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Numerical minimization of energy functionals in continuum mechanics using hp-FEM in MATLAB

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1. Introduction

Energy functionals appearing in various types of problems in science and engineering can be efficiently minimized using the finite element method (FEM). In [3], we introduced several vectorization techniques for an efficient evaluation of the discrete energy gradient and, additionally, applied these techniques for the minimization of hyperelasticity in 2D and 3D using P1 finite elements (piece-wise linear nodal elements defined on triangles/tetrahedra). Recently, our approach has been successfully applied to 2D/3D problems in solid mechanics, namely the resolution of elastoplastic deformations of layered structures or superelastic and pseudoplastic deformations of shape-memory alloys [2].

The hp-FEM is an advanced numerical method based on FEM dating back to the pioneering works of I. Babuška, B. A. Szabó and co-workers in 1980s. It provides increased flexibility and convergence properties compared to the ”conventional” FEM. In particular, hp-FEM on quadrilaterals (in 2D) and hexahedra (in 3D) are usually preferred in structural computations.

This contribution presents and extends results published in [1], where the energy evaluation techniques of [3] are combined with the implementation of rectangular hp-FEM [4] using some techniques, mainly for the construction of hierarchical shape basis functions, taken from [5]. The actual minimization of energies was performed using the trust-region (TR) method available in the MATLAB Optimization Toolbox which was found to be very efficient in the comparison performed in [3]. It requires the gradient of a discrete energy functional and also allows to specify a sparsity pattern of the corresponding Hessian matrix which is directly given by a finite element discretization. The gradient can be evaluated explicitly or numerically using the central difference scheme. A particular hyperelasticity problem was chosen to demonstrate the capabilities of our implementation.

2. Hyperelasticity

Boundary value problems in (non-linear) elastostatics provide examples of vector problem which can be directly dealt with our approach, see [3]. Given a (hyper)elastic body spanning the domain $\Omega \in \mathbb{R}^d$ and subjected to volumetric force, $\mathbf{f}(\mathbf{x})$, the corresponding deformation, $\mathbf{y}(\mathbf{x})$, can be obtained by minimization of the following energy functional:

$$J(\mathbf{y}(\mathbf{x})) = \int_\Omega W\big(\mathbf{F}(\mathbf{y}(\mathbf{x}))\big)\,\mathrm{d}\mathbf{x} - \int_\Omega \mathbf{f}(\mathbf{x}) \cdot \mathbf{y}(\mathbf{x})\,\mathrm{d}\mathbf{x}\,, \tag{1}$$

where $\mathbf{F}(\mathbf{y}(\mathbf{x})) = \nabla \mathbf{y}(\mathbf{x})$ denotes deformation gradient and

$$W(\mathbf{F}) = C_1\big(I_1(\mathbf{F}) - \dim - 2\log(\det \mathbf{F})\big) + D_1(\det \mathbf{F} - 1)^2 \tag{2}$$

is so-called compressible Neo-Hookean energy density with C_1, D_1 being material constants and $I_1(\mathbf{F}) = \|\mathbf{F}\|^2$ denotes the squared Frobenius norm.

We consider a double-beam model given by the following parameters: a 2D hyperelastic domain given by a rectangle $[0, 1] \times [0, 0.25]$ is subjected to a constant volumetric vector force $\mathbf{f} = (0, -2 \cdot 10^7)$ acting in a top-to-bottom direction; zero Dirichlet boundary conditions are applied on the left and right edges. We assume the Young modulus $E = 10^8$ and the Poisson ratio $\nu = 0.3$. Arbitrary, although mutually consistent physical units are considered. For illustration, Fig. 1 shows examples of the corresponding deformed mesh together with the underlying Neo-Hookean density distribution. Fig. 2 depicts a comparison of P1 elements and hp-FEM for the polynomial degrees $p = 1, 2, 3, 4$ (denoted by Q1, Q2, Q3, Q4, respectively) used in our computation. Since we do not know the exact energy value, we use J_{ref} as the smallest of all achieved energy values $J(u)$ obtained in our computation decreased by 10^2. Q2 and Q4 elements are superior to P1, Q1 and Q3 in accuracy with respect to the number of dofs. However, Q2 elements are only slightly better with respect to the evaluation times, while Q4 elements turned out to be the least efficient.

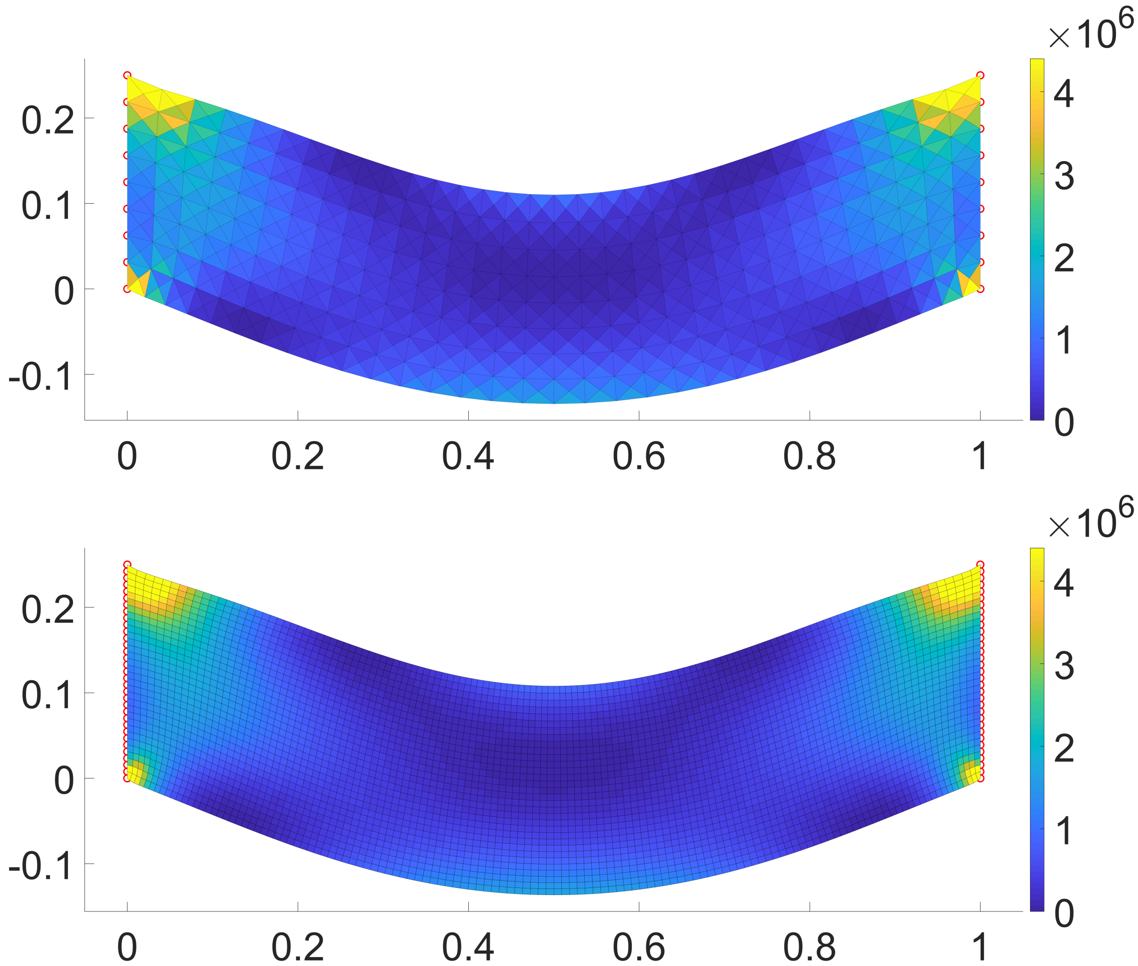

Fig. 1. Deformation and the corresponding Neo-Hookean density distributions for the 2D hyperelastic problem. The top figure corresponds to P1 elements and a computational mesh with 1 024 triangles. The bottom figure corresponds to Q3 elements and a computational mesh with 4 096 rectangles

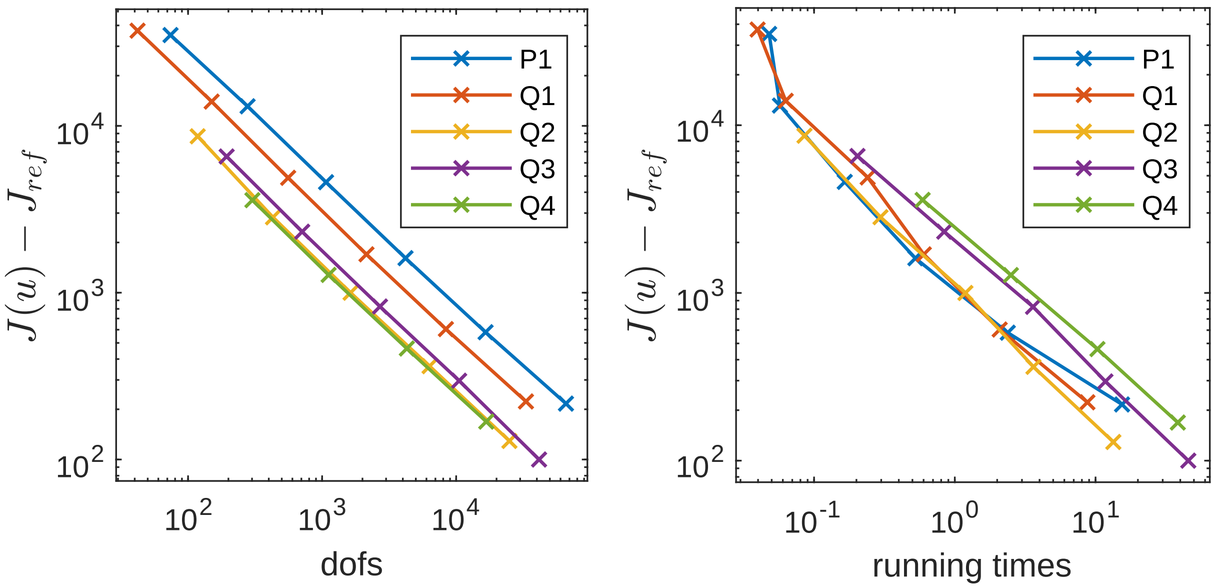

Fig. 2. Performance of hyperelasticity: comparison of elements

3. Conclusions and outlook

The hp-FEM for 2D rectangular elements was successfully incorporated into our vectorized MATLAB code and its improved convergence performance was demonstrated on the particular hyperelasticity problem.

This work contributes to our long-term effort in developing a vectorized finite element-based solvers for energy minimization problems. Since many such problems emerge in science and engineering, the code is designed in a modular way so that various modifications (e.g., in functional types or boundary conditions) can be easily adopted. Our future research directions include implementing the hp-FEM in 3D or tuning the applied minimization algorithms.

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References

[1] Frost, M., Moskovka, A., Valdman, J., Minimization of energy functionals via FEM: Implementation of hp-FEM, LSSC 2023, Lecture Notes in Computer Science, doi: 10.48550/arXiv.2309.13028. (accepted paper)

[2] Frost, M., Valdman, J., Vectorized MATLAB implementation of the incremental minimization principle for rate-independent dissipative solids using FEM: A constitutive model of shape memory alloys, Mathematics 10 (2022) No. 4412.

[3] Moskovka, A., Valdman, J., Fast MATLAB evaluation of nonlinear energies using FEM in 2D and 3D: Nodal elements, Applied Mathematics and Computation 424 (2022) No. 127048.

[4] Moskovka, A., Valdman, J., MATLAB implementation of hp finite elements on rectangles using hierarchical basis functions, PPAM 2022, Lecture Notes in Computer Science (LNCS) 13827 (2023) 287-299.

[5] Szabó, B., Babuška, I., Introduction to finite element analysis, John Wiley & Sons, 2011.