Application of Smoothed Particle Hydrodynamics in biomechanics: advanced procedure for discretization of complex biological shapes into pseudo-particles

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Abstract— **Smoothed Particle Hydrodynamics is meshless numerical method which is based on continuum mechanics approach, capable of analyzing stresses in both solids and fluids as well as stresses that are result of solid-fluid interaction, with very versatile applications, and yet it' is not sufficiently implemented in biomechanics due to difficulties of node grid generation from complex shape objects. This paper presents multiblock procedure for generation of pseudo-particles which are used in Smoothed Particle Hydrodynamics for representation of discretized parts of analyzed continua. This procedure enables creation of evenly sized pseudo-particles even for the very irregular shaped object such are organs, bones or blood vessels which are analyzed in biomechanics.**

I. Introduction

THIS paper deals with the issue of insufficient implementation of Smoothed Particle Hydrodynamics in biomechanics. Smoothed Particle Hydrodynamics (in short SPH) is numerical method originally designed for solving astrophysical problems, which application field was later extended with Computational Fluid Dynamics (CFD), and solid mechanics, by adding strength of materials into SPH equations [1]. SPH is the most popular meshless method based on continuum mechanics approach, which means that every SPH pseudo-particle describes certain part of analyzed continua, similarly to finite elements in Finite Element Method (FEM) [2].

Unlike finite elements, pseudo particles in SPH method are not connected with mesh, which allows simulation of problems with very large deformations. Lack of mesh allows significant changes of analyzed object shape, but it also brings some difficulties in SPH implementation [2]. Many commercial FEM programs have very adaptive algorithms for mesh generation, but since SPH is not commercially wide speeded, it is very difficult to generate appropriate model for complex geometry which is found in biomechanics such are blood vessels, bones, organs. The most common approach in generating SPH nodes is to use the same technique used in generation of FEM mesh, and to generate SPH pseudo-particle in centers of elements or on FEM nodes, but this method neglect the fact that 3D finite elements can be elongated or irregular shaped which means that distance between SPH particles will not be uniform [2]. Although every SPH pseudo-particle can have different size and mass, homogeneous pseudo-particles are more appropriate, especially for CFD calculations. This paper presents novel procedure for generation of nodes (pseudo-particles) from irregular shaped geometry, which will ease application of SPH for biomechanical simulations.

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II. SPH in Biomechanical Analysis

A. Advantages and Disadvantages

SPH method provides possibility for numerical analysis of fluid flow [3], solid deformation [4] and fluid-solid interaction [5] within Lagrangian material framework, which means that motion of fluid (or solid) section is observed. These sections are represented by pseudo-particles and each pseudo-particle of SPH method is similar to an element in FEM method, but since there are no common nodes between pseudo-particles these pseudo-particles can have different neighboring particles throughout analysis which enables better handling of large deformations but requires frequent searches for neighboring particles. To model continuum material (voids and inter-molecular spaces neglected) with pseudo-particles, two approximations are implemented: kernel approximation and particle approximation.

B. Kernel Approximation

The conservation laws of continuum mechanics are expressed in form of partial differential equations which are transformed into integral equations by interpolation function that gives "kernel estimate" of the field variables at point [2]. Exact value of function $f(\mathbf{x})$ in integral form is given with (1)

$$f(\mathbf{x}) = \int_{\Omega} f(\mathbf{x}')\delta(\mathbf{x}-\mathbf{x}')\,d\mathbf{x}' \tag{1}$$

where $f(\mathbf{x})$ represents a function of position vector $\mathbf{x}$ defined in the domain Ω and $\delta(\mathbf{x}-\mathbf{x}')=\begin{cases}1 & \mathbf{x}=\mathbf{x}'\\ 0 & \mathbf{x}\neq\mathbf{x}'\end{cases}$ is the Dirac delta measure. Replacing $\delta(\mathbf{x}-\mathbf{x}')$ with kernel function $W(|\mathbf{x}-\mathbf{x}'|,h)$ where h is the smoothing length, gives us kernel approximation of function $f(\mathbf{x})$

$$\langle f(\mathbf{x})\rangle=\int_{\Omega} f(\mathbf{x}')W(|\mathbf{x}-\mathbf{x}'|,h)\,d\mathbf{x}'. \tag{2}$$

C. Particle Approximation

Another important aspect of SPH is particle approximation [2]. Integral form given in equation (2) is not practical for numerical implementation because analyzed continuum is divided into finite number of pseudo-particles which carry individual mass and occupy individual space. Therefore continuous integral representations given with (2) can be converted to discrete forms of summation over all pseudo-particles within support domain defined by smoothing length h. If the infinitesimal volume $d\mathbf{x}'$ from equation (2) is replaced by finite volume of the particle ΔV_j (where particle mass m_j and particle density ρ_j can be used to define finite volume as $\Delta V_j=m_j/\rho_j$) and if the summation of all particles within support domain is implemented in equation (2) we get discreditized particle approximation of function $f(\mathbf{x})$ for particle i

$$\begin{aligned}\langle f(\mathbf{x}_i)\rangle &\cong \sum_{j=1}^{NNP} f(\mathbf{x}_j)W(|\mathbf{x}_i-\mathbf{x}_j|,h)\,dV_j\\ &=\sum_{j=1}^{NNP}\frac{m_j}{\rho_j}f(\mathbf{x}_j)W(|\mathbf{x}_i-\mathbf{x}_j|,h)\end{aligned} \tag{3}$$

where *NNP* represents number of nearest neighboring particles.

D. Modeling of Viscous Fluid Flow

Total stress tensor $\sigma_{\alpha\beta}$ in viscous fluid [6] (in biomechanical application that would be blood) can be decomposed into hydrostatic pressure p and viscous shear stress ${}^{visc}S_{\alpha\beta}$ (which is result of fluid flow)

$$\sigma_{\alpha\beta}=-p\delta_{\alpha\beta}+{}^{visc}S_{\alpha\beta} \tag{4}$$

where $\delta_{\alpha\beta}$ represent Kronecker delta.

For Newtonian fluids volume viscosity can be neglected, so viscous shear stress can be calculated as

$${}^{visc}S_{\alpha\beta}=\mu\left(\partial_a v_\beta+\partial_a v_\beta-\frac{2}{3}\partial_\gamma v_\gamma\delta_{\alpha\beta}\right)=\mu\varepsilon_{\alpha\beta} \tag{5}$$

where μ represents coefficient of dynamic (shear) viscosity and $\varepsilon_{\alpha\beta}$ is strain rate tensor which for every particle i can be calculated as

$$\begin{aligned}\varepsilon^i_{\alpha\beta}=&\sum_{j=1}^{NNP}\frac{m_j}{\rho_j}v^{ji}_\beta\frac{\partial W^{ij}}{\partial x^i_\alpha}+\sum_{j=1}^{NNP}\frac{m_j}{\rho_j}v^{ji}_\alpha\frac{\partial W^{ij}}{\partial x^i_\beta}\\ &-\left(\frac{2}{3}\sum_{j=1}^{NNP}\frac{m_j}{\rho_j}\mathbf{v}^{ji}\cdot\nabla_i W^{ij}\right)\delta_{\alpha\beta}\end{aligned}. \tag{6}$$

E. Elastic Material Model for Biological Materials

In order to model behavior of elastic solids [7] in biomechanical analysis (such are walls of blood vessels for example), total stress tensor $\sigma_{\alpha\beta}$ is calculated as a sum of hydrostatic pressure p and shear stress $S_{\alpha\beta}$

$$\sigma_{\alpha\beta}=-p\delta_{\alpha\beta}+S_{\alpha\beta}. \tag{7}$$

Shear stress in next time step is calculated by adding its increment to current step value

$${}^{t+\Delta t}S_{\alpha\beta}={}^{t}S_{\alpha\beta}+dt\cdot\frac{dS_{\alpha\beta}}{dt}. \tag{8}$$

Shear stress increment is calculated with

$$\begin{aligned}\frac{dS_{\alpha\beta}}{dt}=&G\left(\dot{\varepsilon}_{\alpha\beta}-\frac{1}{3}\delta_{\alpha\beta}\dot{\varepsilon}_{mm}\right)\\ &+S_{\alpha\gamma}\Omega_{\beta\gamma}+S_{\gamma\beta}\Omega_{\alpha\gamma}\end{aligned} \tag{9}$$

where strain rate tensor is given with

$$\begin{aligned}\dot{\varepsilon}^i_{\alpha\beta}=&\frac{1}{2}\sum_{j=1}^{NNP}\frac{m^j}{\rho^j}\left(v^j_\alpha-v^i_\alpha\right)\frac{\partial W^{ij}}{\partial x^i_\beta}\\ &+\frac{1}{2}\sum_{j=1}^{NNP}\frac{m^j}{\rho^j}\left(v^j_\beta-v^i_\beta\right)\frac{\partial W^{ij}}{\partial x^i_\alpha}\end{aligned} \tag{10}$$

while rotation tensor $\Omega_{\alpha\beta}$ is given with

$$\begin{aligned}\Omega_{\alpha\beta}=&\frac{1}{2}\sum_{j=1}^{NNP}\frac{m^j}{\rho^j}\left(v^j_\alpha-v^i_\alpha\right)\frac{\partial W^{ij}}{\partial x^i_\beta}\\ &-\frac{1}{2}\sum_{j=1}^{NNP}\frac{m^j}{\rho^j}\left(v^j_\beta-v^i_\beta\right)\frac{\partial W^{ij}}{\partial x^i_\alpha}\end{aligned}. \tag{11}$$

III. Generation of SPH Nodes

In FEM nodes define mesh of elements, and every element has the same nodes during whole analysis no matter how deformed it can get. In SPH method nodes define centers of pseudo-particles, which do not have defined neighbors, which allow modeling of significant deformations. Same as the elements in FEM, pseudo-particles can have different mass and volume, but they always have circular or spherical shape [2]. Non-homogenous pseudo-particle size can be a problem because SPH uses Lagrangian framework so motion of fluid section

can differ if some part of the fluid is modeled with one big or several smaller pseudo-particles. To create more homogenous node distribution multiblock concept is used. This concept is developed for FEM [8] and for SPH application is modified so that instead of finite elements, grid of pseudo-particles is created.

Structured mesh generation is the most adequate method for discretising domains into FEM mesh because in this method all internal points are topologically alike, and elements that they form are regular. The method is based on a direct mapping from the solution domain (SD) to computational domain (CD) (Fig. 1a).

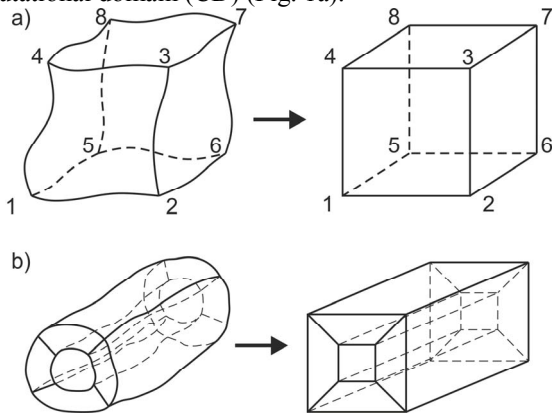

Fig. 1. Mapping of a block from Solution Domain (SD) to Computational Domain (CD) a) single block b) multiblock

Boundary points defined within the SD are used to interpolate the internal points in the CD. The point grid distribution is determined by solving Poisson equation for each coordinate direction. Structured grids use general curvilinear coordinates to create a body fitted mesh. This is an advantage since boundaries can be exactly described and therefore boundary conditions can be accurately modeled. Unfortunately, this approach has some disadvantages, for instance it cannot be used for complicated geometries which are found in biomechanical analysis, so new multiblock or composite grid approach was developed for FEM mesh generation [8] and in this paper its modification to SPH method is presented.

In multiblock approach SD is divided into a set of blocks [9] and every block in SD is mapped onto a Cartesian block in CD (Fig. 1b). Structured mesh techniques are applied to blocks. Blocks are then linked together to produce a much larger mesh. Since multiblock grids are unstructured on the block level, data about block connectivity is required in order to enable merging of block boundary FEM nodes to produce unified FEM mesh, or in case of SPH, to avoid overlapping of particles on block boundaries. The actual SD on which the governing physical equations are solved is a set of connected, regular blocks in CD which are discretized into FEM elements or SPH pseudo-particles. The First step in multiblock approach is definition of blocks' topology. Topology definition means definition of a wireframe model around volumetric model by placing wireframe points, connecting these points, and assigning them to fixed surfaces.

For analyzed biomechanical model (carotid artery bifurcation) user-defined sections can be observed Fig. 2(a).

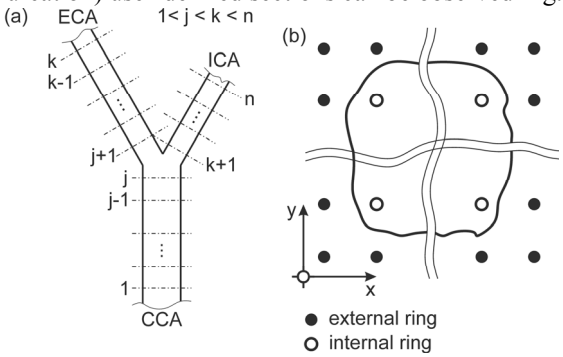

Fig. 2. Vertices of the blocks: (a) sections containing the blocks' vertices and (b) layout of blocks' vertices in each section

For each section maximum dimensions of object are known as well as the coordinates of barycenter point and normal vector direction. This organization of the blocks is observed in each section from the top of the z axis downwards. Blocks' points are placed in the section to form a 2D array and are divided into two groups: external and internal ring (Fig. 2(b)). The external points of the block (external ring) are set to lie in the section and outside of analyzed object at half the maximum dimension of the section from the section center point in directions of local coordinate axes x and y. The internal points of a block (internal ring) are placed inside the analyzed object.

Different blocks' arrangement strategies can be used for all or just some of the points. Number of divisions on the block opposite sides must be equal. For the first blocks' shown on Fig. 2(a) arrangement strategy uses only the external points (external ring) and the number of elements or particles per block' edge is 2 (Fig. 3.

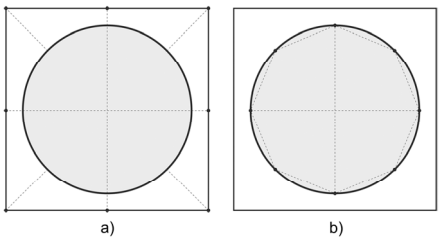

Fig. 3. Mapping from computation to physical domain for straight vessel

Nodes on the surface defined by the point cloud are obtained by projecting the grid points on the point cloud in direction connecting the adequate grid points of opposing edges of the block. Nodes within the domain are constructed by transfinite interpolation (TFI).

If topology with 3x3 blocks is used, this methodology can be implemented for node generation for bimechanical models with branching (Fig. 4).

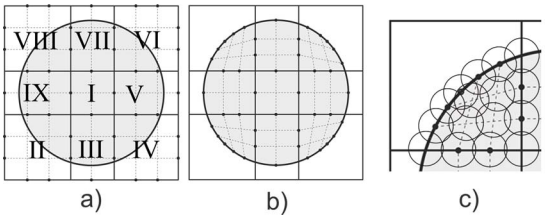

Fig. 4. The first variant: (a, b) Mapping from computational to physical domain in section and (c) generation of SPH pseudo-particles from FEM nodes (detail of upper left corner)

The block marked I denote the central block while other blocks are denoted by II to IX. Three blocks on the left and right are used to describe mesh before and after branch, and three blocks in the middle exists only before the branching. In this case particles have un-homogenous size distribution in the blocks II, IV, VI, and VIII.

To generate the same-sized particles in the entire domain, it is necessary to apply more sophisticated layout of the blocks. One of possible topologies is shown in Fig. 5(a).

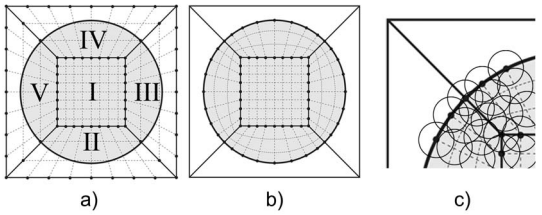

Fig. 5. The second variant: (a, b) Mapping from computational to physical domain in section and (c) generation of SPH pseudo-particles from FEM nodes (detail of upper left corner)

The block marked I denote the central block. Block below, right, above, and left are denoted by II, III, IV, and V respectively.

In this topology, the set of 8 vertices are assigned the smallest number of blocks that provide the proper particle size. Since grid points is always projected in the direction that connects the two corresponding grid points of opposing edges of the block, this way ensures that each unit generates proper nodes for equivalent inter-particle distances. Blocks configuration obtained by the first and second variant of blocks' topology is given on Fig. 6.

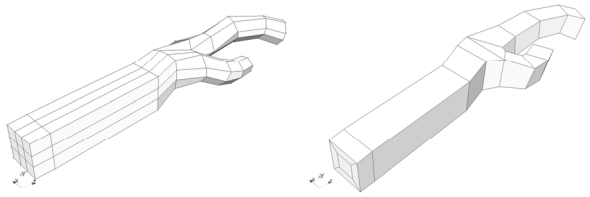

Fig. 6. Blocks' configuration obtained by the a) first b) second variant of blocks' topology

Once the topology definition has been done, grids are produced automatically by stl2sph software, which employs a multiblock meshing scheme for SPH pseudo-particle generation. Resulting model for second variant of topology is shown in Fig. 7.

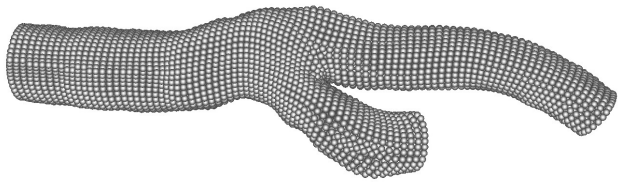

Fig. 7. SPH model of carotid artery bifurcation created by multiblock approach

IV. Conclusion

Difficult discretization of complex geometry continuum into pseudo-particles is one of the main issues faced when implementing SPH in biomechanics which leads to insufficient usage of this very versatile numerical method. This paper presented resolving of this issue by multiblock approach which divides whole geometry into simpler blocks which are then discretized into evenly sized pseudo-particles. Another important issue which will be focus of our future work (which is closely related to work presented in this paper) is definition of loads and boundary condition, because selection of surfaces (on which boundary conditions and loads should be applied) is not as easy as in FEM since SPH pseudo-particles do not have common and external faces like finite elements which are used for surface definition.

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