A UNIT CELL APPROACH TO REDUCE COMPUTATIONAL TIME OF MESHFREE BASED PLANT TISSUE MODELS

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Abstract - Plant tissue modelling and simulation has become one of the popular research topics in the field of computational mechanics. In this regard, numerous numerical modelling techniques are being researched to study real tissue mechanisms with the help of High Performance Computing (HPC). Among such numerical modelling techniques, meshfree methods have a higher capability, particularly in modelling critical plant tissue deformations during drying. However, existing meshfree based models are computationally expensive in modelling real tissues made oat of loge number of cells, limiting their applications in the real world tissues having thousands of cells It is mainly due to the computationally inefficient conventional neighbourhood treatment methods used in above numerical methods. Accordingly, this research oimed to develop o meshfree based unit cell approach which con be used as o bulldog black to model large tissues. Here, a novel Fixed Neighbourhood based SPH (FN-SPH) method was involved to setup a unit cell representing several real cells (seven cells here). Compared to the original tissue with seven cells, the tissue made oat of the unit cell approach resulted in approximately50M of overall computational time reduction, highlighting the capability of this approach in reducing the computational cost in simulating large-scale plant tissues

Keywords - Fixed Neighbourhood based Smoothed Particle Hydrodynamics (FN-SPH), High Performance Computing (HPC), Meshfree Methods, Numerical Modelling, Plant Tissues

I. INTRODUCTION

From the ancient time, drying or dehydration has been used for the preservation of food materials. As moisture escapes from the food material during drying. it undergoes shrinkage and excessive deformations (Bai 2002; Mayor, ?Bowie & Sereno 2011k Compared to the fresh condition, dried version of a given food material usually has a different structure, mechanical properties, nutrients, visual appearance and mouth feel, leading to higher consumer demand. One of the key observations during drying is the structural deformation as influenced by the moisture content reduction and the drying temperature, which leads to heterogeneous tissue morphological alterations (Bai 2002). In order to optimise such dried focd characteristics, it is critical to have a broader understanding of fundamental mechanisms involved (II. C P Karunasena, Gu, et al. 2015b). For this purpose, there have been many numerical models developed so far, which are either based on grid-based modelling methods such as Finite Difference Methods (FDM) and Finite Element Methods (FEM), or meshfree based modelling techniques. In common, these methods have targeted to model the dynamic co-existence of liquid, solid and gas phases, excessive wall deformations and mufti-scale relationship between sub-cellular and bulk plant material deformations (H. C P Kanmasena, Gu, et al. 2015b; Lewicki & Pawlak 2003). However, many recent research findings have revealed that meshfree based modelling approaches are more capable of modelling large tissue deformations during drying, compared to grid based methods (H. C P Karunasena, Gu, et al. 201Sb; H. C P Karunasena, Senadeera, Brawn, et al. 2014a; H. C P Karunasena, Senadeera, Gu, et al. 2014d; Liu et al. 2003). Furthermore, combined grid.based and meshfree methods have also shown promising capability in modelling multi-scale tissue mechanisms (Ghysels et al. 2009; H. C. P. Karunasena et al. 2014c). Also, several types of food • material structures and many advanced physical mechanisms such as case hardening and porosity development during drying have recently been modelled

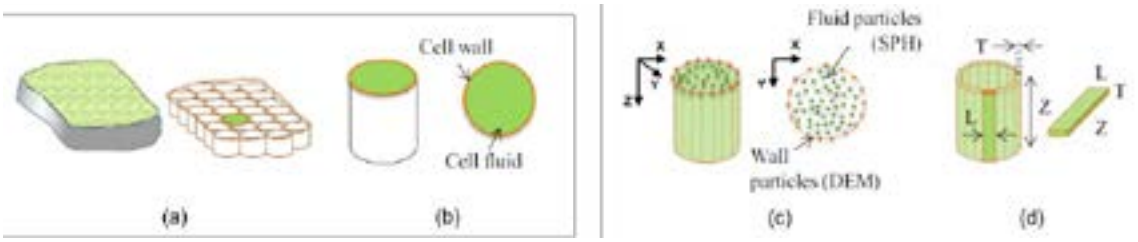

Figure 1. (a) A plant tissue simply represented as an aggregate of cylindrical cells. (b) 2-D model to represent any cylindrical cel (c) Particle scheme used for the 2-D cell model: fluid model based on SPH particles and wall model based on DEM particle (d) discrete elements of the cell wall (H. C. P. Karunasena, Senadeera, Brown, et al. 2014a)

(Bai 2002; H. C P Karunasena, Brown, et al. 2015c; H. C.P. Karunasena et al. 2015a; Van Liedekerke et al. 2011; Rathnayaka Mudlyanselage et al. 2017). Figure 1 presents a basic meshfree based model of a plant cell developed using Smoothed Particle Hydrodynamics (SPH) and the Discrete Element Method (DEM).

However, compared to grid based numerical method; meshfree methods demand higher computational resources and time. Therefore, much attention is currently on improved meshfree based modelling techniques to reduce computational effort. For instance, simulation of the dynamics of a single apple cell just for S ms in real time requires a SDH-OEM based meshfree model to run for at least 200 seconds in a typical personal computer having Intel•CorelMi7.6700, 3.4 GH1 • 8 core processor with 8 GB RAM in Ubuntu. Furthermore, if this model is used to simulate a 1 mm^2 tissue consisting of 178 cells, approximately 10 hours of simulation time would be needed (H. C P Karunasena, Senadeera, Gu, et al. 2014a). If this is so, it may become computationally much difficult to model and simulate a tangible real plant tissue (e.g. 1 cm * 1 cm), having thousands of cells. Accordingly, as the number of cells in a plant tissue increases, the overall computational time increases exponentially, limiting the applicability of current modelling approaches. Anyway, modelling such larger tissue are of much importance to the field since different analysis and predictions are to be done involving realistic tissues of tangible sizes.

In above models, it is commonly observed that more than 50% of the computational time is taken by the All Pair Search (APS) algorithm, which is used for interaction calculations in Nearest Neighbour Particle Searching (NNPS), which is an indispensable part of meshfree based models (Hansani, Karunasena & Sumith 2017; Hansani, Sumith & Karunasena 2016). Although APS is the simplest method to identify neighbour particles, it consumes more time as it checks every particle in the simulation domain for possible neighbourhood interactions, which is repeated in each time step, not like in grid based methods having fixed neighbours (Liu et al. 2003). As a solution, computational time reduction steps have been recently proposed for meshfree based plant tissue models, with the use of Fixed Neighbourhood method (FN) and Cell-Linked List Algorithm (CLLA) (Hansani, Karunasena & Sumith 2017; Hansani, Sumith & Karunasena 2016). However, there are many limitations in these modelling approaches as these models are more focused on micro-scale cellular mechanisms rather than simulating bulk scale mechanisms of larger tissues.

In this background, this research proposes a unit cell approach to conveniently model large plant tissues, which will be described in sections below.

II. NNPS AND FN-SPH BASED SIMULATION

In meshfree methods, Nearest Neighbour Particle Searching (NNPS) is one of the key time-consuming components in the source code of the model. In NNPS, physical properties of a given particle is calculated using the properties of the neighbouring particles. Here, the neighbouring particles are the ones that are located in a distance less than or equal to *2h from the particle of interest*, where h is smoothing length.

In this work, individual seven cells were taken as a unit cell and simulated as a cluster using APS in SPH. Then the

unit cell was setup using the novel Fixed Neighbourhood based SPH method (FN-SPH) also and the two methods were compared both qualitatively and quantitatively. The FN-SPH has characteristics of the grid based methods such as Finite Difference Method (FDM) and Finite Element Method (FEM) and it involves following key steps in its implementation:

1. Place each particle in an enclosed boundary of 3h
2 Store neighbouring particle identities in the computer memory
3 Perform interaction calculations for the above neighbouring particles
4 Run all the iterations and perform all calculations in the model using the selected neighbours

This approach runs under two key assumptions: 1) cell fluid is incompressible and only have low Reynolds number fluid flow conditions, 2) each particle is virtually located in an enclosed circular boundary of radius 3h, where a fixed number of neighbouring particles exist. Therefore, unlike in APS approach, the entire problem domain is not searched during the simulations in each time step, but only the pre-determined neighbouring regions, which is essentially a smaller portion of the whole problem domain (see Figure 2) (Hansani, Karunasena & Sumith n.d.; Hansani, Sumith & Karunasena 2016). This is the main cause for the reduction of the computational time significantly.

III. METHODOLOGY

The FN-SPH based unit cell model was developed based on an existing C++ code (H. C. P. Karunasena, Senadeera, Brown, et al. 2014a), that had been developed for single plant cell simulations. Here, for the convenience of concept validation, a smaller unit cell was involved in this paper, consisting of seven individual cells. In the original model, a single cell was modelled using 96 wall particles and 656 fluid particles. Accordingly, here the unit cell was modelled using 252 wall particles and 1728 fluid particles (see Figure 3) (Hansani, Sumith & Karunasena 2016). Simulations were done using a High-Performance Computer (HPC) having Intel® CoreTM i7-6700, 3.4 GHz × 8 core processor having 32 GB RAM in Ubuntu operating system. Parallel processing was used in the computer code to reduce overall computational time. For visualisation of the model outcomes, the Open Visualisation tool (Ovito), version 1.1.0 was used.

IV. RESULTS AND DISCUSSION

As given in Table 1, when comparing the model outcomes from both approaches, the results are almost same. It implies that the unit cell approach can fundamentally be applied for tissue simulations and predictions.

Figure 4 presents the qualitative results comparing the seven cells and unit cell under varying moisture content. The two set of results indicate that the unit cell has the capability to mimic the gradual deformation and shrinking characteristics displayed by the original seven cell cluster, even with less number of particles and interactions.

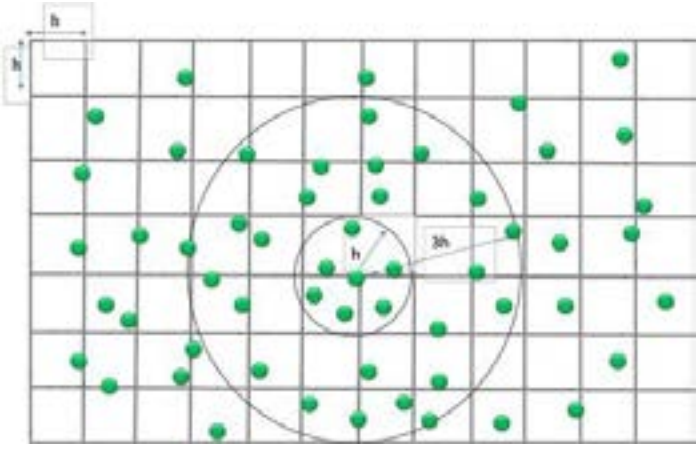

Figure 2. Domain discretisation in FN-SPH based on a circular boundary of radius 3h

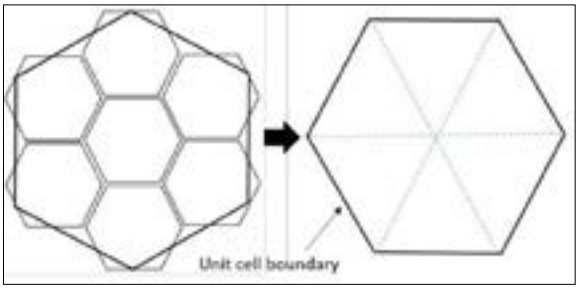

Figure 3. Aggregation of seven cells(left) into a simple unit cell(right)

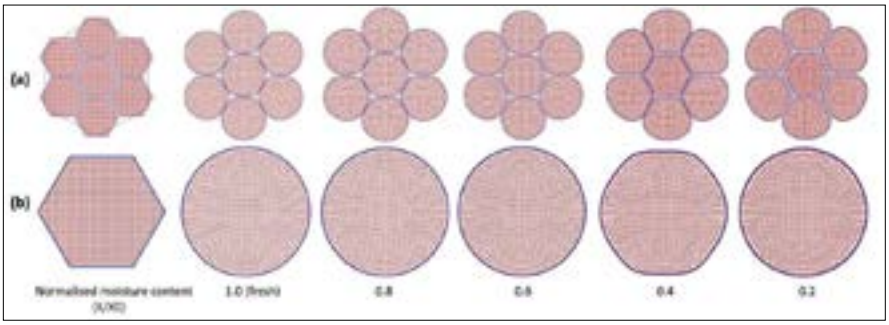

Figure 4. Deformation of a tissue during drying (reduction of the X/X0): (a) a tissue with combined seven cells with APS, and (b) unit cell with FN-SPH used

Table 1. Comparison of model outcomes

Parameter	Tissue with combined seven individual cells	Tissue with the unit cell
Percentage error in model consistency	4.90%	-1.48%
Fluid Final Pressure (kPa)	187.0	189.5
Fluid final density (kgm^{-3})	999.9	999.9
Final stretch ratio	1.0	1.1
Normalized moisture content	1	1
Final cell fluid mass (kg)	2.17389E-09	1.53076E-08
Final cell area (m2)	2.09965E-08	1.47269E-07
Final cell equivalent diameter (μm)	163.5	433.0
Final cell perimeter (μm)	516.4	1360.6
Final cell roundness	0.990	1.000
Final cell elongation	1.008	1.001
Final cell compactness	0.959	0.994
Wall inter-particle force (theory (mN)	1.531	4.111
Wall inter-particle force (SPH) (mN)	1.606	4.050
Wall contraction force due to drying (mN)	-1.452	1.763
Maximum number of interactions per particle	23	29
Minimum number of interactions per particle	14	14
Number of particles with no interactions	0	0
Average number of interactions per particle	17	18

Table 2: Comparison of simulation results of the original tissue model with seven cells using APS, the tissue model with the unit cell approach using FN-SPH method

	A/A₀			D/D₀			P/P₀			R/R₀		
X/X₀	Seven cells	Unit cell	%Error	Seven cells	Unit cell	%Error	Seven cells	Unit cell	%Error	Seven cells	Unit cell	%Error
1	1	1	0	1	1	0	1	1	0	1	1	0
0.8	0.9363	0.9408	0.481	0.9676	0.9699	0.238	0.9732	0.9699	0.339	0.9885	1.0001	1.173
0.6	0.8594	0.8725	1.524	0.927	0.9341	0.766	0.9403	0.934	0.67	0.972	1.0001	2.891
0.4	0.7251	0.7956	9.723	0.8516	0.892	4.744	0.9027	0.8953	0.82	0.89	0.9926	11.53
0.2	0.6891	0.7619	10.56	0.8301	0.8728	5.144	0.8811	0.8729	0.931	0.8876	0.9999	12.55

Table 2 presents the quantitative values such as the normalized cell area (A/A0), ferret diameter (D/D0), perimeter (P/P0) and roundness (R/R0), against the normalised moisture content (X/X0). Here, X, A, D, P and R are the moisture content, area, diameter, perimeter and roundness respectively while X0, A0, D0, P0 and R0 are the initial values of those properties. It is evident that both results are in very good agreement where the maximum percentage error limiting to 12.5%.

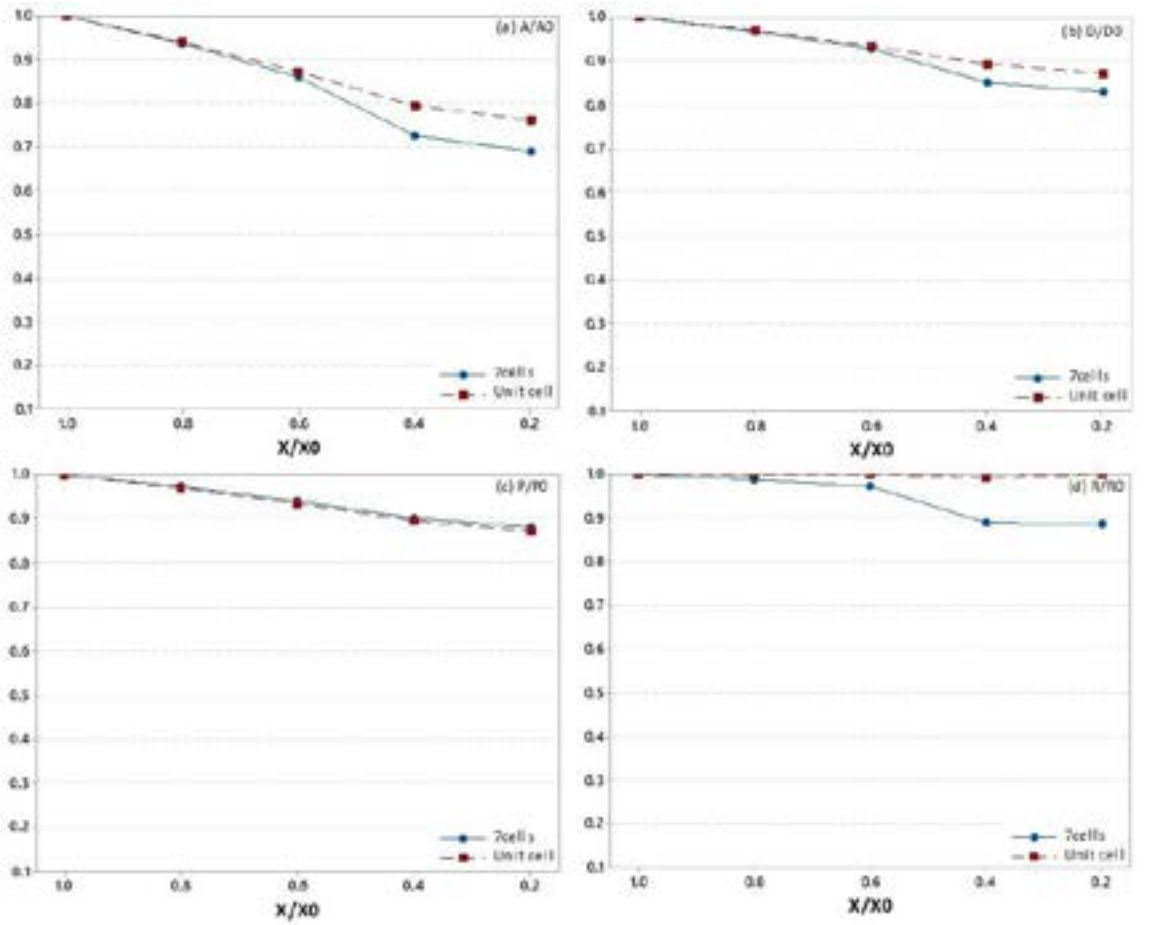

Figure 5. Quantitative results of the simulations of seven cell method and proposed unit cell method comparing with (a) A/A0 - Normalized cell area (b) D/D0 - Normalized cell ferret diameter (c) P/P0 - Normalized cell perimeter (d) R/R0 - Normalized cell perimeter respect to X/X0 – Normalized moisture content

Next, the Figure 6 compares the computational time for both methods. Accordingly, the unit cell approach records an 80% computational time reduction compared to the original model with seven cells. Therefore, the validity of the unit cell approach in order to reduce the computational time is evident. Furthermore, it can be observed that the simulation time is gradually reducing as the cell cluster or the unit cell is getting dried. One of the main reasons for this is the reduced size of the cellular problem domain, where neighbourhood finding become easier since particles are located much closer.

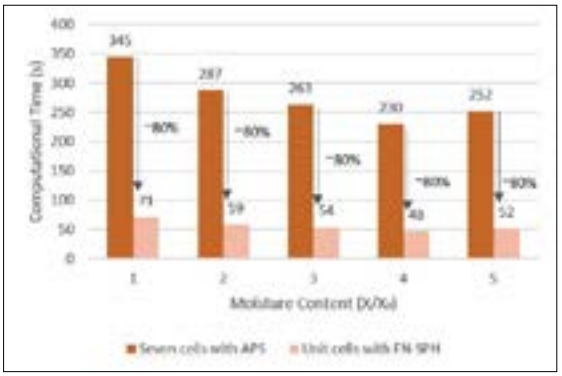

Figure 6. Comparison of the computational time of seven cell and the unit cell implementation. It clearly indicates that the unit cell can reduce the computational time significantly

V. CONCLUSION

This paper presented a unit cell approach by incorporating the FN-SPH approach, which results in about 80% of the computational time reduction compared to original tissue modelling approach involving APS in SPH. The accuracy of predications is also much comparable with the original model predictions. The computational advantage is particularly due to the reduced number of interaction calculations offered by the proposed method, where the whole problem domain is not searched to identify the neighbouring particles, under NNPS in SPH. Accordingly, this can be used in large tissue simulations producing much higher levels of computational advantages. However, the application of the proposed technique is limited to lower Reynold number flow conditions in the fluid flow problem domains, if FN-SPH is used. However, if APS is used instead of FN-SPH for the unit cell approach, the lower Reynold number condition can be avoided, but with additional computational expense. This approach has the potential of applying in many other research areas other than just plant tissue modelling, such as modelling of animal tissues or non-continuum discrete materials in general

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