Received: 15 May 2024 | Revised: 10 September 2024 | Accepted: 11 September 2024

DOI: 10.1002/pamm.202400081

RESEARCH ARTICLE

Using surrogate models to accelerate load step methods for nonlinear finite element problems in hyperelasticity

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Abstract

Finite element methods for displacement problems in hyperelasticity lead to systems of nonlinear equations. These equations are usually solved with Newton's method or a related method. The convergence of Newton's method depends heavily on the proximity of the initial guess to the numerical solution. Load step methods overcome problems with divergence by applying the load in increments, leading to a sequence of sub-problems with initial guesses closer to the numerical solution of each sub-problem, supporting the convergence. The downside of this approach is the high computational effort needed to solve the load steps. Based on a benchmark problem in high-order FEM, we extend traditional load step methods to a new approach exploiting the hierarchical basis used for the spatial discretization of the problem and saving up to 50% of computation time (vs. benchmark).

1 | INTRODUCTION

We consider displacement problems with hyperelastic material models. For an open, connected subset $\Omega \subset \mathbb{R}^3$ the deformation

$$\varphi : \bar{\Omega} \to \mathbb{R}^3$$

under the action of surface (i.e., traction or pressure) and body (i.e., gravity) loads is to be found. In finite element (FE) methods, usually the displacement

$$\mathbf{u} : \bar{\Omega} \to \mathbb{R}^3, \quad \varphi = id + \mathbf{u}$$

is considered instead. Discretizing the problem with finite elements (FEs) leads to a system of nonlinear equations, which is usually solved with Newton's method. The convergence of Newton's method depends on the quality of the initial guess. For displacement problems, the natural choice for an initial guess is the initial configuration of the problem (no displacement). Depending on the magnitude of the load, this may lead to divergence of Newton's method. Typically, this problem is overcome by applying the load in increments, thus generating a sequence of displacement solutions leading to the final solution. This strategy is computationally expensive as it involves solving a sequence of non-linear problems.

Especially for problems with critical points (snap-back/snap-through), arc-length methods [1, 2] may be used. They are based on an unknown scaling of the load. The scaling factor is then added as a degree of freedom (DOF) and Newton's method is applied to the new problem. Another possibility to reduce the computational effort is to modify Newton's method. When used in the context of optimization, Newton's method is typically equipped with step size selection (also called line search) to accelerate the convergence. The behavior of step size selection algorithms for nonlinear equations depends on the properties of the Jacobian and despite their success in optimization problems, they are observed to be challenging to tune for nonlinear systems of equations [3, pp. 287–288]. Another possibility is to modify Newton's method such that the Newton step becomes less expensive. Variants of Newton's method that are suitable for root-finding problems are inexact Newton methods, where the linear system for the Newton step is not solved exactly, but only up to a tolerance for the residual norm, and Quasi-Newton methods like Broyden's method that are based on an approximation of the Jacobian. Recently, nonlinear preconditioning [4] has been proposed as a method that accounts for the different types of nonlinearity in a problem by splitting the DOFs into groups. For displacement problems discretized with FEs the split could be done with respect to locality or the polynomial degree of the FE basis functions on the reference element.

The traditional FE approach, called h-version, is to refine the mesh to make the diameter of the elements smaller. Usually, smaller elements increase the quality of the approximation. In recent years, the p-version of the FE method has gained interest as an alternative to this approach. In this method, the mesh is fixed and the ansatz space on the reference element is enriched with basis functions of higher polynomial degree. The p-version is robust to locking and mesh-distortion and empirically shows exponential rates of convergence [5, 6].

Expanding the FE space with polynomials of higher degree leads to a substantial increase in the number of DOFs, especially for 3D problems. Finding a numerical solution requires solving (linear or nonlinear) systems of equations and the total computation time often behaves like $\mathcal{O}(n^3)$, where n is the number of DOFs. Using load steps further increases the computational effort, as described above.

In this article, we present a method to use solutions for the displacement obtained on low-order models (models with low polynomial degree) as starting vectors for Newton's method on high-order models and therefore reducing the computational effort in load stepping methods for the p-version of the FEM. A similar approach is used in ref. [7] to accelerate the convergence in computing the active mechanical response of an artery wall. In Section 2, we introduce a model problem and how load steps are used to find the displacement. In Section 3, we describe the hierarchical structure of the discretization. Furthermore, we explain how we prolong solutions on low-order models (surrogate models) into higher-order models. We then show the results of our numerical tests using two discretizations of our model problem and finding that a combination of surrogate models and a relaxed tolerance on intermediate load steps reduces the computation time to about 50% (for a coarse mesh) or 60% (for a fine mesh).

2 | NEWTON'S METHOD FOR A BENCHMARK PROBLEM IN NONLINEAR FEM

Cook's membrane, the model problem we selected for our numerical tests, is a standard benchmark problem in computational mechanics. The geometry of the problem is described in Figure 1. For the right Cauchy-Green tensor $\mathbf{C}$ and the deformation gradient $\mathbf{F}$, we assume that the strain energy density is given by

$$\psi(I_{\mathbf{C}}, J) = \frac{\mu}{2}(I_{\mathbf{C}} - 3) + \frac{\lambda}{4}\left(J^2 - 1\right) - \left(\frac{\lambda}{2} + \mu\right)\log J \quad \text{with } I_{\mathbf{C}} = \operatorname{trace}(\mathbf{C}), J = \det(\mathbf{F})$$

and Lamé parameters $\lambda = 432.099$ MPa and $\mu = 185.185$ MPa as in ref. [8]. We discretize the linearization of the weak form in the reference configuration with hexahedral elements, see Figure 2a, leading to a set of equations

$$\mathbf{F}(\mathbf{u}) = \mathbf{0}$$

where $\mathbf{F} : \mathbb{R}^n \to \mathbb{R}^n$ and n is the number of DOF. By using the Neo-Hooke material model we assume a nonlinear stress-strain relationship, thus these equations are also nonlinear. We consider problems with

$$\mathbf{F}(\mathbf{u}) = \mathbf{E}_{ext} - \mathbf{E}_{int}(\mathbf{u}), \tag{1}$$

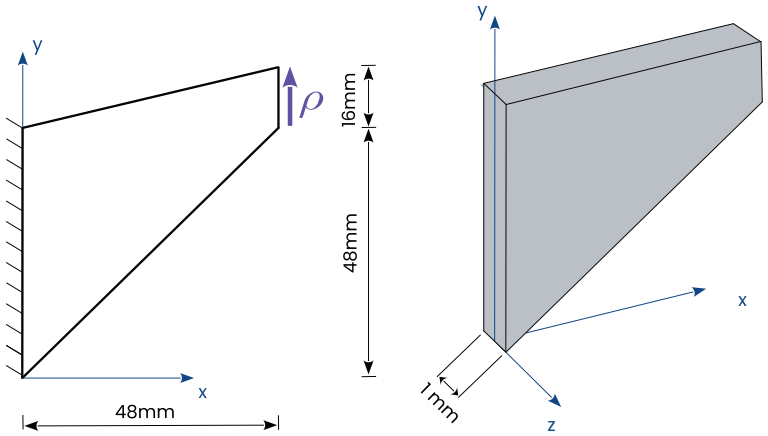
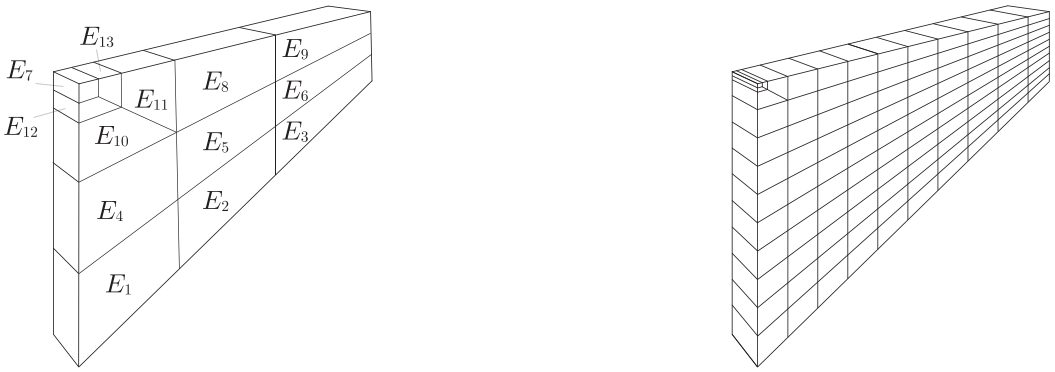


FIGURE 1 Geometry and boundary conditions for Cook's membrane. The elastic block is clamped to a wall on the left-hand side, we set a Dirichlet boundary condition here. On the right-hand side, a traction load is applied in y-direction and modeled with a Neumann boundary condition.



(A) **Mesh 1:** 13 finite elements, refinement towards the upper left corner. (B) **Mesh 2:** 104 finite elements.

FIGURE 2 FE discretization of Cook's membrane. FE, finite element.

where $\mathbf{E}_{ext} \in \mathbb{R}^n$ is the external load vector and $\mathbf{E}_{int}(\mathbf{u})$ is the internal load vector.

The Jacobian of $\mathbf{F}$ at $\mathbf{u}_k$ is denoted as $\mathbf{J}_\mathbf{F}(\mathbf{u}_k)$. For Newton's method, we set the starting vector $\mathbf{u}_0 = \mathbf{0}$ and iterate

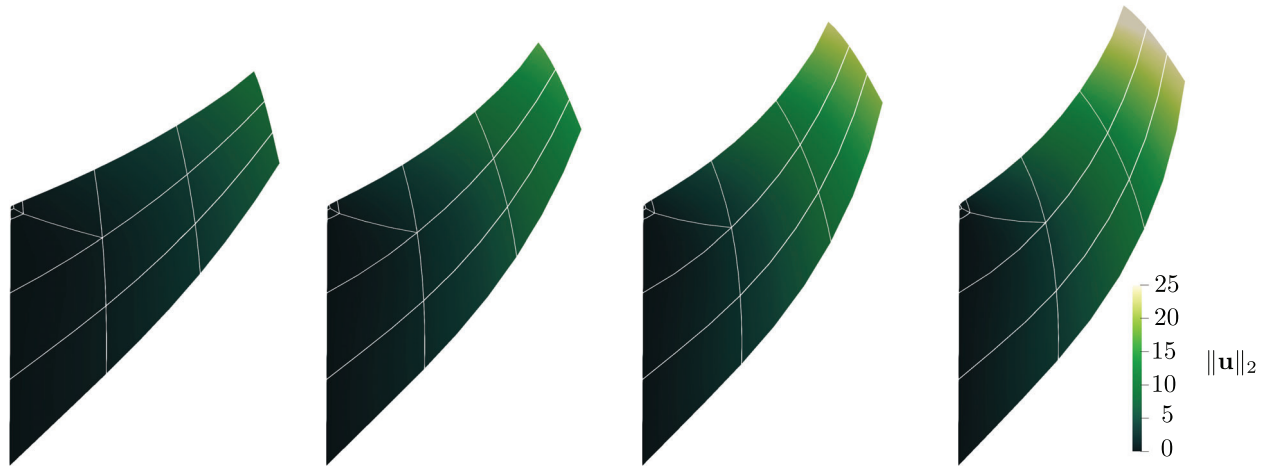
$$\mathbf{J}_\mathbf{F}(\mathbf{u}_k)\mathbf{p}_k = -\mathbf{F}(\mathbf{u}_k), \tag{2}$$

$$\mathbf{u}_{k+1} = \mathbf{u}_k + \mathbf{p}_k, \tag{3}$$

until $k = k_{max}$ or $R(\mathbf{u}_k) := \frac{\|\mathbf{F}(\mathbf{u}_k)\|_2}{\|\mathbf{E}_{ext}\|_2} < tol_{Newton}$. If the iteration is terminated by the second condition, we say that Newton's method has converged and call the final iterate $\mathbf{u}_{ns}$ the (numerical) solution.

The convergence of Newton's method depends heavily on the initial guess and in particular its distance to the solution. Newton's method is known to converge locally quadratic. The higher the applied load ρ, the larger is the displacement generally (since our benchmark problem does not show snap-back or snap-through behavior). For a large displacement, the initial guess $\mathbf{u}_0 = \mathbf{0}$, corresponding to no displacement, is a poor guess and typically leads to divergence of Newton's method.

Typically, in the case of divergence of Newton's method, the load is instead applied in increments, known as load-stepping or force loading, and the (numerical) solution of the previous load step is used as the initial guess for the next load step, see Figure 3. Let $\ell \in \mathbb{N}$ be the number of load steps. The load vector $\mathbf{E}_{ext}$ depends linearly on the magnitude of



(A) Load step 1 (12.5 MPa applied) (B) Load step 2 (25 MPa applied) (C) Load step 3 (37.5 MPa applied) (D) Load step 4 (50 MPa applied)

FIGURE 3 Displacement of Cook's Membrane, computed in $\ell = 4$ load steps. In load step 4, the full load ρ is applied.

the shear load ρ. In case of load increments of same size, the ℓ sub-problems therefore are

$$\mathbf{F}_i(\mathbf{u}) = \frac{i}{\ell}\mathbf{E}_{ext} - \mathbf{E}_{int}(\mathbf{u}), \quad 1 \leq i \leq \ell.$$

The termination condition for Newton's method, see Equation (2), on the subproblems is modified to

$$R_i(\mathbf{u}) := \frac{\|\mathbf{F}_i(\mathbf{u})\|_2}{\frac{i}{\ell}\|\mathbf{E}_{ext}\|_2}.$$

In case of convergence of Newton's method on the first sub-problem $\mathbf{F}_1(\mathbf{u}) = \mathbf{0}$, the numerical solution is set as a starting vector for Newton's method on $\mathbf{F}_2$ and so on. In case of convergence of Newton's method on all of the subproblems, we can summarize this approach as

$${}_{i+1/\ell}\mathbf{u}_0 = {}_{i/\ell}\mathbf{u}_{ns},$$

where the left subscript indicates the current load step (i or $i+1$) and the total number of load steps ℓ.

The classical load-stepping method is intuitive since deformations do not happen "at once" but the position of a particle in time is continuous. From a numerical point of view, the new starting vectors are closer to the solution and therefore facilitate the convergence of Newton's method. However, the computational effort is high, especially in cases where the load increments that lead to convergence need to be small.

3 | SURROGATE MODEL APPROACH

In the following, we present a method to generate starting vectors on the same mesh, but on low-order ansatz spaces. We then increase the polynomial degree while we increase the load. Our goal is to lower the computational effort for the traditional load step approach.

Consider first a numerical solution $\mathbf{u}_{ns}$ for Newton's method, see Equation (2). The vector $\mathbf{u}_{ns}$ defines a FE model for the displacement field of our benchmark problem. Let the index set of the vector be denoted with

$$[n] := \{i \in \mathbb{N}, i \leq n\}.$$

The components I_x, I_y, I_z of the vector are associated with the x, y or z-direction:

$$I_x \cup I_y \cup I_z = [n], I_x \cap I_y = I_x \cap I_z = I_y \cap I_z = \emptyset.$$

The (approximate) displacement $u(x,y,z) = \big(u_x(x,y,z), u_y(x,y,z), u_z(x,y,z)\big)$ of a point $(x,y,z) \in \mathbb{R}^3$ is

$$u_x(x,y,z) = \sum_{i \in I_x} u^{(i)} N_i(x,y,z) \text{ in direction of } x,$$

$$u_y(x,y,z) = \sum_{i \in I_y} u^{(i)} N_i(x,y,z) \text{ in direction of } y \text{ and}$$

$$u_z(x,y,z) = \sum_{i \in I_z} u^{(i)} N_i(x,y,z) \text{ in direction of } z,$$

where the functions

$$N_i : \mathbb{R}^3 \to \mathbb{R}, \quad i \in [n]$$

are the ansatz functions of the FE space. They are compositions of a mapping from a (hexahedral) domain element to the reference element Ω_{st} and a basis function defined on Ω_{st}. The quality of the approximation depends, from an analytical point of view, only on the choice of mapping and shape functions (if we keep the mesh fixed). Our approach is based on using high-order shape functions. In the following, we describe the prolongation of low-order solutions into FE spaces of higher dimension.

Let the set of all basis functions in direction of x, y and z be given by

$$\mathcal{N}_x = \{N_i \mid i \in I_x\}, \quad \mathcal{N}_y = \{N_i \mid i \in I_y\}, \quad \mathcal{N}_z = \{N_i \mid i \in I_z\}, \text{ resp.}$$

We now introduce an additional superscript for the highest polynomial degree p that is used in the ansatz space and denote the sets of basis functions of polynomial degree up to p by

$${}^p\mathcal{N}_x, {}^p\mathcal{N}_y \text{ and } {}^p\mathcal{N}_z.$$

The basis functions of the FE are denoted as

$${}^pN_i(x,y,z).$$

The nonlinear problem $\mathbf{F}$ and its number of DOFs n, see Equation (1), depend on the basis $({}^p\mathcal{N}_x, {}^p\mathcal{N}_y, {}^p\mathcal{N}_z)$. This is expressed by adding a superscript p to the problem so that we now write our nonlinear problem for a FE discretization with polynomial degree p as:

$${}^p\mathbf{F} : \mathbb{R}^{n_p} \to \mathbb{R}^{n_p},$$

$${}^p\mathbf{F}({}^p\mathbf{u}) = \mathbf{0}$$

with $n_p \in \mathbb{N}$, ${}^p\mathbf{u} \in \mathbb{R}^{n_p}$.

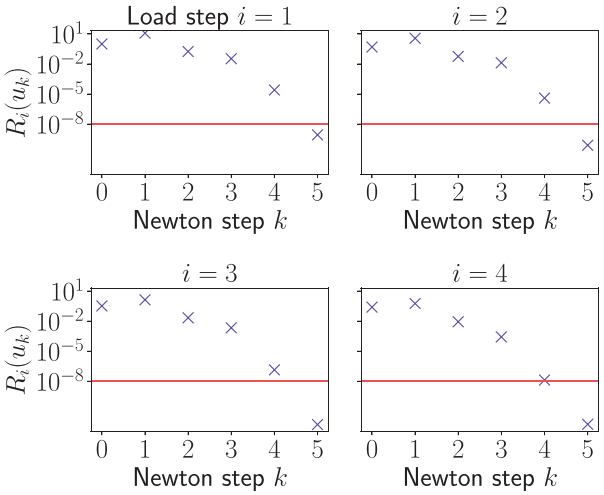
Definition 3.1 (Hierarchical basis). A sequence of bases $({}^p\mathcal{N}_x, {}^p\mathcal{N}_y, {}^p\mathcal{N}_z)$ is called *hierarchical* if

$${}^p\mathcal{N}_x \subset {}^{p+1}\mathcal{N}_x, \quad {}^p\mathcal{N}_y \subset {}^{p+1}\mathcal{N}_y \quad \text{and} \quad {}^p\mathcal{N}_z \subset {}^{p+1}\mathcal{N}_z$$

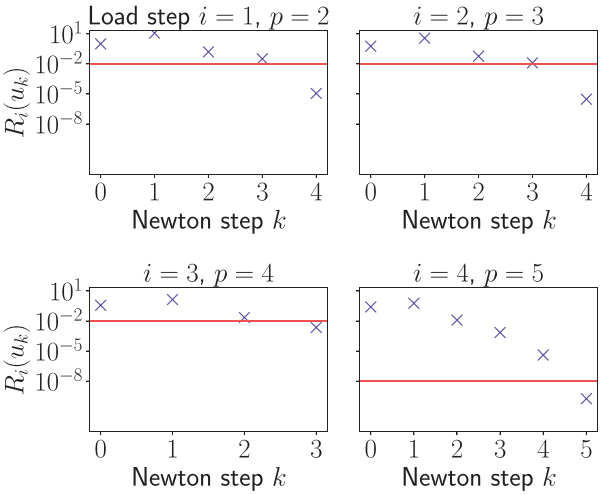
for all $p \in \mathbb{N}$.

Let $({}^1\mathcal{N}_x, {}^1\mathcal{N}_y, {}^1\mathcal{N}_z), ({}^2\mathcal{N}_x, {}^2\mathcal{N}_y, {}^2\mathcal{N}_z), \ldots$ be a sequence of hierarchical bases for an FE problem. Injection of a coefficient vector with respect to $({}^p\mathcal{N}_x, {}^p\mathcal{N}_y, {}^p\mathcal{N}_z)$ into a coefficient vector with respect to $({}^{p+1}\mathcal{N}_x, {}^{p+1}\mathcal{N}_y, {}^{p+1}\mathcal{N}_z)$ is defined as

$${}_{p+1}P_p : \mathbb{R}^{n_p} \to \mathbb{R}^{n_{p+1}}$$



(A) Benchmark: Traditional load step method with $tol_{Newton} = 10^{-8}$.



(B) Surrogate model method. In intermediate load steps, the Newton tolerance is relaxed to 10^{-2}.

FIGURE 4 Convergence of Newton's method for Cook's membrane discretized with 13 finite elements.

$$ {}^{p+1}P_p({}^{p}\mathbf{u})^{(i)} := \begin{cases} {}^{p}\mathbf{u}^{(j)} & \text{if } {}^{p+1}N_i = {}^{p}N_j, \\ 0 & \text{else.} \end{cases} $$

Injection of a coefficient vector with respect to $({}^{p}\mathcal{N}_x, {}^{p}\mathcal{N}_y, {}^{p}\mathcal{N}_z)$ into a coefficient vector with respect to $({}^{q}\mathcal{N}_x, {}^{q}\mathcal{N}_y, {}^{q}\mathcal{N}_z)$ for $q > p$ is then given by

$$ {}_{q}P_p = {}_{q}P_{q-1} \circ {}_{q-1}P_{q-2} \circ \dots \circ {}_{p+1}P_p. $$

We now show how we use injection on our model problem. We consider four load steps and start with an FE model of polynomial degree 2. The first starting vector is

$$ {}^{p=2}_{1/4}\mathbf{u}_0 = \mathbf{0}, $$

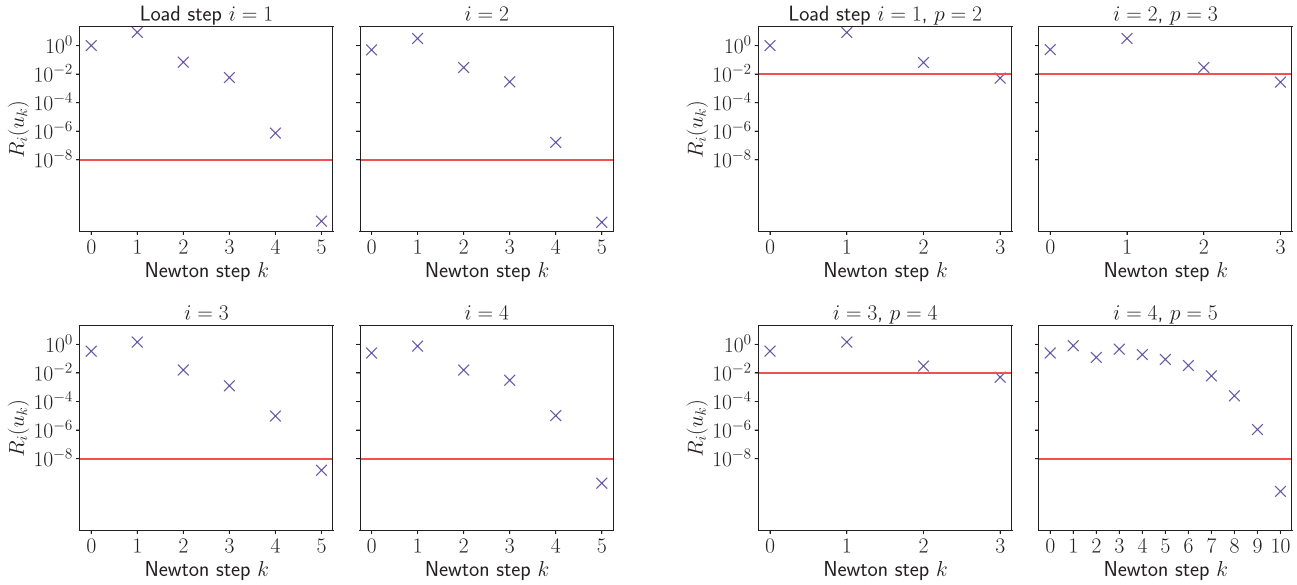
where again the left subscript is added to indicate the current load step (1) and the total number of load steps (4). We apply Newton's method and in case of convergence, we inject the (numerical) solution of the first load step into a model with polynomial degree 3:

$$ {}^{p=3}_{2/4}\mathbf{u}_0 = {}_{3}P_2\left({}^{p=2}_{1/4}\mathbf{u}_{ns}\right). $$

We apply Newton's method and continue like this until we arrive at the final load step and the final polynomial degree (here $p = 5$).

4 | NUMERICAL RESULTS

We compare displacement simulations of Cook's membrane. The applied shear load is $\rho = 50$ MPa for the geometry with 13 elements in Figure 2A and $\rho = 30$ MPa for the refined geometry with 104 elements. The applied loads were chosen such that the benchmark method converges in four load steps for both meshes. For the ansatz functions on the reference element, the trunk space and hierarchical shape functions as defined in ref. [5] are used with a polynomial degree of 5 in the last load step. Both problems cannot be solved using a single load step and therefore require intermediate load steps. The convergence of the traditional load step method can be seen in Figures 4A and 5A. On an Intel Xeon processor



(A) Benchmark: Traditional load step method.

(B) Surrogate model method with relaxed tolerance as described in Figure 4b.

FIGURE 5 Convergence of Newton's method for Cook's membrane discretized with 104 finite elements.

TABLE 1 Degrees of freedom for the two discretizations of Cook's membrane.

Polynomial degree	2	3	4	5
DOF (13 elements)	402	672	1122	1752
DOF (104 elements)	2523	4284	7359	11 748

Abbreviation: DOF, degree of freedom.

TABLE 2 Iterations and relative computation time of load step methods for Cook's membrane (discretization with 13 elements) with different combinations of surrogate model and relaxed tolerance on intermediate load steps.

	Benchmark	Relaxed tolerance			Surr. model	Surr. model + Relaxed tol.		
Intermediate Load step tolerance	10^{-8}	10^{-3}	10^{-2}	10^{-1}	10^{-8}	10^{-3}	10^{-2}	10^{-1}
Final Load step tolerance	10^{-8}	10^{-8}	10^{-8}	10^{-8}	10^{-8}	10^{-8}	10^{-8}	10^{-8}
Total iterations Intermediate load steps	15	12	11	7	15	12	11	7
Iterations Final load step	5	5	5	5	5	5	5	5
Computation time (compared to benchmark)	100%	86.65%	82.7%	66.13%	52.08%	47.58%	45.66%	39.71%

Note: Starting vectors are generated using injection of low-order solutions as described in Section 3.

(E5-2665), it requires a computation time of about 180 s for 13 elements (see Table 2, benchmark column) and 1674 s for 104 elements. The linear systems are solved using the Pardiso solver (Intel Math Kernel Library Version 2022.0.2 for Linux). In Figure 4B, the proposed method using a surrogate model on the first few load steps, as described in Section 3, is shown for the discretization with 13 elements. The first load steps are carried out on low-order FE models and the numerical solutions are injected into a starting vector for the next load step, resulting in convergence of Newton's method on the original problem with the full load (load step 4) and converging in 45.66% of computation time compared to the reference benchmark method. The computational savings are due to two factors: The intermediate load steps are solved with a relaxed tolerance ($tol_{Newton} = 10^{-2}$) and are of smaller size. While in the benchmark problem, four nonlinear problems with 1752 DOFs each are solved, for the surrogate model method, the number of DOFs is substantially lower on intermediate load steps (see also Table 1). Only the nonlinear problem in the last load step is of full size and solved to the strict tolerance 10^{-8}. In Table 2, we compare computation times and number of iterations for different choices of the relaxed tolerance. We see that the number of intermediate iterations increases with a stricter tolerance (10^{-3} and 10^{-8}).

TABLE 3 Iterations and relative computation time of load step methods for Cook's membrane (discretization with 104 elements).

	Benchmark	Relaxed tolerance			Surr. model	Surr. model + Relaxed tol		
Intermediate Load step tolerance	10^{-8}	10^{-3}	10^{-2}	10^{-1}	10^{-8}	10^{-3}	10^{-2}	10^{-1}
Final Load step tolerance	10^{-8}	10^{-8}	10^{-8}	10^{-8}	10^{-8}	10^{-8}	10^{-8}	10^{-8}
Total iterations Intermediate load steps	15	12	9	6		12	9	6
Iterations Final load step	5	5	5	6	Div.	14	10	13
Computation time (compared to benchmark)	100%	86.5%	75.33%	67.12%		83.03%	62.93%	71.39%

The total computation time is less than 55% of benchmark computation time for all considered surrogate model methods on this mesh.

Both factors (surrogate models and relaxed tolerance) have also been tested individually. The surrogate model solved to strict tolerance (see Table 2) leads to a computation time of 52.08% and the relaxed tolerance approach without surrogate models leads to computation times from 66% to 87%, see Table 2. We see that a combination of both strategies yields the best results.

The convergence of the traditional load step method and the surrogate model method with relaxed tolerance on a finer mesh with 104 elements can be seen in Figure 5. We observe that 10 Newton steps are needed for convergence on the last load step in comparison to 5 Newton steps for the traditional load step approach. In Table 3, the computation times for all considered variants for the nonlinear solver are shown. We see that relaxing the tolerance decreases the computation time down to 67%–87% and increases the number of Newton iterations on the last load step only in one case (6 vs. 5). The surrogate model increases the number of Newton iterations in all cases (10−14 vs. 5) and surprisingly even leads to divergence when used without relaxing the tolerance. Here, the numerical solution from the previous load step computed with a strict tolerance, seems to result in a poor starting vector for the last load step. This could be due to locking effects on the low-order models, that is, unphysically small deformations that occur in conforming low-order FEs, or the load step size. In all cases where convergence on the last load step is achieved, we see a decrease in computation time.

5 | CONCLUSION AND OUTLOOK

We used the load step method to find the displacement on two discretizations (coarse and fine mesh) of Cook's membrane. If load steps are used to generate good starting vectors for the final load step, it was found in all considered cases that it is not necessary to solve the intermediate load steps with strict tolerance. In order to save computation time in intermediate load steps, we proposed to use a low-order model and increase the polynomial degree as we increase the load. In all convergent cases, the computation time was decreased compared to the benchmark. However, on the fine mesh, the number of Newton iterations was significantly increased. While the starting vector for the final load step is cheap to generate for low-order models, it remains to be investigated how the choice of polynomial degree and load steps affect the convergence of Newton's method. Future work should also explore the use of different Newton tolerances depending on the load step. Also, different geometries and material models should be considered.

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How to cite this article: Fesefeldt, L., Le Borne, S., Düster, A., & Radtke, L. (2024). Using surrogate models to accelerate load step methods for nonlinear finite element problems in hyperelasticity. *Proceedings in Applied Mathematics and Mechanics*, *24*, e202400081. https://doi.org/10.1002/pamm.202400081