorithm should be able to predict particle positions in the next time step and compare them to actual positions obtained from video sequences. Finally, a complex toolbox will be developed with potential applications in analogical research areas, such as cell tracking in biological structures.

Acknowledgement

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doc. Ing. Anna Jadlovská, PhD.
Department of Cybernetics and Artificial Intelligence
Faculty of Electrical Engineering and Informatics
Technical University of Košice
Letná 9, 042 00 Košice, Slovakia
anna.jadlovska@tuke.sk

Ing. Slávka Jadlovská
Department of Cybernetics and Artificial Intelligence
Faculty of Electrical Engineering and Informatics
Technical University of Košice
Letná 9, 042 00 Košice, Slovakia
slavka.jadlovska@tuke.sk

Bc. Peter Rabatin
Department of Cybernetics and Artificial Intelligence
Faculty of Electrical Engineering and Informatics
Technical University of Košice
Letná 9, 042 00 Košice, Slovakia
rabatinp@gmail.com

RNDr. Mária Šviková, CSc.
High School of St. Thomas Aquinas
Zbrojničná 3, 040 01 Košice, Slovakia
svikova@gmail.com