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Monte Carlo parameterization in the VirtualLeaf framework

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Abstract. The recently developed simulation framework VirtualLeaf uses Metropolis Monte Carlo dynamics for studying plant tissue morphogenesis. Minimizing the energy of the tissue is done by an energy evaluation-only method. We developed a more robust criterion for the energy minimization method for the multivariable and complex systems where the use of a gradient norm is impossible. The proposed criterion is based on checking energy changes in a sliding window of successive energy steps against a threshold value. The advantages of the sliding window criterion are discussed and results obtained by this method are presented. The impact of the choice threshold value on the energy minimization has been studied.

1. Introduction

1.1 Modeling the cell behavior in VirtualLeaf

As indicated in [1, 2], the process of the equilibration of the water relations in plant tissue is significantly faster than turgor regulation and growth processes. That is why the system can be considered in a state of equilibrium at any given time [3, 1, 4]. The process of the equilibration is the balance between intracellular turgor pressure (e.g. due to the water uptake) and counteracting of the cell wall to this pressure. For modelling this state one can directly use the stress-strain relationship using the tensile force within cell walls as done in the CellModeller framework [5] or the more general and widely used energy formalism [1, 3, 6] based implicitly on the force as applied in the VirtualLeaf framework [3].

In VirtualLeaf a tissue is represented by a mesh of cells where a cell is a polygon surrounded by walls (Fig. 1). The wall consists of edges linked by nodes. In VirtualLeaf the cell and tissue behaviors are represented within a generalized energy, i.e. Hamiltonian [3]:

$$E = \lambda_A \sum_{cells} (a_i - A_i)^2 + \lambda_E \sum_{edges} (l_j - L_j)^2 , \qquad (1)$$

where the first term represents the turgor in the cell and the second term represents the resistance of the edges to the turgor, a_i - actual cell area and l_j - actual edge length, A_i - cell area in the absence of counteracting cell wall forces (target area) and L_j - edge lengths of cell wall in the absence of turgor pressure, λ_A - cell compression or expansion resistance parameter and λ_E is a spring constant of the edge.

1.2. Energy minimization in VirtualLeaf

The stable state of the system, i.e. the balance between turgor pressure and cell wall resistance at a certain time is defined by the minimization of the generalized potential. In VirtualLeaf, minimizing the energy of the system is done using the Metropolis Monte Carlo method [7, 8] as shown by the flowchart in Fig.1. One node from the set of nodes is randomly selected and is displaced by distance D in a random direction. It causes geometric changes both in actual area of cells and in actual length of edges that leads to an energy change of the system. The displacement is always accepted if it leads to an energy drop, i.e. $\Delta E_i < 0$. Otherwise, it is rejected. Displacements resulting in an energy increase are accepted with the Boltzmann probability $P(\Delta E_i) = e^{-\Delta E_i/T}$, where T is a parameter of random fluctuation as a noise and rejected otherwise. The conditional acceptance of some positive energy displacements helps avoid getting stuck in local minima.

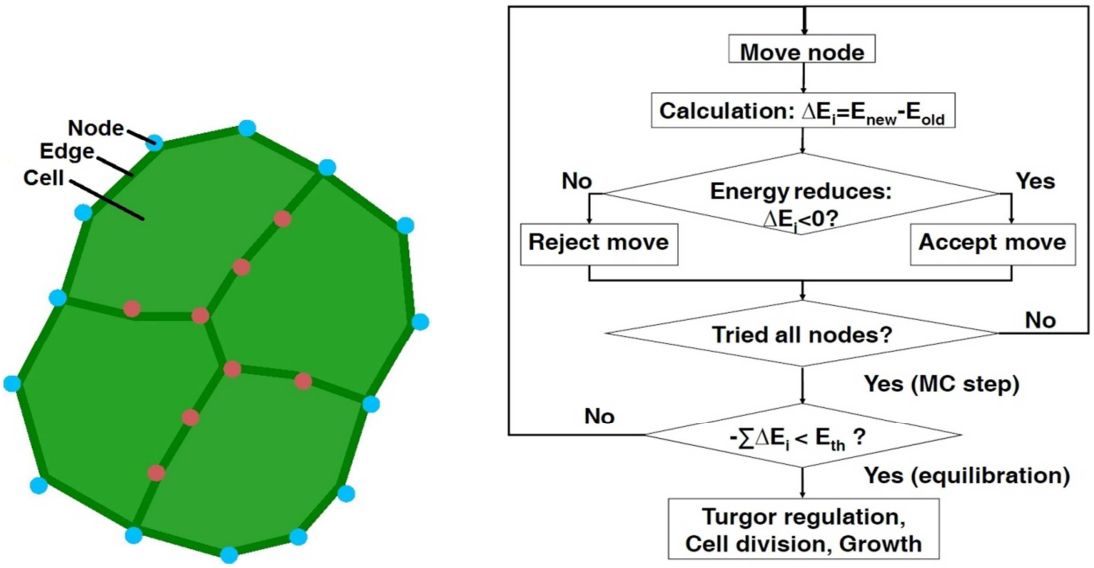

Figure 1. Representation of the tissue (left) and MC energy minimization flowchart (right) in VirtualLeaf.

In this way, iteratively all nodes are attempted to be displaced and it is called one Monte Carlo (MC) step if the number of attempts is equal to the number of nodes in the whole system. The MC step is repeated until the desirable equilibration state of the system, i.e. a sufficient balance between the turgor pressures and cell walls resistances, is reached. At the end of each MC steps the energy change is evaluated by

$$-\sum_{nodes} \Delta E_i < E_{th}, \qquad (2)$$

where E_{th} represents the tolerance of the $|\sum \Delta E_i|$ convergence. If the system satisfies this criterion, then the slower biological processes such as the turgor pressure increase, cell division and cell growth are performed. Otherwise, again the displacements of all nodes are attempted to reach the desirable state of the equilibration.

However, this criterion based on an energy evaluation only method cannot result in the desirable equilibration of the system. That is why our main aim is to elaborate a more robust method for energy minimization in VirtualLeaf.

2. Results and discussion

2.1. Analysing the criteria for energy minimization

One of the robust methods typically used for the energy minimization of a system is the derivative method based on the first derivative of the energy with respect to the geometry of the system when it is available. However, the energy derivatives are not available for the Hamiltonian in Eq. (1) due to its multi-variability, as it consists of the contributions to the energy from various terms, the large number of cells and cell walls. That is why in VirtualLeaf a non-derivative method, i.e. an energy evaluation only method or, more precisely, a “function-only method” [9] is used as a convergence criterion for minimization.

Let's analyse the possible consequences of the VirtualLeaf criterion in an actual simulation. In addition to the VirtualLeaf criterion, we also use the criterion of a predefined maximum number of MC steps that can be configured by the VirtualLeaf user. We have studied the minimization convergence of small (4-cell) and big (287-cell) tissues with 11000 MC steps for the case of the Auxin Growth model of VirtualLeaf. In Fig. 2 we present the total energy of these tissues versus the number of MC steps during one time step. One can see the decrease of the total energy of the tissue during energy minimization, i.e. when the

number of MC steps increases. We should note that when the minimization is close to convergence the energy changes from MC step to MC step should be very small, i.e. the curve in Fig. 2 comes to a plateau. We observed quite fast convergence (~100 MC steps) in the case of the small tissue and slower convergence for the big tissue.

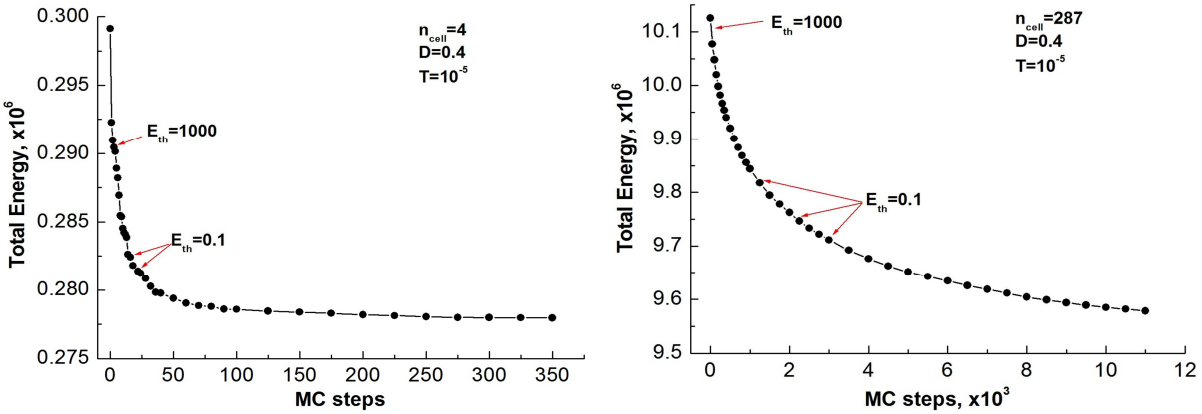

Figure 2. Total energy of the 4-cell (left) and 287-cell (right) tissues versus the MC steps. Arrows correspond to different random seeds.

We also performed MC simulation using the energy evaluation only criterion. When we use E_{th}=1000, it resulted in very early ending of the MC calculation in both cases. With this criterion the system supposedly has reached convergence, though in fact it was far from a converged minimum. As this value of E_{th} was quite large, we have also used E_{th} = 0.1 which is sufficiently small. In this case the system was closer to the converged minimization. However, the convergence obtained with this tolerance became more dependent on the random seeds, which causes some doubt about the robustness of the criterion used in VirtualLeaf.

To find the reason of such sensitivity we studied the energy minimization and convergence of the 287-cell tissue with 11000 MC steps for three random seeds. We present the results of this study in Fig. 3, left. There is almost no difference in these dependencies within the entire interval of MC steps performed which is, indeed, inherent to the stochastic processes. Then we analysed the evolution of the energy difference during energy minimization cycle which we present in Fig. 3, right. We would observe a gradual decreasing of the curve, if we use a gradient of energy.

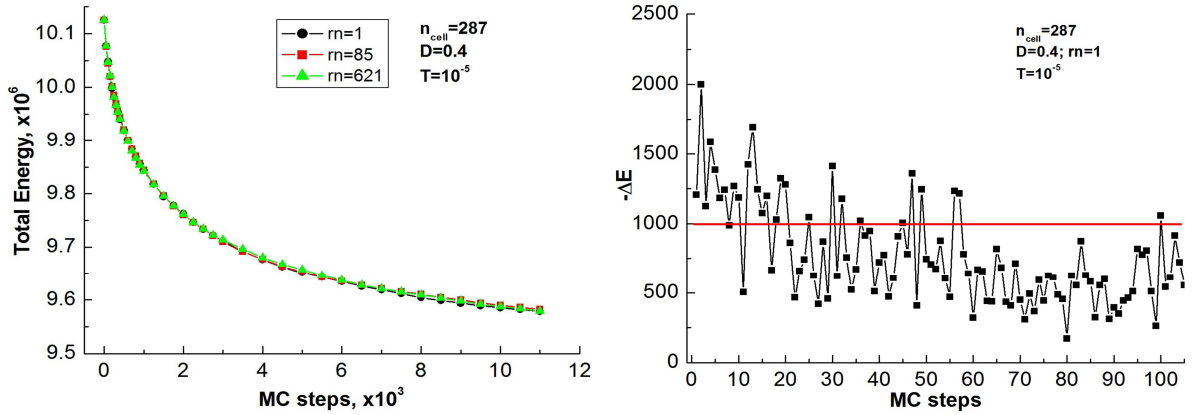

Figure 3. Total energy at various random number (*rn*) seeds (left) and the energy difference (right) versus the number of MC steps for the 287-cell tissue.

However, as the $\sum \Delta E_i$ is used directly instead of any gradient, it increases and decreases with a large deviation even if its mean value decreases with increasing MC steps. As a result, the convergence criterion can be met at any MC steps where $|\Delta E| < E_{th}$. In VirtualLeaf the convergence criterion is considered satisfied at very early MC steps, for instance at *MC step* = 8 (which is sensitive to the random seed), though until *MC step* = 40 the mean value of $|\Delta E|$ is large than E_{th} =1000.

2.2. Modified criteria for energy minimization

As the energy difference is changed around its mean value, we assume that a more correct criterion for convergence in this case is more systematically satisfying the condition of $|\Delta E| < E_{th}$, for instance its satisfaction at a number of consecutive MC steps. For this aim we developed a *sliding window* method. In this method we use the average value of $|\Delta E|$ in *m* consecutive MC steps instead of its single value:

$$\frac{1}{m}\sum^{m}\left(-\sum_{nodes}\Delta E_i\right) < E_{th}. \quad (3)$$

This energy window with width *m* slides step-by-step together with the increasing MC steps as shown in Fig. 4 (left) until the condition in Eq.(3) is satisfied, e.g. until *MC step* = 40 in this case. We have demonstrated that this is a more robust criterion for minimization convergence as the average has a much less erratic behaviour and is not prone to having "false positives" in exhibiting convergence in contrast to (2).

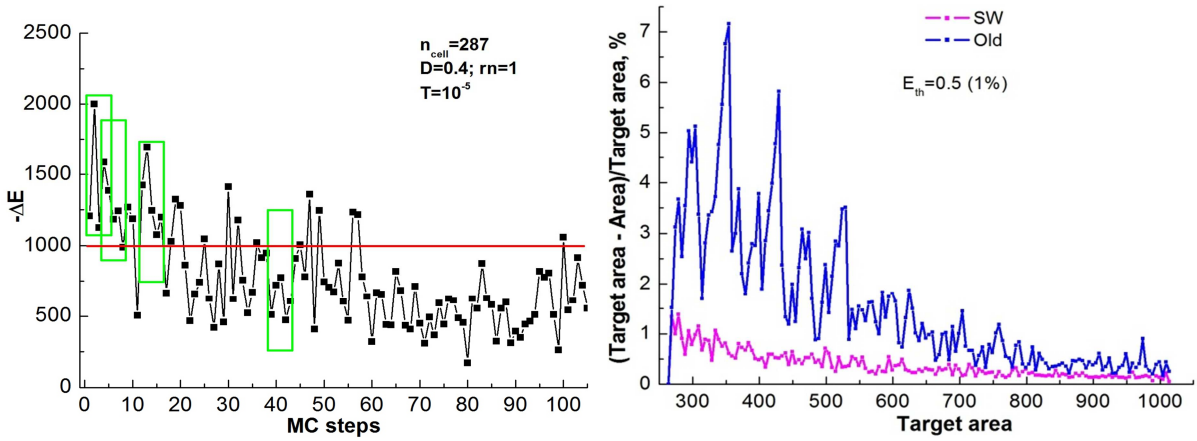

Figure 4. Sliding window (green rectangle) in energy difference versus the MC steps for the 287-cell tissue (left) and comparison of the sliding window (SW) and old criteria for minimization with respect to convergence for the growth of the 2-cell tissue in the Demo1 model of VirtualLeaf (right).

To demonstrate the effect of the modified criterion we plotted in Fig. 4 (left) the difference between the target and actual area versus the target area during tissue growth without any cell division. We took only the first term in Eq. (1) and allowed expansion of the tissue by the systematic increase of the target area at each time step. The width of the sliding window was *m* = 5 MC steps. As threshold value we used E_{th} = 0.5 which corresponds to 1 % of the initial total energy.

In the case of the sliding window we observed a very nice agreement between the predicted minimum and the tolerance value E_{th} at the initial stage of growth. Indeed, one can see the difference between the target and actual area reaches 1 % quickly at the beginning of simulation. Then it decreases as the relation of E_{th} to the total energy decreases due to the increase of the total energy during the tissue growth. However, when we used the old criterion, i.e. (2), there was no agreement in results with the used values of E_{th}: the predicted

values were significantly far from the tolerance, with very big deviations in the entire interval of the growth studied. These results show the disadvantage of the criterion (2) resulting in unpredictable and wrong (unstable) states of the system. At the same time, they demonstrate the robustness of the sliding window criterion in the case of this multivariable system.

2.3. Exploration of MC parameters

As shown in Sec. 2.1, the energy convergence is sensitive to the change of threshold energy E_{th}. We also studied the sensitivity of energy convergence to other parameters such as the length of node displacement D and the random fluctuation parameter T. For the right choice of the values of these parameters we have to answer the next questions: which values are more suitable for the MC energy minimization and what is the criterion for the choice of suitable values?

One can propose the analysis of the system state during time evolution is suitable for this aim. Nevertheless, due to the continuous dynamic changes of the system studied here with processes such as cell division and growth and various terms in Hamiltonian such integrated studies cannot provide adequate answers.

We believe that the best method is the study of the system state directly during the energy minimization cycle. In particular, the total energy evolution of the system used in Sec. 2.1 (see Fig. 2) is a robust way to evaluate the suitability of the values of the parameters. We therefore used this method in our study.

We studied the influence of the length of the node displacement D on the MC energy minimization. We present the results in Fig. 5 (left). Note that until now we presented results with D =0.4. In Fig. 5 (left) one can see that the increase of D (e.g. D =0.7) results in the regression (worsening) of the convergence to the equilibrated state: the total energy of the system decreases more slowly with a large slope in the entire range of the MC steps calculated. However, the decrease of D (e.g. D =0.1) drastically changes the behaviour of this dependence. Indeed, in this case the total energy of the tissue decreases very fast at the beginning MC steps, then it is almost not changed having a plateau of curve in the large range of MC steps which indicates convergence to an energetically stable state of the tissue approximately after $4x10^3$ MC steps. From this plateau one can conclude that the energy of the stable state of this tissue at this time is approximately 9.45×10^6.

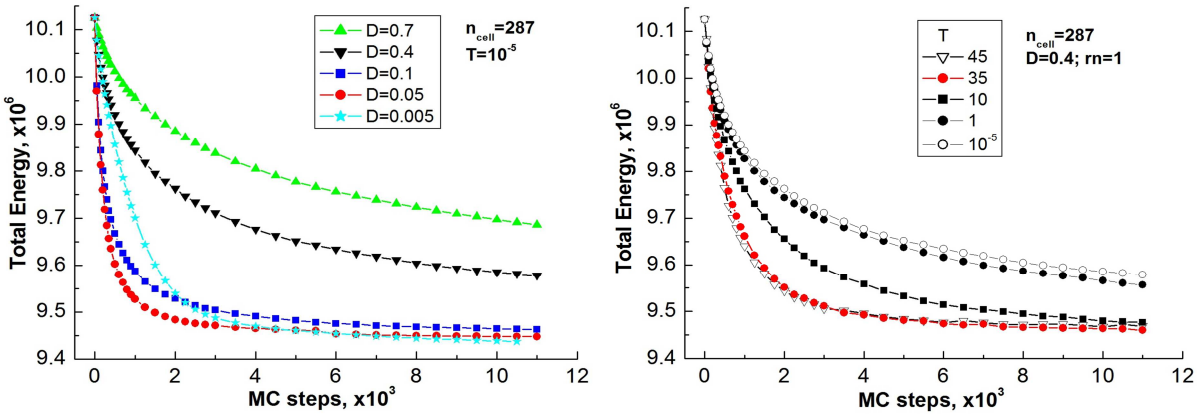

Figure 5: Total energy of the 287-cell tissue versus the number of MC steps for the various values of D (left) and T (right).

Changing D from D =0.1 to D =0.05 does not give a significant effect, just slightly decreases the number of MC steps for reaching convergence. However, a further decrease of D (in particular, D =0.005) results again in the regression of the reaching of the equilibrated state. The reason is that too small node displacements cause too small decrease of the total

energy at per MC step. Hence it requires more MC steps to decrease the energy until to its equilibrium value.

In Fig. 5 (right) we show the influence of T on the energy minimization. One can see that for small values ($T \leq 10$) the increase of T does not give a desirable effect: reaching an equilibrated state requires very long MC calculation. However, further increasing T results in the steepest decreasing energy in early MC steps and thus faster reaching an equilibrated state. We conclude that the use of T =35 is enough in the studied case.

By evaluation of the influence of both D and T on the state of the system we can summarize that the values of E_{th} =0.5, D =0.05 and T =35 are optimal for relatively fast convergence to the equilibrated state in the studied case. Note that though the values of MC parameters are well suited for fast and good convergence, they should be explored in each specific cases, e.g. for different cell sizes, for the cell expansion regime (without division).

3. Conclusions

We analysed the criteria for energy minimization in the Monte Carlo phase in VirtualLeaf simulations. We developed a robust criterion for MC energy minimization in VirtualLeaf - the sliding window criterion. Without this criterion the state of the system found during time evolution and at the final stage can be unpredictable and too far from equilibrium. We have found the sliding window criterion is well suitable for a multi-variable and complex system where the derivative methods are not available such as in this case.

We found that suitable values for the MC parameters can be determined by studying the evolution of the total energy of the system during MC energy minimization. This is a direct, robust and very fast method in comparison with integrated analysis methods. Finding the universal values of parameters suitable for various cases of studies is not easy task or even impossible. However, we developed the robust method for the evaluation of the MC parameter values in order to be sure finding suitable values for MC minimization.

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