M.Sc. Physics of Complex Systems

Cooperative and critical phenomena

Self Assembling Chains: the FCW model

Course
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Introduction

The flexible chainlike walker (FCW) model was presented in 2008 by Takashi Mashiko, from the department of Mechanical Engineering of Shizuoka University. The model is proposed as a minimal model of a deformable moving object and as an extension of the regular random-walk model. In [1] the collective behaviour of a many-body system of FCW's is studied through numerical simulations on a square lattice. The results show that the FCW's exhibit a novelty type of irreversible aggregation, despite the lack of adherence in the model, which had always been assumed in all previous aggregation models. This irreversible aggregation without adherence proves to be an outcome of the deformability of the FCW's. Moreover, other FCW models were presented also by Takashi Mashiko in 2009 [2] and are also reviewed and studied here. These are the smart and the double-headed FCW models. It will be shown that providing the FCW's with some kind of intelligence isn't sufficient to avoid the irreversible aggregation while providing them with two heads is a sufficient condition to remove it.

The FCW model

- **Objects of the model**:
  - **Grid:** $L \times L$ square lattice of L^2 sites.
  - **FCW:** A FCW of lenght l is represented by l serially concatenated particles which occupy adjacent sites of the grid. The 1^{st} particle is said to be the head of the FCW while the l^{th} particle represents its tail.
- **Initialisation**

  FCWs are placed at random positions as initial distribution. Each FCW is put straight horizontally. This is partly for simplicity and partly for avoiding inborn "locking" (explained in the next section).
- **Time evolution**

  These are the rules that each of the FCW's follow at each time step:
  - The head particle chooses one of its four nearest-neighbour sites.
  - If **the site is not occupied** by another particle (of the same FCW or of another one) move the head particle to the selected site. If **the site is occupied** the FCW doesn't move at this time step.
  - Move the rest of the particles following the head. This is to say: the second particle moves to the site the head particle has just left, the third particle moves to the site the second particle has just left, and so on.

  Recall that if the head particle couldn't move, the FCW doesn't move at this time step!
- **Important magnitudes**
  - Density: number of FCW particles normalised by the total number of sites.

$$\rho = Nl/L^2$$

  - Mobility: number of FCW's that have succeeded in moving at that time step normalised by the total amount of FCW's.

$$M(t) = N_{mov}(t)/N$$

Theoretical considerations

Some considerations about the deformability and mobility of the FCW's and can be advanced from a theoretical approach. For $l = 1$ we recover the regular particle-like random walker, for $l = 2$ the FCW's don't change in form (so there is no deformability) but just in direction and for $l \geq 3$ we have full deformable FCW's. Considering a sufficiently large number of FCW's, N, in the equilibrium state of the system it is clear than the probability of occupation of a site of the grid won't depend on wether the site is a nearest-neighbour of a FCW, but only in the overall density of particles. For $l = 1$ each FCW can have 4 nearest-neighbours available, so the mobility (which is the probability that a nearest-neighbour of a FCW is empty) will be given by

$$M_\infty = 1 - \rho \tag{1}$$

In the case of $l \geq 2$, each FCW will have always one of its 4 nearest-neighbours sites occupied by its own "post-head" particle. Then the mobility will be given by

$$M_\infty = \frac{3}{4}(1 - \rho) \tag{2}$$

However it is shown in the results section that the simulations do not agree with Eq. (2) for FCW's of $l \geq 3$. Instead, a phase transition is observed from a moving state (higher-M_∞) to an aggregated state ($M_\infty \sim 0$). This aggregated state, where FCW's do not move, can be explained from the deformability of the FCW's.

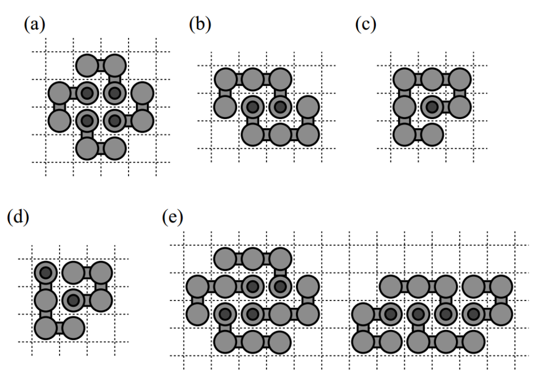


Figure 1: Examples of mutual locking of FCWs. (a) Four-body mutual locking of l=3 FCWs. (b) Two-body mutual locking of l=5 FCWs. (c) Self-locking of an l=8 FCW. (d) Quasi-mutuallocking of l=4 FCWs, where the right one is locked by the left one, while the left one is not completely locked by the right one (but by other FCWs, which are not shown here). (e) Other types of fourbody mutual locking than type (a), possible for l=4 FCWs.

Observing the time variations in detail, we notice that $l = 3$ or longer FCWs sometimes form a scrum when they happen to encounter each other, and get locked by themselves. That is, all four nearest-neighbor sites of the FCWs' head particles are occupied by their own particles. Let us refer to such a situation as "mutual locking." Some examples of mutual-locking patterns are shown in Fig. 1: Four $l = 3$ or longer FCW's can form a fylfot scrum (a). FCW's of $l = 5$ or longer can form couplershaped gridlock when two of them happen to meet (b). Furthermore, if an FCW is long enough ($l \geq 8$), it can lock itself by coiling (c), which is called here "self-locking." In some cases, the locking is not completely mutual, as exemplified in (d), which is, so to speak, "quasi-mutual-locking." Self-locking and quasi-mutual-locking, however, are regarded here as special cases of mutual locking. Once mutual locking takes place, the FCW's concerned cannot move anymore. This causes the irreversibility of the aggregation process. On the other hand, shorter FCW's of $l = 1$ or 2 do not go into mutual locking, no matter how many FCW's happen to gather at once. [1]

Results

Simulations have been done for a $L = 100$ lattice and for FCW's of length $1 \leq l \leq 8$. Mobility has been computed in the equilibrium state for density values in the range $\rho \in [0.01, 0.6]$ with steps of $\rho_i = 0.01$. To ensure that the system reaches the equilibrium for any density, 10^5 time steps have been considered, averaging over the last $5 \cdot 10^4$. Moreover, in order to have better statistics the value of mobility for each density has been averaged over 10 runs.

Fig. 2 shows that the numerical results for $l = 1$ and $l = 2$ agree with the theoretical predictions. On the other hand, the results for $l = 3$ and $l = 4$ show sharp drops from the higher-M_∞ state to the $M_\infty \sim 0$ state, so a phase transition is observed. In addition, $l \geq 5$ FCW's settle down in the $M_\infty \sim 0$ state even when the density ρ is low. It should be recalled that for $l = 3$ and for density values below the critical density (the density value where the transition occurs) the mobility follows the theoretical line. Thus, for small density values the mobility of $l = 3$ FCW's could be predicted with Eq. (2).

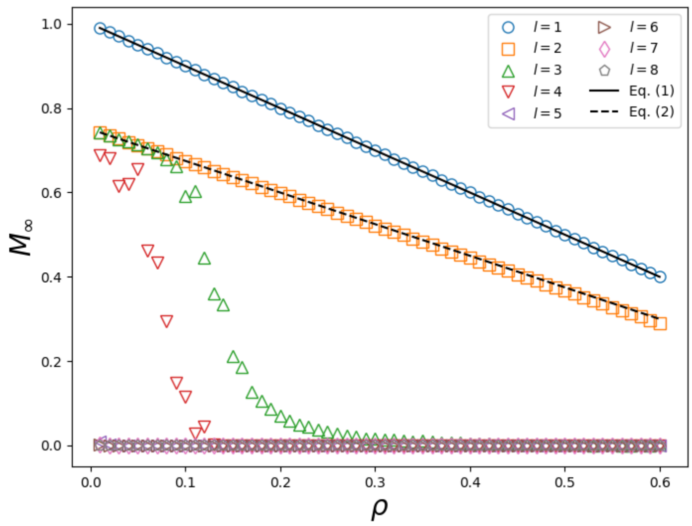
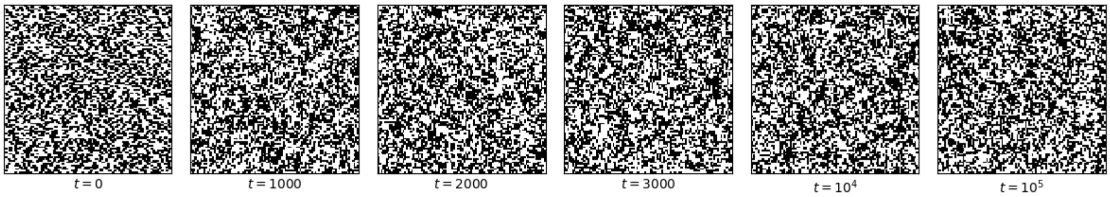


Figure 2: Equilibrium mobility M_∞ as a function of particle density ρ

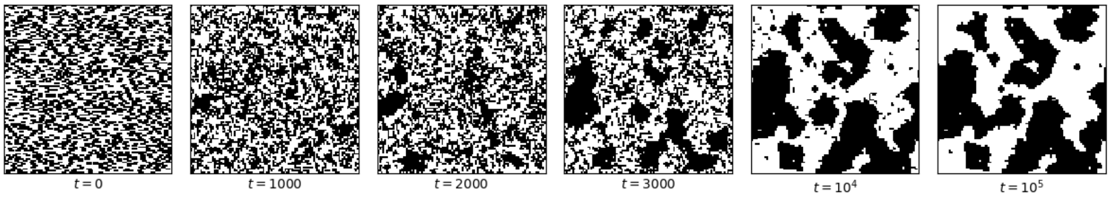
Finally, a qualitative study of the time evolution of the FCW model is presented. To demonstrate and visualise the difference between the rigid shorter FCW's ($l \leq 2$) and the deformable longer FCW's ($l \geq 3$) typical pattern variations with time of $l = 2$ and $l = 3$ FCWs are shown below. The density is the same for both cases: $\rho = 0.5$ (the number of FCW's is $N = 2500$ for $l = 2$ and $N = 1667$ for $l = 3$). The snapshots are of $t = 0$ (initial distribution), 1000, 2000, 3000, 10 000, and 100 000.

As can be observed, Fig. 3(b) shows how for $\rho = 0.5$ and $l = 3$ the system equilibrates in an ordered phase where FCW's don't move. On the other hand, Fig. 3(a) shows a disordered phase for any time and we can appreciate no qualitative changes between the initial distribution and the equilibrium distribution.

Thus, it has been shown that FCWs aggregate spontaneously and irreversibly, though no such adherence is assumed. Adherence is not required for the occurrence of aggregation and the irreversibility results from the mutual locking of FCWs. Therefore, the aggregation mechanism of FCW's is fundamentally different from that of the conventional models. The fact that this novel type of aggregation is possible only for the many-body system of deformable objects strongly suggests the significance of studying such a system as in the present work.



(a) FCW's of $l = 2$



(b) FCW's of $l = 3$

Figure 3: Time evolution of the FCW model for $\rho = 0.5$ and $L = 100$.

The smart FCW model

Now a modification of the FCW model is considered. In this model, the head particle of the FCW's always chooses and move to an unoccupied nearest-neighbours site unless impossible. Thus, this modified model is expected to have higher possibility of moving in comparison with the original FCW model, so the mobility should be higher of that of the original FCW's for all density values. [2]

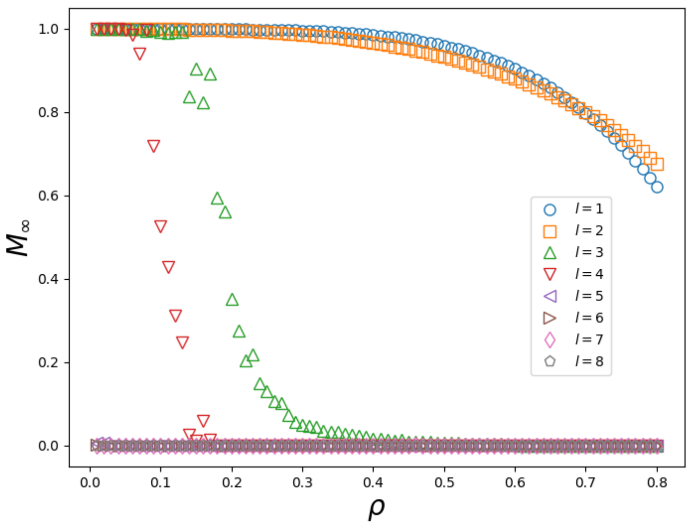


Figure 4: Asymptotic mobility M_∞ as a function of particle density $1 \leq l \leq 8$ for smart FCW's. Each symbol represents the averaged value taken over $5 \cdot 10^4$ time steps in the asymptotic state and over at least 10 runs.

Now the results for the smart FCW's are shown i n Fig. 4 corresponding to Fig. 2. It is clear that for $l = 1$ and $l = 2$ the results no longer agree with the theoretical predictions for the FCW model, as it should be expected. Moreover, now that curves are not linear and the mobility of the smart FCW's is clearly higher than that of the original ones at the same density value ρ, which was also expected. However, the results for $l \geq 3$ are qualitatively the same: a phase transition from the moving state to the aggregated state is observed for $l = 3$ and $l = 4$ while for $l \geq 5$ the system remains always in the aggregated state, even for low density values.

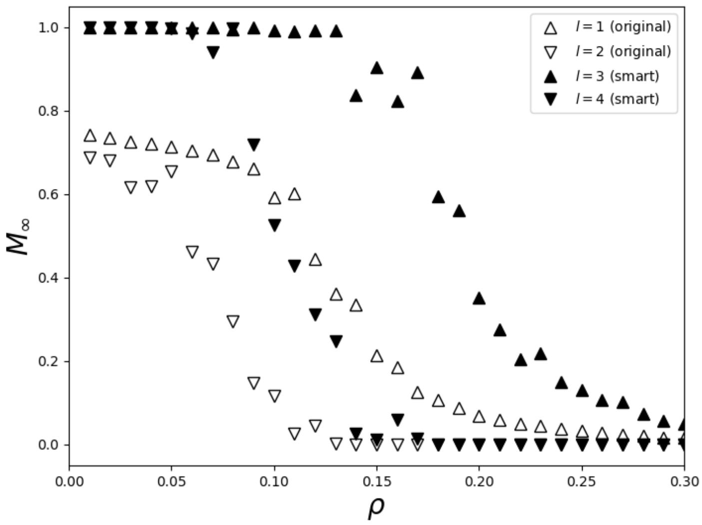


Figure 5: Accurate comparative study of the phase transition in the FCW and smart FCW models

However, comparing more accurately the phase transition for $l = 3$ and $l = 4$ between the FCW and smart FCW models some differences are found. While the values of the critical density at which the transition occurs are nearly the same, the M_∞ values in the moving state are higher than those of the original FCW's, as can be seen in Fig. 5.

The double-headed FCW model

Finally, the last modification of the original FCW model is presented. In this model, the head and the tail particles of each FCW are not fixed but switch with each other randomly at every time step. The randomly-selected head particle chooses one of its four nearest neighbor sites at random and moves to that site if it is vacant, followed by the subsequent particles, as in the case of the original FCW (not the smart FCW). [2]

The results for this model are presented in Fig. 6 corresponding to Fig. 2 and Fig. 4. The first important result is that for $l = 1$ the numerical results agree with that of the original FCW's and the theoretical approach given by Eq. (1). This should be expected as for $l = 1$ the FCW's are point-like particles and it makes no sense to consider a head and a tail. Then, for $l \geq 2$ the mobility of the FCW's no longer agree with that of the original FCW's. Three main differences must be highlighted for these cases. First, there is no longer a phase transition and for all $l \geq 2$ the $M_\infty - \rho$ curves just decrease monotonically as ρ increases. Second, for low density values ($\sim \rho < 0.2$) the curves are close to the theoretical approach for $l = 2$ given by Eq. (2), while for high density values ($\sim \rho > 0.6$) mobility approaches Eq. (1). Finally, all the curves for $l \geq 2$ are close to each other, which means that the length l of the FCW's does not much affect the collective behaviour. This is in contrast to both original and smart FCW models, where the mobility decreased with the increase on the FCW's lenght l going through a phase transition for $l = 3$ and $l = 4$. Thus, this final point seems to be the key point of the no irreversible aggregation of the double-headed FCW model.

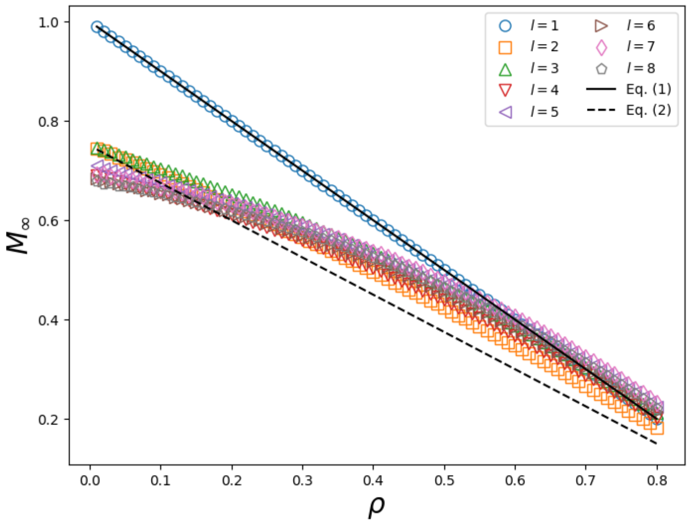


Figure 6: Asymptotic mobility M_∞ as a function of particle density $1 \leq l \leq 8$ for smart FCW's. Each symbol represents the averaged value taken over $5 \cdot 10^4$ time steps in the asymptotic state and over at least 10 runs.

It is important to note that the reason why the double-headed FCWs do not undergo mutual locking is not because they remain in nearly the same positions, without moving effectively, due to the random switching of the head and the tail particles. In a macroscopic time scale, each double-headed FCW surely travels, as does the regular random-walker whose displacement is proportional to the square root of the elapsed time ($\sqrt{t}$). [2]

Conclusions

To conclude, in the present work three different Flexible Chain-like Walker (FCW) models have been reviewed and studied by numerical simulations as a many body system in a square lattice. First, the 'original" FCW model presented in [1] shows a phase transition from a moving state to an aggregated one, where the FCW's basically don't move, for $l = 3$ and $l = 4$. For $l = 1, 2$ the mobility can be predicted with a theoretical approach that gives rise to Eq. (1) for $l = 1$ and Eq. (2) for $l = 2$. For $l \geq 5$ the equilibrium state of the system has been shown to be the aggregated state with 0 mobility. This results where also observed in the smart FCW model, where the FCW's move whenever possible. This shows that the results are robust and unique characteristics of unidirectional, deformable, selfdriven objects. On the other hand, the double-headed FCW model doesn't show irreversible aggregation and the length l of the FCW's does not much affect the collective behaviour of the system. This indicates that bidirectionality prevents self-driven objects from experiencing the mutual locking and thus the irreversible aggregation.

Future work

Further studies motivated by these models could be done in a high dimensional space, where the mutual locking should be more difficult to achieve and, thus, the phase transition should occur for higher FCW's length l.

A Algorithms

The algorithms implemented to perform simulations of the different models presented here can be found at the following GitHub account https://github.com/agimenezromero/FCW-model along with some documentation.

References

[1] Takashi Mashiko. "Irreversible aggregation of flexible chainlike walkers without adherence". In: *Phys. Rev. E* 78 (1 July 2008), p. 011106. DOI: 10.1103/PhysRevE.78.011106. URL: https://link.aps.org/doi/10.1103/PhysRevE.78.011106.

[2] Takashi Mashiko. "Effect of Individual Properties of Flexible Chainlike Walkers in a Many-Body System". In: *The Open Transport Phenomena Journal* 1 (Oct. 2009), pp. 30–34. DOI: 10.2174/1877729500901010030.