Assessing the potential of Jacobian-free Newton-Krylov methods for cell-centred finite volume solid mechanics

Philip Cardiff[1,2,3*] and Ivan Batistić[4]

[1*]School of Mechanical and Materials Engineering, University College Dublin, Ireland.

[2]UCD Centre for Mechanics, University College Dublin, Ireland.

[3]SFI I-Form Centre, University College Dublin, Ireland.

[4]University of Zagreb, University of Zagreb, Croatia.

*Corresponding author. E-mail: philip.cardiff@ucd.ie

Abstract

In this study, we explore the efficacy of Jacobian-free Newton-Krylov methods within the context of finite-volume solid mechanics. Traditional Newton-based approaches to solving nonlinear systems often require explicit formation and storage of the Jacobian matrix, which can be computationally expensive and memory-intensive. The Jacobian-free Newton-Krylov method circumvents this by employing Krylov subspace iterative solvers, such as GMRES, in conjunction with a Newton iteration scheme that approximates the action of the Jacobian through finite difference evaluations. This approach promises significant computational savings, especially for large-scale, complex simulations prevalent in solid mechanics. This article research systematically evaluates the performance of Jacobian-free Newton-Krylov methods by benchmarking them against conventional segregated methods on a suite of test problems, including elastic, plastic, linear and nonlinear geometry deformation scenarios. Key metrics such as convergence rate, computational cost, and robustness are analysed. Additionally, we investigate the impact of various preconditioning strategies on the efficiency of the Jacobian-free Newton-Krylov method. Our findings indicate that Jacobian-free Newton-Krylov methods can achieve comparable/superior/XXX convergence behaviour relative to traditional segregated methods, particularly in cases where YYYY. The results suggest that Jacobian-free Newton-Krylov methods are promising for advancing finite-volume solid mechanics simulations, offering a viable pathway for enhancing computational efficiency and scalability. EMPHASISE: easy to extend segregated frameworks, on contrast to exact Jacobian methods.

Key FV points: - many FV codes were developed around a segregated solution procedure, which requires significant effort to extend to a full Newton method, e.g. in terms of Jacobian assembly, storage, and linear system solution. - this paper examines Jacobian-free Newton-Krylov as a straight-forward extension of the segregated approach, without the need for a full Jacobian based method. - compact approximate Jacobian for preconditioner (more compact than FE approach) - implemented in OpenFOAM, and code and cases are made publicly available.

Keywords: Jacobian-free Newton-Krylov, Finite volume method, GMRES, OpenFOAM

1 Introduction

Finite volume formulations for solid mechanics are heavily influenced by their fluid mechanics counterparts, favouring segregated implicit and fully explicit methods. Segregated approaches, where the governing momentum equation is temporarily decomposed into scalar component equations, offer memory efficiency and simplicity of implementation, but the outer coupling Picard iterations often suffer from slow convergence. Explicit formulations are equally straightforward to implement and offer superior robustness but are only efficient for fast dynamics. In contrast, the finite element community commonly employs Newton-Raphson-type solution algorithms, which necessitate repeated assembly of the exact Jacobian and solution of the resulting block-coupled non-diagonally dominant linear system. Traditional Newton-based approaches, as commonly employed with finite element approaches, often require explicit formation and storage of the Jacobian matrix, which can be computationally expensive and memory-intensive. In addition, from a finite volume perspective, derivation, assembly, storage and solution of the resulting block-coupled system often require major refactoring of existing segregated frameworks or creating entirely new implementations. Consequently, similar block-coupled solution finite volume methods are rare in the literature [**? ? ?**]; The motivation of the current work is to seek (or exceed) the robustness and efficiency of block-coupled Newton-Raphons approaches in a way that can be easily incorporated into existing segregated solution frameworks. To this end, the current article examines the efficacy of Jacobian-free Newton-Krylov methods, where the quadratic convergence of Newton methods can potentially be achieved without deriving, assembling and storing the exact Jacobian.

Jacobian-free Newton-Krylov methods circumvent the need for the Jacobian matrix by combining the Newton-Raphson method with Krylov subspace iterative linear solvers, such as GMRES, and noticing that such Krylov solvers do not explicitly require the Jacobian matrix. Instead, only the action of the Jacobian matrix on a solution-type vector is required. The key step in Jacobian-free Newton-Krylov methods is the approximation of products between the Jacobian matrix and vectors using the finite difference method; that is

$$\mathbf{J}\mathbf{v} \approx \frac{\mathbf{F}(\mathbf{x} + \epsilon\mathbf{v}) - \mathbf{F}(\mathbf{x})}{\epsilon} \tag{1}$$

where $\mathbf{J}$ is the Jacobian matrix, $\mathbf{x}$ is the current solution vector (e.g. nodal displacements), $\mathbf{v}$ is a vector (e.g., from a Krylov subspace), and ϵ is a small scalar perturbation. With an appropriate choice of ϵ (balancing truncation and round-off errors), the characteristic quadratic convergence of Newton methods can be achieved without the Jacobian, hence the prefix *Jacobian-free.* This approach promises significant memory savings over Jacobian-based methods, especially for large-scale, but also potentially for execution time, with appropriate choice of solution components.

A crucial aspect of ensuring the efficiency and robustness of the Jacobian-free Newton-Krylov method is the choice of a suitable preconditioner for the Krylov iterations. This preconditioner is often derived from the exact Jacobian matrix to accelerate convergence in traditional Newton methods. However, we do not have direct access to the full Jacobian matrix in the Jacobian-free approach, necessitating an alternative strategy to approximate its action.

To this end, and to extend existing segregated frameworks, we propose using a compact-stencil approximate Jacobian as the preconditioner. This approximate Jacobian corresponds to the matrix typically employed in segregated approaches; similar approaches are successful in fluid mechanics applications [**? ?**]; however, it is unclear if such an approach is suitable for solid mechanics - a question which we hope to answer in this work. By leveraging this compact-stencil approximate Jacobian, we aim to effectively precondition the Krylov iterations, enhancing convergence while maintaining the memory and computational savings that define the Jacobian-free method. Similarly, if such an approach is efficient, it would naturally fit into existing segregated frameworks, as existing matrix storage and assembly can be reused.

The remainder of the paper is structured as follows: Section 2 summarises a typical solid mechanics mathematical model and its cell-centred finite volume discretisation. Section 3 presents the solution algorithms, starting with the classic segregated solution algorithm, followed by the proposed Jacobian-free Newton-Krylov solution algorithm. The performance of the proposed Jacobian-free Newton-Krylov approach is compared with the segregated approach on several varying benchmark cases in Section 4, where the effect of several factors are examined, including problem dimension, mesh, material model, nonlinear geometry, choice of preconditioner, and other solution parameter. Finally, the article ends with a summary of the main conclusions of the work.

2 Mathematical Model and Numerical Methods

2.1 Governing Equations

WIP

2.2 Cell-Centred Finite Volume Discretisation

WIP

3 Solution Algorithms

3.1 Segregated Solution Algorithm

WIP

3.2 Jacobian-free Newton-Krylov Algorithm

WIP

4 Test Cases

WIP

5 Conclusions

WIP

The main conclusions of the work are:

- WIP
- WIP

Acknowledgments. This work has emanated from research conducted with the financial support of/supported in part by a grant from Science Foundation Ireland (SFI) under Grant number RC2302_2. Philip Cardiff gratefully acknowledges financial support from the Irish Research Council through the Laureate program, grant number IRCLA/2017/45, and the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (Grant agreement No. 101088740). Vikram Pakrashi would also like to acknowledge FlowDyn RDD/966 and SiSDATA EAPA_0040/2022. Additionally, the authors want to acknowledge project affiliates, Bekaert, through the Bekaert University Technology Centre (UTC) at University College Dublin (www.ucd.ie/bekaert), I-Form, funded by SFI Grant Number 16/RC/3872, co-funded under European Regional Development Fund and by I-Form industry partners, NexSys, funded by SFI Grant Number 21/SPP/3756, and the DJEI/DES/SFI/HEA Irish Centre for High-End Computing (ICHEC) for the provision of computational facilities and support (www.ichec.ie). Finally, part of this work has been carried out using the UCD ResearchIT Sonic cluster funded by UCD IT Services and the UCD Research Office.

Appendix A WIP

WIP

References

[1] Griffith, B.P., Goerlich, C.E., Singh, A.K., Rothblatt, M., Lau, C.L., Shah, A., Lorber, M., Grazioli, A., Saharia, K.K., Hong, S.N., Joseph, S.M., Ayares, D., Mohiuddin, M.M.: Genetically Modified Porcine-to-Human Cardiac Xenotransplantation. New England Journal of Medicine **387**(1), 35–44 (2022) https://doi.org/10.1056/NEJMoa2201422 . Publisher: Massachusetts Medical Society _eprint: https://doi.org/10.1056/NEJMoa2201422. Accessed 2023-12-05

[2] Koh, J., Chee, H.K., Kim, K.-H., Jeong, I.-S., Kim, J.-S., Lee, C.-H., Seo, J.-W.: Historical Review and Future of Cardiac Xenotransplantation. Korean Circulation Journal **53**(6), 351–366 (2023) https://doi.org/10.4070/kcj.2022.0351 . Accessed 2023-11-26

[3] Lewis, T.: Milestone Pig-to-Human Heart Transplant May Pave the Way for Broader Trial. https://www.scientificamerican.com/article/milestone-pig-to-human-heart-transplant-may-pave-the-way-for-broader-trial/ Accessed 2023-12-05

[4] Shi, Y., Lawford, P., Hose, R.: Review of Zero-D and 1-D Models of Blood Flow in the Cardiovascular System. BioMedical Engineering OnLine **10**(1), 33 (2011) https://doi.org/10.1186/1475-925X-10-33 . Accessed 2023-12-13

[5] Westerhof, N., Lankhaar, J.-W., Westerhof, B.E.: The arterial Windkessel. Medical & Biological Engineering & Computing **47**(2), 131–141 (2009) https://doi.org/10.1007/s11517-008-0359-2 . Accessed 2023-12-10

[6] Gopalan, C., Kirk, E.: Chapter 2 - The blood vessels. In: Gopalan, C., Kirk, E. (eds.) Biology of Cardiovascular and Metabolic Diseases, pp. 35–51. Academic Press, ??? (2022). https://doi.org/10.1016/B978-0-12-823421-1.00004-4 . https://www.sciencedirect.com/science/article/pii/B9780128234211000044 Accessed 2023-12-10

[7] Burattini, R., Bini, S.: Physiological interpretation of inductance and low-resistance terms in four-element windkessel models: Assessment by generalized sensitivity function analysis. Medical Engineering & Physics **33**(6), 739–754 (2011) https://doi.org/10.1016/j.medengphy.2011.01.012 . Accessed 2023-12-13

[8] Korakianitis, T., Shi, Y.: Numerical simulation of cardiovascular dynamics with healthy and diseased heart valves. Journal of Biomechanics **39**(11), 1964–1982 (2006) https://doi.org/10.1016/j.jbiomech.2005.06.016 . Accessed 2023-12-13

[9] Rudenick, P.A., Bijnens, B.H., Segers, P., García-Dorado, D., Evangelista, A.: Assessment of Wall Elasticity Variations on Intraluminal Haemodynamics in Descending Aortic Dissections Using a Lumped-Parameter Model. PLoS ONE **10**(4), 0124011 (2015) https://doi.org/10.

1371/journal.pone.0124011 . Accessed 2023-12-13

[10] Laubscher, R., Merwe, J., Liebenberg, J., Herbst, P.: Dynamic simulation of aortic valve stenosis using a lumped parameter cardiovascular system model with flow regime dependent valve pressure loss characteristics. Medical Engineering & Physics **106**, 103838 (2022) https://doi.org/10.1016/j.medengphy.2022.103838

[11] Bozkurt, S., Paracha, W., Bakaya, K., Schievano, S.: Patient-Specific Modelling and Parameter Optimisation to Simulate Dilated Cardiomyopathy in Children. Cardiovascular Engineering and Technology **13**(5), 712–724 (2022) https://doi.org/10.1007/s13239-022-00611-9 . Accessed 2023-12-13

[12] Duanmu, Z., Yin, M., Fan, X., Yang, X., Luo, X.: A patient-specific lumped-parameter model of coronary circulation. Scientific Reports **8**, 874 (2018) https://doi.org/10.1038/s41598-018-19164-w . Accessed 2023-12-13

[13] Dash, A., Jain, K., Ghosh, N., Patra, A.: Non-invasive detection of coronary artery disease from photoplethysmograph using lumped parameter modelling. Biomedical Signal Processing and Control **77**, 103781 (2022) https://doi.org/10.1016/j.bspc.2022.103781 . Accessed 2023-12-13

[14] Bjørdalsbakke, N.L., Sturdy, J.T., Hose, D.R., Hellevik, L.R.: Parameter estimation for closed-loop lumped parameter models of the systemic circulation using synthetic data. Mathematical Biosciences **343**, 108731 (2022) https://doi.org/10.1016/j.mbs.2021.108731 . Accessed 2023-12-13

[15] Bozkurt, S.: Mathematical modeling of cardiac function to evaluate clinical cases in adults and children. PLoS ONE **14**(10), 0224663 (2019) https://doi.org/10.1371/journal.pone.0224663 . Accessed 2023-12-14

[16] Pollock, J.D., Makaryus, A.N.: Physiology, Cardiac Cycle. In: StatPearls. StatPearls Publishing, Treasure Island (FL) (2023). http://www.ncbi.nlm.nih.gov/books/NBK459327/ Accessed 2023-12-29

[17] Lelovas, P.P., Kostomitsopoulos, N.G., Xanthos, T.T.: A comparative anatomic and physiologic overview of the porcine heart. Journal of the American Association for Laboratory Animal Science: JAALAS **53**(5), 432–438 (2014)

[18] Crick, S.J., Sheppard, M.N., Ho, S.Y., Gebstein, L., Anderson, R.H.: Anatomy of the pig heart: comparisons with normal human cardiac structure. Journal of Anatomy **193 (Pt 1)**(Pt 1), 105–119 (1998) https://doi.org/10.1046/j.1469-7580.1998.19310105.x

[19] Shah, A., Goerlich, C.E., Pasrija, C., Hirsch, J., Fisher, S., Odonkor, P., Strauss, E., Ayares, D., Mohiuddin, M.M., Griffith, B.P.: Anatomical Differences Between Human and Pig Hearts and Their Relevance for Cardiac Xenotransplantation Surgical Technique. JACC Case Reports **4**(16), 1049–1052 (2022) https://doi.org/10.1016/j.jaccas.2022.06.011 . Accessed 2024-02-25

[20] Andel, C.J., Pistecky, P.V., Borst, C.: Mechanical properties of porcine and human arteries: implications for coronary anastomotic connectors. The Annals of Thoracic Surgery **76**(1), 58–646465 (2003) https://doi.org/10.1016/s0003-4975(03)00263-7

[21] Halaney, D.L., Sanyal, A., Nafissi, N.A., Escobedo, D., Goros, M., Michalek, J., Acevedo, P.J., Pérez, W., Patricia Escobar, G., Feldman, M.D., Han, H.-C.: The Effect of Trabeculae Carneae on Left Ventricular Diastolic Compliance: Improvement in Compliance With Trabecular Cutting. Journal of Biomechanical Engineering **139**(3), 0310121–0310128 (2017) https://doi.org/10.1115/1.4035585 . Accessed 2024-02-27

[22] Rich, N.L., Khan, Y.S.: Anatomy, Thorax, Heart Papillary Muscles. In: StatPearls. StatPearls Publishing, Treasure Island (FL) (2024). http://www.ncbi.nlm.nih.gov/books/NBK557802/ Accessed 2024-02-27

[23] Mao, S.S., Ahmadi, N., Shah, B., Beckmann, D., Chen, A., Ngo, L., Flores, F.R., Gao, Y.l., Budoff, M.J.: Normal Thoracic Aorta Diameter on Cardiac Computed Tomography in Healthy Asymptomatic Adult; Impact of Age and Gender. Academic radiology **15**(7), 827–834 (2008) https://doi.org/10.1016/j.acra.2008.02.001 . Accessed 2024-03-16

[24] Berger, T., Siepe, M., Simon, B., Beyersdorf, F., Chen, Z., Kondov, S., Schlett, C.L., Bamberg, F., Tarkhnishvili, A., Chikvatia, S., Czerny, M., Rylski, B., Kreibich, M.: Pulmonary artery diameter: means and normal limits—assessment by computed tomography angiography. Interactive CardioVascular and Thoracic Surgery **34**(4), 637–644 (2022) https://doi.org/10.1093/icvts/ivab308 . Accessed 2024-03-14

[25] Walpot, J., Juneau, D., Massalha, S., Dwivedi, G., Rybicki, F.J., Chow, B.J.W., Inácio, J.R.: Left Ventricular Mid-Diastolic Wall Thickness: Normal Values for Coronary CT Angiography. Radiology. Cardiothoracic Imaging **1**(5), 190034 (2019) https://doi.org/10.1148/ryct.2019190034

[26] Huang, S.Y., Lin, J.H., Lin, E.C., Yang, P.C., Tsou, H.L.: Effects of birth season, breed, sex, and sire family on cardiac morphology determined in pigs (Sus scrofa domestica) by use of echocardiography. Comparative Medicine **51**(6), 545–549 (2001)

[27] Prince, M.R., Novelline, R.A., Athanasoulis, C.A., Simon, M.: The diameter of the inferior vena cava and its implications for the use of vena caval filters. Radiology **149**(3), 687–689 (1983) https://doi.org/10.1148/radiology.149.3.6647844

[28] Schwein, A., Magnus, L., Markovits, J., Chinnadurai, P., Autry, K., Jenkins, L., Barnes, R., Vekilov, D.P., Shah, D., Chakfé, N., Bismuth, J.: Endovascular Porcine Model of Iliocaval Venous Thrombosis. European Journal of Vascular and Endovascular Surgery **63**(4), 623–630 (2022) https://doi.org/10.1016/j.ejvs.2021.12.022 . Accessed 2024-03-18