Dept of Physics, IIT Delhi

Course Code : PYD411
Project Code : SBBABU1
Academic Year : 2020 - 2021, Semester - I

MODELLING LEAF GROWTH

OM PRAKASH PRAJAPATI (2017PH10835)
PRATYAY PANDE (2017PH10838)

Adviser: Prof. Sujin B. Babu

Signature of student 1:

Om Prakash

Signature of the adviser: ....

Signature of student 2:

pratyay pande

1. Motivation

In this project, we are trying to model the growth of a leaf using concepts of simple physics and light computations. The motivation is to create a light and simple model, and check if the model can successfully represent a real structure of a leaf. Models that currently exist in literature offer a more biological aspect and are computationally expensive, since some involve solving PDEs and a lot of real world factors like atmospheric pressure, humidity, temperature, soil moisture content, etc. are taken into account. We are working to see if this problem can be simplified or if the approach can be simplified if we use simple laws of physics to simulate the growth of the cell.

Almost all of the work done in the project is not inspired by any existing work on this subject, since we are applying the concepts of basic physics in leaf growth. References to literature were made available, and some of the literature that was referenced by us are as follows:

Literature that we took inspiration from are as follows:

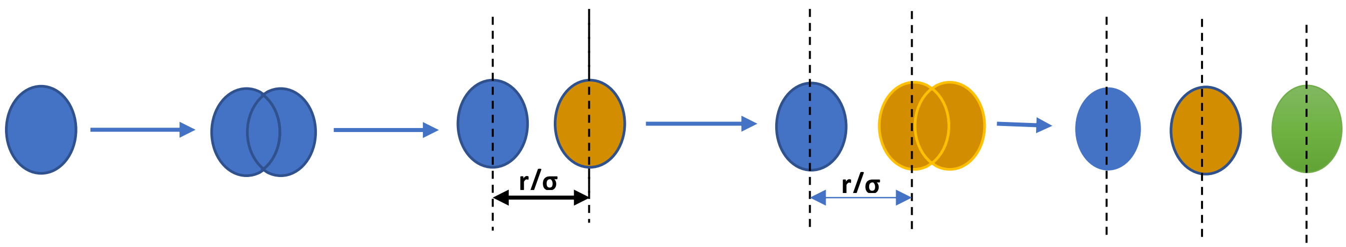
"A leaf area model to simulate cultivar-specific expansion and senescence of maize leaves", J. I. Lizaso, W. D. Batchelor, M. E. Westgate

Currently our working model successfully models the growth of one segment of the leaf. We plan on working on this idea further in order to simulate the growth of cells in the whole leaf taking into account some more factors that we have currently approximated.

2. Computational Setup

Implementation idea:

a) <u>**At Cellular level:**</u>
We assumed that at basic microscopic level the cell division takes place under a fixed potential so that we can monitor the interaction of it with the surrounding layers of cells. In our basic model we assume our leaf structure to be a cell thick and the cellular division rate to be in accordance with the potential. The potential we take is Lennard-Jones potential.



Lennard Jones Potential

In our model, we assumed that the Lennard Jones potential is acting in between any 2 cells. The Lennard Jones potential function is represented as given in the following equation:

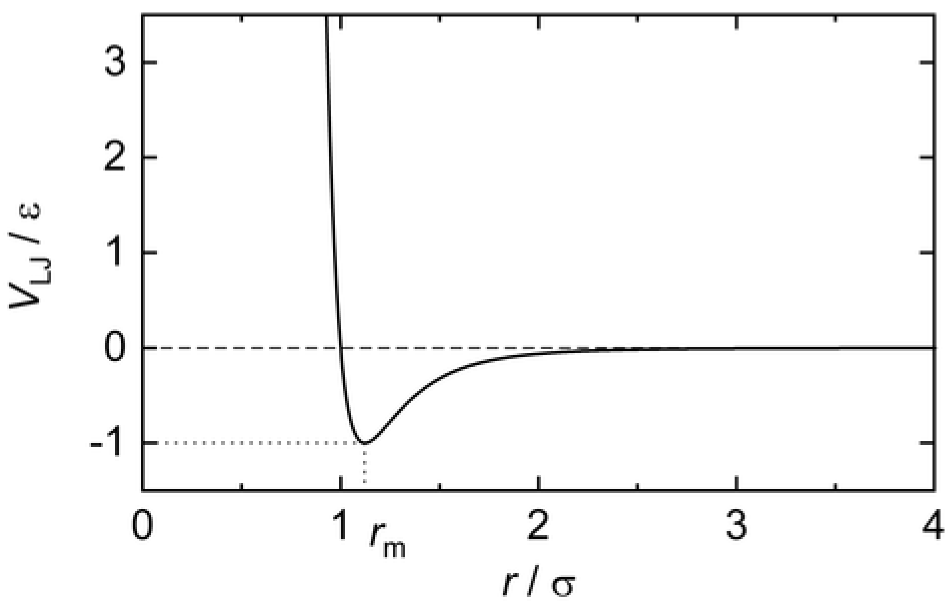
$$V_{\mathrm{LJ}} = 4\varepsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^{6} \right]$$

- As per the given figure, LJ potential is effective only within the range of [1,2].
- So, in order to stay the particles subjected to LJ potential the interparticle distance must be within [1,2].
- We assumed, the distance **r/σ**, to vary from **1 to 2**. Thus, the interparticle distance will decide the rate in a compartment.

The function when plotted gives the graph as mentioned in the diagram given alongside. We can calculate that the graph has a minima at an estimated distance of separation:

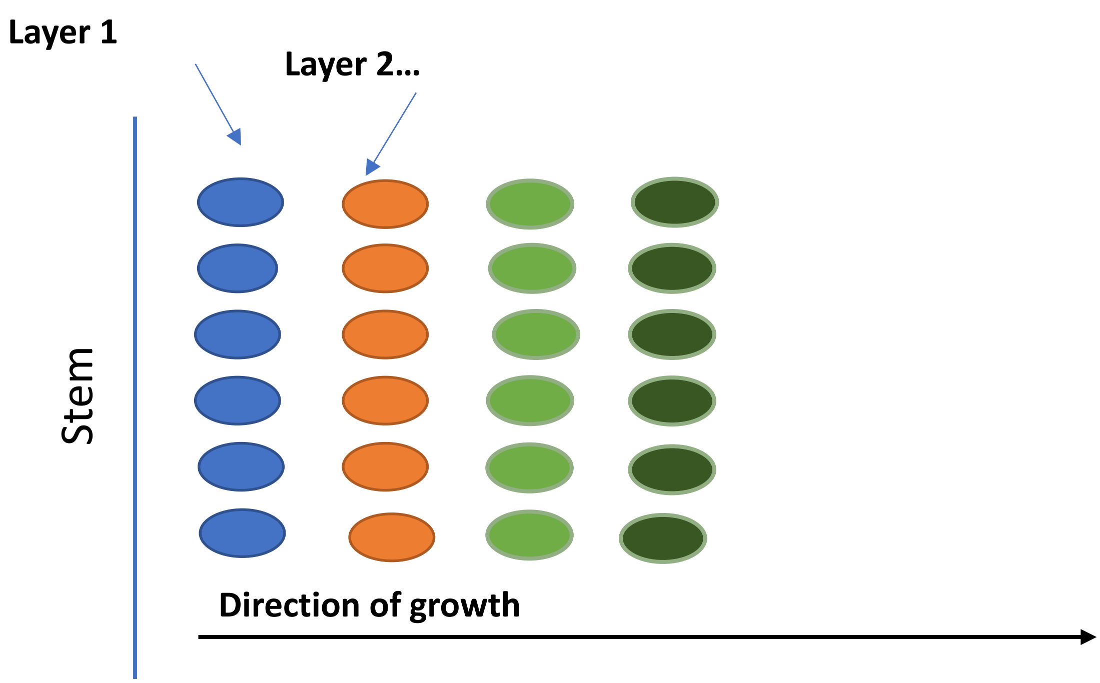
$$\boldsymbol{r_0 = \sigma \times 2^{1/6}}$$

It can also be noted that the Lennard Jones Potential rapidly diminishes at $r = 2r_0$, and becomes negligible (almost vanishes) when $r \approx 2.5r_0$. Hence, it was deduced that when we calculate the potential for one cell of radius r due to the other cells, we can ignore the cells that are beyond the $2.5r_0$. Thus, we can utilise this as an optimisation to the algorithm for calculating the new potential.



First approach idea:

- We take a compartment and take the cell division for n cells in length and m cells across the stem all under LJ potential.
- For compartment 1, we fixed the cell division after layer 2 to take place when it has reached a distance of r/sigma = 1.2(just for analysis).
- Similarly, we can get a large set of r/sigma within [1,2] and different sets of growth too.
- The figure below shows the idea used in the code.



a) **<u>Partition of Leaf:</u>**

We can divide a leaf (at basic level) into a fixed number of compartments/sections for example, let us take a maple leaf and divide it into 6 sections each with different rate of growth. By doing this we achieve a different approach yet quite helpful one in proceeding the simulations.

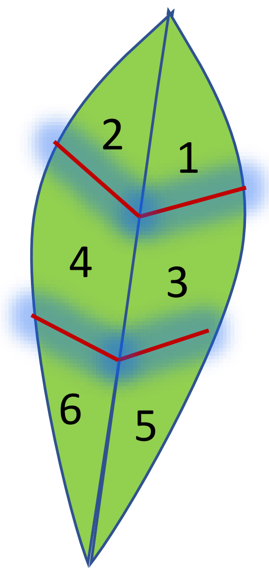
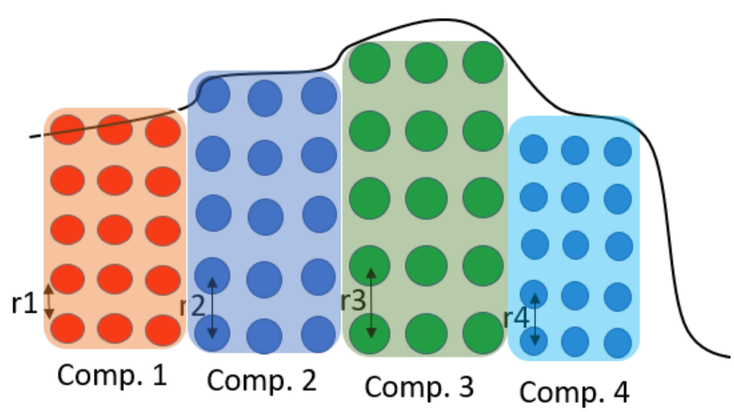


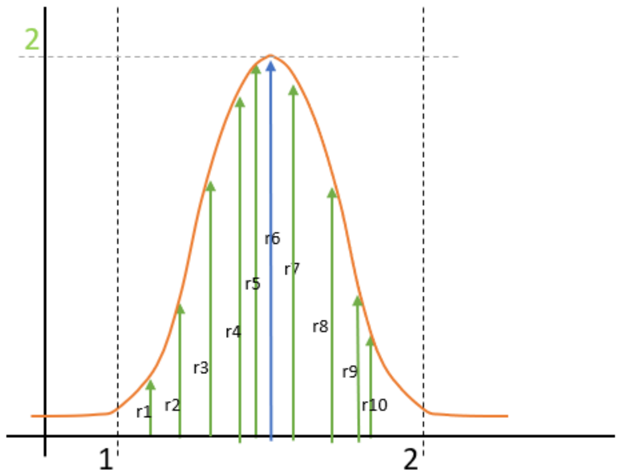
Fig. 1: Compartments in a leaf.

For a good profiled growth, we can assume a lot of compartments inside a leaf so we get the best simulated structure of a leaf. The figure below shows a large number of compartments (each compartment has different coloured cells) with different rate of cellular fission as well as growth that can result in the formation of leaf-like structure.



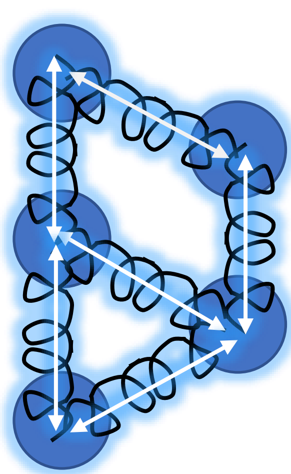
Refining the algorithm to a compartment level:

- If we limit the radii distance to be bounded in [1,2], we can get a Gaussian like distribution of radii values between 1 and 2.
- We can derive those values and use them respectively for different compartments.
- The given fig. 1, shows the radius values.



Drawbacks of this thought model:

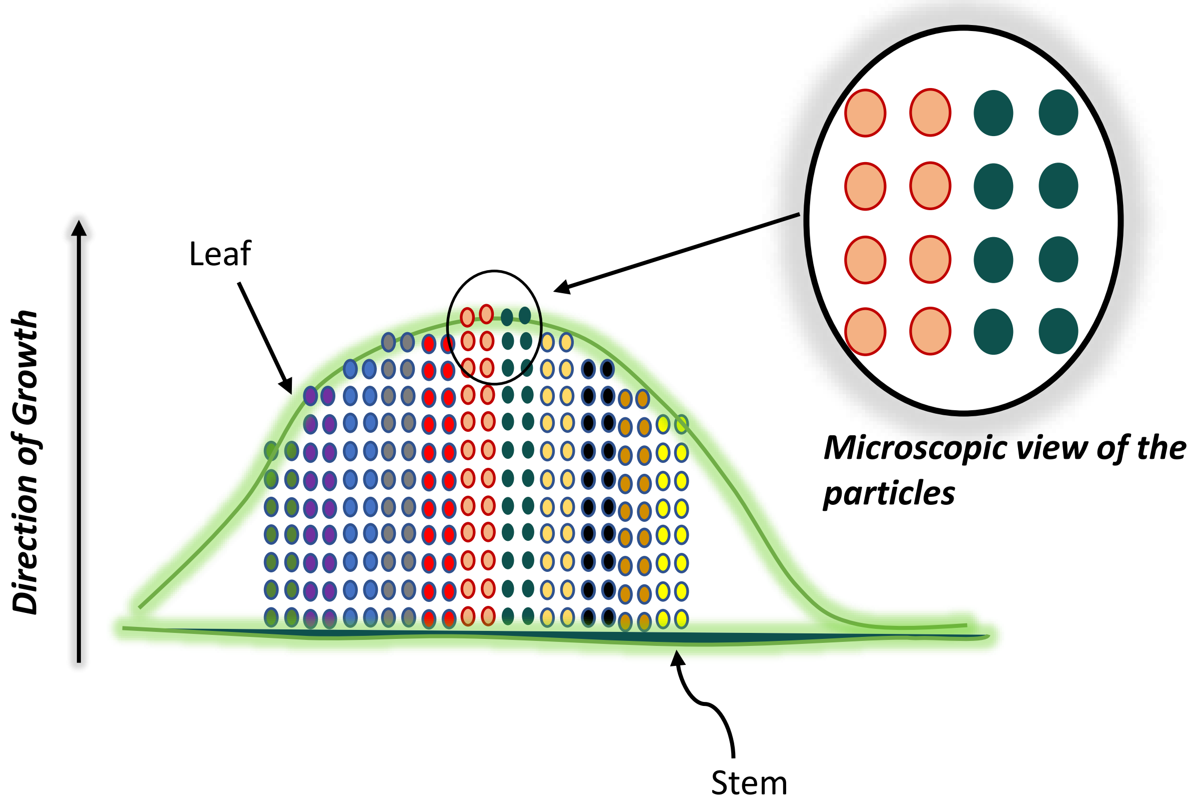
- We did not take the stress or strain by the adjacent atoms of the same as well as different compartments into account.
- A spring model can be an ideal model but the leaf blade posed a serious drawback to this model.



Theory of implementation of the above idea

The rate of growth of each of the compartments built was to be determined using values from a Gaussian, sine or Chi-squared distribution. Thus, the function we choose will be reflected in the shape of the leaf.

In our last version of the code that we built in MATLAB; we involved the live incorporation of the Lennard Jones Potential acting between the cells. After compartmentalising the cells in the leaf, we had eliminated some complications in modelling the leaf growth. For instance, we only need to worry about the lateral growth of each compartment. The current model depicts the growth of one compartment of the leaf whilst taking mitotic cell division and Lennard Jones Potential between the cells into account. The model is portrayed in a 2D graph with the growth in the positive x-direction [since modelling one half of the leaf will be sufficient as we can mirror it to the other half].



Idea is that if we take a large no. of compartments with systematically organised growth rates. We can get a leaf like structure.

The simulation starts with 1 cell having some initial radius $r = \mathbf{r_0}$ with and growth rate **R**. As the cell grows, its radius increases. When the radius r reaches σ/2, the cell undergoes mitotic cell division and 2 new cells having radius $r/2$ are formed. Due to the Lennard Jones potential acting on the whole system, the system will tend to change to the configuration with the minimum potential. To find the minima for each configuration, we calculated the derivative of the Lennard Jones Potential function and calculated its root. To calculate this root, we used the Newton-Raphson Method.

We assumed that the left end of the cells is fixed since it is the main stem, and also took the approximation that in the optimum configuration, the distance between any 2 consecutive cells is the same.

Since the derivative of the function cannot have a defined global maximum, the root is the separation for which the potential is minimum. Using this separation, we calculated the locations of the cells, and thus were able to plot them in a graph.

3. Results and discussion

By application of these ideas, we were able to produce the crude level simulation of the growth of a leaf from its stem. Now, initially when we built the model, we considered the interactions between cells in the lateral direction since the interactions in the longitudinal directions will be cancelled. Hence, our current model assumes the presence of the Lennard Jones Potential in the entire leaf and the cells behave according to the behaviour of the potential.

The figure given in the following page gives an example of one of the earlier results of the model that we have obtained.

Finally, at the time of completion of the project, we have managed to get the final result in the form of a complete bisected image of a leaf. This result only proves that we can model the growth of the leaf using concepts of simple physics within the cells and the idea of the project that we were working on is in fact valid.

There also are images of the results of the final model.

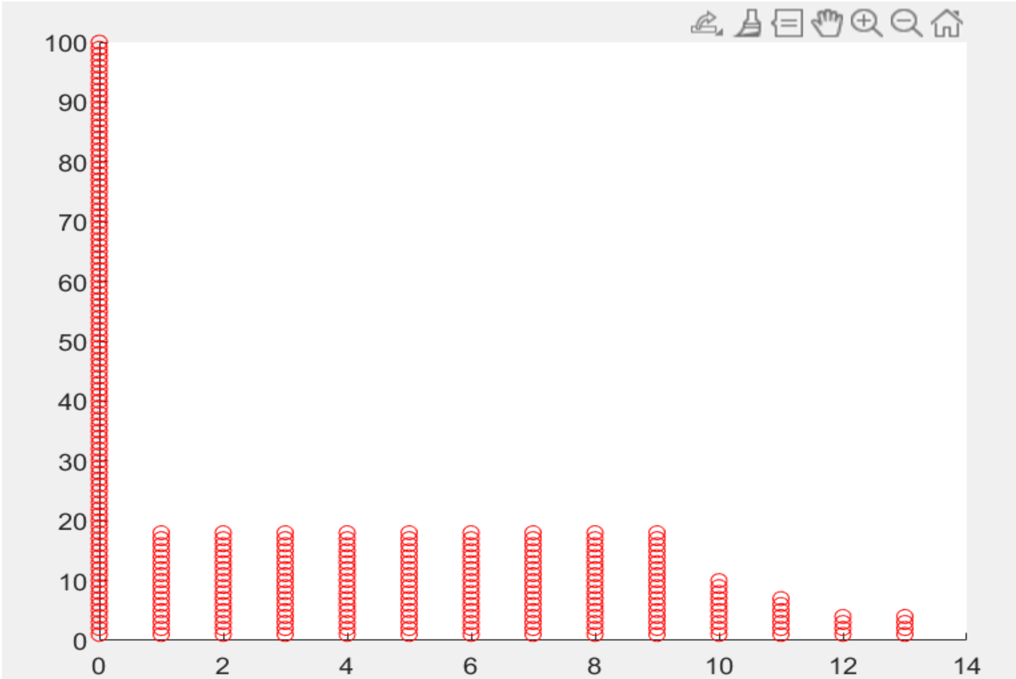


Fig: Initial model depicting the final stage of growth of the half of the leaf

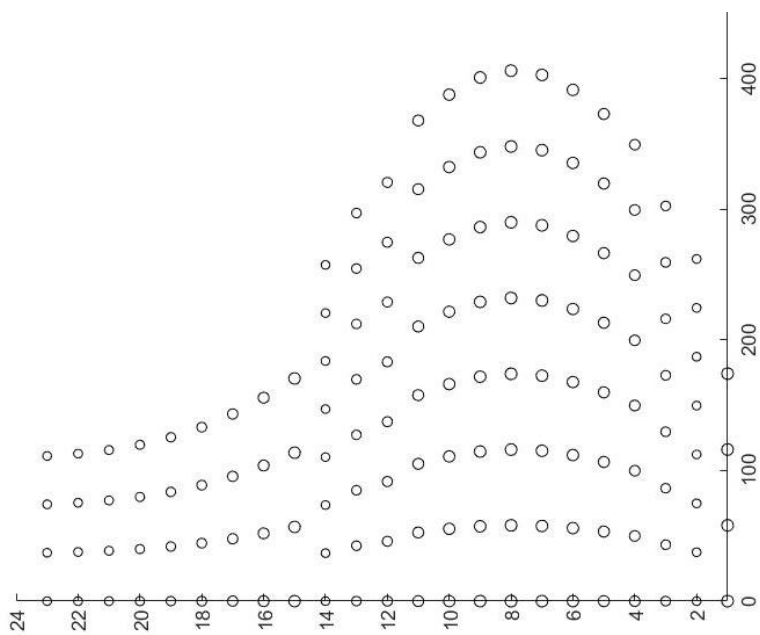


Fig: Final model showing the state of growth of half of a leaf (*peepal*)

Following are some more leaves that we have successfully obtained with this model:

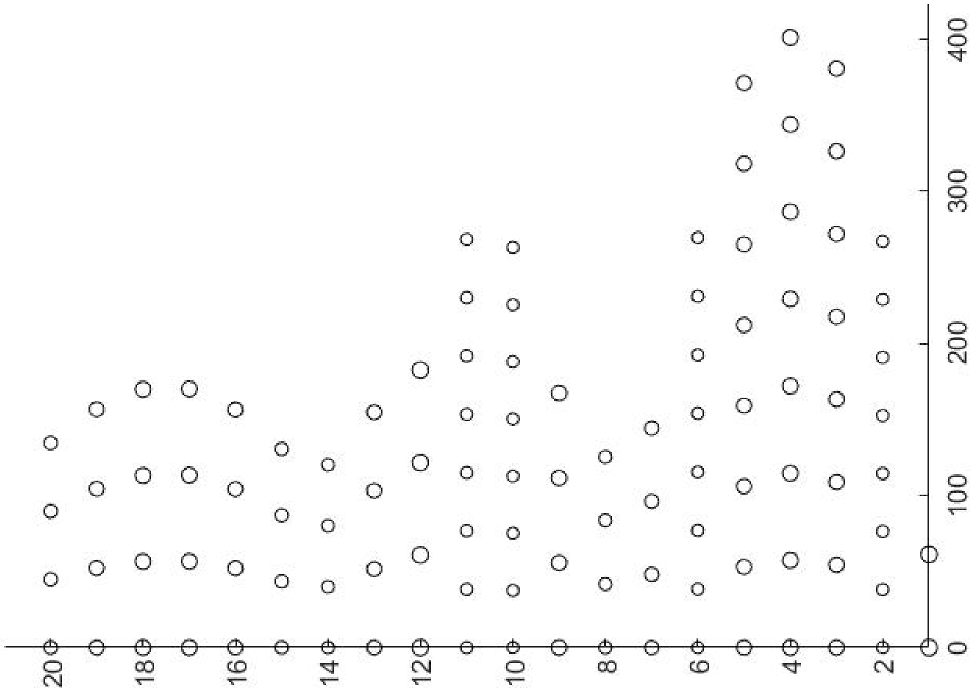


Fig: Attempt to reconstruct half of a neem leaf

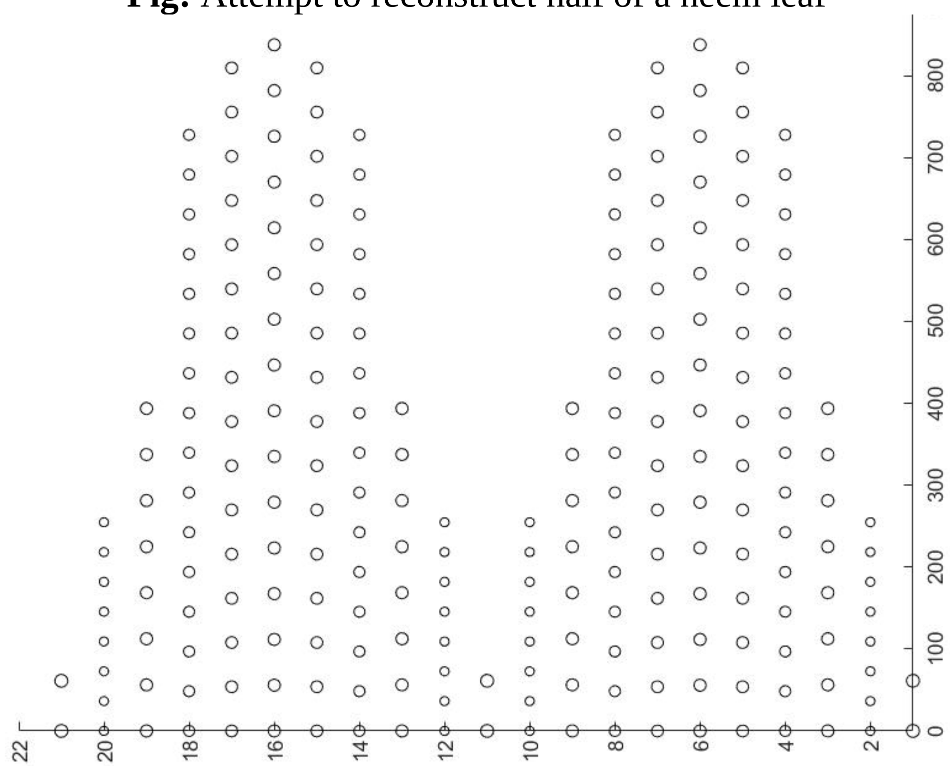


Fig: Another half-leaf that we obtained

4. Conclusions

We observed that model developed by us is feasible and gives acceptable results similar to what is observed in nature. Though a crude model, we can still confirm that this model gives us acceptable results.

The calculations involved are a little computationally expensive since the Newton-Raphson Algorithm needs to be run till convergence for a large number of times. It can possibly be sped up and made more accurate by using GPUs. Since MATLAB uses hardware acceleration (GPU or empty nodes of the CPU) whenever available, the calculations were sped up a little.

5. Future scope

Every project can be made better and better with the incorporation of every feasible idea. The significance of this project is that it proves that we can develop a model for leaf growth using concepts of simple physics, which do not expensive computations that are both time and resource consuming. This provides new ways to model leaf growth that is of utmost significance.

Future work that can be done on this project are immense. One such idea is to implement a Machine Learning Algorithm to check how accurate this model is or even fine-tune the parameters involved in the calculation to give more accurate predictions.

Acknowledgements

We would like to acknowledge Prof. Sujin B. Babu for his supervision in the project and for regularly helping us learn more on this project. We would like to thank him for providing us with the initiative to learn more on modelling leaf growth, and gain more knowledge that would otherwise have had been unknown to us.

References

1. "A leaf area model to simulate cultivar-specific expansion and senescence of maize leaves", J. I. Lizaso, W. D. Batchelor, M. E. Westgate.

2. https://www.researchgate.net/publication/5464518_Plant_Growth_Modelling_and_Applications_The_Increasing_Importance_of_Plant_Architecture_in_Growth_Models

turnitin **Turnitin Originality Report**

MODELLING LEAF GROWTH by Om Prakash Prajapati Pratyay Pande

From Theoretical Fishing (Masters)

Processed on 11-Jan-2021 15:28 IST
ID: 1485667967
Word Count: 1813

Similarity Index	Similarity by Source	
3%	Internet Sources:	3%
	Publications:	3%
	Student Papers:	0%

Sujin B Babu

sources:

1 3% match (Internet from 15-Jul-2019)
https://www.agronomy-journal.org/component/citedby/?doi=10.1051%2Fagro%3A19910101&task=crossref

2 1% match (Internet from 22-Sep-2020)
https://core.ac.uk/display/8306157

paper text:

Dept of Physics, IIT Delhi Course Code : PYD411 Project Code : SBBABU1 Academic Year : 2020 - 2021, Semester - I MODELLING LEAF GROWTH OM PRAKASH PRAJAPATI (2017PH10835) PRATYAY PANDE (2017PH10838) Adviser: Prof. Sujin B. Babu Signature of student 1: Signature of the adviser: .... Signature of student 2: 1. Motivation In this project, we are trying to model the growth of a leaf using concepts of simple physics and light computations. The motivation is to create a light and simple model, and check if the model can successfully represent a real structure of a leaf. Models that currently exist in literature offer a more biological aspect and are computationally expensive, since some involve solving PDEs and a lot of real world factors like atmospheric pressure, humidity, temperature, soil moisture content, etc. are taken into account. We are working to see if this problem can be simplified or if the approach can be simplified if we use simple laws of physics to simulate the growth of the cell. Almost all of the work done in the project is not inspired by any existing work on this subject, since we are applying the concepts of basic physics in leaf growth. References to literature were made available, and some of the literature that was referenced by us are as follows: Literature that we took inspiration from are as follows:

1**"A leaf area model to simulate cultivar-specific expansion and senescence of maize leaves", J. I. Lizaso, W. D. Batchelor, M. E. Westgate**

Currently our working model successfully models the growth of one segment of the leaf. We plan on working on this idea further in order to simulate the growth of cells in the whole leaf taking into account some more factors that we have currently approximated. 2. Computational Setup Implementation idea: a) At Cellular level: We assumed that at basic microscopic level the cell division takes place under a fixed potential so that we can monitor the interaction of it with the surrounding layers of cells. In our basic model we assume our leaf structure to be a cell thick and the cellular division rate to be in accordance with the potential. The potential we take is Lennard-Jones potential. r/σ r/σ Lennard Jones Potential In our model, we assumed that the Lennard Jones potential is acting in between any 2 cells. The Lennard Jones potential function is represented as given in the following equation: • As per the given figure, LJ potential is effective only within the range of [1,2]. • So, in order to stay the particles subjected to LJ potential the interparticle distance must be within [1,2]. • We assumed, the distance r/**σ**, to vary from 1 to 2. Thus, the interparticle distance will decide the rate in a compartment. The function when plotted gives the graph as mentioned in the diagram given alongside. We can calculate that the graph has a minima at an estimated distance of separation: r0 = σ x 2^⅙ It can also be noted that the Lennard Jones Potential rapidly diminishes at r = 2r0, and becomes negligible (almost vanishes) when r ≈ 2.5r0. Hence, it was deduced that when we calculate the potential for one cell of radius r due to the other cells, we can ignore the cells that are beyond the 2.5r0. Thus, we can utilise this as an optimisation to the algorithm for calculating the new potential. First approach idea: • We take a compartment and take the cell division for n cells in length and m cells across the stem all under LJ potential. • For compartment 1, we fixed the cell division after layer 2 to take place when it has reached a distance of r/sigma = 1.2(just for analysis). • Similarly, we can get a large set of r/sigma within [1,2] and different sets of growth too. • The figure below shows the idea used in the code. Layer 1 Layer 2… Stem Direction of growth a) Partition of Leaf: We can divide a leaf (at basic level) into a fixed number of compartments/sections for example, let us take a maple leaf and divide it into 6 sections each with different rate of growth. By doing this we achieve a different approach yet quite helpful one in proceeding the simulations. 2 1 4 3 6 5 Fig. 1: Compartments in a leaf. For a good profiled growth, we can assume a lot of compartments inside a leaf so we get the best simulated structure of a leaf. The figure below shows a large number of compartments (each compartment has different coloured cells) with different rate of cellular fission as well as growth that can result in the formation of leaf-like structure. Refining the algorithm to a compartment level: • If we limit the radii distance to be bounded in [1,2], we can get a Gaussian like distribution of radii values between 1 and 2. • We can derive those values and use them respectively for different compartments. • The given fig. 1, shows the radius values. Drawbacks of this thought model: • We did not take the stress or strain by the adjacent atoms of the same as well as different compartments into account. • A spring model can be an ideal model but the leaf blade posed a serious drawback to this model. Theory of implementation of the above idea The rate of growth of each of the compartments built was to be determined using values from a Gaussian, sine or Chi-squared distribution. Thus, the function we choose will be reflected in the shape of the leaf. In our last version of the code that we built in MATLAB; we involved the live incorporation of the Lennard Jones Potential acting between the cells. After compartmentalising the cells in the leaf, we had eliminated some complications in modelling the leaf growth. For instance, we only need to worry about the lateral growth of each compartment. The current model depicts the growth of one compartment of the leaf whilst taking mitotic cell division and Lennard Jones Potential between the cells into account. The model is portrayed in a 2D graph with the growth in the positive x-direction [since modelling one half of the leaf will be sufficient as we can mirror it to the other half]. Leaf Direction of Growth Blade Microscopic view of the particles of different Stem Idea is that if we take a large no. of compartments with systematically organised growth rates. We can get a leaf like structure. The simulation starts with 1 cell having some initial radius r = r0 with and growth rate R. As the cell grows, its radius increases. When the radius r reaches σ/2, the cell undergoes mitotic cell division and 2 new cells having radius r/2 are formed. Due to the Lennard Jones potential acting on the whole system, the system will tend to change to the configuration with the minimum potential. To find the minima for each configuration, we calculated the derivative of the Lennard Jones Potential function and calculated its root. To calculate this root, we used the Newton-Raphson Method. We assumed that the left end of the cells is fixed since it is the main stem, and also took the approximation that in the optimum configuration, the distance between any 2 consecutive cells is the same. Since the derivative of the function cannot have a defined global maximum, the root is the separation for which the potential is minimum. Using this separation, we calculated the locations of the cells, and thus were able to plot them in a graph. 3. Results and discussion By application of these ideas, we were able to produce the crude level simulation of the growth of a leaf from its stem. Now, initially when we built the model, we considered the interactions between cells in the lateral direction since the interactions in the longitudinal directions will be cancelled. Hence, our current model assumes the presence of the Lennard Jones Potential in the entire leaf and the cells behave according to the behaviour of the potential. The figure given in the following page gives an example of one of the earlier results of the model that we have obtained. Finally, at the time of completion of the project, we have managed to get the final result in the form of a complete bisected image of a leaf. This result only proves that we can model the growth of the leaf using concepts of simple physics within the cells and the idea of the project that we were working on is in fact valid. There also are images of the results of the final model. Fig: Initial model depicting the final stage of growth of the half of the leaf Fig: Final model showing the state of growth of half of a leaf (peepal) Following are some more leaves that we have successfully obtained with this model: Fig: Attempt to reconstruct half of a neem leaf Fig: Another half-leaf that we obtained 4. Conclusions We observed that model developed by us is feasible and gives acceptable results similar to what is observed in nature. Though a crude model, we can still confirm that this model gives us acceptable results. The calculations involved are a little computationally expensive since the Newton- Raphson Algorithm needs to be run till convergence for a large number of times. It can possibly be sped up and made more accurate by using GPUs. Since MATLAB uses hardware acceleration (GPU or empty nodes of the CPU) whenever available, the calculations were sped up a little. 5. Future scope Every project can be made better and better with the incorporation of every feasible idea. The significance of this project is that it proves that we can develop a model for leaf growth using concepts of simple physics, which do not expensive computations that are both time and resource consuming. This provides new ways to model leaf growth that is of utmost significance. Future work that can be done on this project are immense. One such idea is to implement a Machine Learning Algorithm to check how accurate this model is or even fine-tune the parameters involved in the calculation to give more accurate predictions. Acknowledgements We would like to acknowledge Prof. Sujin B. Babu for his supervision in the project and for regularly helping us learn more on this project. We would like to thank him for providing us with the initiative to learn more on modelling leaf growth, and gain more knowledge that would otherwise have had been unknown to us. References 1.

1**“A leaf area model to simulate cultivar-specific expansion and senescence of maize leaves”, J. I. Lizaso, W. D. Batchelor, M. E. Westgate.**

2. https://www.researchgate.net/publication/5464518

2**_Plant_Growth_Modelling_ and_Applications_The_Increasing_Importance_of_Plant_Architecture_in_** Growth **_Models**

2 3 4 5 6 7 8 9 10 11 12 13