Evaluation of a new Implicit Coupling Algorithm for the Partitioned Fluid-Structure Interaction Simulation of Bileaflet Mechanical Heart Valves

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Abstract: The movement of the leaflets of Bileaflet Mechanical Heart Valves (BMHVs) strongly interacts with the surrounding fluid motion and therefore it needs to be modeled through a Fluid-Structure Interaction (FSI) scheme with implicit coupling. Therefore, when using partitioned solvers, a subiteration loop within each time step is needed. The stability of such a scheme depends on the value of the under-relaxation factor. For the simulation of a BMHV, several methods can be used to find such an appropriate under-relaxation factor, like fixed under-relaxation or the dynamically changing Aitken Δ^2 under-relaxation. Also, a stable scheme can be achieved with a newly developed algorithm which uses the Jacobian with the derivatives of the pressure and viscous moments acting on the leaflets with resprect to the angular accelerations of the leaflets. In this paper, this new algorithm is presented and compared to existing coupling schemes. It is shown through numerical experiments that our newly developed algorithm outperforms these existing coupling schemes.

Nowadays, mostly a Bileaflet Mechanical Heart Valve (BMHV) is implanted when human valve replacement is needed. However, current valve designs are not optimal: non-physiological flow phenomena can still occur. Hence, numerical simulations can provide an important research tool for gaining insights into the complex dynamics of a BMHV.

The BMHV is typically simplified and modeled as a rigid casing with two rigid leaflets that rotate around their hinge axes. The movement of these leaflets is governed by Newton's Second Law of Motion:

$$\begin{cases} M_1 = I_1 \cdot \ddot{\theta}_1 \\ M_2 = I_2 \cdot \ddot{\theta}_2 \end{cases} \tag{1}$$

with M_i, I_i and $\ddot{\theta}_i$ indicating, respectively, the pressure (and viscous) moment of the fluid exerted on leaflet *i*, the moment of inertia, and the angular acceleration of leaflet *i*.

The numerical simulation of a Bileaflet Mechanical Heart Valve is a Fluid-Structure Interaction (FSI) problem. The movement of the leaflets strongly interacts with the surrounding fluid motion and therefore it needs to be modeled through a coupling scheme. However, when using partitioned solvers, not every FSI coupling scheme reaches a stable and efficient convergence.

In literature, the instability of explicit FSI coupling schemes for the case of BMHVs is explained by Borazjani et al. (2008). Thus, an algorithm with implicitness between the subiterations was found necessary for strong coupling. This implies the introduction of a subiteration loop within each time step. However, for doing so, a stable and efficient approximation of the subsequent angular acceleration $\ddot{\theta}_i^{n+1,k+1}$ is needed in each subiteration *k*. This can be achieved through an under-relaxation scheme:

$$\ddot{\theta}_i^{n+1,k+1} = \ddot{\theta}_i^{n+1,k} + \omega_i^{n+1,k} \cdot \left(\frac{M_i^{n+1,k}}{I_i} - \ddot{\theta}_i^{n+1,k} \right) \tag{2}$$

which can be rewritten as

$$\ddot{\theta}_i^{n+1,k+1} = \left(1 - \omega_i^{n+1,k}\right) \cdot \ddot{\theta}_i^{n+1,k} + \omega_i^{n+1,k} \cdot \frac{M_i^{n+1,k}}{I_i} \tag{3}$$

If chosen properly, the under-relaxation factor $\omega^{n+1,k}$ stabilizes the solution process of the subiterations as described by Borazjani et al. (2008).

For the simulation of a BMHV by partitioned solvers, several methods can be used to find such an appropriate under-relaxation factor. In this paper, an evaluation of such techniques is performed and a new algorithm is introduced. Subsequently, we will discuss the use of a "fixed" under-relaxation factor and a "dynamic" under-relaxation factor. In the "fixed" case, the factor is kept at a constant value during the entire time cycle, as described by Le Tallec et al. (2001) for an industrial shock absorber valve. For the dynamically

changing under-relaxation factor, a best fitted factor value is obtained in each time step. Typically the Aitken Δ² under-relaxation is used, as applied by Borazjanie et al. (2008). The factor is in each subiteration k>1 given by

$$\omega_i^{n+1,k} = \omega^{n+1,k} = -\frac{\left(\overrightarrow{\ddot{\theta}^{n+1,k}} - \overrightarrow{\ddot{\theta}^{n+1,k-1}}\right)^T \left(\overrightarrow{r^{n+1,k}} - \overrightarrow{r^{n+1,k-1}}\right)}{\left(\overrightarrow{r^{n+1,k}} - \overrightarrow{r^{n+1,k-1}}\right)^T \left(\overrightarrow{r^{n+1,k}} - \overrightarrow{r^{n+1,k-1}}\right)} \quad (4)$$

wherein

$$\overrightarrow{\ddot{\theta}^{n+1,k}} = \begin{bmatrix} \ddot{\theta}_1^{n+1,k} \\ \ddot{\theta}_2^{n+1,k} \end{bmatrix} \quad \text{and} \quad \overrightarrow{r^{n+1,k}} = \begin{bmatrix} \frac{M_1^{n+1,k}}{I_1} - \ddot{\theta}_1^{n+1,k} \\ \frac{M_2^{n+1,k}}{I_2} - \ddot{\theta}_2^{n+1,k} \end{bmatrix} \quad (5)$$

Subsequently, these techniques are compared with the new coupling scheme that we've recently developed. This algorithm is based on the prediction of the moments for the new coupling iteration with a numerically computed Jacobian, as introduced by Dumont et al. (2007) for one leaflet, but extended to two leaflets:

$$\begin{cases} M_1^{n+1,k} + \frac{\partial M_1}{\partial \ddot{\theta}_1}\left(\ddot{\theta}_1^{n+1,k+1} - \ddot{\theta}_1^{n+1,k}\right) + \frac{\partial M_1}{\partial \ddot{\theta}_2}\left(\ddot{\theta}_2^{n+1,k+1} - \ddot{\theta}_2^{n+1,k}\right) = I_1 \cdot \ddot{\theta}_1^{n+1,k+1} \\ M_2^{n+1,k} + \frac{\partial M_2}{\partial \ddot{\theta}_1}\left(\ddot{\theta}_1^{n+1,k+1} - \ddot{\theta}_1^{n+1,k}\right) + \frac{\partial M_2}{\partial \ddot{\theta}_2}\left(\ddot{\theta}_2^{n+1,k+1} - \ddot{\theta}_2^{n+1,k}\right) = I_2 \cdot \ddot{\theta}_2^{n+1,k+1} \end{cases} \quad (6)$$

This Jacobian is numerically derived from our flow solver by leaflet perturbations. The components of the Jacobian are derivatives of the pressure (and viscous) moments acting on the leaflets with respect to the accelerations of the leaflets. Instead of calculating this Jacobian every time step, the Jacobian can be extrapolated from previous time steps and a recalculation of the Jacobian is done only when needed.

The above mentioned techniques are implemented in FLUENT and used to simulate the same setting of a 3D BHMV. This allows a comparison of their stability and efficiency. The 3D geometry consists of a straight tube upstream of the valve, and Valsalva sinuses downstream of the valve, as visualized in Figure 1. An inlet aortic flow pulse is imposed, with a constant pressure at the outlet boundary. The valve is initially set in the closed position.

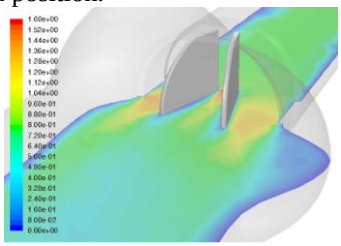

Figure 1: Velocity Magnitude Contours at peak systole (t = 0.125s), visualized on a longitudinal section

Simulations are conducted for different values of the fixed under-relaxation factor namely 0.05, 0.15, 0.25 and 0.285 resulting in resp. 17, 3, 20 and 107 subiterations for the first time step. So, the value of 0.15 can be seen as the optimum. However, as soon as the valve is a few degrees opened, with this optimum value for the first time step, approximately 11 subiterations per time step are needed to achieve convergence.

When using Aitken, a under-relaxation factor of 0.15 was also found for the first time step. However, in the following time steps, the factor value steeply increases until (after approximately 80 time steps with Δt=0.00025s) a stable value of approximately 0.35 is hold, achieving convergence within 3 a 4 subiterations during valve opening.

However, when setting the fixed under-relaxation factor to this optimal value of 0.35 for the entire time cycle, this leads to divergence in the first time step.

Therefore, the results indicate that the dynamic under-relaxation technique outperforms the fixed under-relaxation. This was expected because the fixed factor is a trade-off value that needs to allow stability throughout the entire time cycle, in contrast to the dynamic factor which can be optimized for each specific time step (and subiteration) of the time cycle.

Finally, the dynamically varying techniques are compared against each other. The opening phase of the valve, from t = 0s to t = 0.125s (peak systole), is simulated by 500 time step. On average, Aitken needs 3.2 subiterations per time step, while convergence is achieved in 2.7 subiterations per time step when using the new method which uses the Jacobian.

Thus, during the opening phase of the valve, Aitken Δ² under-relaxation is found more expensive than the the new method using the Jacobian.

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