Abstract In this work, we propose a multigrid preconditioner for Jacobian-free Newton-Krylov (JFNK) methods. Our multigrid method does not require to store any representation of the Jacobian at any level of the multigrid hierarchy. As it is common in standard multigrid methods, the proposed method also relies on three building blocks: transfer operators, smoothers, and a coarse level solver. In addition to the restriction and prolongation operator, we also use a projection operator to transfer the current Newton iterate to a coarser level. The three-level Chebyshev semi-iterative method is employed as a smoother, as it has good smoothing properties and does not require the representation of the Jacobian matrix. We replace the direct solver on the coarsest-level with a matrix-free Krylov subspace method, thus giving rise to a truly Jacobian-free multigrid preconditioner. We will discuss all building blocks of our multigrid preconditioner in detail and demonstrate the robustness and the efficiency of the proposed method using several numerical examples.

1 Introduction

The numerical solution of partial differential equations (PDEs) is often carried out using discretization techniques, such as the finite element method (FEM), and typically requires the solution of a nonlinear system of equations. These nonlinear systems are often solved using some variant of the Newton method, which utilizes a sequence of iterates generated by solving a linear system of equations. However, it can be quite challenging to form these linear systems, as it might be computationally
expensive, or even impossible to assemble a Jacobian matrix. In addition, in some cases, storing a Jacobian might become prohibitive due to memory limitations.

The Jacobian-free Newton Krylov (JFNK) methods exploit the finite difference method to evaluate the action of a Jacobian on a vector, without requiring the knowledge of the analytical form of Jacobian and still retains local quadratic convergence of the Newton method. Even though JFNK methods are quite effective, the convergence properties of the Krylov subspace methods deteriorate with increasing problem size. Hence, it is desirable to reduce the overall computational cost by accelerating the convergence of the Krylov methods. To this end, many preconditioning strategies have been proposed in the literature, see e.g., [5]. Ideally, we would employ multigrid (MG) as a preconditioner since it is known to have optimal complexity, in particular for elliptic PDEs. Unfortunately, it is not straightforward to incorporate the MG method into the JFNK framework, as the standard implementations of the MG method rely on a matrix representation of the Jacobian.

In this work, we propose a matrix-free geometric multigrid preconditioner for the Krylov methods used within the JFNK framework. The proposed method exploits the finite difference technique to evaluate the action of Jacobian on a vector on all levels of multilevel hierarchy. Additionally, we employ polynomial smoothers which can be naturally extended to a matrix-free framework. Compared to other matrix-free MG preconditioners proposed in the literature, e.g., [1, 2, 6, 7], our method does not require the knowledge of the analytical form of Jacobian, and no additional modifications are required in the assembly routine to compute the action of a Jacobian on a vector.

2 Jacobian-free Newton-Krylov methods

The Newton method is the most frequently used iterative scheme for solving nonlinear problems. Newton method is designed to find a root \( x^* \in \mathbb{R}^n \) of some nonlinear function \( F(x^*) = 0 \), given as \( F: \mathbb{R}^n \rightarrow \mathbb{R}^n \). The iteration process has the following form:

\[
x^{(k+1)} = x^{(k)} + \alpha \delta x^{(k)}, \quad \text{for } k = 0, 1, 2, \ldots,
\]

where \( \alpha > 0 \) denotes a line-search parameter and \( \delta x^{(k)} \) denotes a Newton direction. The correction \( \delta x^{(k)} \) is obtained by solving the following linear system of equations:

\[
J(x^{(k)}) \delta x^{(k)} = -F(x^{(k)}),
\]

where \( J(x^{(k)}) = \nabla F(x^{(k)}) \). In the context of this work, we assume that the \( \nabla F \) is obtained as a gradient of some energy functional \( \Psi \), i.e., \( F(x^{(k)}) \equiv \nabla \Psi(x^{(k)}) \). In this way, the Jacobian \( J \) will be a symmetric matrix, which in turn allows us to use a multigrid preconditioner.

In the JFNK methods [5], the solution process is performed without explicit knowledge of the Jacobian \( J \). Instead, the application of a Jacobian to a vector is approximated using the finite difference scheme, given as

\[
J(x^{(k)})u \approx \frac{F(x^{(k)} + \epsilon u) - F(x^{(k)})}{\epsilon},
\]
where we choose $\epsilon = \frac{1}{n\|u\|_2} \sum_{i=1}^{n} \sqrt{\epsilon(1+|\lambda_i^{(k)}|)}$ and $\epsilon$ denotes the machine precision.

2.1 Matrix-free Multigrid Preconditioner

The multigrid method is one of the most efficient techniques for solving linear systems of equations stemming from the discretization of the PDEs. The method relies on a hierarchy of nested finite element spaces $\mathcal{V}_0 \subset \mathcal{V}_1 \subset \cdots \subset \mathcal{V}_L$. In case of geometric multigrid methods, the hierarchy of spaces $\{\mathcal{V}_\ell\}_{\ell=0}^L$ is constructed using a hierarchy of nested meshes $\{T_\ell\}_{\ell=0}^L$, which encapsulate the computational domain $\Omega$. Through the following, we use the subscript $\ell = 0, \ldots, L$ to denote a level, where $L$ denotes the finest level and 0 denotes the coarsest level. We denote the number of unknowns on a given level as $\{n_\ell\}_{\ell=0}^L$.

The multigrid method relies on three main ingredients. Firstly, a set of transfer operators is required to pass the information between the subsequent levels of the multilevel hierarchy. Secondly, suitable smoothers are needed to damp the high-frequency components of the error associated with a given level $\ell$. Finally, an appropriate coarse level solver is required to eliminate the low-frequency components of the error. As the JFNK methods are inherently matrix-free, these ingredients have to be adapted, such that they give rise to a matrix-free multigrid preconditioner.

Transfer Operators: In the standard multigrid method, the interpolation $I^\ell_{\ell-1} : \mathbb{R}^{n_{\ell-1}} \rightarrow \mathbb{R}^{n_\ell}$ and restriction $R^\ell_{\ell-1} : \mathbb{R}^{n_\ell} \rightarrow \mathbb{R}^{n_{\ell-1}}$ operators are employed to prolongate the correction to a finer level and restrict the residual to a coarser level, respectively. The presented multigrid method requires an evaluation of the action of a Jacobian on a vector on all levels of the multilevel hierarchy. Therefore, the current Newton iterate also has to be transferred to the coarser levels. To this aim, we employ a projection operator $P^\ell_{\ell-1} : \mathbb{R}^{n_\ell} \rightarrow \mathbb{R}^{n_{\ell-1}}$. In our numerical experiments, we use $R^\ell_{\ell-1} := (I^\ell_{\ell-1})^T$ and $P^\ell_{\ell-1} = 2^{-d}(I^\ell_{\ell-1})^T$, where $d$ denotes the spatial dimension in which the problem is defined.

Smoothers: We utilize the three-level Chebyshev semi-iterative method [2], as its implementation does not require explicit matrix representation. This method is convergent if all eigenvalues of the Jacobian lie within a bounded interval. Our aim here is to reduce only the high-frequency components of the error associated with a given level $\ell$. Therefore, we focus on the interval $[0.06\lambda_\ell, 1.2\lambda_\ell]$, where $\lambda_\ell$ is an estimated largest eigenvalue of the Jacobian on the level $\ell$. We estimate eigenvalue $\lambda_\ell$ at the beginning of each Newton iteration. More precisely, we employ the Power method, which we terminate within 30 iterations or when the difference between the subsequent estimates is lower than $10^{-2}$. As an initial guess for the Power method, a random vector is provided at the first Newton step. While for the subsequent Newton steps, we utilize the eigenvector associated with the largest eigenvalue, obtained during the previous eigenvalue estimation process, as an initial guess.
The coarse level solver: In the traditional multigrid method, a direct solver is used to eliminate the remaining low-frequency components of the error on the coarsest level. In the Jacobian-free framework, we replace the direct solver with a Krylov-subspace method, e.g., CG method. However, to obtain an accurate solution, a large number of iterations may require. To reduce the amount of work, we employ a preconditioner based on the limited memory BFGS (L-BFGS) quasi-Newton method [8]. The L-BFGS preconditioner is created during the very first call to the CG method by storing a few secant pairs. Following [8], we collect the secant pairs using the uniform sampling method, which allows us to capture the whole spectrum of the Jacobian.

By design, the CG method is suitable for solving the symmetric positive definite systems. When solving the non-convex problems, the arising linear systems might be indefinite, which can render the CG method ineffective. To ensure the usability of the CG method, we propose a few modifications. Firstly, we terminate the iteration process, as soon as the negative curvature is encountered [9]. At this point, we also compute the Rayleigh quotient, given as \( \lambda_c = \left( \begin{array} {c|c} p^T A p & p^T p \\ \hline p^T p & p \\ \end{array} \right) \), which gives an estimate of the eigenvalue encountered at the current iterate (that will be also negative). Secondly, we shift the whole spectrum of the Jacobian by adding a multiple of identity, given as \( A_s = A + (-\lambda_c) I \), where \( I \) denotes an identity matrix. The shifting strategy is applied recursively, until the modified \( A_s \) becomes positive definite. Please note, the application of the \( A_s \) to a vector can be trivially evaluated in the Jacobian-free framework.

The multigrid algorithm equipped with the shifting strategy is described in Algorithm 1.

**Algorithm 1: Jacobian-free Multigrid - \( V(v_1, v_2) \)-cycle**

1. Function: \( s_\ell \leftarrow \text{MG}(x_\ell^{(k)}, F(x_\ell^{(k)}), b_\ell, \ell) \)
2. \( s_\ell \leftarrow 0 \); \hfill \text{= Initialize correction}
3. if \( \ell \not= 0 \) then
4. \( s_\ell \leftarrow \text{Smoothing}(s_\ell, x_\ell^{(k)}, F(x_\ell^{(k)}), b_\ell, v_1) \); \hfill \text{= Pre-smoothing}
5. \( r_{\ell-1} \leftarrow R_{\ell-1}^{-1}(b_\ell - J(s_\ell)) \); \hfill \text{= Restrict the residual}
6. \( x_\ell^{(k)} \leftarrow p_{\ell-1}^{-1} r_{\ell-1} \); \hfill \text{= Restrict Newton iterate}
7. \( e_{\ell-1} \leftarrow \text{MG}(x_{\ell-1}^{(k)}, F(x_{\ell-1}^{(k)}), r_{\ell-1}, \ell - 1) \); \hfill \text{= Recursion}
8. \( s_\ell \leftarrow s_\ell + I_{\ell-1}^{-1} e_{\ell-1} \); \hfill \text{= Update the correction}
9. \( s_\ell \leftarrow \text{Smoothing}(s_\ell, x_\ell^{(k)}, F(x_\ell^{(k)}), b_\ell, v_2) \); \hfill \text{= Post-smoothing}
10. else
11. \( \lambda_{c_0} \leftarrow 0 \); \hfill \text{= Initialize shifting factor}
12. \( s_0, \lambda_c \leftarrow \text{CG}(s_0, x_0^{(k)}, F(x_0^{(k)}), r_0, \lambda_{c_0}, v_e) \); \hfill \text{= Coarse level solver}
13. while \( \lambda_c < 0 \) do
14. \[ \lambda_c \leftarrow \min(\lambda_c, \lambda_{c_0}) \]; \hfill \text{= Update shifting factor}
15. \( s_0, \lambda_c \leftarrow \text{CG}(s_0, x_0^{(k)}, F(x_0^{(k)}), r_0, \lambda_{c_0}, v_e) \); \hfill \text{= Shifted CG solver}
3 Numerical Experiments

In this section, we investigate the performance of the proposed MG preconditioner through three numerical examples: 

**Bratu:** Let us consider a domain \( \Omega := (0, 1)^2 \). The solution of Bratu problem is obtained by solving the following energy minimization problem:

\[
\min_{u \in H^1(\Omega)} \Psi_B(u) = \int_{\Omega} \left(\frac{1}{2} ||\nabla u||^2 - \lambda \exp(u)\right) dx,
\]

such that \( u = 0 \) on \( \Gamma \),

where we choose \( \lambda = 5 \) and \( \Gamma = \partial \Omega \) denotes the boundary. In our experiments, the mesh \( T_0 \) is triangular and consists of 25 elements in each direction.

**Minimal Surface:** We consider again a domain \( \Omega := (0, 1)^2 \). This experiment aims to find the minimal area of the surface by solving the following convex minimization problem:

\[
\min_{u \in H^1(\Omega)} \Psi_M(u) = \int_{\Omega} \sqrt{1 + ||\nabla u||^2} dx,
\]

such that \( u = 0 \) on \( \Gamma_{D_1} \),

\[
u = x(1-x) \quad \text{on} \quad \Gamma_{D_2},
\]

where, \( \Gamma_{D_1} = \{ [0, 1] \cup [1, y] \} \) and \( \Gamma_{D_2} = \{ (x, 0] \cup (x, 1] \} \). We consider mesh \( T_0 \) as in the previous example.

**Hyperelasticity:** At the end, we investigate a finite strain deformation of a beam, \( \Omega = (0, 10) \times (0, 1) \times (0, 1) \), with the rotational deformation applied on the boundaries \( \Gamma_{D_1} = \{ 0 \} \times [0, 1] \times [0, 1] \), and \( \Gamma_{D_2} = \{ 10 \} \times [0, 1] \times [0, 1] \). We consider Neo-Hookean material model, and seek for the displacement field \( u \) by solving the following non-convex minimization problem:

\[
\min_{u \in [H^1(\Omega)]^3} \Psi_N(u) = \int_{\Omega} \left( \frac{\mu}{2} (I_C - 3) - \mu \ln(J) + \frac{\lambda}{2} (\ln(J))^2 \right) dx,
\]

such that \( u = \vec{0} \) on \( \Gamma_{D_1} \),

\[
u = u_2 \quad \text{on} \quad \Gamma_{D_2},
\]

where \( u_2 = (0, 0.5(0.5 + (y - 0.5) \cos(\pi/6) - (z - 0.5) \sin(\pi/6) - y), 0.5(0.5 + (y - 0.5) \sin(\pi/6) + (z - 0.5) \cos(\pi/6) - z)) \). Here, \( J := \det(F) \) denotes the determinant of the deformation gradient \( F := I + u \). The first invariant of the right Cauchy-Green tensor is computed as \( I_C := \text{trace}(C) \), where \( C = F^T F \). For our experiment, Lamé parameters \( \mu = \frac{E}{2(1 + \nu)} \) and \( \lambda = \frac{\nu E}{(1 + \nu)(1 - 2\nu)} \) are obtained by setting value of Young’s modulus \( E = 10 \) and Poisson’s ratio \( \nu = 0.3 \). On the coarse level, the domain is discretized using hexahedral mesh, denoted as \( T_0 \), with 10 elements in \( x \)-directions and 1 element in \( y \) and \( z \) directions.
3.1 Convergence study

We solve the proposed numerical examples using the inexact JFNK (IN) method with a cubic backtracking line-search algorithm [3]. At each IN iteration, the search direction is required to satisfy \[ \| J(x^{(k)}) \delta x^{(k)} + F(x^{(k)}) \| \leq \eta^{(k)} \| F(x^{(k)}) \|, \]
where \( \eta^{(k)} = \min(0.5, \| F(x^{(k)}) \|) \). The algorithm terminates if \( \| F(x^{(k)}) \| < 10^{-6} \). The arising linear systems are solved using three different solution strategies: the CG method without any preconditioner (CG), the CG method with L-BFGS preconditioner (CG-QN), and the CG method with the multigrid preconditioner (CG-MG). The L-BFGS preconditioner is constructed during the first inexact Newton iteration by storing 20 secant pairs. The MG preconditioner has a form of a V-cycle and performs 5 pre-smoothing and 5 post-smoothing steps. On the coarse level, we use the CG-QN method with the spectral shift, which is activated only if the negative curvature is encountered. We employ shifting factor \( \gamma = 5 \), in Algorithm 1. The coarse level solver terminates if \( \| r_0 \| < 10^{-12} \), or if the maximum number of iterations, given by the number of unknowns, is reached.

The performance of all solution strategies is evaluated for increasing problem size on successively finer refinement levels. The refinement levels are denoted by \( L_0, L_1 \ldots, L_5 \), where \( L_0 \) denotes the coarse level, equipped with mesh \( T_0 \) and FE space \( V_0 \). The number of levels in the multilevel hierarchy is increased with the refinement level, e.g., MG employs 2 levels for the \( L_1 \) refinement level and 6 levels for the \( L_5 \) refinement level. We assess the performance of the methods by measuring the number of required gradient evaluations (GE). In multilevel settings, the number of effective gradient evaluations is computed as \( \text{GE} = \sum_{\ell=0}^{L} 2^{-d(L-\ell)} \text{GE}_\ell \), where \( \text{GE}_\ell \) denotes the number of gradient calls on a given level \( \ell \).

We note, the discretization of the minimization problem is performed using the finite element framework libMesh [4], while the presented solution strategies are implemented as a part of the open-source library UTOPIA [10].

**Influence of different preconditioners on the performance of the JFNK method:** Table 1 and 2 illustrate the performance of the IN method with different linear solvers. As we can see, for the smaller problems \( L_1, L_2 \), the IN method with the CG and the CG-QN outperforms the IN method with the CG-MG method. However, as the problem size increases, the IN method with CG-MG is significantly more efficient than with CG or CG-QN. For instance, for the Bratu example and \( L_5 \) refinement level, the CG-MG method outperforms the other methods by an order of magnitude.

The nonlinearity of the Bratu problem is not affected by the problem size and therefore the number of IN iterations remains constant for all refinement levels. We can also observe that the behavior of the CG-MG method is level independent. The number of required gradient evaluations is therefore bounded after few refinements, as the cost of the coarse level solver becomes negligible. The same behavior can not be observed for the minimal surface problem, as this problem is strongly nonlinear and the nonlinearity of the problem grows with increasing problem size. Due to this reason, the number of IN iterations and the total gradient evaluations also increases for the minimal surface problem. However, we note, that increase is more prevalent.
Table 1: The number of total gradient evaluations required in inexact JFNK method.

| Levels | Bratu | Minimal surface | Hyperelasticity |
|--------|-------|-----------------|-----------------|
|        | CG    | CG-MG           | CG              | CG-QN | CG-MG | CG    | CG-QN | CG-MG |
| L1     | 176   | 107             | 264             | 360   | 229   | 596   | 467   | 546   |
| L2     | 367   | 233             | 253             | 835   | 501   | 567   | 626   | 655   |
| L3     | 767   | 476             | 244             | 2009  | 1170  | 662   | 1349  | 1464  |
| L4     | 1582  | 1097            | 239             | 3544  | 2201  | 782   | 1971  | 1954  |
| L5     | 3377  | 2345            | 238             | 6154  | 4316  | 931   | –     | –     |

Table 2: The total number of inexact JFNK iterations (# IN), the total number of CG-MG iterations (# CG-MG), and the average number of gradient evaluations per total linear iteration (# AGE).

| Levels | Bratu                      | Minimal surface                  | Hyperelasticity                   |
|--------|----------------------------|----------------------------------|-----------------------------------|
|        | # IN | # CG-MG | # AGE | # IN | # CG-MG | # AGE | # IN | # CG-MG | # AGE |
| L1     | 3    | 7      | 39.32 | 6    | 13     | 45.85 | 9    | 28     | 34.66 |
| L2     | 3    | 9      | 28.25 | 7    | 18     | 31.51 | 5    | 15     | 25.12 |
| L3     | 3    | 9      | 27.10 | 8    | 25     | 26.50 | 5    | 20     | 20.95 |
| L4     | 3    | 9      | 26.61 | 9    | 32     | 24.45 | 5    | 39     | 18.76 |
| L5     | 3    | 9      | 26.55 | 9    | 41     | 22.79 | –    | –      | –     |

Table 3: The total number of inexact JFNK iterations (# IN), the total number of CG-MG iterations (# CG-MG), and the total number of gradient evaluations (# GE) with CG, CG-QN, and shifted CG-QN methods. The experiment was performed for the hyperelasticity example.

| Levels | CG                      | CG-QN                  | Shifted CG-QN |
|--------|-------------------------|------------------------|---------------|
|        | # IN | # CG-MG | # GE | # IN | # CG-MG | # GE | # IN | # CG-MG | # GE |
| L1     | 9    | 3010   | 51094 | 9    | 130    | 2057 | 9    | 28     | 868  |
| L2     | 5    | 16     | 44866 | 5    | 1017   | 14814 | 5    | 15     | 372  |
| L3     | 5    | 21     | 1265  | 5    | 26     | 512  | 5    | 20     | 426  |
| L4     | 6    | 39     | 733   | 6    | 39     | 733  | 5    | 39     | 733  |

For IN method equipped with the CG or the CG-QN methods than with the CG-MG method.

For the hyperelasticity example, the stored energy functional is non-convex hence the negative curvature is quite often encountered on the coarse level. We notice that with increasing problem size, the negative curvature is encountered fewer times. As a consequence, a huge amount of coarse level gradient evaluations is required to shift the spectrum of the Jacobian for smaller problems. Therefore, the average number of gradient evaluations per CG-MG decreases as the problem size increases, as we can observe in Table 2. Nevertheless, IN method equipped the CG-MG outperforms the CG and the CG-QN methods, see Table 1. Interestingly, the use of the L-BFGS preconditioner is less effective, as on the first IN iteration, the CG method terminates before the whole spectrum of the Jacobian can be captured.
Effect of the coarse level solver on the performance of the multigrid:

Due to the non-convexity of the stored energy function, for the hyperelasticity problem, it becomes essential to shift the spectrum of the Jacobian on the coarse level to retain the performance of the multigrid preconditioner. If only CG or CG-QN method is used, the total number of effective gradient evaluations blows up, as we can see in Table 3. This is due to the fact, that the coarse level solver (CG/CG-QN method) terminates as soon as the negative curvature is encountered. Therefore, the low-frequency components of the error are not eliminated and the multigrid preconditioner becomes unstable. In contrast, if we employ the shifting strategy, the multigrid preconditioner becomes stable and the total number of the gradient evaluations grows in proportion with the number of required linear iterations.

In conclusion, the performed experiments demonstrate that the proposed Jacobian-free multigrid is a robust and stable preconditioner when applied to problems of various types. Additionally, we observe level-independence behavior, if the nonlinearity or non-convexity of the problem is not influenced by the discretization parameter.

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