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Comparison of a Fixed-grid and ALE Methods on Modelling Fluid-Structure Interaction of the Aortic Valve

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Comparison of a Fixed-grid and ALE Methods on Modelling Fluid-Structure Interaction of the Aortic Valve

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Abstract

This study aimed at assessing the robustness of a fixed-grid fluid-structure interaction (FSI) method (Multi-Material Arbitrary Lagrangian Eulerian; MM-ALE) to modelling the 2D native aortic valve dynamics, and comparing it to the Arbitrary Lagrangian Eulerian (ALE) method. For the fixed-grid method, the explicit finite element solver LS-DYNA was utilized, where two independent meshes for the fluid and structure were generated and the penalty method was used to handle the coupling between the fluid and structure domains. For the ALE method, the implicit finite element solver ADINA was used where two separate conforming meshes were used for the valve structure and the fluid domains. The comparison demonstrated that both FSI methods predicted accurately the valve dynamics, fluid flow, and stress distribution, implying that fixed-grid methods can be used in situations where the ALE method fails.

Keywords:

aortic valve, fluid-structure interaction, Arbitrary Lagrangian Eulerian, Fixed-grid FSI, Finite Element.

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Introduction

Computational modelling of the heart valves was firstly introduced about four decades ago. Due to the limitations of the computational resources and numerical methods at the time, these early studies utilized simplified geometries, loads, material models and analyses. Computational simulation of the native heart valves is a valuable tool that enables the understanding of normal and diseased valve function and can, subsequently, assist in tailoring surgical intervention for the specific underlying pathology [1]. In addition, patient-specific models can be used to evaluate the disease state and progression, with a view to assisting clinicians towards individualized treatment and intervention [2]. Computational models can play a significant role in optimizing the design of new prosthetic valves by considerably reducing the cost and time required for assessment and evaluation [1,3]. Moreover, computational models of the native heart valves can provide important stress-strain input for optimizing the culturing/conditioning of tissue-engineered heart valves in bioreactors using physiologically relevant mechanical/ hemodynamic stimuli.

Early computational models of the heart valves were focused on either the structural analysis, where the blood flow was not considered and the transvalvular pressure was applied to the valve surface [4-8], or computational fluid dynamics (CFD) of the blood flow, where the leaflets were fixed in a fully or partially open position [9-13]. A numerical model that closely represents the physiological **behaviour** of heart valves should incorporate the motion of the leaflets, valve annulus dilation, and blood flowing through the valve. Such numerical model requires coupling the solutions of the governing equations for structural deformation and fluid flow, using an FSI methodology. Comparison of FSI and Structural models of a polymeric heart valve found that the FSI method is more appropriate to predict the valve **behaviour** [14]. With advances in computer technology and numerical methods, FSI method has been implemented in many computational software. In general, the FSI method can be categorized into two approaches, including the Arbitrary Lagrangian Eulerian (ALE), or dynamic-mesh, and the fixed-mesh (Eulerian) methods. In the ALE method, the fluid and the structure parts share boundaries and the fluid elements move according to the structure deformation. In this method, each element has only one type of material (fluid or solid). The ALE method has been reported to be the most accurate method since no interpolation algorithm is required and conformed fluid and structure meshes are used. For heart valves FSI simulation, the ALE method has been successfully applied to model the function of bileaflet mechanical heart valves during the cardiac cycle, with the leaflets considered as rigid bodies [15-18]. The main drawback of this method has been reported to be its inability to cope with contact when the leaflets coapt during diastole. Owing to this, this method fails in the FSI **modelling** of tissue valves (natural and bioprosthetic), where the leaflets are very flexible and contact each other during diastole. Therefore, this method has mainly been used to only model tissue valve function during systole [19,20]. On the other hand, fixed-grid methods (Eulerian), in which the fluid mesh remains unchanged, have been shown to be capable of solving FSI problems, where complex geometries undergo large deformations and different structural components come into contact. However, this method has been reported to be less accurate than the ALE method due to the interpolation method used to account for the fluid and structure interaction at the interface. Different fixed-grid methods have been proposed to study FSI of natural or bioprosthetic aortic valves. These have included the immersed boundary (IBM) [21,22], sharp-interface immersed boundary method [23], sharp-interface level set method [24], fictitious domain [25-27] and Multi-Material Arbitrary Lagrangian Eulerian (MM-ALE) [28-32] methods. The MM-ALE method allows for multiple materials in an element and, therefore, more stable and robust and allows for additional flexibility over the other fixed-grid methods. This method has been implemented in the commercial finite element software **LS-DYNA** for decades and has been used to simulate FSI of different engineering applications.

The present work was aimed at assessing the **reliability, robustness and accuracy of the MM-ALE (fixed-grid) method in modelling the FSI of the natural aortic valve, against the ALE method, which represents the benchmark in FSI modelling, being widely accepted as the most accurate and reliable method for solving FSI problems. Therefore, the aim of this study was not to fully characterize the aortic valve dynamics, which**

would have required a much more rigorous validation against physical experiments than the one presented here, but rather to assess the level of accuracy of the MM-ALE method against the benchmark. A comprehensive validation against *in vivo* and *in vitro* data of their aortic valve model was conducted in a previously published study by the authors, which developed a full 3D FSI model of the aortic valve using the MM-ALE method [33]. In that study, a good agreement was found between the 3D FSI aortic valve model and *in vivo* and *in vitro* data. However, that study also highlighted discrepancies between the MM-ALE model and the experimental results. Owing to this, the present study investigated whether these discrepancies were due to the accuracy of the solver, by comparing the MM-ALE method to the ALE one. Providing that the fixed-grid method can produce accurate and reliable results, it would be a more straightforward and more easily applicable method for simulating the aortic valve dynamics than the ALE method, since the latter demonstrated significant shortcomings in handling large deformations and coaptation areas in complex geometries, such as the aortic valve. The comparison between the two methods was performed in terms of the valve dynamics, fluid flow, and stress distribution, using a realistic 2D aortic valve geometry. Due to the limitations of the ALE method, a 2D approach rather than a 3D one was preferred, since the latter would have significantly enhanced the shortcomings of the ALE method and increased the complexity in mesh generation and adaptation, without increasing the accuracy of the comparison, or any potential disagreement between the two methods.

Material and Methods

For the ALE method, the finite element software ADINA (ADINA R&D, Inc., Watertown, MA) was used, whereas for the MM-ALE method the LS-DYNA software (LSTC, Livermore, CA) was used. A simplified 2D geometry of the aortic valve was generated by considering the valve consisting of two sinuses and three leaflets. In addition, the valve was assumed to be symmetric about its central line and, therefore, only one leaflet was considered in the numerical simulations. The 2D valve geometry was generated in accordance with the parameters reported in [34,35] for an adult human (Table 1). The initial configuration of the valve was assumed to be at the end-diastolic phase.

In both the MM-ALE and ALE methods the fluid was modelled as laminar incompressible and Newtonian, with a density and viscosity within the physiological range of 1000 kg/m³ and 0.004 Pa·s [36], respectively. In LS-DYNA, FSI coupling is only available for the compressible solver however the incompressibility of the fluid was maintained in LS-DYNA by keeping Mach number below 0.3 as will be discussed below [37]. The leaflet and the aortic wall were assumed to be linear elastic with Young's modulus of 200 kPa and 300 kPa [8], respectively, and a Poisson's ratio of 0.49.

For the ALE method two conforming meshes were generated, one for the fluid domain and the other for the valve structure (Figure 1a). In this method, the continuity and Navier-Stokes equations were reformulated by replacing the convective velocity v_i with $v_i - v_i^g$, where v_i^g represented the grid velocity [38]:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial x_i} (v_i - v_i^g) = -\rho \frac{\partial v_i}{\partial x_i} \quad (1)$$

$$\frac{\partial \rho v_i}{\partial t} + \frac{\partial \rho v_i}{\partial x_j} (v_j - v_j^g) = -\frac{\partial p}{\partial x_i} + \mu \frac{\partial}{\partial x_j} \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) + F_i \quad (2)$$

In these equations, $v_i^g = 0$ corresponds to the Eulerian formulation and $v_i^g = v_i$ corresponds to the Lagrangian formulation [38]. Moreover, μ represents the shear viscosity. The fluid domain was discretized using 2D flow-condition-based interpolation (FCBI) elements [39]. The solution of the FCBI elements satisfies the mass and momentum conservation, and it uses a linear function for the velocity interpolation and a bilinear function for the pressure interpolation. The fluid domain was divided into six sections to

1
2 ensure proper meshing during the FSI computation without using the mesh adaptation capability in ADINA.
3 Similarly to the fluid domain, the solid domain was also divided into six sections and discretized using plain
4 strain elements.
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8 “[insert Figure 1]”

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10 Figure 1. Computational meshes of the fluid domain and valve structure, and the coupled fluid and valve
11 structure meshes as used in the (a) ALE solver (ADINA) and (b) MM-ALE solver (LS-DYNA).
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14 The fluid and structure equations were coupled using a monolithic solver in ADINA, which combined the
15 fluid and structure matrices into one large matrix, which was then solved using the Newton-Raphson
16 iteration method. The maximum number of FSI iterations at each time step was set to 100 with a relative
17 force and displacement/velocity tolerance of 0.001 as the FSI convergence criteria. A mesh sensitivity study
18 for the ALE method was conducted using two mesh sizes: i) Mesh-I with 6072 fluid elements and 123 solid
19 elements; ii) Mesh-II with 18560 fluid elements and 436 solid elements, which was more than three times
20 denser than Mesh-I. For the mesh sensitivity study, the aortic wall was fully constrained. The mesh
21 dependence was studied using the radial and axial (with reference to the aortic root) displacements of the
22 leaflet, as well as the outlet axial fluid velocity as shown in Figure (2a & 2b). The results were found to be
23 mesh independent and Mesh-I was used for the comparison study, since it had fewer elements and the
24 results could be obtained in a shorter time compared to the Mesh-II model.
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26
27 In addition, the effect of time discretization was assessed using three different time steps: i) 0.005s; ii)
28 0.0025s; iii) 0.001s (Figure 2c & 2d). The simulations showed that the reduction of the time step induced
29 leaflet oscillations during closing. Moreover, the general leaflet behaviour, as well as the magnitude and
30 trend of the velocity, remained the same regardless of the time steps. Therefore, it was concluded that a
31 time step of 0.005s was sufficient to capture the valve dynamics and fluid flow through the valve in a
32 reasonable computational time.
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38
39 Table 1. Dimensions of the 2D aortic valve model [34;35].
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Parameter	Value
Base radius (R_b)	12 mm
Sinus radius (R_s)	17.5 mm
Sinus height (H_s)	21 mm
Aortic valve height (L)	39 mm
Aortic wall thickness (t_w)	2 mm

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54 For the fixed-grid MM-ALE method two independent meshes for the fluid (blood) and the structure (valve)
55 were generated as can be seen in Figure 1b. This method used a Split-Operator method to split the
56 computation in each time step into two steps. Firstly, the conservation equations were solved in the
57 Lagrangian formulation by setting the mesh velocity to the fluid velocity, which effectively turned off the
58 advection in the equations of motion. At this step, the elements moved with the material and the changes
59 in the internal energy and velocity that occurred due to the external and internal forces were computed.
60 The equilibrium equations of the momentum and energy became [40, 41]:

$$\frac{\partial \rho v_i}{\partial t} = -\frac{\partial \sigma_{ij}^f}{\partial x_j} + F_i \quad (3)$$

$$\frac{\partial e}{\partial t} = \sigma_{ij}^f \frac{\partial v_i}{\partial x_j} + F_i v_i \quad (4)$$

In this formulation, $\sigma_{ij}^f = -p\delta_{ij} + \mu\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right)$ and e represent the internal energy. The second step was the advection step, in which all nodes were remapped back to their initial positions and the transport of internal energy, mass and momentum through the element boundaries were computed. The transport equations of a variable ϕ for the advection step were:

$$\frac{\partial \phi}{\partial t} + (v_i - v_i^g) \frac{\partial \phi}{\partial x_i} = 0 \quad (5)$$

$$\phi(x_i, 0) = \phi_0(x) \quad (6)$$

The fluid mesh was created as a simple rectangular domain by excluding the valve structure (Figure 1b). In addition, two fluid parts were added to the fluid domain to represent the inlet and outlet reservoirs. The FSI coupling was activated using the *CONSTRAINED_LAGRANGE_IN_SOLID card. The penalty method was used to track the relative displacement between the Lagrangian structure and the Eulerian fluid with appropriate number of coupling points on the Lagrangian structure. In the penalty method, the Eulerian parts were defined as masters while the Lagrangian parts as slaves. The mesh sensitivity of the MM-ALE method was assessed using a fully constrained aortic wall and three different meshes: i) Model-A with 921 fluid elements and 115 solid elements; ii) Model-B with 962 fluid elements and 458 solid elements; iii) Model-C with 1820 fluid elements and 458 solid elements. The mesh dependence was studied using the radial and axial (with reference to the aortic root) displacements of the leaflet, as well as the outlet axial fluid velocity as shown in Figure 3a & 3b. Mesh independence was achieved using 962 8-node brick elements for the fluid domain and 458 8-node brick elements for the valve structure (Model-B).

"[insert Figure 2]"

Figure 2. Mesh sensitivity (a, b) and (c) and time step sensitivity (c, d) studies for the ALE method (ADINA).

The mesh and time step sensitivities studies were conducted by comparing the radial and axial (with reference to the aortic root) displacements of the leaflet (a, c), and the outlet axial fluid velocity (b, d). Mesh-I: 6072 fluid elements and 123 solid elements; Mesh-II: 18560 fluid elements and 436 solid elements.

In LS-DYNA, the time step was found to be proportional to the speed of sound. For that, speed of sound was reduced from its physiological values of 1500 m/s to 20 m/s to reduce the computation time. In the present work two FSI simulations with a fully constrained aortic wall were performed to assess the effect of reducing the fluid sound speed in the MM-ALE solver. In the first model, the fluid sound speed was set to its physiological value of 1500 m/s while in the second model the speed of sound was reduced to 20 m/s and the fluid compressibility was kept low (Mach number < 0.3). The results showed good agreement between the two sound speed values (Figure 3c & 3d). However, the computation time was considerably different. Using a sound speed of 20 m/s, one cycle was solved in 5.95 hours, whereas using a sound speed of 1500 m/s the time taken for one cycle to be solved was 16.82 hours. Thus, all computations were conducted using the speed of sound of 20 m/s.

“[insert Figure 3]”

Figure 3. Mesh sensitivity (a, b) and speed of sound sensitivity (c, d) studies for the MM-ALE method (LS-DYNA). The mesh and speed of sound sensitivity studies were conducted by comparing the radial and axial (with reference to the aortic root) displacements of the leaflet (a, c) and the outlet axial fluid velocity (b, d). Model-A: 962 fluid elements and 115 solid elements; Model-B: 921 fluid elements and 458 solid elements; Model-C: 1820 fluid elements and 458 solid elements.

At the inlet, a pulsatile velocity waveform with a peak systolic velocity of 0.6 m/s was prescribed (Figure 4), which even though it was lower than the average peak aortic flow, it was within the physiological range [42]. The low peak value was chosen in order to keep the flow in the laminar regime. A symmetry boundary condition was applied at the symmetry line, and a zero normal traction was prescribed at the outlet. The heart rate was assumed to be 60 bpm, so the period of the cardiac cycle was 1s. No-slip FSI boundary conditions were applied at the boundaries of the aortic root and leaflet. At the fluid/solid interface the displacement compatibility and traction equilibrium were enforced. Leaflet coaptation was modelled as a frictionless contact of the leaflet with a fixed rigid part along the symmetry line. In order to avoid element discontinuity in the ALE method during leaflet coaptation, an offset distance of 0.05 mm was applied between the leaflet and the rigid part.

In order to facilitate the comparison between the ALE and MM-ALE methods, and minimize the differences between the two cases, the study kept all physical quantities and properties the same in both solvers (aortic valve root geometry and dimensions, boundary conditions and material properties). However, and since the two solvers have different ways to numerically discrete the model in space and time, the numerical differences could not be avoided.

“[insert Figure 4]”

Figure 4. The pulsatile velocity waveform applied at the inlet in both the MM-ALE and ALE methods.

Results

The FSI simulations with the ALE and MM-ALE methods were performed for three cardiac cycles. The results of the radial displacement of the leaflet for the three cycles for the two methods are shown in Figure 5. For both methods, the results of the second and third cycles were almost identical, indicating that periodicity was achieved within 3 cycles. Owing to this, the comparison between the ALE and the MM-ALE methods was conducted using the third cycle results. The radial displacements of the leaflet tip predicted by ALE and MM-ALE methods were compared to the *in vivo* measurements of canine aortic valve radial displacement reported by Thubrikar [34], (Figure 6). In general, both the ALE and MM-ALE methods predicted similar leaflet displacement during systole, and they were both in good agreement with the *in vivo* data. Nevertheless, discrepancies were seen between the numerical and the *in vivo* results, which can be attributed to the anatomical and physiological differences between canine and human. Indeed, the diastolic pressure of the canine model is between 50-80 mmHg and the systolic between 120-150 mmHg, which is rather hypertensive compared to the case of the healthy adult human (80/120 mmHg, diastolic/systolic), which was simulated in the FSI model. Moreover, the method used to measure leaflet displacements in the experimental canine model employed radiopaque markers placed on the leaflets, which could have also impacted on the results of the experimental study. In addition, in FSI models the duration of the cardiac cycle was assumed to be one second, which resulted in longer ejection time compared to the *in vivo* data.

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“[insert Figure 5]”

Figure 5. Comparison of the radial leaflet displacements of three cardiac cycles predicted by the ALE (ADINA; a) and MM-ALE (LS-DYNA; b) methods.

“[insert Figure 6]”

Figure 6. Comparison of the radial displacements of the leaflet tip predicted by the ALE (ADINA) and MM-ALE (LS-DYNA) methods to the *in vivo* experiments reported by Thubrikar [34].

The comparison between the ALE and MM-ALE methods was carried out using the radial and axial displacements of the tip of the leaflet, the outlet axial fluid velocity at the **centre**, the dilation of the aortic wall at the top end of the sinus, and the Von Mises stress distribution across the leaflet. In general, the motion of the aortic valve during the cardiac cycle can be divided into three phases, including a rapid opening phase, open phase and a rapid closing phase [34]. In general, both methods demonstrated a fair agreement in predicting the radial and axial leaflet displacement during the cardiac cycle (Figure 7a). However, the MM-ALE method overestimated the radial displacement of the leaflet during peak systole by about 20% compared to the ALE method. In addition, leaflet oscillations were observed following leaflet coaptation for the results of the MM-ALE method. These were attributed to the smaller time step used in the explicit solver to ensure numerical stability. The same **behaviour** was observed in the ALE solver using smaller time steps (results not shown); however, the trend was similar. During diastole, the MM-ALE and the ALE methods predicted different leaflet **behaviours**. Following valve closure, the ALE method predicted that the leaflet remained in its axial position until the end of the cardiac cycle, but for the MM-ALE method predicted that the leaflet reached its minimum axial position and then moved gradually upwards until the end of the cardiac cycle. This can be attributed to the offset used in the ALE method to prevent elements overlapping during leaflet coaptation. The opening/closing characteristics of the two methods were compared in terms of the rapid valve opening time (RVOT), rapid valve closing time (RVCT), and ejection time (ET) as shown in Figure 7b. Both methods predicted very comparable opening and closing characteristics of the aortic valve. The maximum difference between the two methods was about 6%.

During the cardiac cycle, the aortic root dilates inward and outward according to the pressure in the valve. In this work, we compared the aortic valve root dilation from a point at the top of the sinus. The study found, both methods predicted similar oscillatory aortic wall motion during systole (Figure 7c). The wall dilation starts before the leaflets start to open by about 30 ms. During diastole, the oscillations predicted by the ALE method disappeared after 0.6 s and the aortic wall remained at its position until the end of the cycle. However, the MM-ALE predicted oscillations for the whole duration of the cardiac cycle, although their amplitude was small after valve closure. This can also be attributed to the smaller time step used in the MM-ALE method. In terms of the axial velocity at the outlet, the MM-ALE method underestimated the maximum velocity by about 6% compared to the ALE method. However, a good general trend was observed in both methods (Figure 7d).

“[insert Figure 7]”

Figure 7. Comparison between the ALE (ADINA) and MM-ALE (LS-DYNA) methods in terms of the (a) radial and axial leaflet displacements, (b) opening/closing characteristics (RVOT: rapid valve opening time; RVCT: rapid valve closing time; ET: ejection time), (c) aortic root dilation at the top end of the sinus of the aortic valve and (d) the outlet axial fluid velocity .

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2 The von-Mises stress distributions on the leaflet at the peak systole and at early diastole are presented in
3 Figure 8. Generally, a good agreement was found between the ALE and MM-ALE results. The maximum Von
4 Mises stresses at the peak systole and early diastole were predicted close to the leaflet attachment region
5 in both methods. However, at early diastole, another region of high von Mises stresses was predicted in the
6 belly region due to the leaflet coaptation. Both methods predicted comparable stress magnitude at the
7 belly during the systole and early diastole as shown in Figure 9. However, the ALE method was found to
8 predict higher von Mises stress in the belly region during coaptation (Figure 9). This is due to different
9 contact methods used in the two solvers.
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14 “[insert Figure 8]”

15 Figure 8. Von-Mises stress (Pa) distribution across the aortic valve leaflet using the MM-ALE (LS-DYNA; a, c)
16 and the ALE (ADINA; b, d) methods, at the fully open (a, b) and fully closed (c, d) leaflet positions.
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20 Since the ALE method was implemented in the implicit solver ADINA, its computation time was significantly
21 faster compared to the MM-ALE method in the explicit solver LS-DYNA. In ADINA the computation time for
22 one cardiac cycle of the aortic valve was about 5 minutes, while LS-DYNA required more than 5 hours to
23 accomplish one cardiac cycle in Intel Core i7, 3.1 GHz, 8 Gb RAM (Table 2). Nevertheless, this difference was
24 mainly due to different time discretization schemes in the finite element solvers and not due to the FSI
25 methods. The explicit solver (LS-DYNA) required smaller time step to satisfy the stability conditions, which
26 was about 6000 times smaller than the time step used in the implicit solver (ADINA).
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32 Figure 9. Von-Mises stress at the belly region during the cardiac cycle predicted by the ALE (ADINA) and
33 MM-ALE (LS-DYNA) methods.
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37 Table 2. Time steps and the computational time for the 2D aortic valve predicted by ADINA and LS-DYNA.

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Solver	Time step (s)	Computation time (min)
ADINA	5.00E-03	3.89
LS-DYNA	8.35E-07	329

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48 Discussion

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50 FSI modelling of the natural heart valves involves large deformations and complex geometries, which pose
51 certain constraints on the ALE method. Dynamic elements can become extremely distorted when the
52 leaflets undergo large deformations/displacements during the cardiac cycle. These can, consequently,
53 affect the accuracy of the model, or in some cases, lead to the termination of the computation due to
54 element overlapping. Owing to this, fixed-grid methods have been widely used as an alternative in the FSI
55 modelling of heart valves. The main advantage of fixed grid method is in the easiness of mesh generation
56 process by generating two independent meshes for the fluid and solid domains. However, fixed-grid
57 methods are known to be less accurate than the ALE method due to the use of interpolation methods at
58 the interfaces.
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The present work assessed the MM-ALE method in modelling the mechanics of the aortic valve by comparing to the ALE method. The study considered a simplified 2D aortic valve root geometry with physiological boundary conditions. For the ALE method, the implicit finite element software ADINA was used, and care was taken during mesh generation to prevent element overlapping and discontinuity. On the other hand, the explicit finite element software LS-DYNA was considered for the MM-ALE method, which employed nonconforming meshes. In this work, the valve fluid domain was generated as a rectangular shape by ignoring the valve structure. The FSI solver in LS-DYNA is a compressible solver, therefore, the time step was found to mainly depend on the speed of sound. The speed of sound was reduced from its physiological values of 1500 m/s to 20 m/s to reduce the computation time. However, the incompressibility of the flow was maintained by keeping the Mach number below 0.1. A study was conducted to evaluate the effect of speed of sound reduction and found that the reduction had a minor effect on the FSI results; however, the computation time was reduced by a factor of three.

A comparison study of the valve dynamics was conducted to validate the FSI models of the ALE and MM-ALE methods. The comparison study was conducted using the *in vivo* data of the canine valve dynamics [34]. In the *in vivo* study, the valve dynamics was quantified by measuring the leaflet displacement in the radial direction by placing radiopaque markers on the leaflet tips [34]. However, the purpose of the comparison study was not to develop an accurate model of the canine aortic valve, but to give the degree of relevance and accuracy of the computational simulation results to model the dynamics of the native valve. Despite the anatomical and physiological differences between the models and the *in vivo* data, both FSI models were able to capture the overall trend and magnitude of valve dynamics during the cardiac cycle.

Both methods seem to be bit slower than the *in vivo* measurements [34] during the opening and closing phases. These differences can be attributed to the lower input velocity and simplified 2D aortic valve geometry used in the present study. In addition, the differences can be attributed to the physiological differences present between the canine aortic valves used in the study by Thubrikar [34] and the adult human aortic valve geometry used in the present study.

Furthermore, a comparison study was conducted between the MM-ALE and ALE methods based on the aortic valve dynamics, fluid flow, and stress distribution. Although some discrepancies were found between the two methods, overall the results of both FSI methods were found to be comparable and in good agreement. MM-ALE method was found to overestimate the radial leaflet displacement during peak systole by about 20% higher compared to ALE method. During diastole, the leaflet remained coapted in ALE model, while in MM-ALE model the leaflet moved gradually upward until the beginning of the systole phase. This can be due to the different contact models used in the two solvers. With regards to the velocity at the outlet, the maximum difference between the two solvers was about 8%. Both solvers were found to predict the opening/closing characteristics with minor differences. MM-ALE method was found to overestimate RVOT, RVCT and ET by about 6.1%, 5.7% and 1.3 %, respectively compared to ALE. In addition, both methods predicted very similar aortic wall dilation during early systole. In ALE solver the aortic wall oscillations disappeared after 0.6 s, however, MM-ALE solver predicted oscillations to the end of the cycle. With regards to the stress distributions in the valve, both solvers showed comparable stress distributions during the cardiac cycle. The stress magnitude in leaflet was found to be highly affected by the leaflet's dynamics and coaptation. At early diastole both solvers predicted the same von-Mises stress value, however differences can be found during the coaptation. For the ALE method the leaflets remained almost at constant position consequently the stress value remained high during diastole. However, for the MM-ALE the stress dropped gradually as the leaflet moving upward during the diastole. The difference in the leaflet dynamics during diastole could be attributed to different contact methods used in the two solvers.

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Conclusions

This study was conducted to evaluate and assess the ability of the MM-ALE fixed-grid method to model the FSI of heart valves by comparing its results to those of the current benchmark, which is the ALE method. The valve dynamics, fluid flow and stress distribution on the valve were used to compare the two methods. The study found that the MM-ALE method was able to efficiently predict the blood-valve interaction.

Conflict of interest

The authors have no conflict of interest.

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Figure Captions

Figure 1. Computational meshes of the fluid domain and valve structure, and the coupled fluid and valve structure meshes as used in the (a) ALE solver (ADINA) and (b) MM-ALE solver (LS-DYNA).

Figure 2. Mesh sensitivity (a, b) and (c) and time step sensitivity (c, d) studies for the ALE method (ADINA). The mesh and time step sensitivities studies were conducted by comparing the radial and axial (with reference to the aortic root) displacements of the leaflet (a, c), and the outlet axial fluid velocity (b, d). Mesh-I: 6072 fluid elements and 123 solid elements; Mesh-II: 18560 fluid elements and 436 solid elements.

Figure 3. Mesh sensitivity (a, b) and speed of sound sensitivity (c, d) studies for the MM-ALE method (LS-DYNA). The mesh and **speed of sound** sensitivity studies were conducted by comparing the radial and axial (with reference to the aortic root) displacements of the leaflet (a, c) and the outlet axial fluid velocity (b, d). Model-A: 962 fluid elements and 115 solid elements; Model-B: 921 fluid elements and 458 solid elements; Model-C: 1820 fluid elements and 458 solid elements.

Figure 4. The pulsatile velocity waveform applied at the inlet in both the MM-ALE and ALE methods.

Figure 5. **Comparison of the radial leaflet displacements of three cardiac cycles predicted by the ALE (ADINA; a) and MM-ALE (LS-DYNA; b) methods.**

Figure 6. Comparison of the radial displacements of the leaflet tip predicted by the ALE (ADINA) and MM-ALE (LS-DYNA) methods to the *in vivo* experiments reported by Thubrikar [34].

Figure 7. Comparison between the ALE (ADINA) and MM-ALE (LS-DYNA) **methods** in terms of the (a) radial and axial leaflet displacements, (b) opening/closing characteristics (RVOT: rapid valve opening time; RVCT: rapid valve closing time; ET: ejection time), (c) aortic wall dilation at the top end of the sinus of the aortic valve and (d) the outlet axial fluid velocity .

Figure 8. **Von-Mises stress (Pa) distribution across the aortic valve leaflet using the MM-ALE (LS-DYNA; a, c) and the ALE (ADINA; b, d) methods, at the fully open (a, b) and fully closed (c, d) leaflet positions.**

Figure 9. **Von-Mises stress at the belly region during the cardiac cycle predicted by the ALE (ADINA) and MM-ALE (LS-DYNA) methods.**

Figure 1. Computational meshes of the fluid domain and valve structure, and the coupled fluid and valve structure meshes as used in the (a) ALE solver (ADINA) and (b) MM-ALE solver (LS-DYNA).

364x130mm (300 x 300 DPI)

Figure 2. Mesh sensitivity (a, b) and (c) and time step sensitivity (c, d) studies for the ALE method (ADINA).

The mesh and time step sensitivities studies were conducted by comparing the radial and axial (with reference to the aortic root) displacements of the leaflet (a, c), and the outlet axial fluid velocity (b, d). Mesh-I: 6072 fluid elements and 123 solid elements; Mesh-II: 18560 fluid elements and 436 solid elements.

191x130mm (300 x 300 DPI)

Figure 3. Mesh sensitivity (a, b) and speed of sound sensitivity (c, d) studies for the MM-ALE method (LS-DYNA). The mesh and speed of sound sensitivity studies were conducted by comparing the radial and axial (with reference to the aortic root) displacements of the leaflet (a, c) and the outlet axial fluid velocity (b, d).

191x129mm (300 x 300 DPI)

Figure 4. The pulsatile velocity waveform applied at the inlet in both the MM-ALE and ALE methods.

76x55mm (300 x 300 DPI)

Figure 5. Comparison of the radial leaflet displacements of three cardiac cycles predicted by the ALE (a; ADINA) and MM-ALE (b; LS-DYNA) methods.

196x68mm (300 x 300 DPI)

Figure 6. Figure 6. Comparison of the radial displacements of the leaflet tip predicted by the ALE (ADINA) and MM-ALE (LS-DYNA) methods to the in vivo experiments reported by Thubrikar [34].

77x56mm (300 x 300 DPI)

Figure 7. Comparison between the ALE (ADINA) and MM-ALE (LS-DYNA) methods in terms of the (a) radial and axial leaflet displacements, (b) opening/closing characteristics (RVOT: rapid valve opening time; RVCT: rapid valve closing time; ET: ejection time), (c) aortic wall dilation at the top end of the sinus of the aortic valve and (d) the outlet axial fluid velocity .

167x118mm (300 x 300 DPI)

Figure 8. Von-Mises stress (Pa) distribution across the aortic valve leaflet using the MM-ALE (LS-DYNA; a, c) and the ALE (ADINA; b, d) methods, at the fully open (a, b) and fully closed (c, d) leaflet positions.

175x151mm (300 x 300 DPI)

Figure 9. Von-Mises stress at the belly region during the cardiac cycle predicted by the ALE (ADINA) and MM-ALE (LS-DYNA) methods.

78x55mm (300 x 300 DPI)