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Explicit interface tracking of moving Red Blood Cells in finite volume mesh.

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Abstract

Advances in medical science have seen a growth in the virtual modelling of rheological-blood systems. Current studies of rheological systems are predominantly based on simplified empirical characterisations of non-Newtonian fluids [5]. To gain a more in-depth understanding of these processes, explicit modelling of red blood cells, their movement, collisions and fluid dynamic interactions are necessary. Here, we seek to explicitly model the bi-concave disc shape of red blood cells and track their movement against the background of non-moving finite volume mesh. This was achieved using an interface tracking method [7] developed in-house in Fortran95. Explicit Lagrangian tracking of blood cells carries the potential for finite element analysis (FEA) simulations of cell structures and the modelling of fluid-structure interactions.

Introduction

Human blood is a complex mixture of plasma, red blood cells (erythrocytes), platelets (thrombocytes) and white blood cells (leukocytes). The mixture is predominantly composed of plasma at 55% and red blood cells (RBCs) at 45% (the hematocrit value). Plasma, a mixture of water, dissolved proteins, glucose, hormones and carbon dioxide, behaves like a Newtonian fluid. However, RBCs as a mixture with plasma exhibit non-linear flow characteristics due to the RBC's deformable biconcave disc-shape which flex and stretch elastically as a result of applied fluid and boundary forces. RBCs' membrane consists of a lipid bilayer of fatty molecules that is attached to a cytoskeleton structure and filled with a haemoglobin solution. RBCs typically measure 8µm in diameter and 2µm in thickness [1]. In the process of circulation, RBCs must flow through both large arteries as well as small capillary blood vessels, some of which are only 3µm in diameter. The properties of RBCs have been investigated in a number of experiments, namely in micro pipette aspirations [3], RBC deformations by optical tweezers [6] and membrane response due to thermal fluctuations. These experiments concluded RBC membranes demonstrated viscoelastic properties. Due to the complex interaction between flow dynamics and RBC viscoelasticity, a higher level of detail can be obtained if the transient fluid-structure interactions of RBCs and flow were deterministically modelled without the use of empirically derived closure expressions.

Jafari et al. [8] numerically investigated the tendency for RBCs to aggregate into 'stacks of discs' in the narrow confines of capillaries by using a VOF representation of RBCs. The VOF model did reveal the tendency for RBCs to aggregate but as the simulation progressed it was clear that the high shear rate of capillary flows was too strong for the VOF interface to resist and the RBC would lose its shape. It was obvious an FEA model was needed to calculate the balance of forces between the applied stress and the RBC structure's restoring force.

AlMomani et al. [1] used the level set method to model RBCs and the Immersed Boundary (IB) method to simulate the Fahraeus-Lindquist effect whereby RBCs migrate to the centre of the blood vessel and platelets migrate to the wall, thus changing the blood's effective viscosity. His results were promising, showing the tendency for RBC centre-line migration to increase with increasing hematocrit value though admittedly the results were for very slow flows of Re = 1.0 and in two dimensions.

Fedosov et al. [4] developed a complex model of the RBC where the viscoelastic lipid bilayer was modelled as a separate entity from the haemoglobin mixture held within. By using an FEA-like 2D triangular lattice, known as dissipative particle dynamics (DPD) modelling, the membrane viscoelasticity, membrane bending resistance and membrane thermal fluctuations could be simulated with accuracies close to experimental results and better than theoretical predictions which assumed simplified ellipsoid RBC shapes. When a Poiseuille flow velocity field was applied to RBC DPD structure, the bi-concave disc stretched into a parachute form in agreement with experimental observations. Fedosov noted that the DPD model could be coupled with Lattice Boltzmann (LB) or Immersed Boundary (IB) flow solvers in future work to create a fully coupled fluid-structure FEA-CFD model of blood rheology. Given this detailed understanding of the RBC structure, its membrane elasticity as well as internal structural dynamics, a detailed, high-fidelity meshing technique is the natural advancement for capturing the underlying physics at work. Here, we outline a dynamic meshing technique which provides surface mesh necessary for calculating membrane stresses, as well as the ability to generate the 'cut cells' necessary for finite-volume style CFD simulations.

Intersection Marker method for multiphase CFD applications

Explicit interface tracking in two-phase flows have been achieved in a variety of forms, including massless particle methods and by using the level-set mathematical function [9]. However, these methods may not be suitable for the direct importation of 2D FEA surface meshes into regular 3D hexahedral Eulerian mesh required for finite-volume CFD simulations. Presently, we have developed [7] a hybrid Lagrangian-Eulerian front-tracking method called the intersection-marker (ISM) method which tracked the 2D surface as a Lagrangian but remeshed the surface within each control volume for each timestep so that both positional accuracy, surface continuity and volume conservation were preserved. It was realised that apart from having developed a detailed interface tracking algorithm for deformable surfaces, the method was ideally suited for importing FEA-like triangular mesh for immersed-boundary type CFD simulations.

The ISM interface tracking method works by representing a closed 2D surface as a collection of discrete interfaces residing within their respective control volumes. The interface of 3 to 6 sides is subdivided into triangular surfaces for higher accuracy. Also, it is necessary to represent the basic interface as triangular elements because a triangular surface subjected to a twisting vector field will always recover a quantifiable planar surface.

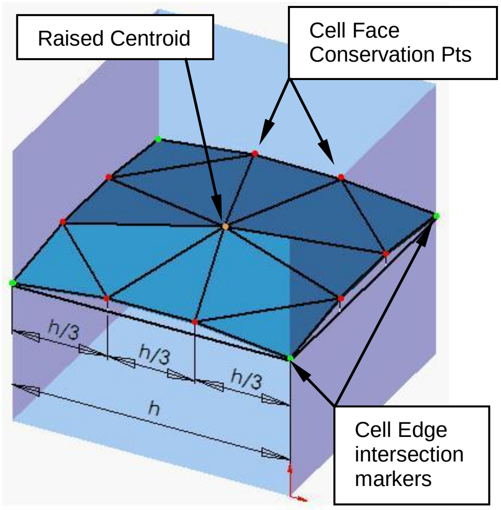

Figure 1. Intersection-marker (ISM) representation of a 2D interface in a regular hexahedral control volume.

Figure 1 shows a four sided interface modelled using the ISM method. The interface is made up of its component points, (1) the intersection markers where the interface crosses the control volume cell edges, (2) the cell face conservation points which allow composite curves to be modelled, and (3) the raised centroid whose position is calculated to satisfy volumetric conservation. Also present but not shown is the 'surface normal' that is orientated perpendicular to a Least-Squares-Fit-Plane calculated from the combination of intersection markers. The normal vector is pointed outwards from the material surface to differentiate which portion of the cut volume contains the tracked void fraction. Calculation of the void fraction is by summing the triangular columns as evaluated by multiplying the triangular base area with the column's centroidal height.

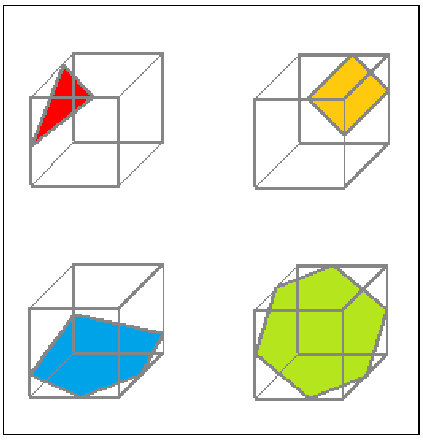

Figure 2. Four examples of different ISM combinations.

The ISM method identifies the type of interface inhabiting a cell by the combination of cell-edge intersections that interface makes. As discussed in the previous paper [7], a basic set of planar-type interfaces: 8 intersection marker combinations for 3 sided interfaces, 15 for 4 sided, 24 for 5 sided and 4 for 6 sided; (total 51 combinations, Figure 2) provided a standard look-up table for algorithmic identification. However, more intersection-marker combinations were encountered after rigorous testing. These new combinations included non-planar-type interfaces.

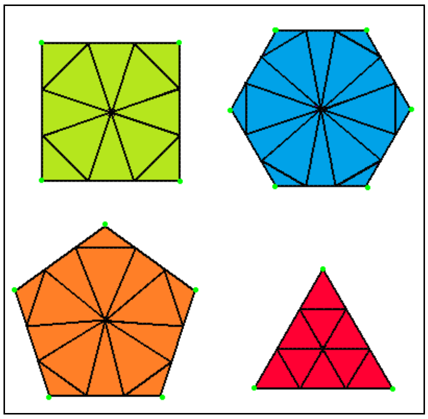

Figure 3. Polygon subdivision strategies for ISM interface modelling.

Twenty four new combinations were found for 6-sided interfaces which were twisted from the planar position. Another 24 combinations were found when 'saddle shaped' 6 sided surfaces were encountered. Moreover, the standard layouts of interface subdivision (Figure 3.) required modification for high aspect-ratio four-sided interfaces and for five-sided interfaces where one side is grossly concave side (Figure 4.). These new layouts were necessary to prevent the modelled interface from collapsing and folding onto itself.

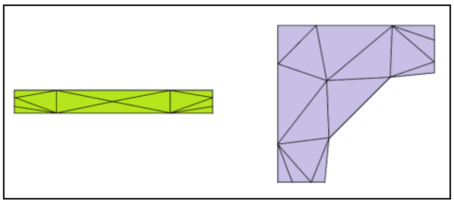

Figure 4. Modified polygon subdivisions for irregular-shaped interfaces.

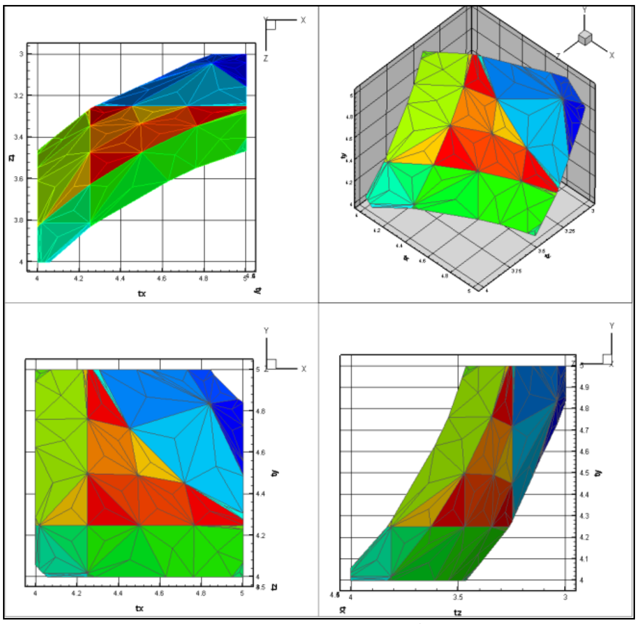

Figure 5: Typical composite interface within a control volume before remeshing

FEA Mesh Importation.

Given a 2D triangular surface-mesh, we want to convert this into a 3D volume mesh suitable for finite volume solutions. The process of FEA mesh importation is conducted in two steps. First, each triangular surface is projected to a 3D Eulerian space of regular hexahedrons. Each triangle mapped onto the Eulerian mesh may intersect a number of control volumes. The algorithm keeps a tally of all triangular surfaces necessary for reconstructing the composite interface of each 'interface cell.' (Figure 5.) The cell-edge intersections these triangles make with each Eulerian control volume also identifies the type of interface that will reside in each interface volume. Knowing the triangles necessary for the reconstruction of each interface cell,

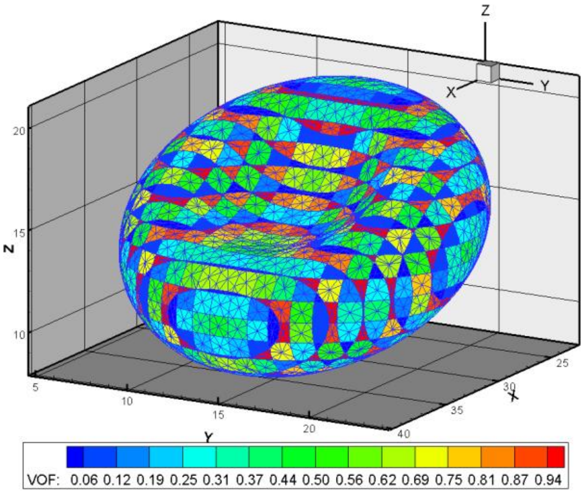

Figure 6. 2D Interface tracking of a disc-shaped RBC inside regular cube mesh. Compound curvatures inside unit-volume mesh are displayed in Volume of Fraction (VOF) contours.

the algorithm conducts a second-pass to (1) remesh the points of the poly-line on each cell-face to only two 'face points'. The remeshed polyline becomes a trapezoid in a calculation similar to Aulisa's 2D interface tracking method [2] and (2) calculating the position of the 'raised-centroid' so that that the volume of the composite interface before remeshing is equal to the volume of the remeshed interface.

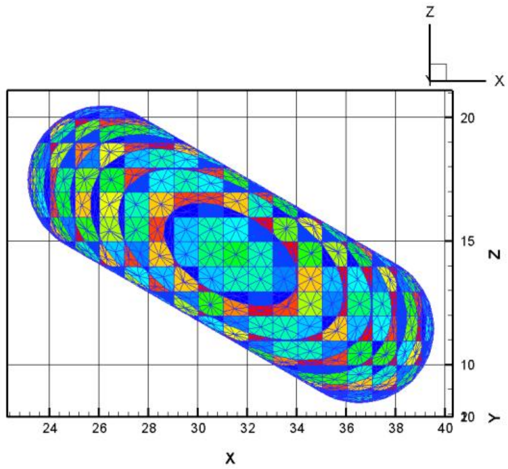

Figure 7. Side view of RBC interface model.

Results: mapping of the FEA mesh.

To benchmark the accuracy of the interface tracking algorithm, we generated a RBC disc to test the translational and rotational mapping of the FEA mesh to the CFD mesh. We did this knowing that a RBC disc is more difficult to model than a disc, possessing both concave and convex surfaces with both sharp and subtle interface curvatures. And it is for this reason that we found the extra interface topologies as noted earlier. However, it can be reported that the method works quite well, conserving a ~1400 unit volume disc of diameter 18 unit and height of 6 units, to within a value of $1\text{x}10^{-7}$ unit volume. (Figure 6.) Due to the limitations of floating point calculations and global tolerance issues in meshing and remeshing, there are inevitably small

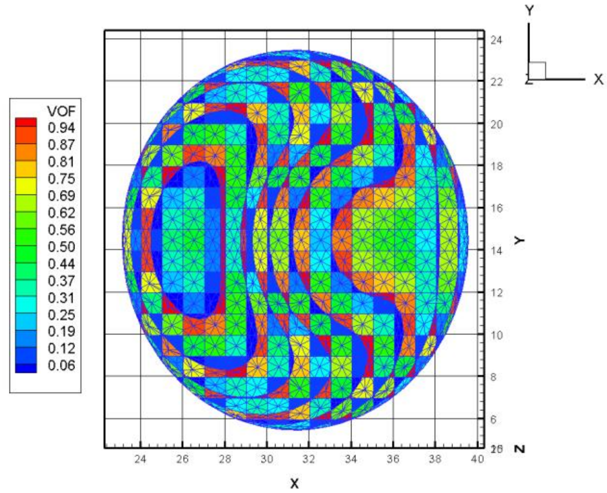

Figure 8. Top view of RBC mapped to CFD mesh showing each interface clearly within the bounds of its own control volume.

discrepancies that arise from the many scalar and vector operations made in the calculation. On a cell-by-cell basis, this discrepancy is so small as to have a negligible effect on the void fraction calculation necessary for mass and momentum conservation. Furthermore, since all positions of the RBC's interface are mapped from the original interface, small volumetric errors do not propagate throughout the transient simulation.

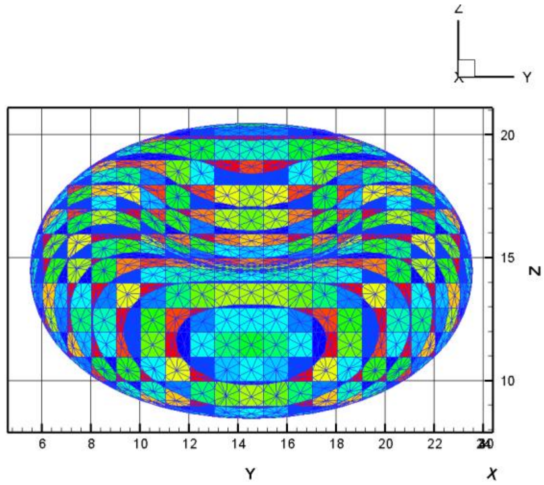

Figure 9. Front view of RBC interface model in finite volume mesh.

Advection of RBC model.

Advection of the RBC model can be done in a variety of ways. The simplest method, where no internal or membrane stresses are taken into account, would use the velocity field as calculated by the flow solver, to directly map the points of the interface to its new location. The advection of interface points inside each control volume is calculated using the tri-linear interpolation method. Eight points of the vector field, positioned on the vertices of each control volume, are used as the input parameters of the tri-linear interpolation. In this manner the interface position is updated for each successive timestep.

A more sophisticated manner of advecting the interface would be to calculate the surface pressure integral of the RBC; then feed that information into the 3D FEA model as laid out the initial RBC mesh to calculate for RBC deformation / deflection; then finally to calculate for the net movement of the RBC as a result of the net force applied on the RBC through its centroid. All points on the RBC are thus translated to their new position as calculated in the net movement.

Conclusions and future work.

The Intersection Marker (ISM) method for interface tracking was used to import a 2D-surface FEA mesh into a 3D hexahedral mesh to ultimately model red blood cell (RBCs) movements in an immersed boundary CFD simulation. Progress to this point has been successful with the method demonstrating a high degree of detail and accuracy. The level of detail allow many options for the research to proceed. The fluid domain internal and external of the RBC membrane can be decoupled and solved separately. Likewise, the pressure information as calculated by the flow solver can be used to calculate for RBC deflection in a FEA simulation. This would entail the communication of stresses from the fluid flow to the FEA mesh, resulting in FEA mesh deflection which would be fed back into the CFD mesh allowing for coupled FEA-CFD fluid structure interaction. Conversely, a single-fluid approach can be adopted for simplicity in manipulating the interface. More research and investigation is needed to ascertain what the optimal solution may be.

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