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AUGMENTED LAGRANGIAN APPROACH FOR QUASI-INCOMPRESSIBLE CARDIAC MECHANICS

Joventino O. Campos[a], Rodrigo W. dos Santos[a,b], Joakim Sundnes[c] and Bernardo M. Rocha[a,b]

[a]*Programa de Pós Graduação em Modelagem Computacional, Universidade Federal de Juiz de Fora, Rua José Lourenço Kelmer, S/n - Martelos, Juiz de Fora - MG, Brasil, ppg.modelagemcomputacional@ufjf.edu.br, http://www.ufjf.br/pgmc*

[b]*Departamento de Ciência da Computação, Universidade Federal de Juiz de Fora, Rua José Lourenço Kelmer, S/n - Martelos, Juiz de Fora - MG, Brasil, depto.computacao@ufjf.edu.br, http://www.ufjf.br/deptocomputacao*

[c]*Simula Research Laboratory, University of Oslo, Martin Linges vei 25, 1364 Fornebu, post@simula.no, http://www.simula.no*

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Abstract. Computational models of heart mechanics have a large potential for application in medical research, and may give improved understanding of heart physiology and of important clinical problems such as heart failure. From the mathematical point of view, the passive mechanical behaviour of the heart can be described using the finite deformation theory from the field of solid mechanics. The tissue is typically modeled as an anisotropic, non-linear, hyperelastic and either incompressible or nearly incompressible material. Incompressibility is often enforced using a penalty function, which is known to dramatically change the conditioning of the stiffness matrix. For high penalty parameters, the condition number increases and the performance of iterative solvers will decrease. In this work we apply the Augmented Lagrangian approach with a mixed three field finite element formulation to incorporate quasi-incompressibility. This approach allows smaller penalty parameters, which is expected to result in linear systems with better numerical properties. Another advantage of the approach is that it offers complete control of the volumetric change during a simulation, which is not possible using the standard penalty formulation. The performance of the different approaches are examined using a set of problems from a cardiac mechanics benchmark.

1 INTRODUCTION

Computational modeling of cardiac electromechanical activity is a subject of substantial medical and scientific interest, which may contribute to increased understanding of several phenomena associated with heart physiology and pathology. Furthermore, there is increasing interest in applying computational models to study and optimize new therapies for cardiac disease, and for development of new drugs (Trayanova and Winslow, 2011). However, accurate modeling of heart physiology is a challenging problem, since it is a complex multiscale and multiphysics problem, which necessitates close interaction between numerous mathematical models.

Computational models focusing only on mechanical aspects of heart function have also led to considerable insight. One area of particular interest is the complex phenomena of heart failure, which is a mechanical dysfunction where the heart progressively loses its pumping ability (Mann and Bristow, 2005). However, although pure mechanical models, and in particular passive mechanics models, are considerably simpler than the coupled electro-mechanics problem, they still represent a substantial computational challenge. The tissue behavior is typically modeled as hyper-elastic, and is strongly non-linear, orthotropic and nearly incompressible. These are all factors known to be challenging for numerical solution of the equations.

Several independent simulation codes have been developed for cardiac mechanics, and a benchmark recently described in Land et al. (2015) represents a first attempt at comparing and verifying these solvers. The benchmark tests relevant aspects including pressure loading and anisotropic and spatially varying material properties. Within this context, only a few studies have focused on increasing the efficiency and robustness of cardiac mechanics simulations. For instance, Land et al. (2012) uses strategies to reduce the total number of full Newton iterations, such as strain prediction, modified Newton methods and matrix-free solvers. Hadjicharalambous et al. (2014) presents the weakly penalized form of the problem, while Sundnes et al. (2014) focuses on efficient linearization of coupled active and passive mechanics problems.

As noted above, heart tissue is normally modeled as incompressible or nearly incompressible, which is known to cause numerical difficulties such as locking and an ill-conditioned stiffness matrix. The finite element literature includes a large number of alternative methods for handling nearly incompressible systems, one being the Augmented Lagrangian method (Glowinski and Le Tallec, 1989; Simo and Taylor, 1991; Weiss et al., 1996). To our knowledge this strategy has never been applied in cardiac mechanics, and may potentially improve computational performance by reducing the condition number of the stiffness matrix and thereby improving the convergence of iterative solvers. In the present work we evaluate the performance of the Augmented Lagragian approach, and compare it to alternative formulations of nearly incompressible problems. The methods are compared by applying them to the test cases proposed in Land et al. (2015).

2 MATHEMATICAL MODEL

The model that describes cardiac tissue deformation is based on continuum mechanics theory for finite deformations (Javier Bonet, 2008). The boundary value problem is defined as follows: given the body forces $\mathbf{B}$ and the boundary conditions $\bar{\mathbf{u}}$ and $\bar{\mathbf{T}}$, find the displacement field $\mathbf{u}$ such that:

$$\begin{cases} \mathrm{Div}(\mathbf{FS}) + \mathbf{B} = 0, & \text{in } \Omega_0, \\ \mathbf{u} = \bar{\mathbf{u}}, & \text{on } \partial\Omega_0^D, \\ \mathbf{FSN} = \bar{\mathbf{T}}, & \text{on } \partial\Omega_0^N. \end{cases} \tag{1}$$

Here, $\mathbf{S}$ is the second Piola-Kirchhoff tensor, $\mathbf{F} = \mathbf{I}+\text{Grad}(\mathbf{u})$ is the deformation gradient tensor, $\bar{\mathbf{u}}$ are the precribed displacements and $\bar{\mathbf{T}}$ is the first Piola-Kirchhoff traction vector prescribed on the boundary $\partial\Omega_0^N$, which has normal vector $\mathbf{N}$.

Assuming that the material is hyperelastic, the stress can be derived from a strain energy function:

$$\mathbf{S}_p = 2\frac{\partial \Psi}{\partial \mathbf{C}}, \tag{2}$$

where $\mathbf{C} = \mathbf{F}^T\mathbf{F}$ is the right Cauchy-Green tensor. The form of the strain energy Ψ depends on the material considered. We will consider two different material laws, one is the classical Neo-Hookean material, with

$$\Psi = \frac{\mu}{2}(I_1 - 3) - \mu(\ln J) + \frac{\lambda}{2}(\ln J)^2, \tag{3}$$

where μ and λ are material constants. The other material we used is a typical cardiac constitutive model which is transversely isotropic and was proposed by Guccione et al. (1995). Its strain energy function is given by

$$\Psi = \frac{c}{2}(e^Q - 1), \tag{4}$$

and

$$Q = b_f E_{11}^2 + b_t(E_{22}^2 + E_{33}^2 + E_{23}^2 + E_{32}^2) + b_{fs}(E_{12}^2 + E_{21}^2 + E_{13}^2 + E_{31}^2) \tag{5}$$

where E_{ij} are components of the Green-Lagrange strain tensor $\mathbf{E}$ in a local orthonormal coordinate system with cardiac fibers aligned in the $\mathbf{e}_1$-direction, and where C, b_f, b_t, b_{fs} are material parameters. The Guccione et al. (1995) constitutive law was implemented and validated in our code using a procedure described by Urquiza et al. (2010).

3 METHODS

The models presented above are to be solved using the finite element method. In this section we present the formulation for nearly incompressible problems, the mixed three-field formulation used in this work, and finally the Augmented Lagrangian approach used to improve the iterative solver performance.

3.1 Nearly incompressible formulation

To apply the finite element method we need to establish the variational form of the problem. We adopt a quasi-incompressible formulation, where the deformation gradient and its respective deformation measures are separated into isochoric and volumetric parts. We define $\bar{\mathbf{F}} = J^{-1/3}\mathbf{F}$, $\bar{\mathbf{C}} = \bar{\mathbf{F}}^{\mathbf{T}}\bar{\mathbf{F}} = J^{-2/3}\mathbf{C}$, where $\bar{\mathbf{F}}$ is associated with the isochoric deformation which satisfies $\det \bar{\mathbf{F}} = 1$ and $\bar{\mathbf{C}}$ which is the isochoric part of the right Cauchy-Green deformation tensor.

The strain energy function in its decoupled form is given by

$$\Psi(\mathbf{C}) = \Psi_{\text{iso}}(\bar{\mathbf{C}}) + \Psi_{\text{vol}}(J), \quad \text{with} \quad \Psi_{\text{vol}}(J) = \frac{\kappa}{2}(J(\mathbf{u}) - 1)^2, \tag{6}$$

where the volumetric term $\Psi_{\text{vol}}(J)$ depends on the parameter $\kappa > 0$, also known as bulk modulus. The total potential energy is given by $\Pi_p(\mathbf{u}) = \Pi_p^{\text{int}}(\mathbf{u}) + \Pi^{\text{ext}}(\mathbf{u})$, where the contributions

from the internal and external potential part of the energy are defined, respectively, as

$$\Pi_p^{\text{int}}(\mathbf{u}) = \int_{\Omega_0} [\mathbf{\Psi}_{vol}(J) + \mathbf{\Psi}_{iso}(\bar{\mathbf{C}})] dV, \tag{7}$$

$$\Pi^{\text{ext}}(\mathbf{u}) = -\int_{\Omega_0} \mathbf{B} \cdot \mathbf{u} dV - \int_{\partial\Omega_0^N} \bar{\mathbf{T}} \cdot \mathbf{u} dS, \tag{8}$$

where $\mathbf{B}$ denotes the external applied body forces and $\bar{\mathbf{T}}$ the external applied traction. Note that this formulation corresponds to the standard penalty formulation of the problem where the material is treated as nearly incompressible and a large value of the penalty parameter κ prevents significant volumetric changes.

3.2 Mixed three-field formulation

Usually in order to avoid the problem known as the locking of the finite element solution, alternative finite element procedures are employed such as mixed formulation or stabilization techniques. In the present work we used a mixed three-field finite element formulation which was proposed by Simo, Taylor and Pister (STP) (Simo et al., 1985; Simo and Taylor, 1991) which has been used successfully in biomechanics (Gasser et al., 2006).

This formulation considers the displacement field $\mathbf{u}$, the pressure p and the dilatation $\tilde{J}$ as independent variables. Here the element-wise scalar variable $\tilde{J}$ is such that $J = \tilde{J}$ will be satisfied on each finite element in a mean sense. Thus, the following energy functional of the variational formulation is introduced

$$\Pi_{STP}(\mathbf{u}, p, \tilde{J}) = \int_{\Omega_0} \left[\Psi_{\text{iso}}(\overline{\mathbf{C}}) + \Psi_{\text{vol}}(\tilde{J}) + p(J(\mathbf{u}) - \tilde{J}) \right] dV + \Pi_{\text{ext}}(\mathbf{u}), \tag{9}$$

where the $J = \tilde{J}$ constraint is imposed through p, Ψ_{vol} is the same as previously defined and $\Pi_{\text{ext}}(\mathbf{u})$ is the the external contribution, as defined in equation (8). Here we choose a $Q1 - Q0 - Q0$ mixed finite element discretization for $\mathbf{u}$, p and $\tilde{J}$, that is, piecewise linear elements for displacement and constant piecewise elements for the scalar fields p and $\tilde{J}$. One attractive point of this formulation is that static condensation of p and $\tilde{J}$ can be performed at the element level, which leads to a reduced problem in terms of the displacement field only.

3.3 Augmented Lagrangian

Although the mixed three field FE formulation is robust and efficient, it still requires a high value for the κ parameter to prevent significant volumetric changes. This increases the ill-conditioning of the stiffness matrix and may result in poor performance of iterative solvers. Here the Augmented Lagrangian (ALG) approach was used for the treatment of quasi-incompressibility constraint within a finite elasticity setting. This approach was first introduced within finite elasticity context by Glowinski and Le Tallec (1982, 1984), and since then have been used successfully by others (Simo and Taylor, 1991), including in a work by Weiss et al. (1996) where a biomechanics problem was solved using the STP mixed three-field finite element formulation.

In the Augmented Lagrangian approach for quasi-incompressibility another Lagrange multiplier μ is added on each finite element to enforce the element-wise constraint $\det \mathbf{F} = 1$. This multiplier is computed in an iterative fashion by

$$\mu_{k+1} = \mu_k + \xi(\det\mathbf{F} - 1), \tag{10}$$

where ξ is a chosen constant. This iterative procedure is usually known as Uzawa algorithm. When combined with the STP mixed formulation, we only enforce the $\det \mathbf{F} = 1$ constraint in a mean sense, considering the constraint on the variable $\tilde{J}$ introduced by the mixed formulation, instead of using $J = \det \mathbf{F}$. With this approach we can control the volumetric changes within an element to any desired accuracy, which allows a reduction in the penalty parameter κ from the volumetric term Ψ_{vol} of the strain energy, which in turn alleviates the ill-conditioning of the stiffness matrix.

The functional of the Augmented Lagrangian method is

$$\Pi_{ALG}(\mathbf{u}, p, \tilde{J}, \mu) = \int_{\Omega_0} \left[\Psi_{\text{iso}}(\overline{\mathbf{C}}) + \Psi_{\text{vol}}(\tilde{J}) + p(J - \tilde{J}) \right] dV + \Pi_{\text{ext}} + \int_{\Omega_0} \mu(\tilde{J} - 1)\, dV, \quad (11)$$

which is discretized using piecewise linear elements for displacements and piecewise constants for the other variables. Here, $\tilde{J}$ and p are statically condensed and the Lagrange multiplier μ is computed using the Uzawa iteration via equation (10).

This way we can enforce incompressibility without using a high global value for κ, since the multiplier is locally computed on each element to enforce $\tilde{J} = 1$. Only those elements violating a specified criterion will have its multiplier μ increased to satisfy the criterion, as shown in Algorithm 1.

Algorithm 1: Augmented Lagragian algorithm

```
Set Lagrange multiplier μ_0 = 0
while full load not reached yet do
    Apply load increment
    k = 0
    do
        Use Newton iteration to solve the nonlinear problem (1)
        foreach finite element e that do not satisfy |J̃ − 1| < tol do
            Update Lagrange multiplier as μ^e_{k+1} = μ^e_k + ξ(J̃ − 1)
        end
        k = k + 1
    while there exists elements e such that |J̃ − 1| > tol
end
```

We applied two different numerical methods to solve the linear systems resulting from the discretization. A reference solution was obtained with a direct solver from the MUMPS package Amestoy et al. (2000), while the performance of the formulations within the context of iterative methods was tested using the GMRES solver with BoomerAMG, an Algebraic Multigrid (AMG) preconditioner (Henson and Yang, 2002).

4 COMPUTATIONAL EXPERIMENTS

In order to assess the performance of the Augmented Lagrangian approach for cardiac mechanics, we present computer simulations results for two differents problems. The first one is a well known problem in computational mechanics, which is Cook's membrane, whereas the second problem is from the cardiac mechanics benchmark proposed by Land et al. (2015).

4.1 Cook's membrane

This problem is commonly used to evaluate the convergence properties of finite element methods when the material is considered incompressible or quasi-incompressible (de Souza Neto et al., 2005). The geometry and dimensions of the problem are presented in Figure 1. The nodes on the left face had its displacements restricted and a vertical load $F = 6.25$ was applied on the right face. The Neo-Hookean model was used to describe the material response, with the following parameters: thickness is $h = 1mm$, material coefficients $\mu = 80.1938$ and $\kappa = 400942$. Note that we used a high value used for the penalty parameter, like in de Souza Neto et al. (2005), in order to restrict significant volumetric changes.

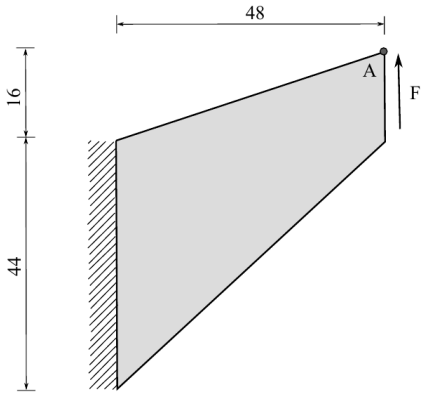


Figure 1: Cook's membrane problem.

The vertical displacement at point A was observed for successively refined meshes to evaluate the finite element convergence. We compared the performance of the STP formulation and ALG approach. When using high values for the penalty parameter, in the STP formulation, the performance of Krylov iterative solvers usually decay.

Figure 2 presents three different scenarios using these solvers, where the direct method was used as a reference. We note that both formulations converge. Note that the ALG solution is only slightly different from the STP solution in some points. The maximum difference between ALG and STP solutions is about 0.37%, which is in accordance with results found by de Souza Neto et al. (2005) for another FE formulation.

Our focus was on the comparison of the numerical performance of the iterative solver when a different FE formulation was used, that is, with and without the ALG approach. Simulations using different values of penalty parameter for the ALG formulation were carried out, where the value $\kappa = 400942$ was used as a reference.

The performance of the solution without and with ALG is presented in the Table 1 in terms of Newton iterations and mean number of GMRES iterations to achieve convergence in each load increment. Runtime measurements (see Table 2) indicate that, by using the ALG with a reduced value for κ, the solver can be up to three times faster in this testcase.

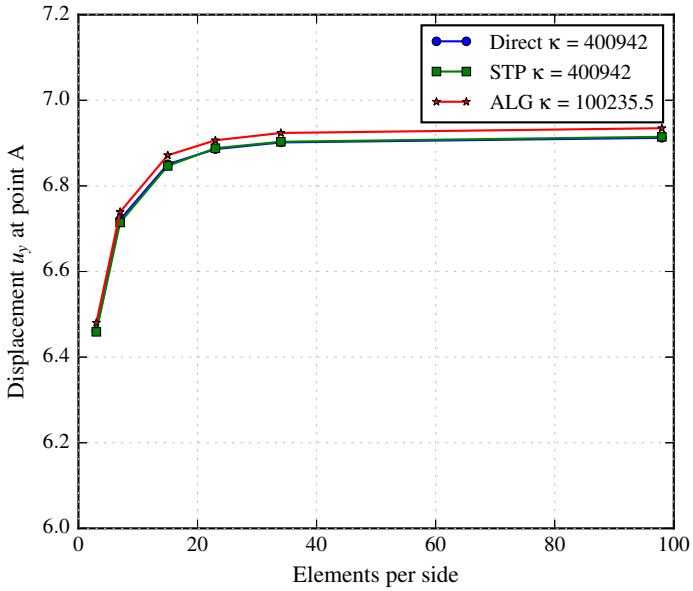


Figure 2: Cook problem convergence.

Table 1: Comparison of the solver performance with and without ALG approach.

Increment	Newton Iterations		GMRES Iterations	
	STP	ALG	STP	ALG
1	19	17	20.0	15.6
2	17	16	18.9	13.1
3	17	17	19.6	12.1
4	18	17	18.9	11.3
5	19	17	19.1	12.0
6	15	17	18.0	11.4
7	17	13	17.5	12.4
8	18	13	18.0	12.9
9	15	12	17.4	12.7
10	15	12	17.0	12.5
11	14	13	17.4	12.9
12	15	12	17.3	12.9
13	14	12	16.9	12.9
14	13	12	17.2	12.6
15	13	13	17.2	12.3
16	14	12	16.9	12.7
17	15	14	16.7	12.3
18	13	12	16.5	12.3
19	16	12	16.1	12.1
20	15	11	15.9	12.1

The Table 2 shows the solver performance without ALG using $\kappa = 400942$ and with ALG with κ reduced by a factor of 4 for different mesh refinements.

Note that the solution with ALG performed less iterations during the GMRES solution which

resulted in a smaller total execution time. In this case the solution was about $3\times$ faster than the solution without ALG. This happened because the penalty parameter could be reduced with ALG, which resulted in linear systems better conditioned and easier to solve for GMRES, without loosing control over the desired degree of incompressibility to be satisfied in the elements.

Table 2: Runtime measurements, in seconds, of STP using $\kappa = 400942$ and ALG with κ reduced by a factor of 4.

Elements per side	STP	ALG
27	41.48	16.87
112	192.14	73.70
525	822.47	286.67
1219	2057.46	725.68
2754	5569.56	1715.28
11267	26837.78	8764.35

4.2 Cardiac mechanics benchmark problem

A benchmark problem was proposed by Land et al. (2015) for the validation of implementations of cardiac mechanics simulations. The domain consists of a deforming rectangular beam. This problem tests pressure-type forces, the correct implementation of fiber direction and the transversely isotropic constitutive law for cardiac tissue. The Guccione et al. (1995) model was used with the following parameters: $C = 2$ kPa, $b_f = 8$, $b_t = 2$ and $b_{fs} = 4$. The fiber direction was considered constant along the long axis, i.e. $(1, 0, 0)$. The left face ($x = 0$) was fixed in all directions and a pressure of $0.004kPa$ was applied to the entire bottom face ($z = 0$).

The geometry was discretized using hexahedral elements, as shown in Figure 3. ALG simulations used a mesh with $120 \times 12 \times 12$ elements, resulting in a total of 60840 degrees of freedom. In simulations without ALG a mesh with $220 \times 22 \times 22$ elements and 349140 degrees of freedom was used.

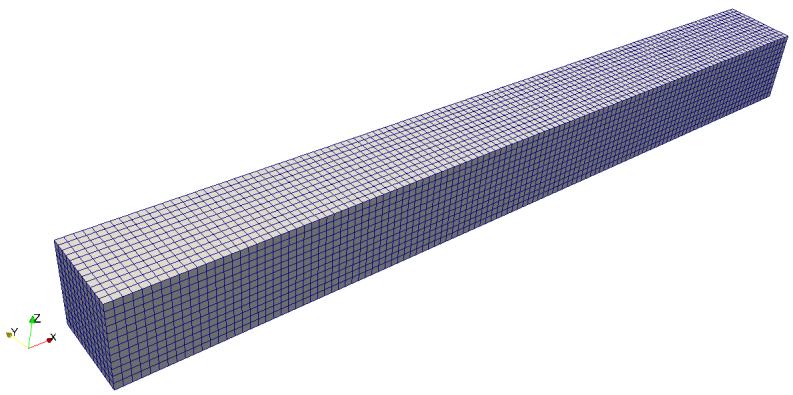


Figure 3: Benchmark geometry discretization.

Figure 4 presents the z-deflection at point $(10, 0.5, 1)$ for the codes tested in Land et al. (2015) and for our code (Cardiax) using iterative method with ALG and direct solver without

ALG. We computed the mean value of the displacements found by the benchmark codes and found a value of 4.1615. The result obtained by our code using the direct method without ALG differed 0.29% from the mean value, whereas the result obtained using the iterative solver with ALG differed only 0.03% from the mean displacement.

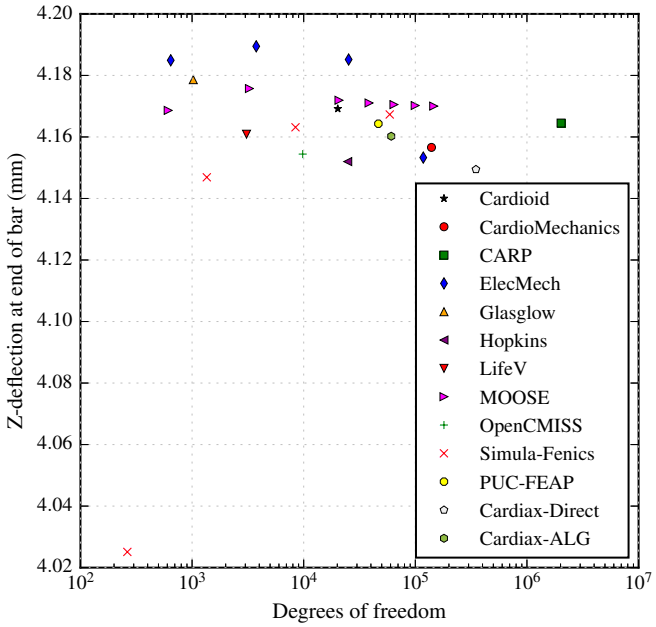
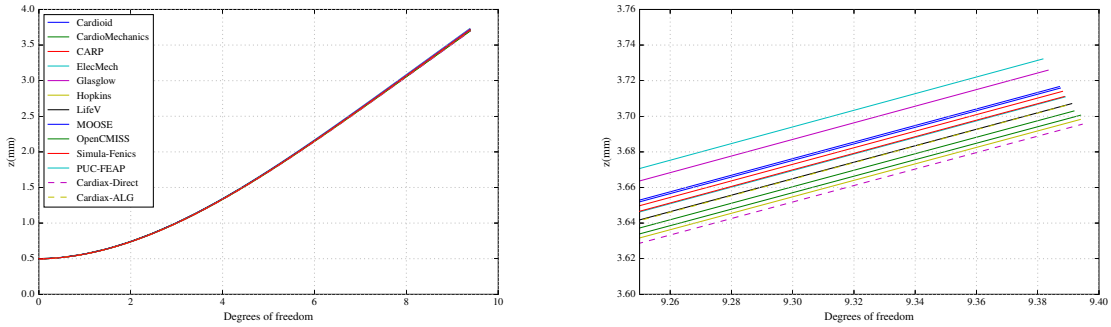


Figure 4: Z-deflection convergence in the benchmark problem.

Figure 5 shows the deformation of line $(x, 0.5, 0.5)$ for each code. It is possible to note that all codes presented close results, but a very small difference among them can be seen in Figure 5(b).



(a) (b)

Figure 5: Left: deformation of a line $(x, 0.5, 0.5)$ for each code; Right: details for the end of the bar.

Figure 6 shows the results of strain computed at some points for the codes that uses similar formulations to Cardiax (low order FE, check details at Land et al. (2015)). The results found

by Cardiax with and without ALG were close to the others presented codes, likewise in above experiments.

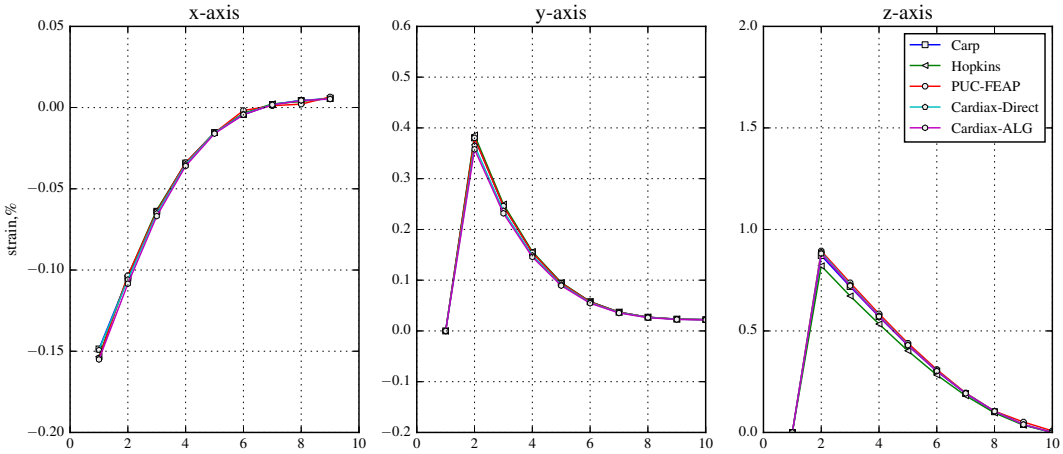


Figure 6: Strain along the line in direction of $x-$, $y-$ and $z-$axes.

Table 3 shows Newton iterations and mean number of GMRES iterations to achieve convergence in each load increment. Note that ALG approach presented a better performance, since it required less Newton iterations in some load increments and less GMRES iterations in all increments.

Table 3: Comparison of the solver performance with and without ALG approach using a mesh of $220 \times 22 \times 22$ hexahedral elements.

Increment	Newton Iterations		GMRES Iterations	
	STP	ALG	STP	ALG
1	5	4	28	14.2
2	4	4	21.2	15.5
3	4	4	23	14
4	4	4	24.8	17
5	4	4	19	16.8
6	5	4	33.8	13.5
7	5	4	34.8	16
8	4	4	32	15.5
9	5	5	46.4	15.2
10	4	4	26.8	14.2
11	4	5	21.2	15.2
12	4	5	27	15.2
13	5	5	37.8	19.2
14	4	6	29	16.8
15	5	5	37.4	18.2
16	4	5	26.5	16
17	5	5	24	18.6
18	4	4	29.2	17.5
19	5	6	29.6	16.7
20	5	6	31.6	21.8

The Cardiax code presented satisfactory results for this benchmark problem, which shows that ALG approach can be used to solve cardiac mechanics problem, improving the performance of the simulations.

4.3 Discussion

The presented results show that the ALG approach can improve the performance of iterative solvers (here we only assessed the performance of GMRES with AMG preconditioner). This strategy reduces the value of the penalty parameter κ, which decreases the ill-conditioning of the stiffness matrix thereby improving the convergence of iterative methods. Furthermore, with the ALG approach one is able to control the incompressibility *a priori*, i.e., we can choose a tolerance (see Algorithm 1) for element-wise volume change that the ALG solution procedure has to satisfy. In the standard penalty formulation this is not possbile *a priori*. We have to choose a value for κ and we will only know the volumetric changes after a post-processing of the solution.

For the cardiac benchmark problem studied here, a small value for the volumetric changes in the elements was obtained with $\kappa = 100$ without ALG (see Table 4). However, in order to illustrate the control over volumetric changes with ALG, we carried out simulations varying κ in both STP and ALG formulations. The ALG simulations were performed considering a tolerance of 10^{-2}. As expected, all the ALG results satisfied this criterion. For the STP formulation, we note, however, that as we reduced κ a more significant volumetric change can be observed, specially for $\kappa < 40$. This also shows that the simulation with ALG using $\kappa/4$ can achieve the

level of volume change as the standard STP formulation with the original value of the penalty parameter.

Table 4: Maximum element-wise volume change.

κ	STP	ALG
10	0.0225757	0.00984744
20	0.0146401	0.0096956
30	0.0111155	0.00981326
40	0.00907006	0.0090695
50	0.00771548	0.00771658
60	0.00674607	0.00674564
70	0.0060127	0.00601191
80	0.00543654	0.00543523
90	0.00496796	0.00496889
100	0.00458284	0.00458245

With a reduction by a factor of 4 in κ we could achieve good results in the cardiac benchmark problem and, at the same time, obtain good performance within the iterative solver. The data from Table 4 shows that we can further reduce it, keeping the desired level of incompressibility and achieve good results.

To summarize, we remark that, depending on the problem characteristics (geometry, loadings, material model) and on the desired accuracy, further reduction of the penalty parameter can yield an even better performance during the preconditioned iterative solution.

5 CONCLUSIONS

This work applied the Augmented Lagrangian to a mixed three field variational formulation to solve cardiac mechanics problems. We presented results for two different problems to first validate the ALG approach for cardiac mechanics using a benchmark problem with reference solution and then to study its numerical performance. The Cardiax code presented satisfactory results for the benchmark experiments, which shows that ALG approach can be used to solve cardiac mechanics problem.

Our preliminary results also showed that the ALG formulation had satisfactory convergence results in the benchmark problems and achieved a better numerical performance in all cases. It was shown that this approach can improve the numerical properties of the problem, consequently improving the simulations perfomance when iterative solvers are used. More importantly, this approach obtained an improved performance without significantly affecting volumetric changes by defining an a priori tolerance to be satisfied.

Future research includes assessing the performance of the ALG for two others problems in cardiac benchmark that use a more detailed geometry of the left ventricle and results in a more complex deformation pattern. We also plan to study the effect of different preconditioners when combined with the ALG formulation.

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