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Reliable Simulation Techniques  
in Solid Mechanics.



## **SPP-1748 Benchmark Collection**

### **Cook's membrane: Hyperelasticity and finite elastoplasticity**

J. Schröder, A. Düster, A. Schwarz, W. Garhuom, S. Hubrich, M. Igelbücher, N. Viebahn

### **Incompressible block under constant partial load**

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### **Analysis of a thin plate**

H. R. Bayat, S. Wulffinghoff, S. Reese

# A selection of benchmark problems in solid mechanics and applied mathematics: Part I

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## Abstract

In this contribution we provide benchmark problems in the field of computational solid mechanics. In detail, we want to address classical fields as incompressibility, thin structures and plasticity at finite deformations. The explicit setups of the benchmarks are described and the numerical schemes are introduced. For the computations the various participating groups use different (mixed) Galerkin finite element formulations and we provide some of the applied material laws in code form online. This paper is the first part of benchmarks, which were developed within the Priority Programme of the German Research Foundation 'SPP 1748 Reliable Simulation Techniques in Solid Mechanics - Development of Non-Standard Discretisation Methods, Mechanical and Mathematical Analysis'.

**Keywords:** numerical benchmark problems, finite element method, hyperelasticity, incompressibility, finite strain plasticity, shell structures

## 1 Introduction

Solving partial differential equations on complex geometries is perhaps one of the most important scientific achievement of the last decades. Analytical or manufactured solutions of such differential equations, e.g. from engineering or economics, is in most cases not available. Therefore, computer-aided numerical algorithms play an important role. At this point we mention that the rapid development of the available computing power contributes significantly to the success of these numerical methods. An end to this progress is currently not conceivable and becomes even more important due to the capabilities to address challenging multiphysics applications. Popular numerical methods are, for example, mesh-free methods, the finite volume method, finite differences, isogeometric analysis and - with possibly the greatest impact - the finite element method. In this field, the German Priority Program 1748 (DFG SPP 1748) *Reliable Simulation Techniques in Solid Mechanics. Development of Non-standard Discretization Methods, Mechanical and Mathematical Analysis* is located. The main goal of this priority program was the development of modern non-conventional discretization methods based e.g. on mixed finite elements or discontinuous Galerkin formulations, including mathematical analysis for geometrically as well as physically non-linear problems in the areas of incompressibility, anisotropies and discontinuities to name a few. Typical problems especially in the field of geometric and material nonlinearities are for instance insufficient stress approximations due to unsuitable approximation spaces as well as weak convergence behavior due to stiffening effects or mesh distortions. Similar problems arise in crack or contact problems, where the local determination of discontinuities as well as their development play an important role in many fields of application.

This paper presents the first of two parts of benchmark collections which were compiled within the SPP 1748. In the first two benchmarks we show results on hyperelastic and elasto-plastic problems at finite strains. Different (mixed) finite element technologies and p-FEM are used to obtain convergent results for certain displacement and stress values for Cook's membrane and an incompressible block problem. In the third benchmark problem - a thin as well as a thick plate - the convergence behavior was investigated. For this purpose, both shell and continuum finite element technologies are used.

## 2 Cook's membrane: Hyperelasticity and finite elastoplasticity

In the first part of this benchmark, the Cook's membrane is investigated by applying a hyperelastic material model (Section 2.3) while in the second part a finite  $J_2$  elastoplastic material model is used (Section 2.4). To this end, different element formulations are investigated by showing displacement and stress convergence studies. Furthermore, the locking effect due to the incompressibility constraint is examined.

### 2.1 Geometry and boundary conditions

Cook's membrane, a tapered cantilever see Cook [1974], combines bending and shearing. The left-hand side of the domain is clamped and a constant shear load in vertical direction is applied on the right-hand side. The thickness of the Cook's membrane is chosen to be 1 mm. The geometry and boundary conditions are illustrated in Figure 2.1.

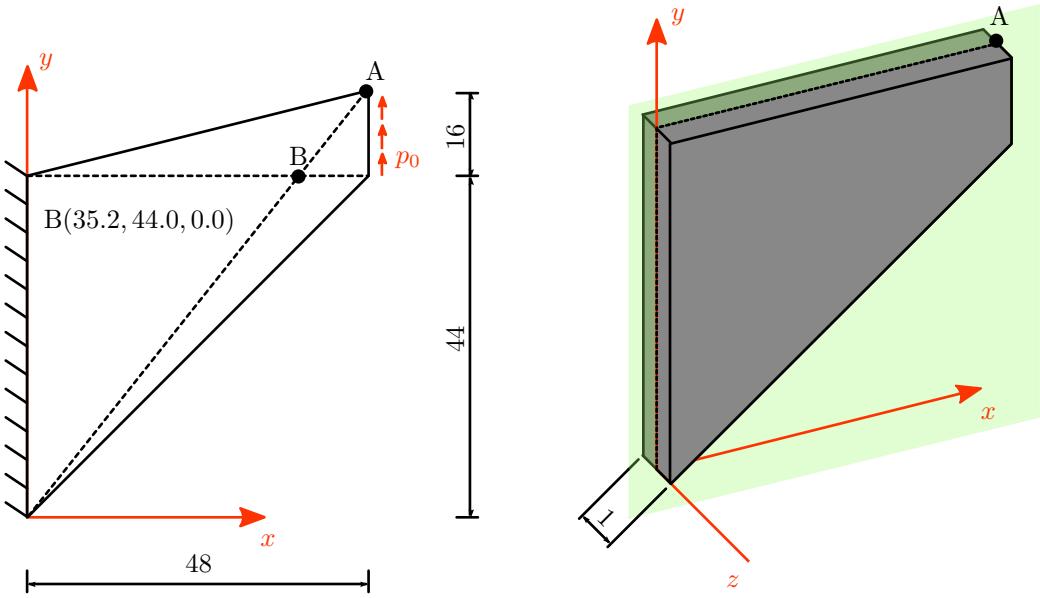


Figure 2.1: Cook's membrane (all dimensions in mm)

## 2.2 Element formulations

Five different element formulations are used in this study. Two formulations are based on triangular (2D) or tetrahedral (3D) shaped elements. The first one applies a pure displacement based formulation with quadratic shape functions (in the following denoted as  $T_2$ ) and the second one is a mixed formulation with an additional constant field for the pressure and volume dilatation (denoted with  $T_2P_0$ ), see e.g. Boffi et al. [2013]. The third and fourth formulation are based on hexahedral shaped elements with a first order polynomial interpolation of the displacements (represented by  $H_1$ ) and a mixed formulation with a piecewise constant pressure field (denoted with  $H_1P_0$ ), see e.g. Boffi et al. [2013]. Furthermore, the three-dimensional problem is discretized also with hexahedral elements, which are used within a  $p$ -extension ( $p$ -FEM) based on the trunk space utilizing hierachic shape functions, see Szabó and Babuška [1991] and Düster et al. [2017].

## 2.3 Cook's membrane for hyperelasticity

**2.3.1 Hyperelastic material model** In the following we use two polyconvex strain-energy functions. The first function reads

$$\psi_1 = \frac{\mu}{2}(I_C - 3) + \frac{\lambda}{4}(J^2 - 1) - \left(\frac{\lambda}{2} + \mu\right)\ln J, \quad (2.1)$$

where  $\lambda$  and  $\mu$  constitute the Lamé parameters,  $J = \det \mathbf{F}$  the determinant of the deformation gradient  $\mathbf{F}$  and  $I_C = \text{tr } \mathbf{C}$  the first principal invariant of the right Cauchy-Green tensor  $\mathbf{C} = \mathbf{F}^T \mathbf{F}$ , see e.g. Ciarlet [1988]. The 2nd Piola Kirchhoff stress tensor  $\mathbf{S} = 2\partial_{\mathbf{C}}\psi$  can be computed from the strain-energy function  $\psi_1$  as follows

$$\mathbf{S} = \frac{\lambda}{2}(J^2 - 1)\mathbf{C}^{-1} + \mu(\mathbf{1} - \mathbf{C}^{-1}), \quad (2.2)$$

here  $\mathbf{1}$  denotes the second-order identity tensor. The material parameters  $(\lambda, \mu)$  as well as the load  $p_0$  are given in Table 2.1.

Parameter	$\lambda$	$\mu$	$p_0$
MPa	432.099	185.185	20

Table 2.1: Material parameters and applied load for  $\psi_1$ 

The second strain-energy function under consideration is based on a split into an isochoric  $U(J)$  and unimodular  $W(I_{\tilde{C}}, II_{\tilde{C}})$  part

$$\psi_2 = U(J) + W(I_{\tilde{C}}, II_{\tilde{C}}), \quad (2.3)$$

see Hartmann and Neff [2003] and Netz et al. [2013]. The principal invariants of the unimodular right Cauchy-Green tensor

$$\tilde{\mathbf{C}} = (\det \mathbf{C})^{-1/3} \mathbf{C} \quad (2.4)$$

are given with

$$I_{\tilde{C}} = \text{tr } \tilde{\mathbf{C}} \quad \text{and} \quad II_{\tilde{C}} = \text{tr}(\text{Cof } \tilde{\mathbf{C}}). \quad (2.5)$$

Following Hartmann and Neff [2003] we choose the isochoric and unimodular parts of the strain energy as

$$U(J) = \frac{\kappa}{50} (J^5 + J^{-5} - 2) \quad (2.6)$$

and

$$W(I_{\tilde{C}}, II_{\tilde{C}}) = \alpha(I_{\tilde{C}}^3 - 27) + c_{10}(I_{\tilde{C}} - 3) + c_{01}(II_{\tilde{C}}^{3/2} - 3\sqrt{3}). \quad (2.7)$$

The 2nd Piola Kirchhoff stress tensor for  $\psi_2$  can be computed as follows

$$\mathbf{S} = JU'(J)\mathbf{C}^{-1} + 2J^{-2/3} \left( (W_{,1} + W_{,2}I_{\tilde{C}})\mathbf{I} - W_{,2}\tilde{\mathbf{C}} - \frac{1}{3}(W_{,1}I_{\tilde{C}} + 2W_{,2}II_{\tilde{C}})\tilde{\mathbf{C}}^{-1} \right) \quad (2.8)$$

with

$$W_{,1} = \partial W / \partial I_{\tilde{C}} = 3 \alpha I_{\tilde{C}}^2 \quad \text{and} \quad W_{,2} = \partial W / \partial II_{\tilde{C}} = c_{01} (3/2) II_{\tilde{C}}^{(1/2)}. \quad (2.9)$$

The material parameters used for the second strain-energy function ( $\alpha, c_{10}, c_{01}, \kappa$ ) as well as the load  $p_0$  are given in Table 2.2.

Parameter	$\alpha$	$c_{10}$	$c_{01}$	$\kappa$	$p_0$
MPa	$3.67 \cdot 10^{-3}$	0.1788	0.1958	1000	0.25

Table 2.2: Material parameters and applied load for  $\psi_2$ 

Furthermore, a Fortran77 code for the computation of the 2nd Piola Kirchhoff stress tensor and the material tangent  $\mathbf{C} = 2\partial_{\mathbf{C}}\mathbf{S}$  will be provided online under (DOI XXX) with the subroutines:

```
SUBROUTINE mate1(v,F,\[Lambda],\[Mu],S,Cmat)
SUBROUTINE mate2(v,F,\[Kappa],\[Alpha],c10,c01,S,Cmat)
```

Here, the input parameters are the deformation gradient ( $\mathbf{F}$  as  $3 \times 3$  field) as well as the material parameters. The output parameters are the 2nd Piola Kirchhoff stress tensor ( $\mathbf{S}$  as  $3 \times 3$  field) and the material tangent ( $\mathbf{Cmat}$  as  $3 \times 3 \times 3 \times 3$  field). For further details on the material model and the solution of hyperelastic problems, the reader is referred to Hartmann and Neff [2003], Düster et al. [2003] and Wriggers [2008].

**2.3.2 Analysis for the 2D plane strain case** In the following the convergence of the spatial discretization in terms of the vertical tip displacement  $u_y$  of the upper right node (point A, see Figure 2.1) is compared. The meshes are uniformly refined by increasing the number of elements per edge. An exemplary mesh with triangular elements is depicted in Figure 2.2a. Furthermore, for  $\psi_1$  a mesh consisting of 13 hexahedral elements with two refinements towards the singularity is used and for  $\psi_2$  a mesh with 15 hexahedral elements with three refinements, as depicted in Figure 2.2b and 2.2c, respectively. The discretization is based on the trunk space utilizing 3D hierachic shape functions. The plane strain conditions are enforced by suppressing the displacements in  $z$ -direction at the front ( $z=0.5\text{mm}$ ) and reverse side ( $z=-0.5\text{mm}$ ) of the hexahedral meshes. In the following, we will consider both strain-energy functions  $\psi_1$  and  $\psi_2$ . An uniform and isotropic increase of the polynomial degree  $p = 1, 2, 3, \dots$  of the shape functions yields the results depicted in Figures 2.3a and 2.3b, which are plotted together with the displacements computed with the formulations  $T_2$  and  $T_2P_0$  for triangular elements. Furthermore, the results of the vertical displacement of point A are given in Tables 2.3 and 2.4.

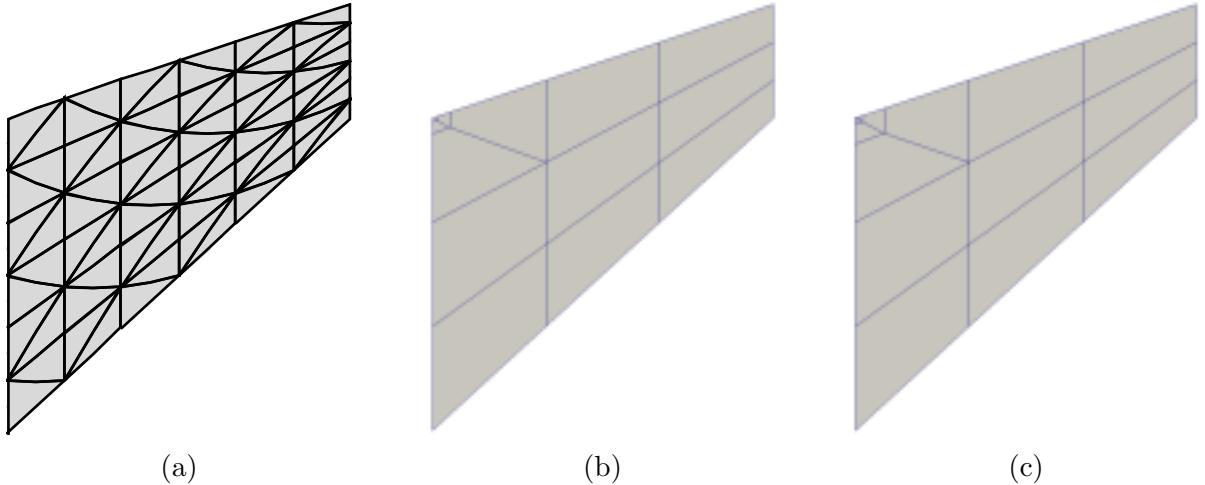


Figure 2.2: Spatial discretization: (a) triangular mesh  $T_2$  and  $T_2P_0$  with 169 nodes (b) hexahedral mesh consisting of 13 elements with two refinements towards the singularity (c) hexahedral mesh consisting of 15 elements with three refinements towards the singularity

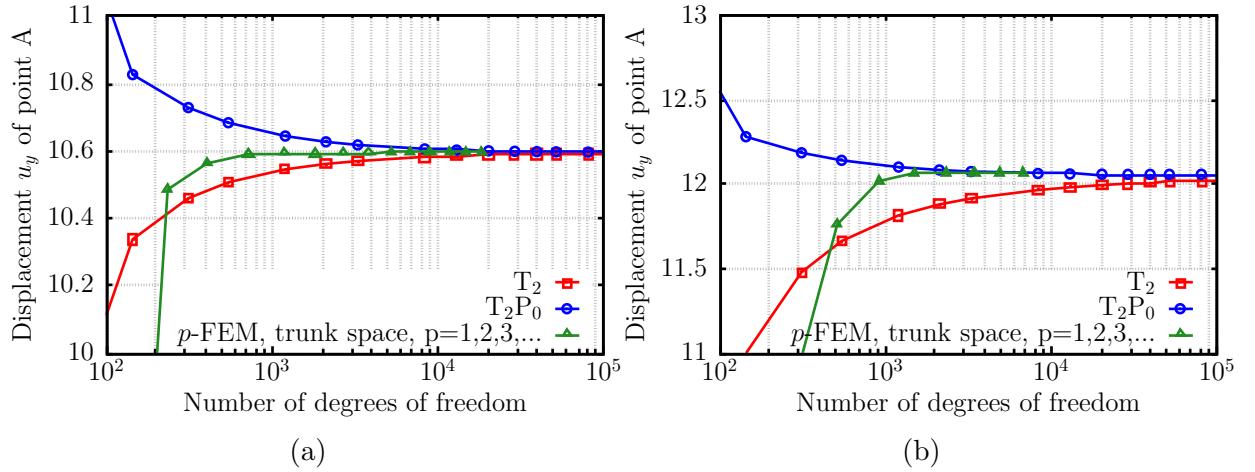


Figure 2.3: Cook's membrane: (a) Convergence of displacement  $u_y$  at point A for  $\psi_1$  (b) Convergence of displacement  $u_y$  at point A for  $\psi_2$

DOFs	$p$ -FEM	DOFs	$T_2$	$T_2P_0$
64	7.891541025	40	9.806907690	11.33745362
234	10.48552788	144	10.33773586	10.82618213
404	10.56281735	312	10.45943835	10.72849326
718	10.59074586	544	10.50672306	10.68358929
1176	10.59357161	1200	10.54536129	10.64401742
1817	10.59279059	3280	10.56978840	10.61771743
2680	10.59340608	8320	10.58101595	10.60584469
3804	10.59418029	12960	10.58432907	10.60250393
5228	10.59459431	20200	10.58680812	10.60010611
6797	10.59483724	39480	10.58943610	10.59772491
8892	10.59500708	51520	10.59020842	10.59707501
11690	10.59512663	80400	10.59124759	10.59625734
14704	10.59521520	115680	10.59191221	10.59578301
18213	10.59528994			

Table 2.3: Convergence of the displacement component  $u_y$  of point A for  $\psi_1$  – for the  $p$ -FEM the hexahedral mesh with 13 elements was used with  $p = 1, \dots, 14$

DOFs	$p$ -FEM	DOFs	$T_2$	$T_2P_0$
80	4.612355002	40	9.014811424	12.92227556
296	10.92119119	144	10.99908813	12.28386453
512	11.76326359	312	11.47965327	12.18887324
914	12.02094058	544	11.66479626	12.14388054
1502	12.06638464	1200	11.81742103	12.10409815
2327	12.07011195	3280	11.91767938	12.07732488
3440	12.06983163	8320	11.96768623	12.06585178
4892	12.07060838	12960	11.98386546	12.06309408
6734	12.07068959	20200	11.99686238	12.06151976
		39480	12.01212534	12.06077186
		51520	12.01710034	12.06087947
		80400	12.02438600	12.06144138
		115680	12.02957600	12.06218674

Table 2.4: Convergence of the displacement component  $u_y$  of point A for  $\psi_2$  – for the  $p$ -FEM the hexahedral mesh with 15 elements was used with  $p = 1, \dots, 9$

Figure 2.4 shows the contour plot of the  $\sigma_{xx}$  stresses for the strain-energy function  $\psi_1$ . Here, the results of the  $T_2$  and the  $T_2P_0$  element are depicted in Figure 2.4a and 2.4b, respectively. Figure 2.4c shows the contour plot of the  $\sigma_{xx}$  stresses for the  $p$ -FEM analysis using 13 hexahedral elements and the order of the Ansatz  $p = 11$ . In Figure 2.5 the stress distribution for the strain-energy function  $\psi_2$  is depicted. It shows the  $\sigma_{xx}$  stresses for the  $T_2$  and the  $T_2P_0$  element in Figure 2.5a and 2.5b, respectively. To this end, the stress values are linearly extrapolated from the integration points to the nodal points. Stress oscillations can be recognized in the case of the displacement based element. The  $\sigma_{xx}$  stress distribution of the  $p$ -FEM solution is plotted in Figure 2.5c. Here, a mesh with 1026 hexahedral elements is used and  $p = 9$  to achieve a smooth solution of the stress distribution.

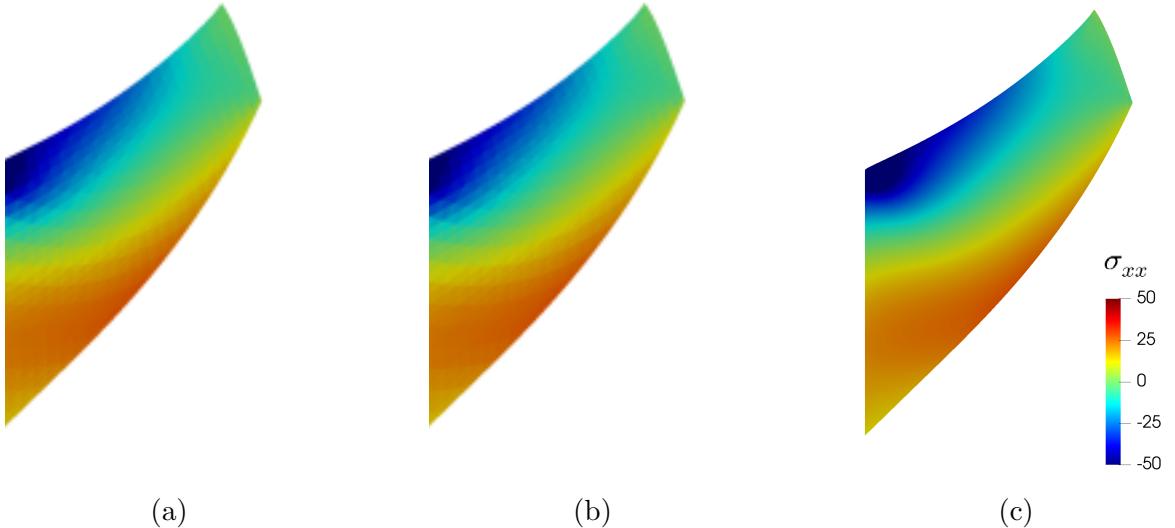


Figure 2.4: Contour plot of the  $\sigma_{xx}$  stresses for  $\psi_1$ : (a)  $T_2$  and (b)  $T_2P_0$  with 4704 DOFs (c)  $p$ -FEM solution with 104 hexahedral elements and  $p = 5$

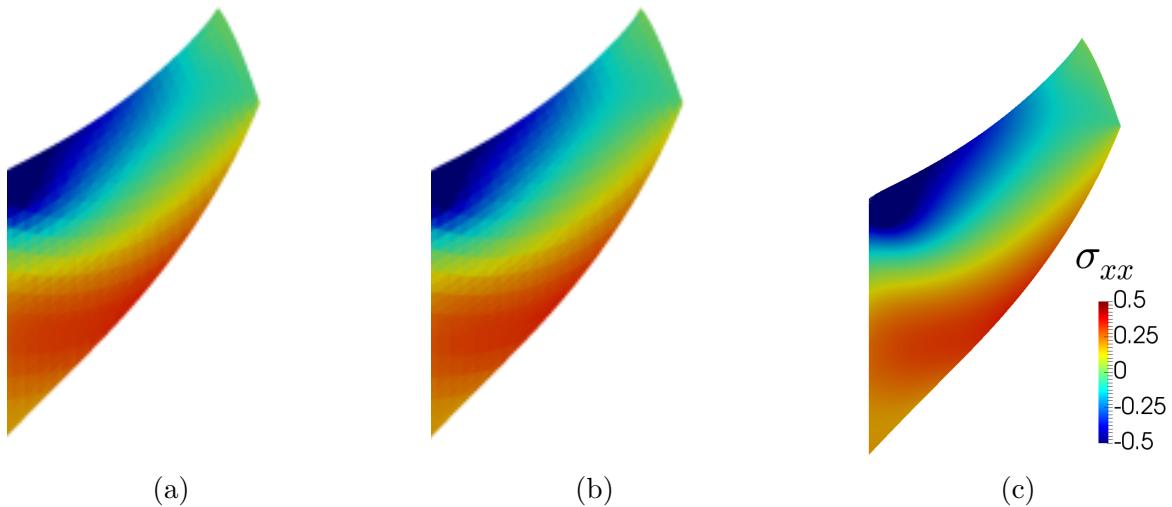


Figure 2.5: Contour plot of the  $\sigma_{xx}$  stresses for  $\psi_2$ : (a)  $T_2$  and (b)  $T_2P_0$  with 4704 DOFs  
(c)  $p$ -FEM solution with 1026 hexahedral elements and  $p = 9$

**2.3.3 Analysis for the 3D case** For the three-dimensional problem we choose the same constitutive model, geometry and boundary conditions analogous to the 2D setting. However, instead of plane strain conditions we consider stress-free out-of-plane surfaces, i.e. the front and reverse side of Cook’s membrane are not constrained. Again, an uniform and isotropic  $p$ -refinement is performed utilizing the hexahedral mesh with 13 elements for  $\psi_1$  and the hexahedral mesh with 15 elements for  $\psi_2$  as depicted in Figure 2.2b and 2.2c, respectively. The symmetry in  $z$ -direction is exploited by choosing one element layer of thickness 0.5 mm. In Figures 2.6a and 2.6b the convergence of the displacement component  $u_y$  at point A is depicted together with the results obtained with the  $T_2$  and  $T_2P_0$  formulations for tetrahedral elements applying also a mesh layer thickness of 0.5 mm. The corresponding numbers are also depicted in Tables 2.5 and 2.6.

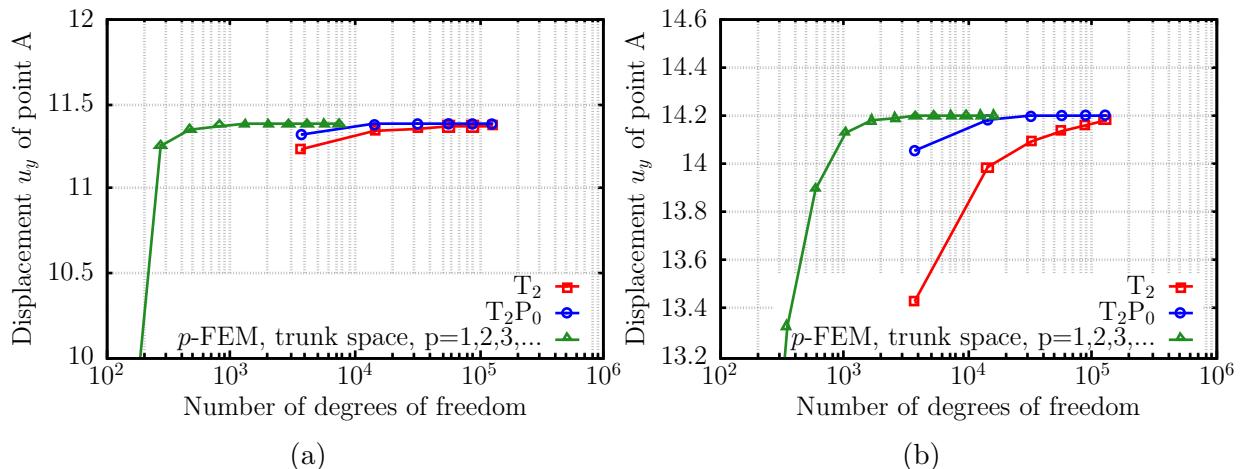


Figure 2.6: Cook's membrane: (a) Convergence of displacement  $u_y$  at point A for  $\psi_1$  (b) Convergence of displacement  $u_y$  at point A for  $\psi_2$

DOFs	$p$ -FEM	DOFs	$T_2$	$T_2P_0$
80	8.434841171	3696	11.23495734	11.32089255
273	11.25351064	14304	11.34322180	11.37919731
466	11.35019765	31824	11.36205916	11.38423863
811	11.37604404	56256	11.36902825	11.38463195
1308	11.37813487	87600	11.37244952	11.38429459
1996	11.37823068	125856	11.37441412	11.38385850
2914	11.37933932			
4101	11.38030765			
5596	11.38083980			
7438	11.38113537			

Table 2.5: Convergence of the displacement component  $u_y$  at point A for  $\psi_1$  – for the  $p$ -FEM the hexahedral mesh with 13 elements was used with  $p = 1, \dots, 10$

DOFs	$p$ -FEM	DOFs	$T_2$	$T_2P_0$
100	5.714955523	3696	13.43185080	14.05810063
345	13.32938972	14304	13.98978503	14.18590622
590	13.89773326	31824	14.09575681	14.20058990
1031	14.13196099	56256	14.13898227	14.20412407
1668	14.18459516	87600	14.16307381	14.20517718
2552	14.19396764	125856	14.18356606	14.20539492
3734	14.19852431			
5265	14.20118387			
7196	14.20253217			
9578	14.20330321			
12462	14.20377868			
15899	14.20409718			

Table 2.6: Convergence of the displacement component  $u_y$  at point A for  $\psi_2$  – for the  $p$ -FEM the hexahedral mesh with 15 elements was used with  $p = 1, \dots, 12$

**Influence of incompressibility:** In this section, we investigate the influence of the incompressibility level on the convergence of the different discretizations. To this end, we keep the same material parameters and load as before and only change the Lamé's parameter  $\lambda$  for the first free energy function  $\psi_1$  and the bulk modulus  $\kappa$  for the second free energy function  $\psi_2$ . The values of Poisson's ratio are approximated considering the corresponding relations for homogeneous isotropic linear materials, see Table 2.7 and 2.8. Consequently, Poisson's ratio for  $\psi_1$  is computed as

$$\nu = \frac{\lambda}{2(\lambda + \mu)} \quad (2.10)$$

and for  $\psi_2$  as

$$\nu = \frac{3\kappa - 2G}{6\kappa + 2G}, \quad (2.11)$$

whereas according to Hartmann and Neff [2003] the shear modulus is defined as

$$G = 54\alpha + 2c_{10} + 3\sqrt{3}c_{01}. \quad (2.12)$$

$\lambda$ in MPa	432.099	750	9260	92600	926000
$\nu$	0.35000	0.40099	0.49020	0.49900	0.49990

Table 2.7: Lamé's parameter  $\lambda$  and Poisson's ratio  $\nu$  for  $\psi_1$ 

$\kappa$ in MPa	4	8	80	800	8000
$\nu$	0.32614	0.40772	0.49023	0.49902	0.4999

Table 2.8: Bulk modulus  $\kappa$  and Poisson's ratio  $\nu$  for  $\psi_2$ 

In order to investigate the influence of the increasing incompressibility level, we study the convergence of the tip displacements. The reference solutions of the tip displacement  $u_y$  at point A are computed by the  $p$ -FEM discretization using 13 elements for  $\psi_1$  and 15 elements for  $\psi_2$ . The corresponding values are given in Table 2.9 and 2.10. Figure 2.7 depicts the convergence of the normalized displacement  $u_y/u_{y,\text{ref}}$  for both strain-energy functions  $\psi_1$  and  $\psi_2$  computed with the different finite element formulations.

$\lambda$ in MPa	432.099	750	9260	92600	926000
$u_{y,\text{ref}}$ in mm	11.38113537	11.15639736	10.78267246	10.74641606	10.74061099

Table 2.9: Reference tip displacement considering strain energy  $\psi_1$ 

$\kappa$ in MPa	4	8	80	800	8000
$u_{y,\text{ref}}$ in mm	15.10420474	14.67075231	14.24783555	14.20432703	14.20075829

Table 2.10: Reference tip displacement considering strain energy  $\psi_2$ 

## 2.4 Cook's membrane for elastoplasticity

In this section we use the same setup as depicted in Figure 2.1. Furthermore, we consider only the 3D case.

**2.4.1 Finite  $J_2$  elastoplastic material model** First, a short summary of the governing equations for the underlying material model will be given which is based on the  $J_2$  flow theory of elastoplasticity for finite strain including a nonlinear isotropic hardening. For a detailed overview about the theory the interested reader is referred to Simo [1988; 1992; 1998] and Simo and Miehe [1992].

For the material model the deformation gradient  $\mathbf{F}$  is decomposed into an elastic  $\mathbf{F}_e$  and a plastic  $\mathbf{F}_p$  part by applying a multiplicative split

$$\mathbf{F} = \mathbf{F}_e \mathbf{F}_p. \quad (2.13)$$

Assuming  $J_2$  von Mises plasticity the plastic deformation only depends on the deviatoric part of the stress tensor. Based on the multiplicative split in Eq. (2.13) the elastic deformation gradient reads  $\mathbf{F}_e = \mathbf{F} \mathbf{F}_p^{-1}$ , thus, the elastic right Cauchy-Green tensor  $\mathbf{C}_e$  can be formulated as

$$\mathbf{C}_e = \mathbf{F}_p^{-T} \mathbf{C} \mathbf{F}_p^{-1}, \quad (2.14)$$

and the elastic left Cauchy-Green tensor  $\mathbf{b}_e$  as

$$\mathbf{b}_e = \mathbf{F} \mathbf{C}_p^{-1} \mathbf{F}^T, \quad (2.15)$$

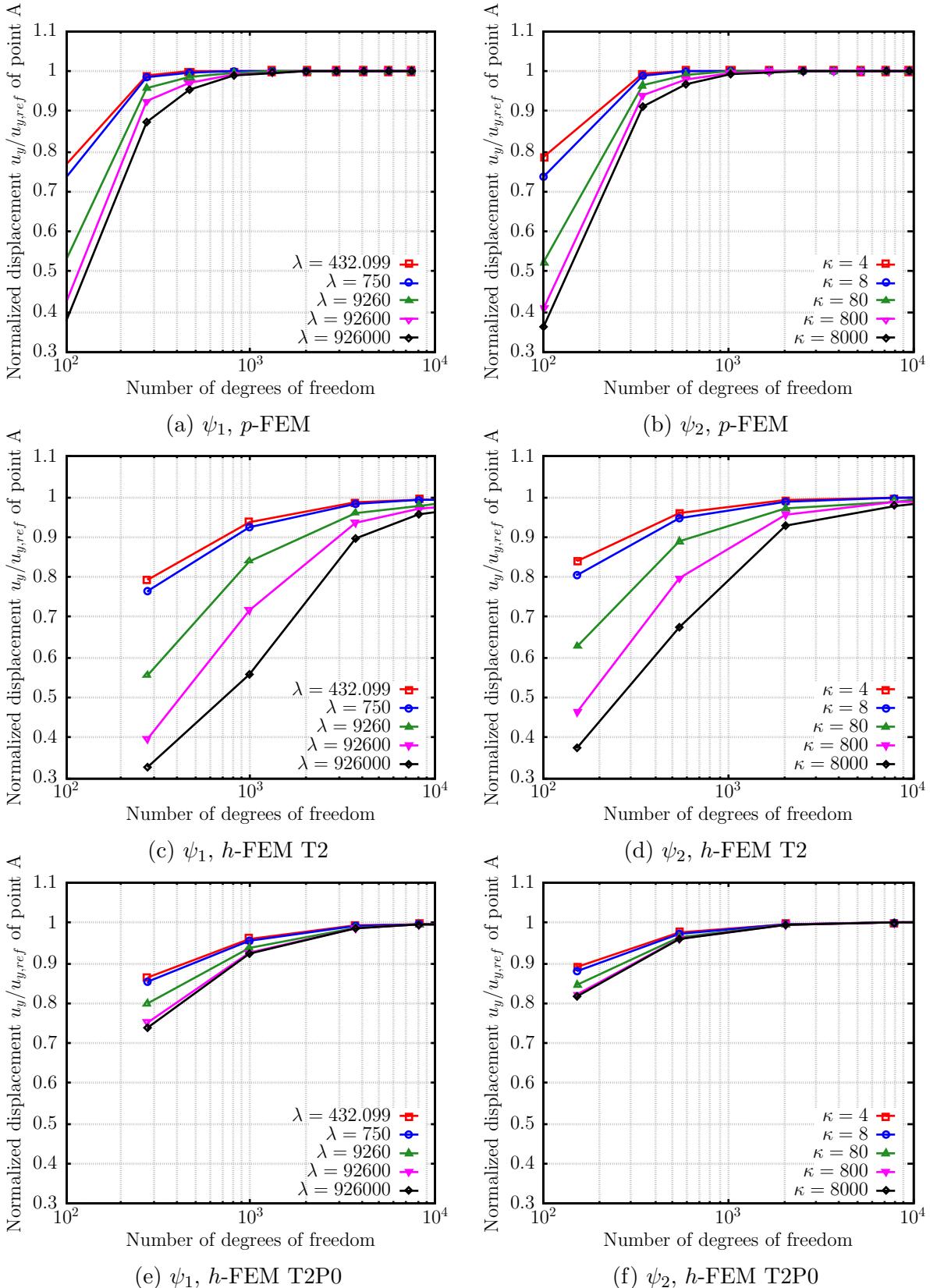


Figure 2.7: Locking behavior considering the normalized displacement  $u_y/u_{y,\text{ref}}$  of point A computed with the different finite element formulations

where  $\mathbf{C}_p = \mathbf{F}_p^T \mathbf{F}_p$  defines the plastic right Cauchy-Green tensor.

An isotropic compressible Neo-Hookean material behavior is assumed for the elastic part of the deformation utilizing the following strain-energy function

$$\psi_e = \frac{\lambda}{4} (III_{C_e} - 1 - \ln III_{C_e}) + \frac{\mu}{2} (I_{C_e} - 3 - \ln III_{C_e}). \quad (2.16)$$

In (2.16),  $\lambda$  and  $\mu$  define the Lamé constants and  $I_{C_e}$  and  $III_{C_e}$  denote the first and third invariant of the elastic right Cauchy-Green tensor  $C_e$  or the elastic left Cauchy-Green tensor  $b_e$  as follows

$$I_{C_e} = \text{tr} C_e \quad \text{and} \quad III_{C_e} = \det C_e \quad \text{or} \quad I_{b_e} = \text{tr} b_e \quad \text{and} \quad III_{b_e} = \det b_e. \quad (2.17)$$

The 1st and 2nd Piola-Kirchhoff as well as the Cauchy and Kirchhoff stress tensors read

$$\mathbf{P} = \frac{\partial \psi_e}{\partial F_e}, \quad \mathbf{S} = 2 \frac{\partial \psi_e}{\partial C_e}, \quad \boldsymbol{\sigma} = \frac{2}{J_e} \mathbf{F}_e \frac{\partial \psi_e}{\partial C_e} \mathbf{F}_e^T, \quad \boldsymbol{\tau} = 2 \frac{\partial \psi_e}{\partial b_e} b_e. \quad (2.18)$$

The yield criterion of the plasticity model reads

$$\Phi(\boldsymbol{\tau}, \bar{\alpha}) = \sqrt{\frac{3}{2} \mathbf{s} : \mathbf{s}} - K(\bar{\alpha}) \quad \text{with} \quad \mathbf{s} = \boldsymbol{\tau} - \frac{1}{3} \text{tr}(\boldsymbol{\tau}) \mathbf{1}. \quad (2.19)$$

In Eq. (2.19)  $\bar{\alpha}$  denotes the hardening variable,  $\mathbf{s}$  defines the deviatoric part of the Kirchhoff stress tensor  $\boldsymbol{\tau}$ , and  $K(\bar{\alpha})$  describes the hardening which consists of a linear and an exponential part as follows

$$K(\bar{\alpha}) = Y_0 + H\bar{\alpha} + (Y_\infty - Y_0) (1 - e^{-\delta\bar{\alpha}}), \quad (2.20)$$

see e.g. Simo [1998]. Here,  $Y_0$  denotes the initial yield stress,  $H$  the linear hardening parameter,  $Y_\infty$  the saturation stress, and  $\delta$  the hardening exponent. In accordance to Simo and Miehe [1992], the evolution of the plastic flow as well as the internal variable reads

$$-\frac{1}{2} \mathcal{L}_v b_e = \gamma \frac{\partial \Phi}{\partial \boldsymbol{\tau}} b_e \quad \text{and} \quad \dot{\bar{\alpha}} = -\gamma \frac{\partial \Phi}{\partial K(\bar{\alpha})}. \quad (2.21)$$

Here,  $\mathcal{L}_v b_e$  denotes the Lie derivative of the elastic left Cauchy-Green tensor  $b_e$  and  $\gamma \geq 0$  is the non-negative plastic multiplier. Based on the principle of maximum dissipation, this follows by enforcing stationarity conditions for the Lagrange functional, which is constructed as an optimization problem with the constraint condition ( $\Phi = 0$ ), depending on the Dissipation inequality and the yield criterion in relation with  $\gamma$ .

Furthermore, Eq. (2.15) can be inserted into the plastic flow formula in Eq. (2.21) to obtain,

$$\dot{\mathbf{C}}_p^{-1} = -2\gamma \mathbf{F}^{-1} \frac{\partial \Phi}{\partial \boldsymbol{\tau}} \mathbf{F} \mathbf{C}_p^{-1}, \quad (2.22)$$

which is then used for the algorithmic treatment of the model. Finally, the material model is complemented by the Kuhn-Tucker conditions

$$\Phi \leq 0, \quad \gamma \geq 0, \quad \Phi\gamma = 0, \quad (2.23)$$

describing loading and unloading. For the integration of the internal variable  $\dot{\bar{\alpha}}$ , a backward Euler scheme is used. For the plastic variable  $\dot{\mathbf{C}}_p$  an exponential map algorithm within an implicit time integration scheme is applied as follows

$$\bar{\alpha}_{n+1} = \bar{\alpha}_n + \Delta_t \gamma, \quad (2.24)$$

$$(\mathbf{C}_p^{-1})_{n+1} = \mathbf{F}_{n+1}^{-1} \exp[-2\Delta_t \gamma \frac{\partial \Phi_{n+1}}{\partial \boldsymbol{\tau}_{n+1}}] \mathbf{F}_{n+1} (\mathbf{C}_p^{-1})_n, \quad (2.25)$$

which was introduced by Weber and Anand [1990] and Eterovic and Bathe [1990]. Here,  $\Delta_t \gamma$  denotes the increment of the plastic multiplier. The material parameters used in this benchmark as well as the load  $p_0$  are given in Table 2.11.

$\lambda$	$\mu$	$Y_0$	$Y_\infty$	$H$	$\delta$	$p_0$
110.743 MPa	80.194 MPa	450.0 MPa	715.0 MPa	129.24 MPa	16.93	350.0 MPa

Table 2.11: Material parameters and applied load

As in the hyperelastic case the convergence of the spatial discretization in terms of the vertical tip displacement  $u_y$  of the upper right node (point A, see Figure 2.1) is studied. As initial discretization a mesh consisting of 104 hexahedral elements with two refinements towards the singularity at the top left corner is used, as depicted in Figure 2.8a. Again, we take advantage of symmetry and apply just one layer of elements of thickness 0.5mm. The starting mesh for the  $H_1$  and  $H_1P_0$  formulations is depicted in Figure 2.8b, whereas in case of the  $T_2$  and  $T_2P_0$  each hexahedral element is subdivided into five tetrahedral elements, taking also advantage of symmetry in thickness direction. In the case of the  $h$ -FEM approach, the elements are uniformly refined in in-plane direction. In contrast, for the  $p$ -FEM the discretization is based on the trunk space utilizing hierachic shape functions. An uniform and isotropic increase of the polynomial degree  $p = 1, \dots, 8$  of the shape functions yields the results depicted in Figure 2.9a, which are plotted together with the displacements computed with the formulations  $T_2$ ,  $T_2P_0$ ,  $H_1$  and  $H_1P_0$ . Furthermore, the results of the vertical displacement of point A are given in Table 2.12. Furthermore, a Fortran77 code for the computation of the 1st Piola Kirchhoff stress tensor and the material tangent  $\mathbf{A} = \partial_{\mathbf{F}} \mathbf{P}$  will be provided online under (DOI XXX) with the subroutine:

```
SUBROUTINE mate(v,niter,MatIO,FI0,h1,SubIterationTolerance,P,Amat,h2,error)
```

DOFs	$p$ -FEM	DOFs	$H_1$	$H_1P_0$	DOFs	$T_2$	$T_2P_0$
570	6.67213	630	7.08243	12.9631	921	11.5843	12.4056
2002	13.5791	2420	10.1830	13.3946	3524	13.4128	13.5667
3434	13.6521	9480	12.2640	13.5958	13776	13.6750	13.7045
6040	13.6790	21180	12.9299	13.6491	54464	13.7016	13.7198
9799	13.6898	37520	13.2212	13.6703	122064	13.7080	13.7238
15033	13.6985	70730	13.4215	13.6860	—	—	—
22051	13.7059	131250	13.5360	13.6936	—	—	—
31162	13.7070	—	—	—	—	—	—

Table 2.12: Convergence of the displacement component  $u_y$  at point A

**Von Mises stress convergence:** In the following, we study the convergence behavior of the von Mises stress. In doing so, we use the same meshes as in the previous section. In Figure 2.9b the von Mises stress at point B is plotted over the number of degrees of freedom. The corresponding numbers are also depicted in Table 2.13. Figure 2.10a shows the contour plot for the von Mises stress  $\sigma_{vM}$  and 2.10b the equivalent plastic strain  $\bar{\alpha}$  for  $p = 6$  at the last load step.

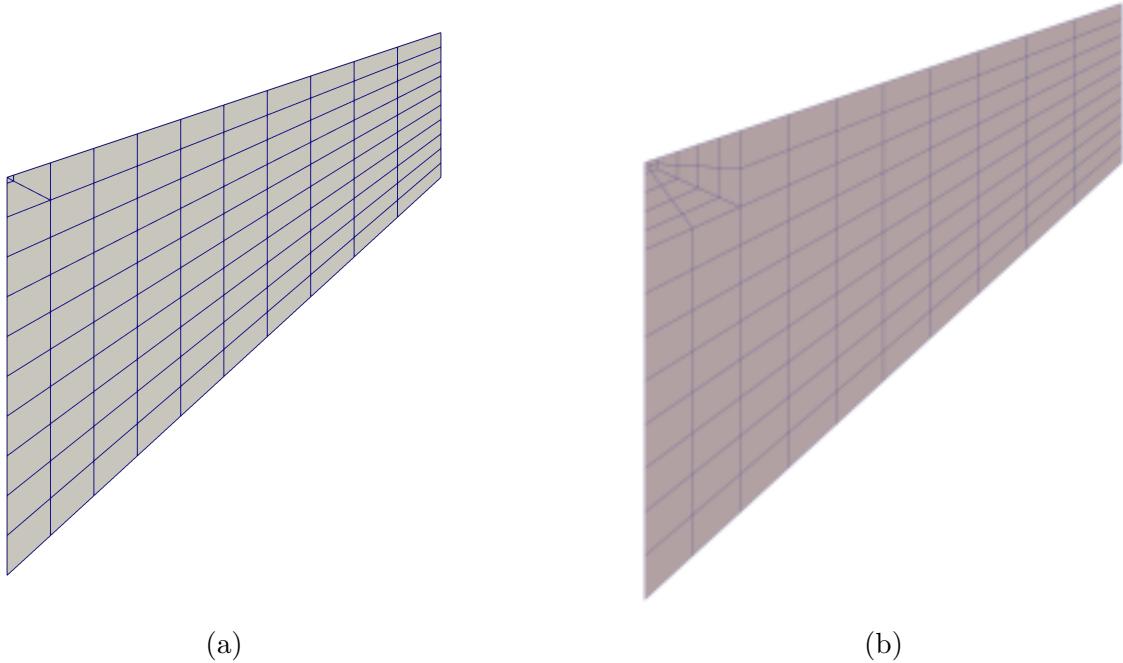


Figure 2.8: Spatial discretization: (a) a mesh consisting of 104 hexahedral elements with two refinements towards the singularity used for the  $p$ -FEM computations (b) the starting mesh for the  $H_1$  and  $H_1P_0$  formulations

DOFs	$p$ -FEM	DOFs	$H_1$	$H_1P_0$	DOFs	$T_2$	$T_2P_0$
570	619.505	630	589.469	610.345	921	659.692	647.006
2002	599.683	2420	609.480	602.642	3524	615.844	609.117
3434	598.359	9480	614.556	598.425	13776	598.334	597.072
6040	596.807	21180	610.269	597.656	54464	597.441	597.339
9799	597.214	37520	606.473	597.616	122064	596.884	596.798
15033	597.327	70730	602.896	597.434	—	—	—
22051	596.939	131250	600.484	597.310	—	—	—
31162	597.078	—	—	—	—	—	—

Table 2.13: Convergence of the von Mises stress  $\sigma_{vM}$  at point B

**Convergence study using different load steps:** In the following we study the influence of the total number of load steps used to apply the load. To this end, the displacement  $u_y$  at point A and the von Mises stress  $\sigma_{vM}$  at point B are investigated. In doing so, we use the same mesh like in the previous section, as depicted in Figure 2.8a applying a polynomial degree of  $p = 5$  based on the trunk space utilizing hierachic shape functions. In Figures 2.11a and 2.11b, the displacements as well as the von Mises stress are plotted over the number of load steps chosen to apply the prescribed load. The corresponding numbers are also depicted in Table 2.14.

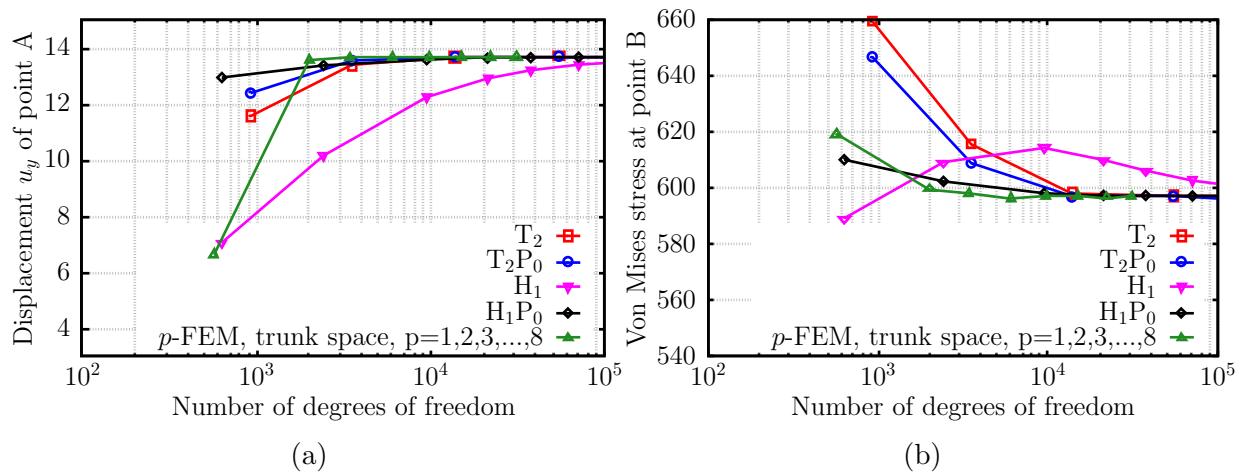


Figure 2.9: Cook's membrane: (a) Convergence of displacement  $u_y$  at point A (b) Convergence of von Mises stress  $\sigma_{vM}$  at point B

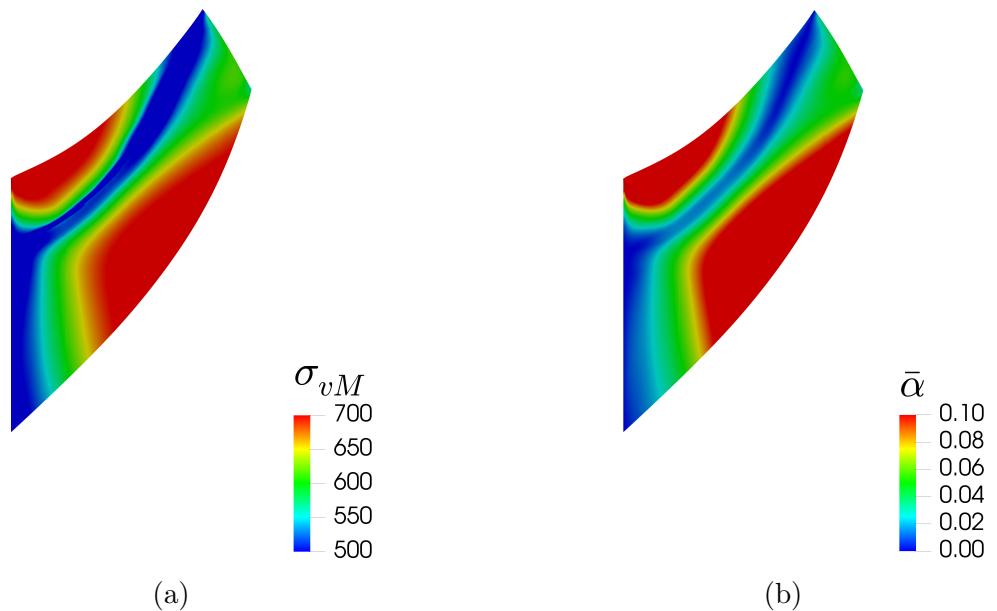


Figure 2.10: Cook's membrane contour plots for  $p$ -FEM (a) von Mises stress  $\sigma_{vM}$  (b) equivalent plastic strain  $\bar{\alpha}$ , for  $p = 6$  at the last load step

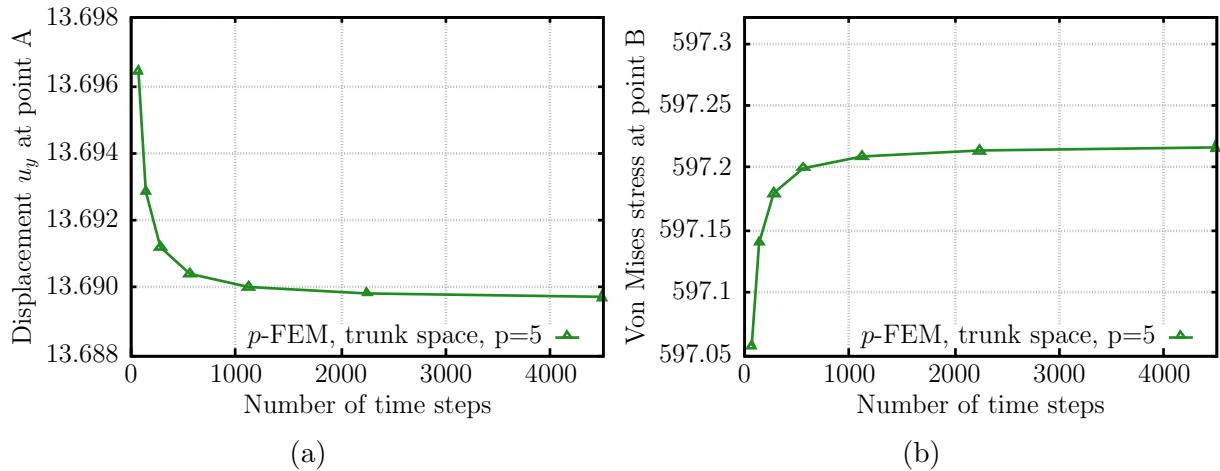


Figure 2.11: Convergence study for different load steps using  $p$ -FEM,  $p = 5$  (a) displacement  $u_y$  at point A (b) von Mises stress  $\sigma_{vM}$  at point B

load steps	$u_y$	$\sigma_{vM}$
70	13.6964	597.058
140	13.6928	597.140
280	13.6912	597.180
560	13.6904	597.200
1120	13.6900	597.209
2240	13.6898	597.214
4480	13.6897	597.216

Table 2.14: Convergence of the displacement component  $u_y$  at point A and the von Mises stress  $\sigma_{vM}$  at point B for different numbers of load steps using  $p = 5$

**Remark** The software used in this study are AceGen and AceFEM (Korelc [1997; 2002], Korelc and Wriggers [2016]) as well as in-house codes AdhoC<sup>4</sup> (Düster and Kollmannsberger [2010]) and AdhoC++ which are jointly developed at the Technical University of Munich and the Hamburg University of Technology.

### 3 Incompressible block under constant partial load

In this benchmark, a cube is subject to a vertical load on part of its upper surface. This benchmark poses two challenges for a FEM simulation in a geometrically non-linear setting:

- two line-singularities induced by a jump in the Neumann boundary condition which intersect in a point,
- almost incompressible material.

The benchmark allows to asses the performance of (high-order) displacement-based and mixed finite elements.

### 3.1 Geometry and boundary conditions

The system is depicted in 3.1.

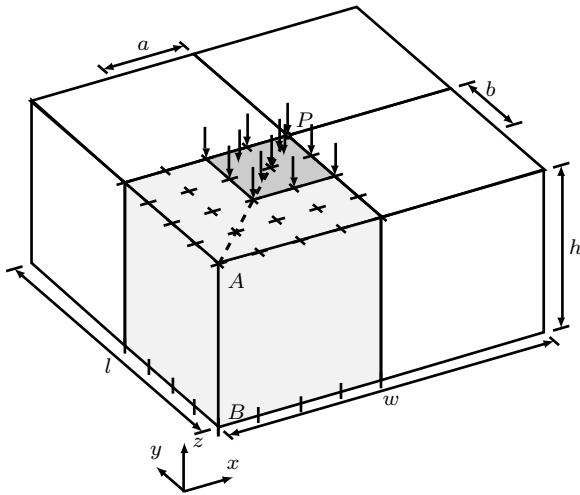


Figure 3.1: Quasi-incompressible cube with partial load.

Its dimensions are given in 3.1.

Table 3.1: Dimensions of the problem.

$h$ in mm	$w$ in mm	$l$ in mm	$a$ in mm	$b$ in mm	$q$ in MPa
50	100	100	25	25	3.0

At the upper surface of the block, i.e. at  $z = h$ , displacements are fixed in both  $x$ - and  $y$ -direction. The bottom of the block, i.e. at  $z = 0$ , is fixed in  $z$ -direction.

Due to axial symmetry of loads and boundary conditions, computations were only carried out on the quarter of the block marked in light gray. To this end, homogeneous Dirichlet boundary conditions were additionally applied on the symmetry planes such that at  $x = 0.5w$ , displacements were fixed in  $x$ -direction and at  $y = 0.5l$  displacements were fixed in  $y$ -direction.

Furthermore, the block is partially loaded with a constant surface load  $q$  on the area defined by  $a$  and  $b$ . The area in dark gray, thus, bears a mixed Dirichlet-Neumann boundary condition. These boundary conditions are chosen according to a similar test presented in Reese et al. [2000].

### 3.2 Hyperelastic material model

We consider a deformation  $\varphi(\mathbf{X}, t)$  which maps points in the initial configuration to the current or deformed configuration. This deformation can be computed using the coordinates of the initial configuration and the displacement field:  $\varphi(\mathbf{X}, t) = \mathbf{X} - \mathbf{u}(\mathbf{X}, t)$ . Using this deformation map, the deformation gradient can be computed as:

$$\mathbf{F} = \text{Grad } \varphi(\mathbf{X}, t) = \text{Grad}(\mathbf{X} - \mathbf{u}(\mathbf{X}, t)) = 1 + \mathbf{H}(\mathbf{X}, t) \quad (3.1)$$

where  $\mathbf{H}(\mathbf{X}, t)$  is the displacement gradient. The volume change  $J$  is given by the determinant of the deformation gradient:  $J = \det \mathbf{F}$  and the right Cauchy-Green-tensor is defined by:  $\mathbf{C} = \mathbf{F}^T \mathbf{F}$ . Based on these quantities, the following isotropic strain energy function  $W(\varphi)$  is used in this benchmark

$$W(\varphi) = \frac{\mu}{2}(\text{tr } \mathbf{C} - 3 - 2 \ln J) + \frac{\lambda}{2}(J - 1)^2 \quad (3.2)$$

The material parameters used in this benchmark are given in 3.2. They lead to a nearly incompressible material with a Poisson ratio of  $\nu = 0.4983$ .

Table 3.2: Material parameters

$\lambda$ in MPa	$\mu$ in MPa
499.92568	1.61148

### 3.3 Discretization and Results

An overall impression of the deformation is provided in 3.2 which depicts the displacement magnitude in the deformed configuration along with the wireframe of the corresponding hexahedral discretization in its initial configuration.

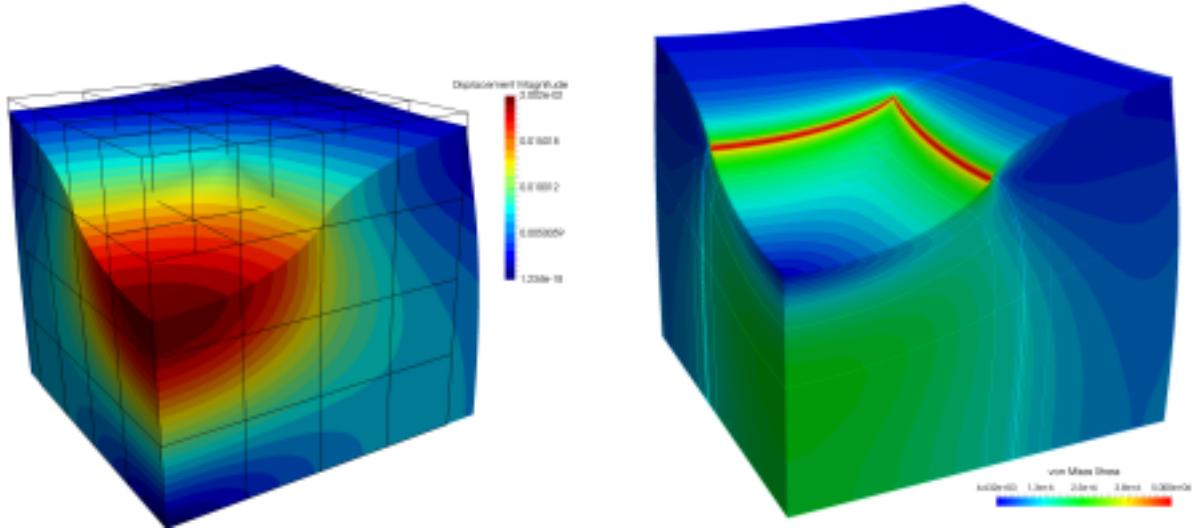


Figure 3.2: Overall impression of results

left: displacement magnitude on a fixed mesh of  $4 \times 4 \times 4$  elements;

right: von Mises stress on a  $8 \times 8 \times 8$  mesh of  $p = 8$ , geometrically graded towards the traction boundary.

The convergence of the vertical displacement in  $z$ -direction at point  $P$ ,  $u_z(P)$ , versus the degrees of freedom (DOF) of the discretization was investigated for the finite elements H1/EI9, H1, H2, H1/P0, O2/P1, H1/E9 (see e.g. Wriggers [2008]) on regular meshes. Here  $4 \times 4 \times 4$ ,  $8 \times 8 \times 8$ ,  $16 \times 16 \times 16$  and  $32 \times 32 \times 32$  elements were used for the elements H1, H1/EI9, H1/P0 and H1/E9 with linear ansatz functions. For the hexahedral element

Table 3.3:  $|u_z(P)|$  for given element types, Dirichlet BC with DOF elimination.<sup>1</sup>

$n_{dofs}$	H1EI9	H1	H2	H1P0	O2P1	H1E9	TSCG
260	19.09	7.78	18.32	19.87	19.80	20.00	20.14
1800	19.98	13.17	19.54	20.02	19.93	20.05	20.10
13328	20.01	17.54	19.98	20.01	19.97	0	20.03
102432	20.00	19.52	20.01	20.00	19.98	0	20.01

<sup>1</sup> The number of degrees of freedom for H1-elements is given. The results for all other elements are computed on the same uniform meshes with the same number of nodes as the corresponding H1-element which leads roughly to the same number of unknowns.

H2 (27 nodes) and the tetrahedral element O2/P1with quadratic ansatz functions the number of elements was reduced such that the number of nodes was the same as for the elements with linear ansatz. The used elements are based on following ideas:

- **H1:** Classical hexahedral displacement based element with linear ansatz and  $2 \times 2 \times 2$  nodes.
- **H2:** Classical hexahedral displacement based element with quadratic ansatz and  $3 \times 3 \times 3$  nodes.
- **H1/E9:** Hexahedral mixed type ansatz with assumed enhanced strain fields and linear displacements. The element uses  $2 \times 2 \times 2$  nodes and has 9 internal degrees of freedom related to the enhanced modes. These mode can be eliminated at element level using Schur complement techniques, details can be found in Simo and Armero [1992].
- **H1/EI9:** Hexahedral mixed type ansatz with assumed enhanced strain fields and linear displacements, like H1/E9. However the enhanced strain modes are included here as a stabilization of a constant strain element, see Mueller-Hoeppe et al. [2009].
- **H1/TSCG:** Hexahedral mixed type ansatz with 12 assumed enhanced strain fields and linear displacements. This element has a special stabilization to avoid hour-glassing of H1/E9, see Korelc et al. [2010].
- **H1/P0:** Hexahedral mixed element with linear ansatz for the displacement field and discontinuous constant pressure field at element level.
- **O2/P1:** Tetrahedral mixed element with quadratic ansatz for the displacement field and continuous linear pressure field.

The results are presented in 3.3 and 3.3. Since all these elements are developed using AceGen, see Korelc and Wriggers [2016], they exhibit quadratic convergence within the Newton-Raphson solution algorithm. Both enhanced strain elements and the mixed O2/P1 and the H1/P0 elements are softer than the H2 element. All elements except the H1/E9 element converge practically to the same solution. For the H1/E9 element, solutions can only be obtained for the two coarsest meshes. For finer mesh resolutions the H1/E9 element depicts nonphysical hourglass instabilities.

Table 3.4:  $|u_z(P)|$  for  $p$ -extension on a  $4 \times 4 \times 4$  mesh, isotropic trunk space, Dirichlet conditions implemented with a penalty method.

$p$	$n_{dofs}$	$ u_z(P) $
1	375	7.656
2	1275	19.637
3	2175	19.998
4	3795	19.956
5	6135	19.986
6	9387	19.999
7	13743	20.010
8	19395	20.018
9	26535	20.020
10	35355	20.022

Furthermore, a purely displacement based high-order finite element using the integrated Legendre basis functions described in Szabó et al. [2004] (trunk space) was used and a  $p$ -extension was carried out on a fixed mesh with  $4 \times 4 \times 4$  elements. The results are depicted in 3.3 and 3.4. It can be observed that the pure displacement formulation

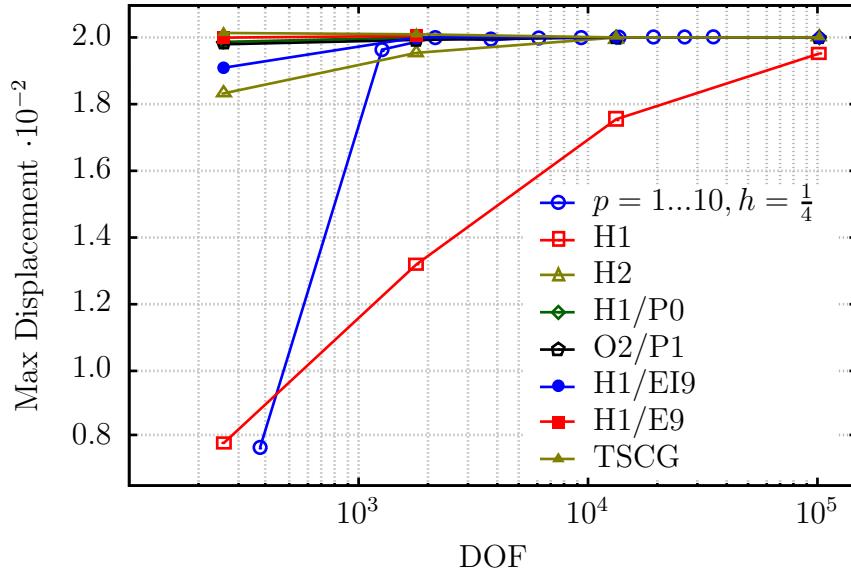


Figure 3.3: Displacement at point  $P$  in  $z$ -direction ( $u_z(P)$ ) for different element formulations and discretizations

locks for  $p = 1$  on the  $h$ -refined meshes. This is expected for this nearly incompressible problem. However, locking may be controlled by increasing the order the finite elements as demonstrated by the curve given by a  $p$ -extension on a fixed mesh with  $4 \times 4 \times 4$  elements.

For the high-order finite element using the integrated Legendre basis functions, additionally the stress component  $P_{zz}$  and the von Mises stress are measured along the diagonal line  $A - P$  at  $z = h$ . The results on a discretization with  $8 \times 8 \times 8$  pure displacement

based elements of  $p = 10$  are given in 3.4 and 3.5. The expected stress is zero at the homogeneous part of the Neumann boundary until it jumps to the value of the load  $q$  under the load surface. The discretization is only able to capture this jump approximately even though the discretization was geometrically propagated with a factor of 0.15 towards the singularity for this particular case.

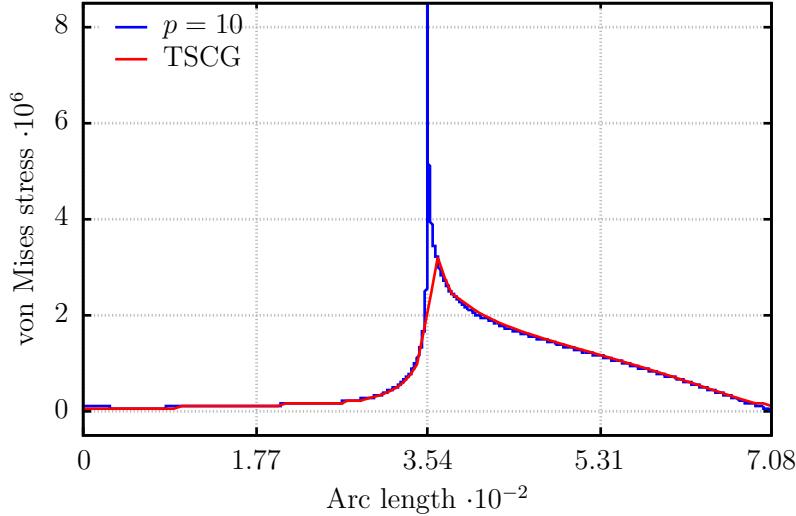


Figure 3.4: Von Mises stress along diagonal from point  $P$  to point  $A$  on top face for the isotropic trunk space of order  $p = 10$  on a  $8 \times 8 \times 8$  mesh, geometrically graded towards the traction boundary and for a  $64 \times 64 \times 64$  mesh of TSCG elements.

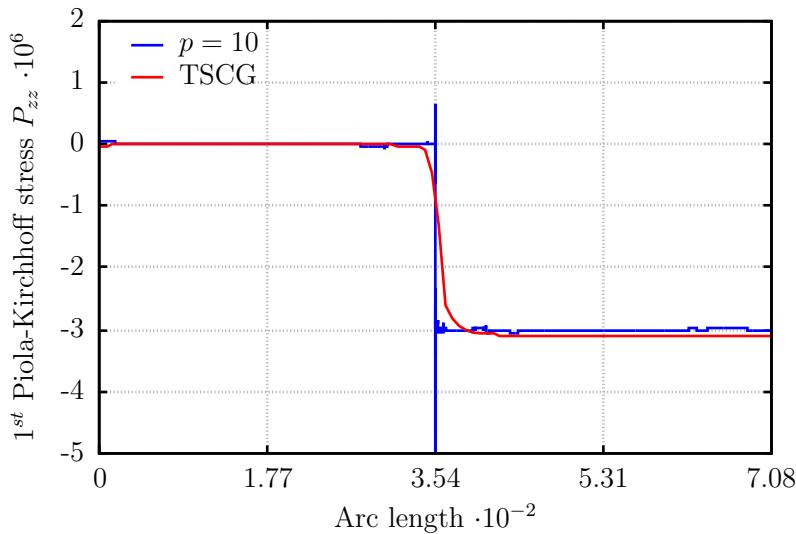


Figure 3.5:  $1^{st}$  Piola-Kirchhoff stress component  $P_{zz}$  along diagonal from point  $P$  to point  $A$  on top face for the isotropic trunk space of order  $p = 10$  on a  $8 \times 8 \times 8$  mesh, geometrically graded towards the traction boundary and for a  $64 \times 64 \times 64$  mesh of TSCG elements.

## 4 Analysis of a thin plate

For the analysis of the complex thin geometries, such as shell and plate structures, various finite element methods have been developed to deliver accurate and efficient simulations. In this section, a study on the performance of three different element formulations is established for a thin plate. To this end, the thickness of the plate is varied from a thick to a very thin plate. Accordingly, two solid finite element methodologies as well as a solid-shell finite element technology are exploited.

### 4.1 Problem definition

A square thin plate is to be investigated in this benchmark (see Korelc et al. [2010]). It is clamped at all four sides (refer to Equation 4.1) and is loaded by a distributed load of  $q = 0.0002 \text{ MPa}$ . Geometry, boundary conditions and loading of the plate in 3D are illustrated in Figure 4.1. The thickness of the plate  $h$  is a variable parameter for later investigations, whereas the side lengths  $a$  of the square are constant and equal to 1 mm.

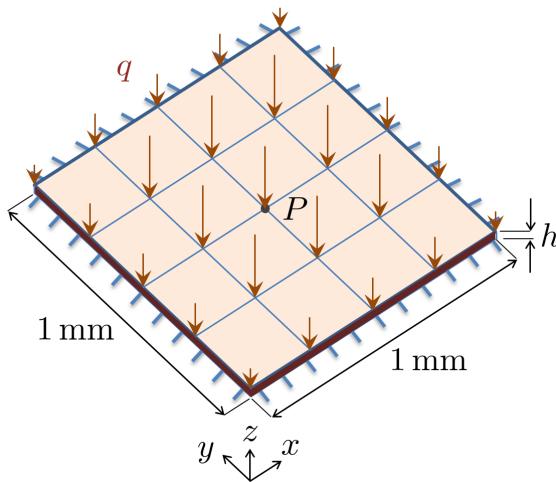


Figure 4.1: Geometry, boundary conditions and loading of the thin plate.

The corresponding boundary conditions read as follows:

$$\begin{aligned} x = 0 : u &= v = w = 0, \\ x = a : u &= v = w = 0, \\ y = 0 : u &= v = w = 0, \\ y = a : u &= v = w = 0, \end{aligned} \tag{4.1}$$

where  $u$ ,  $v$  and  $w$  are the displacements in  $x$ ,  $y$  and  $z$ -directions, respectively.

### 4.2 Material model

In the present work, a Neo-Hooke model for isotropic hyper-elastic material behavior is applied. The material parameters are  $\Lambda = 144.2307692 \text{ MPa}$  and  $\mu = 96.1538 \text{ MPa}$  (corresponding to  $E = 250 \text{ MPa}$  and  $\nu = 0.3$ ). The strain energy function  $W$  is given by

$$W = \frac{\mu}{2}(\text{tr}\mathbf{C} - 3) - \mu \ln(\sqrt{\det\mathbf{C}}) + \frac{\Lambda}{4}(\det\mathbf{C} - 1 - 2 \ln(\sqrt{\det\mathbf{C}})), \tag{4.2}$$

where  $\mathbf{C} = \mathbf{F}^T \mathbf{F}$  is the right Cauchy-Green-tensor with  $\mathbf{F}$  denoting the deformation gradient (see Reese and Wriggers [2000]).

The same plate is examined for the case of linear elasticity with the thickness  $h = 0.01$  mm ( $a/h = 100$ ) in the work of Bayat et al. [2018] and Bayat et al. [2018]. In the aforementioned studies, different conforming and non-conforming element formulations are compared in terms of rate of convergence with respect to mesh refinement level.

### 4.3 Finite element technologies

Three different finite element methods are applied in this work. The first solid element formulation is the standard eight-node tri-linear Q1 brick element with eight Gauss points. Furthermore, an eight-node tri-linear solid element (Q1SP) with reduced integration (one Gauss point in the center of the element) and hourglass stabilization technique is applied. This element formulation is well-known for its performance in overcoming the problems concerned with shear as well as volumetric locking (please refer to Reese and Wriggers [2000] and Reese [2005]). Finally, an eight-node solid-shell (Q1STS) finite element with reduced integration (one integration point) within the shell plane and at least two integration points over the thickness is used (Schwarze and Reese [2009; 2011]). Similar to the Q1SP element formulation, this element benefits from enhanced assumed stains (EAS). However, in addition to the Q1SP element, the transverse shear and curvature thickness locking are additionally addressed by the employment of the assumed natural strain (ANS) concept.

### 4.4 Convergence study

In order to investigate the convergence rate of different element formulations, the vertical displacement  $w_P$  at the point  $P$  on the upper side of the middle of the surface is investigated, see Figure 4.1. To this end, different thicknesses  $h$ , different number of elements  $n_e$  and  $n_z$  in the planar directions ( $x$  and  $y$ ) as well as in the out-of-plane direction ( $z$ ) are considered. The ratio between the length and thickness of the plate ( $a/h$ ) is varied by 20, 50, 100, 200, 500 and 1000 to cover a wide range of thick to thin plates.

Figure 4.2 shows the deformed plate with 10 times magnified displacements.

**4.4.1 Influence of the number of elements in thickness direction** First, the influence of the number of elements in thickness direction on the displacement convergence rate is studied for the two finite element technologies Q1SP and Q1STS for the given aspect ratio  $a/h = 100$ . Figure 4.3 shows the influence of the number of elements ( $n_z$ ) in thickness direction on the deflection  $w_P$  of the plate at the point  $P$  for different number of elements ( $n_e$ ) in planar directions. In addition, the vertical displacements of the point  $P$  are given for the specific planar discretization  $n_e = 32$  in Table 4.1.

Table 4.1: Deflection  $w_P$  at the central point of the plate ( $a/h = 100$ ) for different number of elements in the thickness direction with 32 elements in the planar directions ( $n_e = 32$ ).

$n_z$	1	2	4	8	16	32
Q1SP: $w_P$ in $\mu\text{m}$	9.4099	8.4309	8.2019	8.1453	8.1312	8.1276
Q1STS: $w_P$ in $\mu\text{m}$	8.1761	8.1417	8.1350	8.1335	8.1331	8.1330

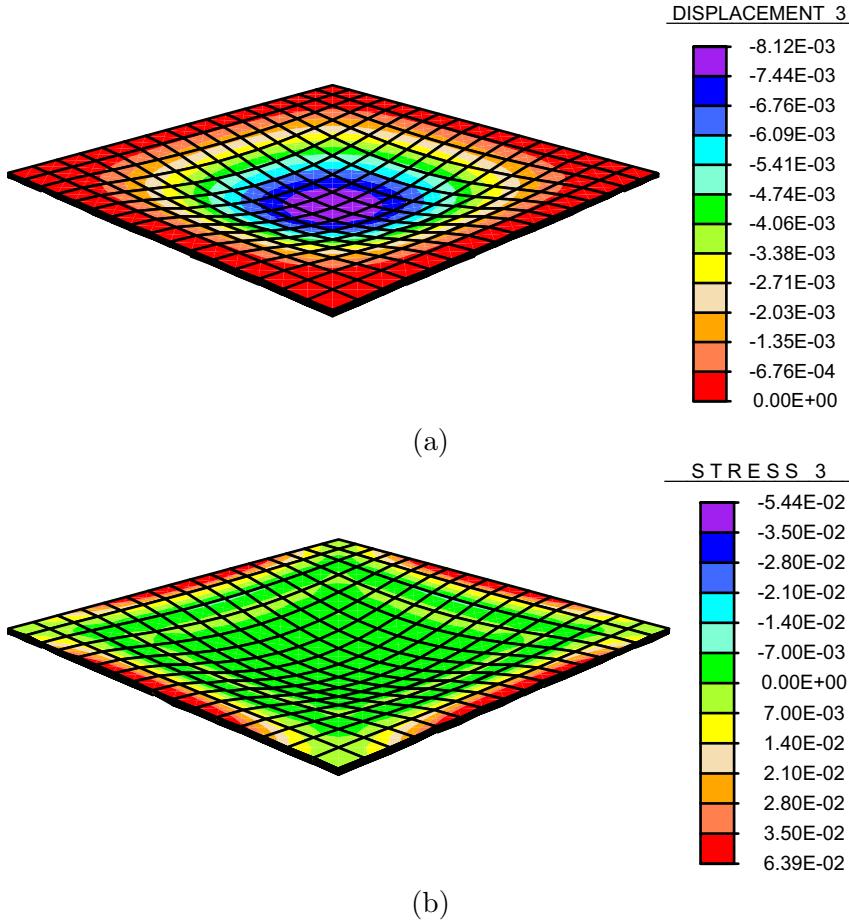


Figure 4.2: (a) Displacement contour and (b) stress distribution of the deformed plate in  $z$ -direction (10 times magnified displacements). The geometrical aspect ratio  $a/h = 100$  and the mesh size  $n_e \times n_z = 16 \times 8$  are set.

According to Figure 4.3, both solid and solid-shell element formulations converge with very few number of elements in thickness direction as long as enough number of elements in the planar directions are used. The difference between the performance of these two element formulations lies mainly in the application of only one element in the thickness direction. For a single element in  $z$ -direction, the Q1SP element formulation shows still a deviation from the converged solution. This is expected because one uses only one Gauss point in the thickness direction in this shell structure. The error of the Q1STS element technique for  $n_z = 1$  is small. This is due to the fact that the latter approach benefits from possessing two or more integration points in the thickness direction.

The hourglass stabilization can be chosen constant. In this way, the deformation of the element is not considered. Another option is to take the deformation of the element into account and change the hourglass stabilization based on the deformed element configuration. To maintain quadratic convergence in the Newton iterations, the stabilization must be kept constant within the load step. This action could bring about a dependency of the solution on the number of load steps (Reese et al. [2017]). To examine this dependency, the convergence behavior of two element formulations with respect to the number of the load steps within a pseudo time range (1 sec) of a calculation is plotted in Figure 4.4. The sensitivity of the results to the size of the load step is negligible as the estimated

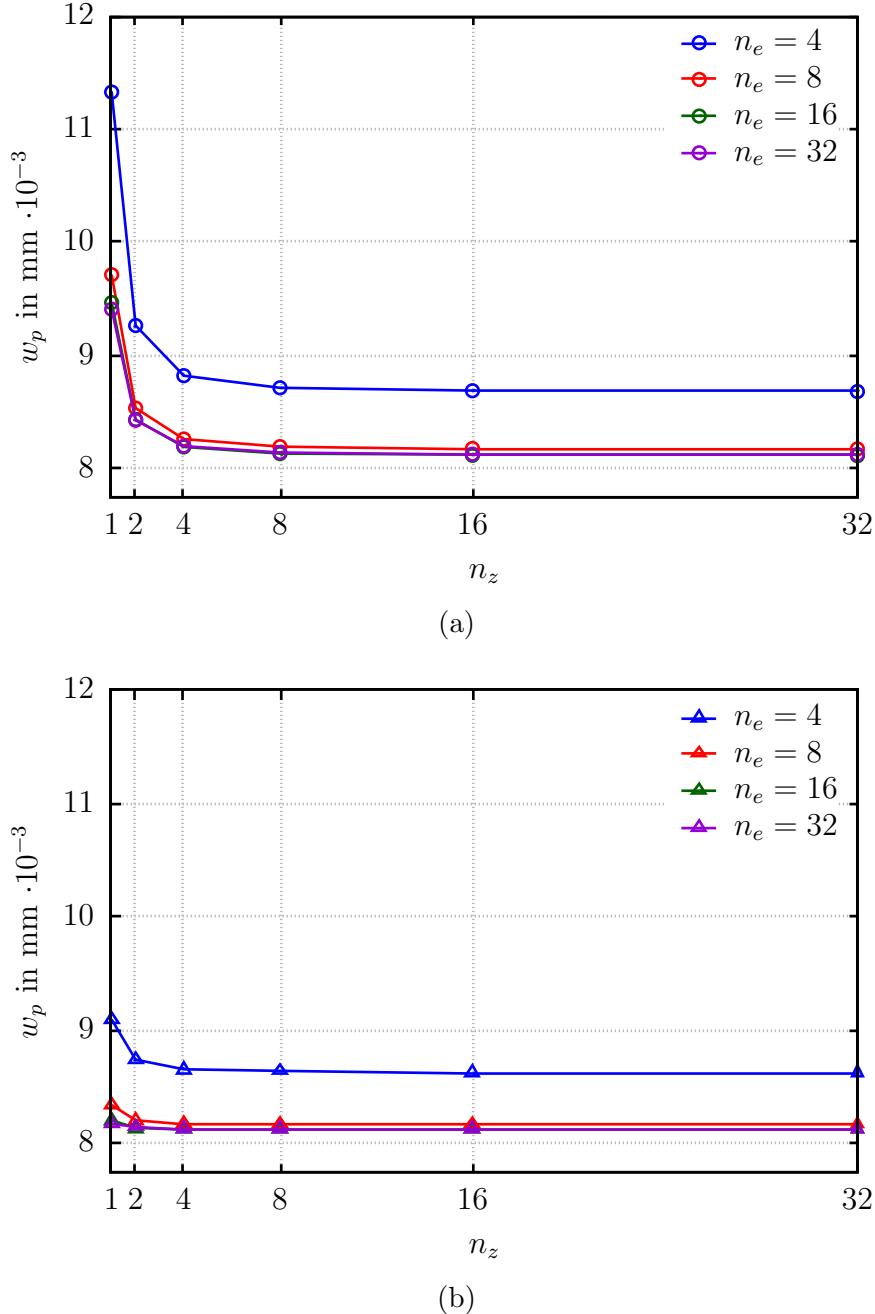


Figure 4.3: Deflection  $w_P$  at the central point of the plate for different number of elements in planar and thickness directions ( $a/h = 100$ ). (a) Q1SP element formulation, (b) Q1STS element formulation with 3 integration points in thickness direction.

relative error ( $|(w_p - w_{P,conv})/w_{P,conv}| \times 100$ ) lies around 1% for having only five load steps. Nonetheless, both element formulations converge quadratically in each load step as expected.

**4.4.2 Influence of the geometrical aspect ratio** The relative displacement  $w_p/w_{P,conv}$  at the point  $P$  with respect to the converged solution  $w_{P,conv}$  is investigated for thick as well as thin plates in Figure 4.5 and Figure 4.6, respectively. The  $x$ -axis of theses figures describes the mesh refinement in the planar directions as follows:

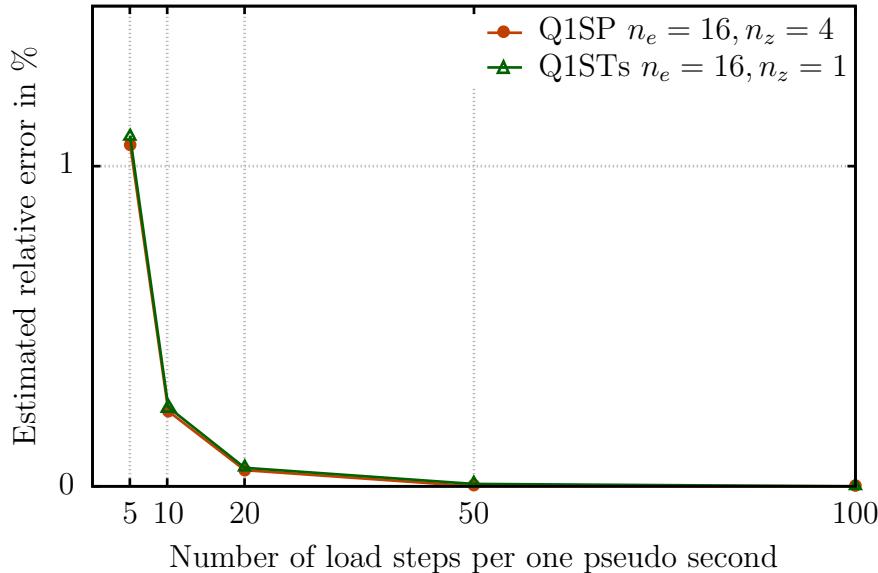


Figure 4.4: Estimated relative error of the point  $P$  with  $a/h = 100$  against different number of load steps in one pseudo second.

$4 \times 4$ ,  $8 \times 8$ ,  $16 \times 16$  and  $32 \times 32$ , indicating the number of elements in  $x$  and  $y$ -direction, respectively.

Figure 4.5 pictures the behavior of different element formulations for thick plates. In our examples, this implies the geometrical aspect ratio  $a/h \geq 50$  with  $a/h = 100$  lying between the thick and thin plate regimes. The Q1STS element formulation overcomes the problem of transverse shear locking with very few number of elements (almost one) in  $z$ -direction due to the application of assumed natural strain (ANS) concept. On the other hand, The Q1SP element needs more elements in the thickness direction to correctly capture the shear deformations. Only few number of elements in the planar directions are used for these two elements since these elements eliminate shear locking effects. On the contrary, the Q1 element observes severe locking due to the presence of shear locking in spite of the refinement of the mesh.

For much thinner structures (here,  $a/h \leq 200$  illustrated in Figure 4.6), the transverse shear deformations become negligible and thus transverse shear locking effects tend to disappear. In other words, for too high aspect ratios ( $a/h = 1000$ ), the shell becomes a membrane in our example. This means that the need for the ANS concept in the solid-shell element formulation becomes less pronounced. As a result, both solid (Q1SP) and solid-shell (Q1STS) element formulations tend to perform similarly. Unlike the outstanding convergence rate of these two element formulations, the Q1 element shows still severe shear locking effects. However, by making the structures excessively thinner, the convergence rate of the Q1 element shows a slight increase. This can be due to the fact that by changing the geometries from shell to membrane, the bending stresses start to decrease.

Finally, the vertical displacement  $w_P$  at the point  $P$  is plotted for different geometrical aspect ratios in Figure 4.7. The size of the mesh is set to the coarsest level which is necessary for the Q1SP and Q1STS element formulations to converge. For these mesh refinement levels, the Q1 elements show severe locking effects.

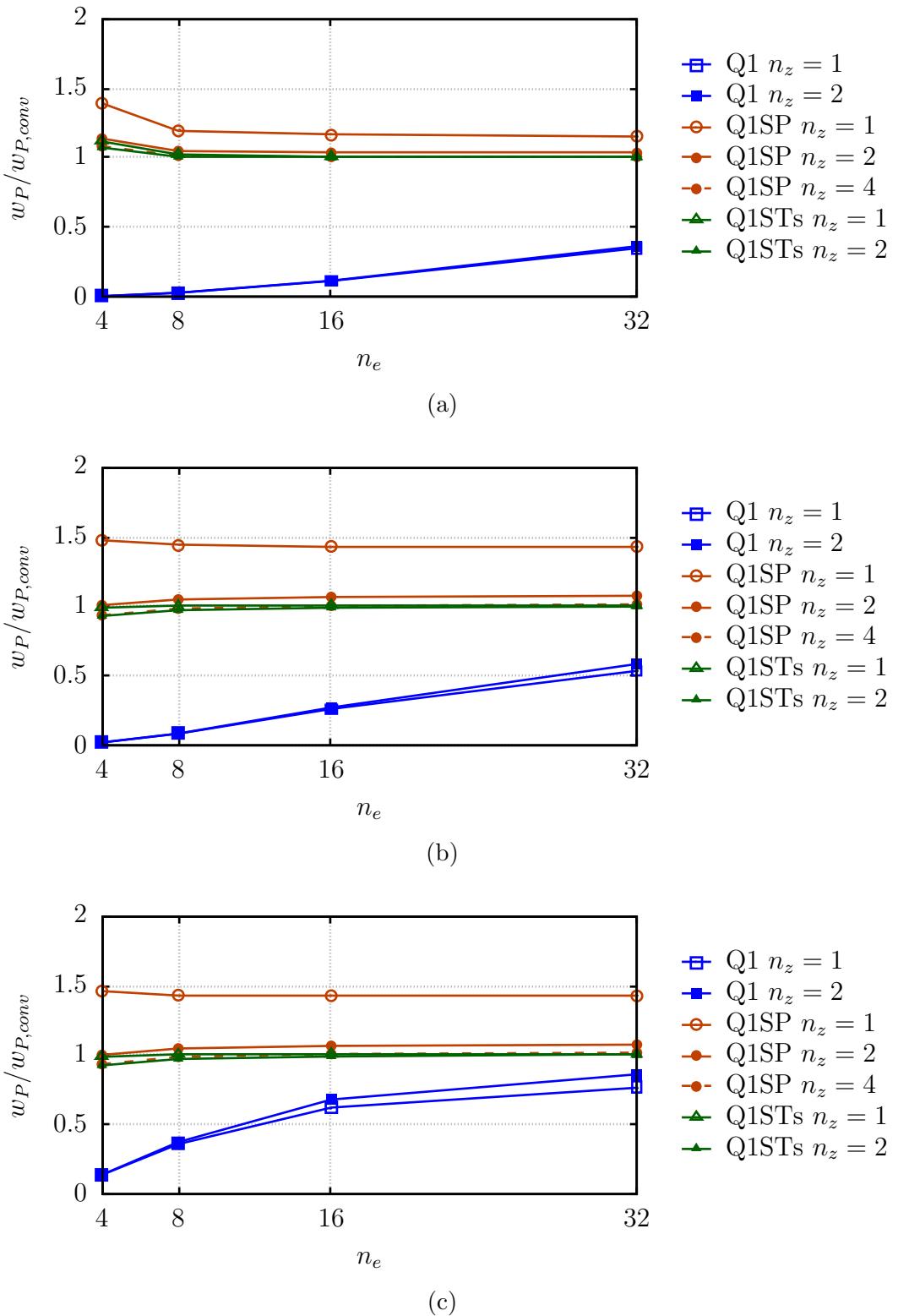


Figure 4.5: Deflection at the central point of the thick plate for different number of elements ( $n_e$ ) in planar directions. (a)  $a/h = 100$ , (b)  $a/h = 50$  and (c)  $a/h = 20$ .

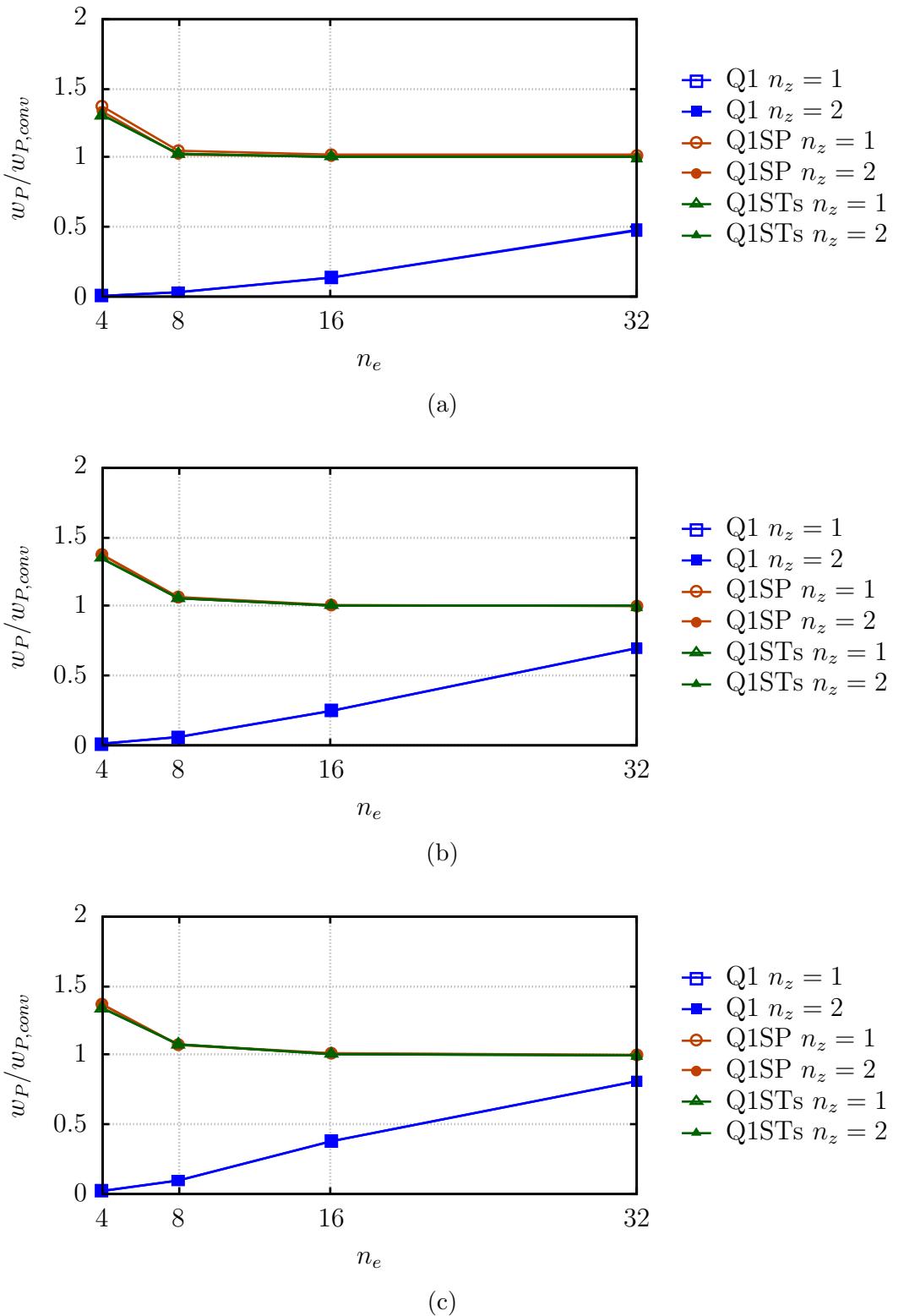


Figure 4.6: Deflection at the central point of the thin plate for different number of elements ( $n_e$ ) in planar directions. (a)  $a/h = 200$ , (b)  $a/h = 500$  and (c)  $a/h = 1000$ .

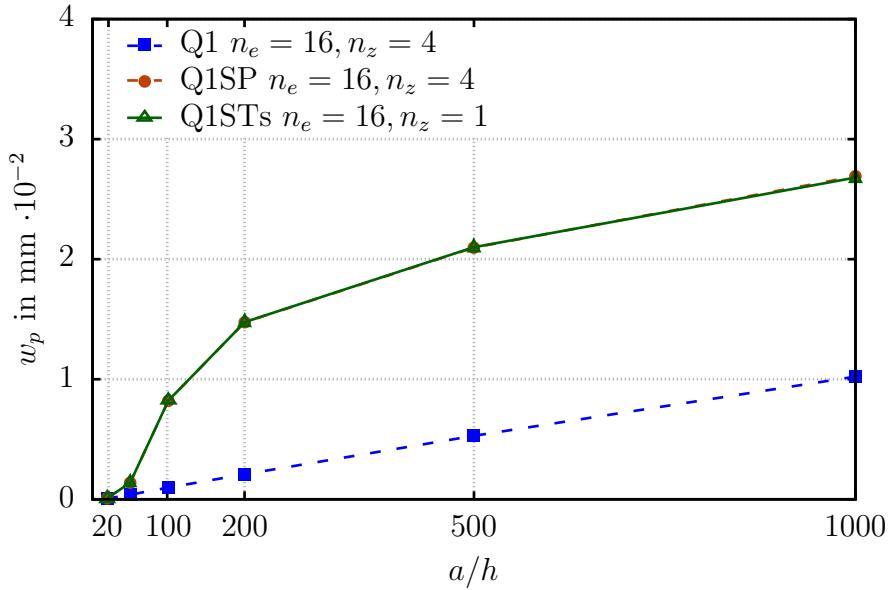


Figure 4.7: Vertical displacement  $w_P$  at the point  $P$  with different thicknesses  $h$

## 5 Conclusion

In the first two benchmarks we provide results on hyperelastic and elasto-plastic problems at finite strains. Different (mixed) finite element technologies as well as  $p$ -FEM was used in order to obtain convergent results for certain displacement and stress values for the Cook's membrane and an incompressible block problem. In benchmark problem in Section 4, the convergence behavior of a thin as well as a thick plate with a distributed load was investigated. Two different finite element technologies, namely solid and solid-shell were applied in addition to the standard Q1 finite element formulation. It was shown that due to the shell structure of the problem, the standard finite element method observes severe locking whereas the other methods show an outstanding convergence rate with respect to the mesh refinement.

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Deutsche Forschungsgemeinschaft  
Schwerpunktsprogramm 1748  
Reliable Simulation Techniques  
in Solid Mechanics.



## **SPP-1748 Benchmark Collection Part II**

### **Material Interfaces**

M. Kästner, P. Hennig, S. Kollmannsberger, M. Elhaddad, D. D'Angella, E. Rank

### **Phasefield model for brittle fracture**

R. Müller, Ch. Kuhn

### **Quasi-static Pressure-driven Cavity**

T. Heister, K. Mang, M. Walloth, T. Wick, W. Wollner

# A selection of benchmark problems in solid mechanics and applied mathematics: Part II

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## Abstract

In this work, we provide benchmark problems in the field of computational solid mechanics and fracture. In detail, we address the classical fields elasticity, incompressibility, and material interfaces. For this we describe explicit setups of the benchmarks and introduce the numerical schemes. For the computations the participating groups use different Galerkin finite element and isogeometric analysis formulations. Some programming codes are available open-source. The output is measured in terms of carefully designed quantities of interest that allow for a comparison of other models, discretizations, and implementations. Furthermore, computational robustness is shown in terms of mesh refinement studies. This paper is the second part of benchmarks, which were developed within the Priority Programme of the German Research Foundation 'SPP 1748 Reliable Simulation Techniques in Solid Mechanics - Development of Non-Standard Discretisation Methods, Mechanical and Mathematical Analysis'.

**Keywords:** Benchmark; Computational Solid Mechanics; Quantities of Interest; Finite Elements; Isogeometric Analysis

## 1 Introduction

Solving partial differential equations on complex geometries is perhaps one of the most important scientific achievement of the last decades. Analytical or manufactured solutions of such differential equations, e.g. from engineering or economics, is in most cases not available. Therefore, computer-aided numerical algorithms play an important role. At this point we mention that the rapid development of the available computing power contributes significantly to the success of these numerical methods. An end to this progress is currently not conceivable and becomes even more important due to the capabilities to address challenging multiphysics applications. Popular numerical methods are, for example, mesh-free methods, the finite volume method, finite differences, isogeometric analysis and - with possibly the greatest impact - the finite element method.

In this field, the German Priority Program 1748 (DFG SPP 1748) *Reliable Simulation Techniques in Solid Mechanics. Development of Non-standard Discretization Methods, Mechanical and Mathematical Analysis* is located. The main goal of this priority program was the development of modern non-conventional discretization methods based e.g. on mixed finite elements or discontinuous Galerkin formulations, including mathematical analysis for geometrically as well as physically non-linear problems in the areas of incompressibility, anisotropies and discontinuities to name a few. Typical problems especially in the field of geometric and material nonlinearities are for instance insufficient stress approximations due to unsuitable approximation spaces as well as weak convergence behavior due to stiffening effects or mesh distortions. Similar problems arise in crack or contact problems, where the local determination of discontinuities as well as their development play an important role in many fields of application.

This paper presents the second of two parts of benchmark collections which were compiled within the SPP 1748. Three benchmarks were designed and shall serve as future reference for comparisons with other discretizations, nonlinear and linear solution algorithms. Specifically, the first benchmark concentrates on material interfaces that lead to high gradients or singularities. Therein, two discretization methods, finite elements and isogeometric analysis are compared. In the second benchmark, a phase-field method is applied for two- and three-dimensional propagating fractures. Lastly, again a phase-field fracture benchmark is provided. Therein, the fracture is subject to a constant pressure.

For this setting, even manufactured solutions are known and taken as reference values. In all configurations, all necessary data are provided to reproduce our findings. These data include reference values, computations on mesh hierarchies and various quantities of interest.

## 2 Material interfaces

This collection of benchmarks pose the challenge of resolving material interfaces as well as high gradients or singularities induced by them. Especially discretization methods that avoid geometry conforming meshes, as presented e.g. in [Düster et al. 2017, Joulaian and Düster 2013, Hennig et al. 2019] will find interesting challenges in the presented two-dimensional benchmarks. Some extensions towards three dimensions can be found in [Elhaddad et al. 2017].

In the following benchmarks, the convergence is measured by the relative error in the total energy with respect to the reference solution

$$\|e\|_{\mathcal{U}} = \sqrt{\frac{|\mathcal{U}_{\text{ex}} - \mathcal{U}|}{\mathcal{U}_{\text{ex}}}} \cdot 100\%, \quad (2.1)$$

where  $\mathcal{U}_{\text{ex}}$  and  $\mathcal{U}$  denote the exact and approximated energy, respectively. For a linear elastic problem  $\mathcal{U} = \frac{1}{2} \int_{\Omega} \boldsymbol{\sigma} : \boldsymbol{\varepsilon} d\Omega$  and for a heat conduction problem  $\mathcal{U} = \frac{1}{2} \int_{\Omega} \kappa \nabla u \cdot \nabla u d\Omega$ .

Two types of discretization methods, Isogeometric Analysis (IGA) [Cottrell et al. 2007] and  $p$ -FEM [Szabó and Babuška 1991], are used to provide reference solutions for the energy  $\mathcal{U}_{\text{ex}}$  on locally refined conforming meshes. Curved geometries are represented in IGA using NURBS or B-splines while the blending function method [Szabó and Babuška 1991] is used in the  $p$ -version of the finite element method. The unknown field variable is approximated in IGA using Bézier extraction of truncated hierarchical B-splines [Hennig et al. 2016] in combination with a safe refinement strategy [Hennig et al. 2017]. In  $p$ -FEM geometrically graded meshes are used. In those cases where no analytic solution is available, improved energy values are obtained by the extrapolation technique described in [Szabó and Babuška 1991].

In the following, all material and geometric parameters are given in consistent units.

### 2.1 Circular Inclusion

This benchmark is to test the representation of stress and strain fields across a material interface. The solution on the rest of the domain is smooth and optimal convergence rates should be achieved easily once the discontinuity introduced by the material interface is resolved properly. An analytical solution is available.

**2.1.1 System** The two-dimensional plane strain problem is governed by the partial differential equations of linear elastostatics without body load. Given in the strong form

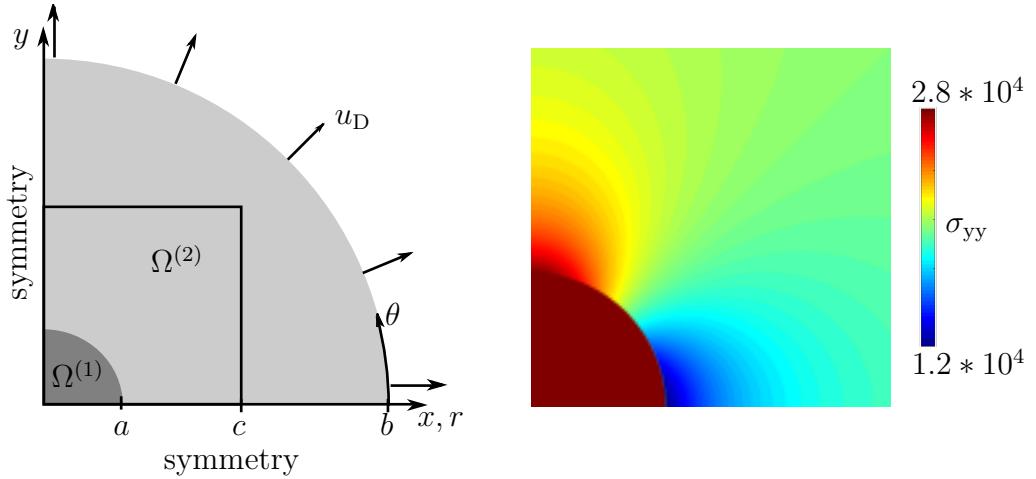


Figure 2.1: Circular inclusion problem: Model problem with domain and boundary condition as well as stress solution for  $\sigma_{yy}$  is illustrated in marked part of the domain.

of the boundary value problem it reads:

$$\nabla \cdot \boldsymbol{\sigma}^{(i)} = \mathbf{0} \quad \forall \mathbf{x} \in \Omega^{(i)}, \quad i = 1, \dots, n, \quad (2.2a)$$

$$\boldsymbol{\sigma}^{(i)} = \mathbb{C}^{(i)} : \boldsymbol{\varepsilon}(\mathbf{u}^{(i)}) \quad \forall \mathbf{x} \in \Omega^{(i)}, \quad i = 1, \dots, n, \quad (2.2b)$$

$$\boldsymbol{\varepsilon}(\mathbf{u}^{(i)}) = \frac{1}{2} \left( \nabla \mathbf{u}^{(i)} + \nabla \mathbf{u}^{(i)\top} \right) \quad \forall \mathbf{x} \in \Omega^{(i)}, \quad i = 1, \dots, n, \quad (2.2c)$$

where  $\Omega^{(1)}, \Omega^{(2)} \subset \mathbb{R}^2$  are defined in Figure 2.1,  $\boldsymbol{\sigma}^{(i)}$  is the stress tensor,  $\mathbb{C}^{(i)}$  the plane strain elastic material tensor,  $\boldsymbol{\varepsilon}$  the strain tensor, and  $\mathbf{u}^{(i)}$  is the displacement vector of the sub-domain  $\Omega^{(i)}$ . The circular inclusion  $\Omega^{(1)}$  has material parameters  $E_1, \nu_1$  and a radius  $a$  that is embedded in an isotropic and linear elastic ( $E_2, \nu_2$ ) disc  $\Omega^{(2)}$  with radius  $b$ . A radial displacement is applied on the outer boundary as depicted in fig. 2.1. The problem can be solved analytically under plane strain conditions leading to the displacement field in polar coordinates [Sukumar et al. 2001]

$$u_r = \begin{cases} \left[ \left( 1 - \frac{b^2}{a^2} \right) \alpha + \frac{b^2}{a^2} \right] r & \text{for } 0 \leq r \leq a \\ \left( r - \frac{b^2}{r} \right) \alpha + \frac{b^2}{r} & \text{for } a \leq r \leq b \end{cases} \quad (2.3)$$

$$u_\theta = 0 \quad (2.4)$$

with

$$\alpha = \frac{(\lambda_1 + \mu_1 + \mu_2)b^2}{(\lambda_2 + \mu_2)a^2 + (\lambda_1 + \mu_1)(b^2 - a^2) + \mu_2 b^2} \quad (2.5)$$

and the Lamé parameters  $\lambda$  and  $\mu$ . The strains are given by  $\epsilon_r = u_{r,r}$  and  $\epsilon_\theta = \frac{u_r}{r}$  and the stresses by  $\sigma_r = 2\mu\epsilon_r + \lambda(\epsilon_r + \epsilon_\theta)$  and  $\sigma_\theta = 2\mu\epsilon_\theta + \lambda(\epsilon_r + \epsilon_\theta)$ .

To reduce the computational effort, the problem is only solved on a square with dimension  $c$  cut out of the cylinder. This setting eases the application of boundary conditions and thereby avoids additional error sources, especially if embedded domain methods with a regular background mesh are used. Homogeneous Dirichlet boundary conditions are applied at the lower and left edge of the square in  $y$  and  $x$  direction, respectively. Neumann

Table 2.1: Circular inclusion problem: Dimensions of the domain in fig. 2.1.

$a$	$b$	$c$
3	15	8

Table 2.2: Circular inclusion problem: Material parameters.

$E^{(1)}$	$\nu^{(1)}$	$E^{(2)}$	$\nu^{(2)}$
$1 \times 10^4$	0.3	$1 \times 10^5$	0.3

Table 2.3: Circular inclusion problem: The strain energy  $\mathcal{U}$  and corresponding degrees of freedom DOF are given for the  $p$ -FEM and IGA ( $p = 4$ ) computation.

$p$ -FEM		IGA, $p_4$	
DOF	$\mathcal{U}/10^6$	DOF	$\mathcal{U}/10^6$
20	1.234078137645319	201	1.239852423077503
194	1.239851448235106	379	1.239852433716069
884	1.239852433865278	903	1.239852433865204
1796	1.239852433865801	2623	1.239852433865802

boundary conditions are applied at the upper and right edge of the square using the analytical stresses.

The dimensions are given in table 2.1 and the material parameters in table 2.2. The analytically computed strain energy is

$$\mathcal{U}_{\text{ex}} = 1.239852433865801 \times 10^6 .$$

**2.1.2 Discretization and Results** An overall impression of the stress state  $\sigma_{yy}$  is provided in fig. 2.1. The jump of the stresses at the material interface is clearly visible.

The  $p$ -FEM discretization uses 5 elements. The circular shape at their boundary is represented exactly using the blending function method, c.f. fig. 2.2. The solution is obtained by keeping the element mesh fixed and uniformly increasing the polynomial degree of the basis functions of each element (uniform  $p$ -refinement).

The IGA discretization is based on 7 NURBS-patches using at least a bi-quadratic basis that allows for an exact geometric representation of the circular inclusion, c.f. fig. 2.2. The basis is  $C^0$ -continuous along the material interface. Due to the absence of singularities and the mild stress concentration, an uniform mesh refinement under constant polynomial degrees was carried out in the convergence studies.

The results of the convergence study are shown in table 2.3 and illustrated in fig. 2.3. It is clearly visible that due to the  $C^0$ -continuous basis along the material interface and the absence of singularities, all methods are able to reproduce optimal convergence rates. For both methods,  $p$ -FEM and IGA with  $p = 4$ , only 1000 degrees of freedom are needed to compute a strain energy that equals the analytically computed strain energy except for the last digit.

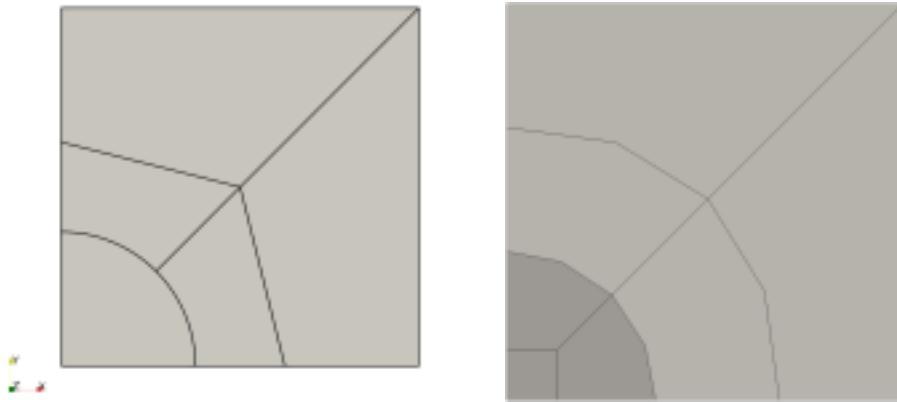


Figure 2.2: Circular inclusion problem: Initial mesh for p-FEM (left) and IGA (right) discretization are illustrated. Please note that the NURBS mesh represents the circle exactly. Linear approximation results from post processing only.

Table 2.4: Elliptical inclusion problem: Dimensions of the domain.

$L$	$r_x$	$r_y$
2	$\sqrt{0.125}$	$0.15r_x$

Table 2.5: Elliptical inclusion problem: Material parameters and traction load.

$E^{(1)}$	$\nu^{(1)}$	$E^{(2)}$	$\nu^{(2)}$	$ \hat{\mathbf{t}} $
$210 \times 10^3$	0.3	$210 \times 10^4$	0.3	100

## 2.2 Elliptical Inclusion

The second benchmark is a linear elastic plane stress problem of an embedded elliptical inclusion. The high aspect ratio of the ellipse leads stress concentrations that have to be resolved.

**2.2.1 System** The model problem is again defined by eq. (2.2), where  $\mathbb{C}^{(i)}$  is the plane stress material tensor,  $\Omega^{(2)}$  is an elliptical inclusion with material parameters  $E_1$ ,  $\nu_1$  and aspect ratio  $r_y/r_x$  that is embedded into a quadratic plate  $\Omega^{(1)}$  with material parameters  $E_2$ ,  $\nu_2$  and dimension  $L$ . The domain and boundary conditions are given in fig. 2.4. The dimensions and material properties are depicted in table 2.4 and table 2.5, respectively. The disc has a loose bearing on the lower and left side and a traction load  $\hat{\mathbf{t}}$  is applied to the right side of the disc.

**2.2.2 Discretization and Results** To validate the extrapolated reference energy, the convergence of the solution is measured in the energy norm for  $p$ -refinement in a FE analysis and for  $h$ -refinement in an isogeometric analysis.

In the case of IGA, 12 patches are used to discretise the computational domain. The elliptical shape of the material interface is represented exactly using NURBS. To properly

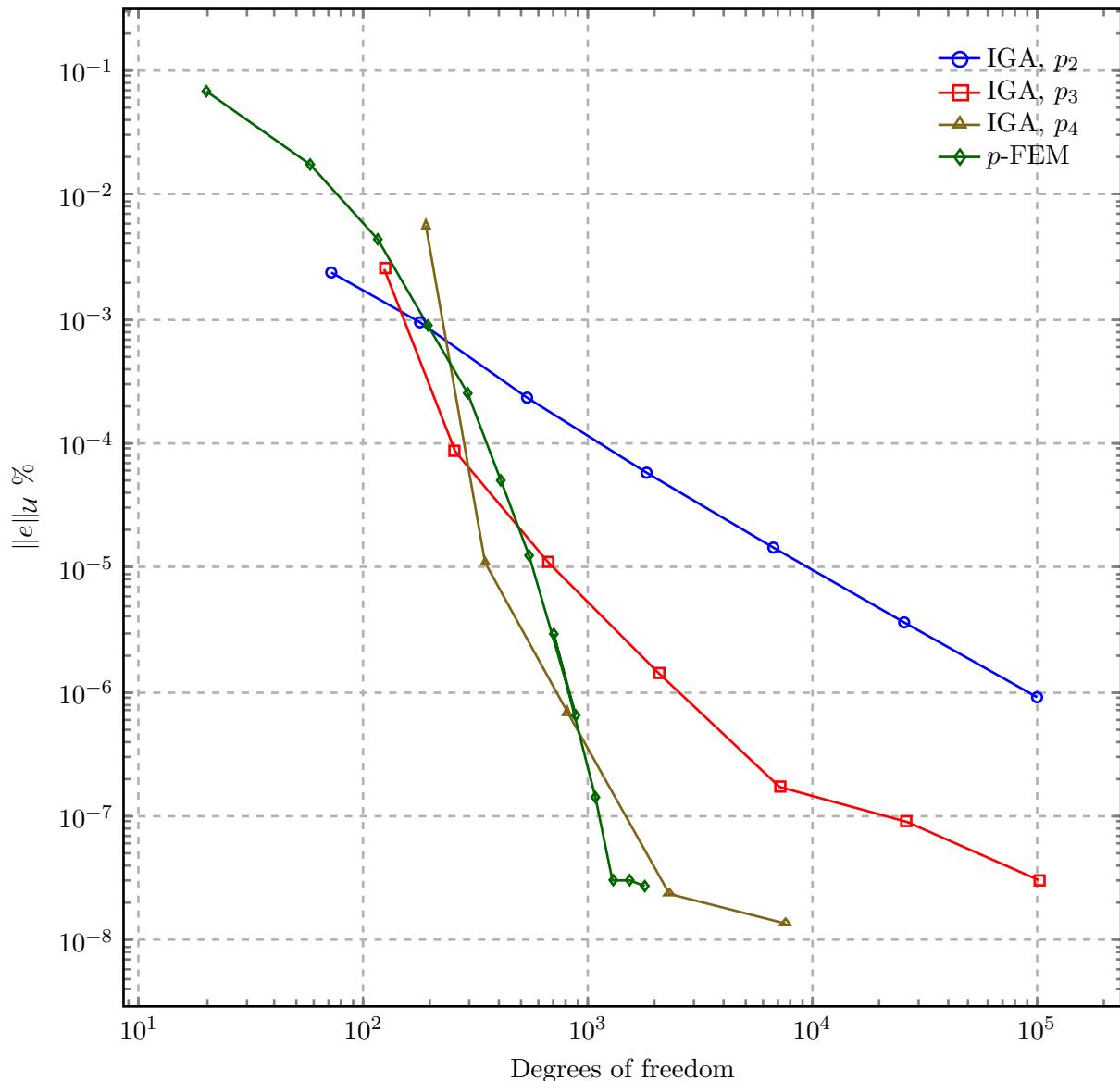


Figure 2.3: Circular inclusion problem: Convergence of total energy.

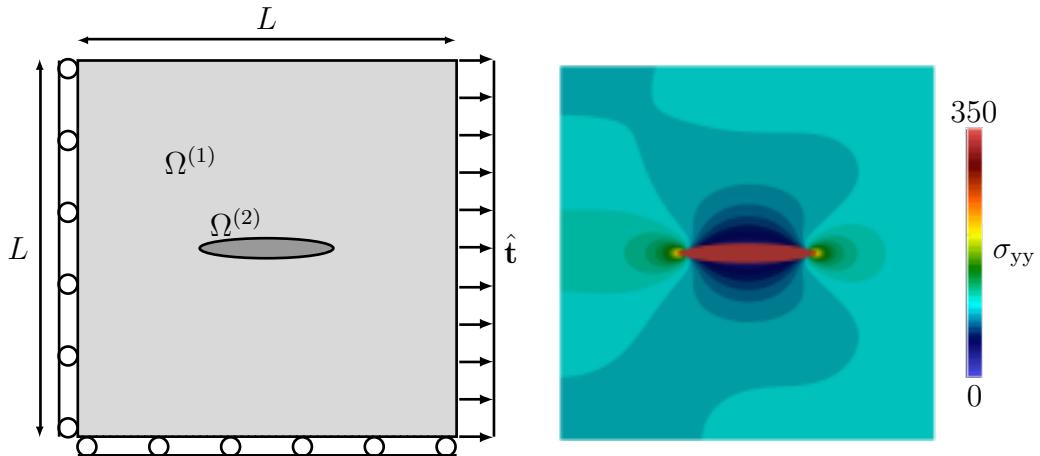


Figure 2.4: Elliptical inclusion problem: Model problem with domain and boundary condition as well as stress solution for  $\sigma_{yy}$  is illustrated.

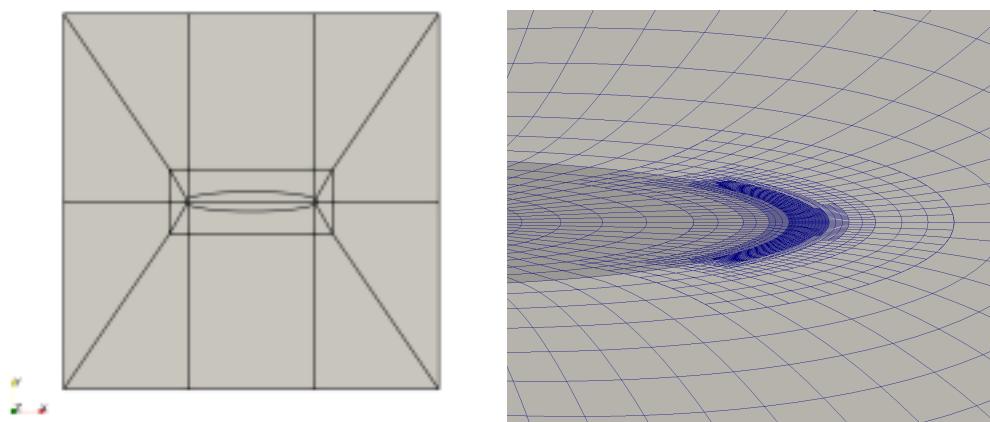


Figure 2.5: Elliptical inclusion problem: Initial mesh for P-FEM (left) and locally refined mesh for IGA (right) discretization are illustrated. In IGA the mesh is refined towards the stress concentration at the material interface.

Table 2.6: Elliptical inclusion problem: The strain energy  $\mathcal{U}$  and corresponding degrees of freedom DOF are given for the  $p$ -FEM and IGA ( $p = 6$ ) computation.

$p$ -FEM		IGA, $p_6$	
DOF	$\mathcal{U}/10^{-2}$	DOF	$\mathcal{U}/10^{-2}$
1934	9.1012391771635864	4785	9.101254710960735017
5302	9.1013093250777097	5323	9.101304183498346023
10334	9.1013110991904414	6553	9.101310846723154046
17030	9.1013111641365024	9347	9.101311158196075112
25390	9.1013111663629354	22059	9.101311166401243602
35414	9.1013111664396851	59127	9.101311166441683475

resolve the stress concentration, the mesh is refined using Bézier extraction of truncated hierarchical B-splines [Hennig et al. 2016] as illustrated in fig. 2.5 on the right. To allow for well graded meshes, a safe refinement strategy is used [Hennig et al. 2017]. Starting from an initial mesh of 768 elements, seven refinement steps are performed for three different polynomial degrees. To also refine the vicinity of the stress concentration, the maximum number of hierarchical levels in a computation is restricted to four.

In the case of  $p$ -FEM, the domain is discretized by a mesh composed of 26 elements with blended edges conforming to the material interface. The mesh is spatially graded towards the stress concentration due to the high curvature of the interface at the major axis of the ellipse. The solution  $\sigma_{yy}$  and the graded meshes are depicted in figs. 2.4 and 2.5. To obtain a reference solution, the energy computed for a discretization with polynomial degrees  $p = 30$  and  $p = 47$  is extrapolated. The extrapolated value is

$$\mathcal{U}_{\text{ex}} = 9.10131116644128 \times 10^{-2} .$$

As shown in table 2.6 and illustrated in fig. 2.6, both discretization methods converge to the extrapolated reference energy.

### 2.3 Inclusion with a corner

The third benchmark is a linear Poisson problem with a sharp inclusion adapted from [Yosibash 1997]. The re-entrant corner at the material interface leads to a singularity in the solution.

**2.3.1 System** This benchmark is governed by the Poisson equation:

$$\kappa^{(i)} \nabla^2 \phi^{(i)} = -1 \quad \forall \mathbf{x} \in \Omega^{(i)} \quad (2.6)$$

$$\phi = 0 \quad \forall \mathbf{x} \in \Gamma_D, \quad (2.7)$$

where  $\phi^{(i)}$  denotes the temperature,  $\kappa^{(i)}$  the thermal diffusivity,  $\Omega^{(i)}$  and  $\Gamma_D$  are defined as shown in fig. 2.7. The dimensions and material properties are given in table 2.7 and table 2.8, respectively. Here, the material interface  $\Gamma_{12}$  has a sharp corner, inducing a vertex singularity. Moreover, the intersection of the material interface with the Dirichlet

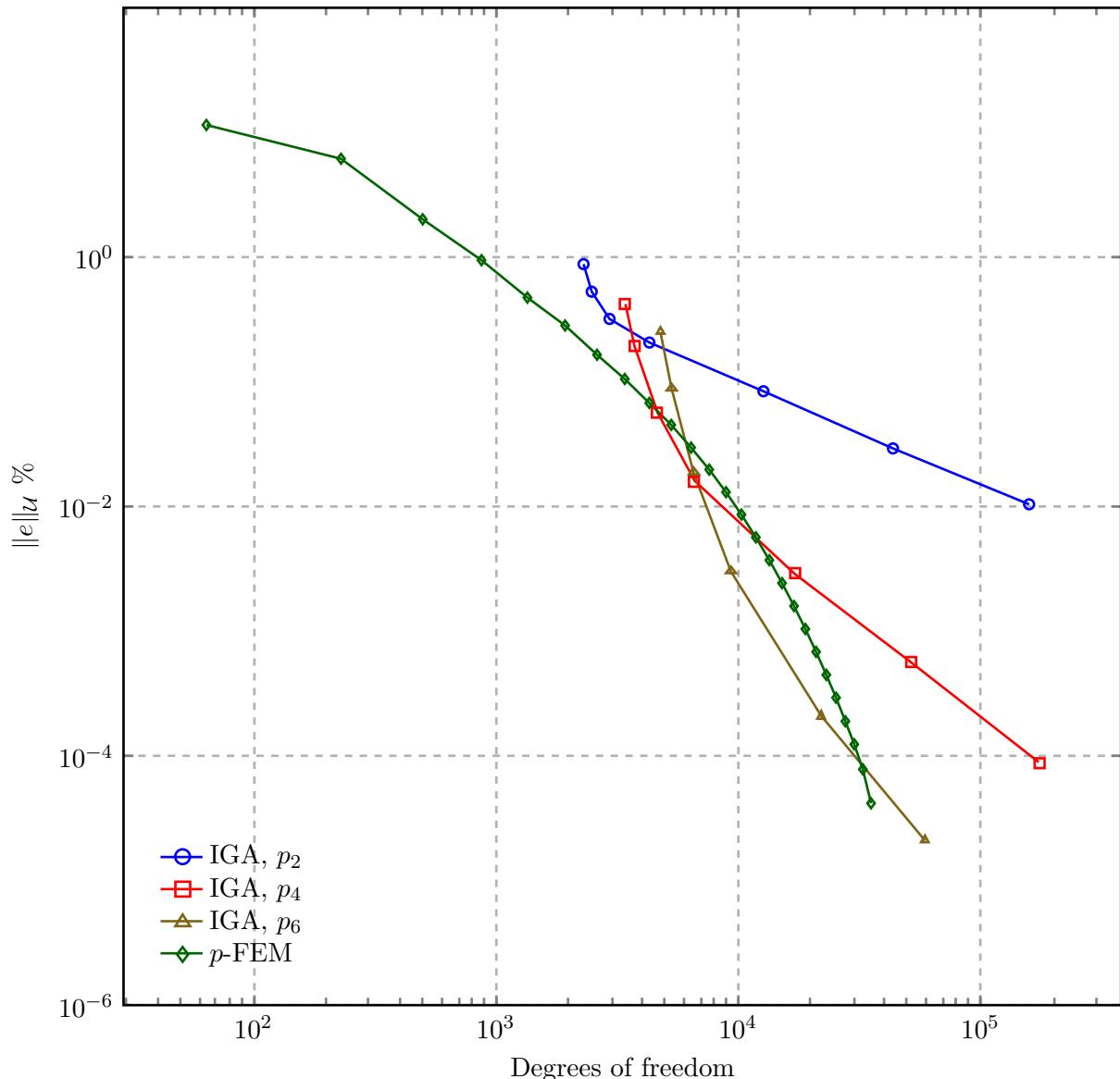


Figure 2.6: Elliptical inclusion problem: Convergence in energy norm

Table 2.7: Inclusion with a corner: Dimensions of the domain in fig. 2.7.

$R$	$\vartheta$
1	$\pi/2$

Table 2.8: Inclusion with a corner: Material parameters and traction load.

$k^{(1)}$	$k^{(2)}$
1	10

boundary  $\Gamma_D$  introduces two additional weak singularities where the solution exhibits reduced continuity.

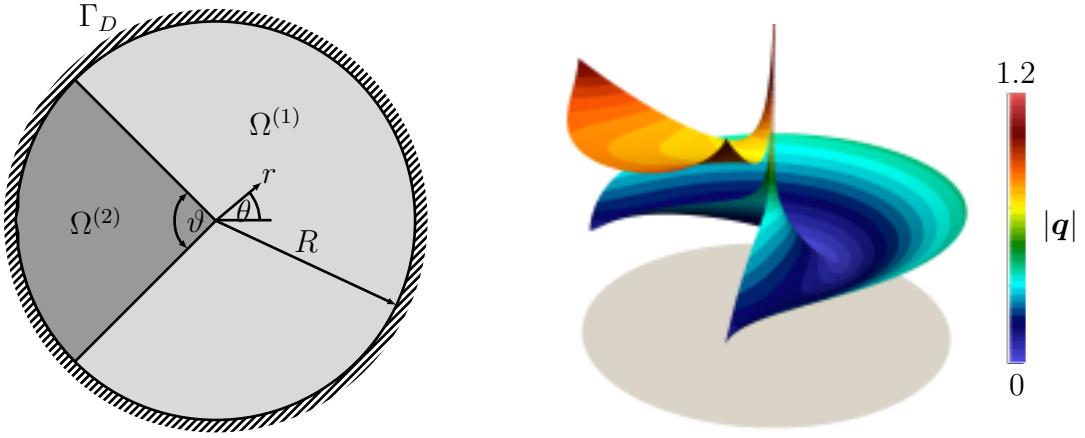


Figure 2.7: Inclusion with a corner: model problem with domain and boundary condition as well as heat flux magnitude is illustrated.

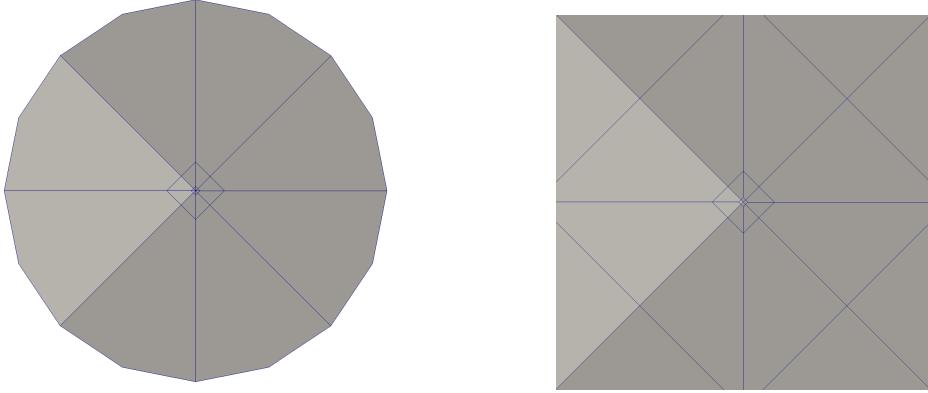


Figure 2.8: Inclusion with a corner: The initial mesh for IGA (left) consists of 28 patches and is locally refined towards the singularity (zoom on the right). The NURBS mesh represents the outer circle exactly. The visible linear approximation results from post processing only.

The exact solution to this problem is given in polar coordinates  $(r, \theta)$  by [Kellogg 1974] :

$$\phi(r, \theta) = A_1 r^{\lambda_1} h_1(\theta) + A_2 r^{\lambda_2} h_2(\theta) + \mathcal{O}(r^2), \quad (2.8)$$

where  $A_1$  and  $A_2$  are scalar constants,  $h_1(\theta)$  and  $h_2(\theta)$  are smooth sinusoidal functions and

$$\lambda_1 = 0.731691779, \quad \lambda_2 = 1.268308221. \quad (2.9)$$

**2.3.2 Discretization and Results** The domain is discretized by 28 NURBS patches with at least quadratic polynomial degree to exactly represent the circular outer boundary of the domain, see fig. 2.8. The initial mesh is locally refined towards the singularity at the re-entrant corner. Due to the local pre-refinement, uniform refinement was applied in the convergence study of the IGA discretization.

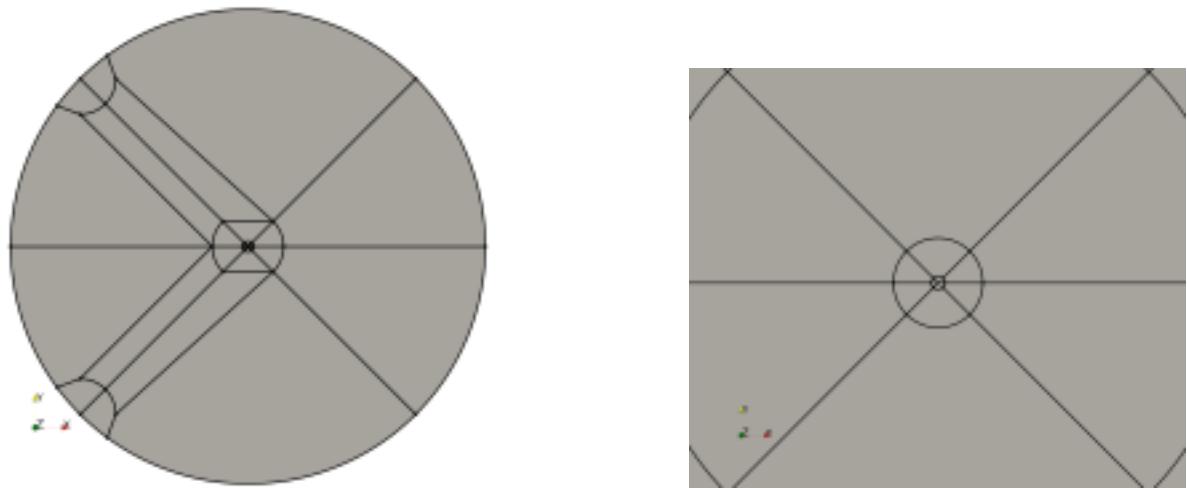


Figure 2.9: Inclusion with a corner: The initial mesh for  $p$ -FEM (left) is locally refined towards the singularity (zoom on the right).

Table 2.9: Inclusion with a corner: The energy  $\mathcal{U}$  and corresponding degrees of freedom DOF are given for the  $p$ -FEM and IGA ( $p = 5$ ) computation.

$p$ -FEM		IGA, $p_5$	
DOF	$\mathcal{U}/10^{-1}$	DOF	$\mathcal{U}/10^{-1}$
41	0.74283160340255783	321	0.83969400295
581	1.0168282915873117	457	0.95680748948
2281	1.0168442811407008	801	1.00201905312
5101	1.0168443147188094	1777	1.01334969314
9041	1.0168443154555366	4881	1.01606662635
14101	1.0168443156940091	15697	1.01668762623
20281	1.0168443158052781	55761	1.01681988939
31651	1.0168443158835522	209617	1.01684404869

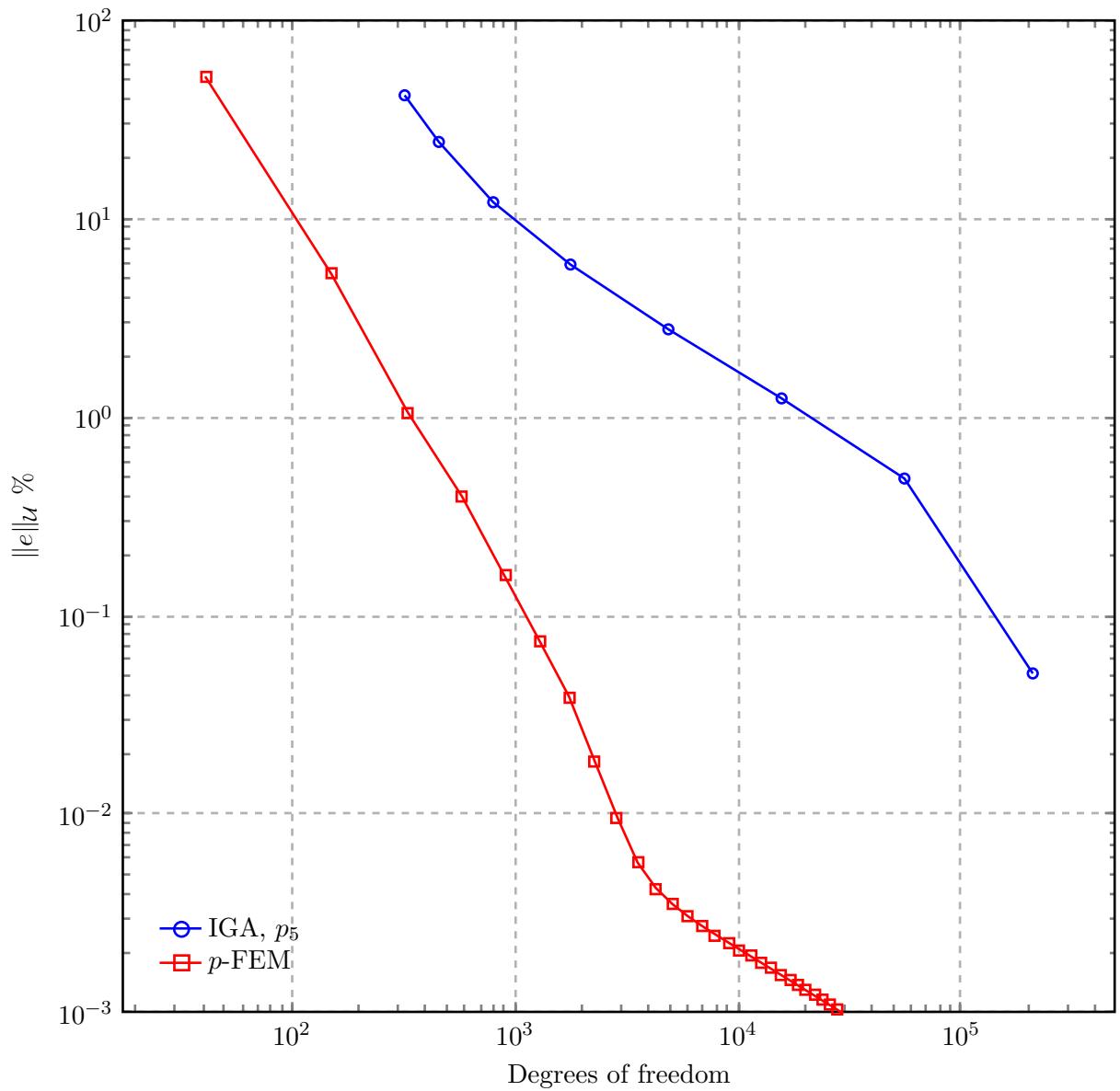


Figure 2.10: Inclusion with a corner: Convergence in energy norm.

The  $p$ -FEM discretization is depicted in fig. 2.9. As in the previous examples, the mesh is conforming to material interface and the domain boundary is exactly represented by means of the blending function method. The mesh is graded geometrically towards the singularity located at the re-entrant corner, see fig. 2.9. The problem is solved by keeping the mesh fixed and performing a uniform  $p$ -extension.

For this example, the extrapolated reference energy is given by

$$\mathcal{U}_{\text{ex}} = 1.016844315974886 \times 10^{-1}.$$

The convergence of the  $p$ -FEM and the IGA discretizations shown in table 2.9 and illustrated in fig. 2.10. In this case the grading of the  $p$ -FEM mesh towards the singularities considerably improves the accuracy per degree of freedom.

### 3 Phase field model for brittle fracture

#### 3.1 Mathematical model

Phase field models for fracture were introduced by the seminal works of Francfort and Marigo [1998], Bourdin et al. [2000], Bourdin [2007]. Initially developed as a regularized version of the fracture mechanical treatment of cracks in the spirit of Griffith, recent extensions treat dynamic and inelastic fracture processes. In order to provide a robust setup for different numerical schemes and discretization methods, the proposed benchmarks are straightforward and disregard special problems concerning the distinction between tension and compression, as well as subtleties in the evolution equation. Details on these issues can for example be found in Kuhn [2012].

With these preliminary remarks, we state the governing differential equations, which follow the original work of Bourdin [2007]. Starting point is the free energy density of the system

$$\Psi(\boldsymbol{\varepsilon}, s) = (s^2 + \eta)W(\boldsymbol{\varepsilon}) + \mathcal{G}_c \left( \frac{1}{4\epsilon}(1-s)^2 + \epsilon|\nabla s|^2 \right) \quad (3.1)$$

which depends on the strain field  $\boldsymbol{\varepsilon}$  and the fracture field  $s$ . The meaning of  $s$  is the following: If  $s = 1$  the material is intact, while  $s = 0$  represents the fully broken material. The parameters  $\mathcal{G}_c$  and  $\epsilon$  describe the cracking resistance (related to the fracture toughness) and the width of the regularization zone. The parameter  $\eta$  models the residual stiffness of the fully broken material ( $s = 0$ ). The residual stiffness is required to ensure a non vanishing stiffness in a static analysis. In (3.1)  $W(\boldsymbol{\varepsilon})$  represents the elastic strain energy density. If an isotropic material behavior is assumed the strain energy density can be expressed with the help of the two Lamé constants  $\lambda$  and  $\mu$  by

$$W(\boldsymbol{\varepsilon}) = \frac{1}{2}\lambda(\text{tr } \boldsymbol{\varepsilon})^2 + \mu \boldsymbol{\varepsilon} : \boldsymbol{\varepsilon} \quad \text{with} \quad \boldsymbol{\varepsilon} = \frac{1}{2}(\nabla \mathbf{u} + \nabla^T \mathbf{u}) \quad (3.2)$$

where  $\boldsymbol{\varepsilon}$  is the linearized strain, and  $\mathbf{u}$  represents the displacement field. The ":" in (3.2) indicates the scalar product between two second order tensors, and "tr" is the trace of a second order tensor. The free energy density (3.1) defines the stress  $\boldsymbol{\sigma}$  via

$$\boldsymbol{\sigma} = \frac{\partial \Psi}{\partial \boldsymbol{\varepsilon}} = (s^2 + \eta)(\lambda \text{tr } \boldsymbol{\varepsilon} \mathbf{1} + 2\mu \boldsymbol{\varepsilon}) \quad (3.3)$$

where  $\mathbf{1}$  is the second order identity tensor. The stress has to satisfy the equilibrium condition

$$\operatorname{div} \boldsymbol{\sigma} = \mathbf{0}, \quad (3.4)$$

with "div" as the divergence. Thus volume forces are neglected. The static mechanical problem has to be supplied with proper boundary conditions, either Dirichlet conditions

$$\mathbf{u} = \mathbf{u}^* \quad \text{on } \partial\mathcal{B}_u \quad (3.5)$$

with prescribed displacements  $\mathbf{u}^*$  on the displacement boundary  $\mathcal{B}_u$ , or Neumann conditions

$$\boldsymbol{\sigma} \mathbf{n} = \mathbf{t}^* \quad \text{on } \partial\mathcal{B}_\sigma \quad (3.6)$$

with prescribed traction  $\mathbf{t}^*$  on the traction boundary  $\mathcal{B}_\sigma$ . The vector  $\mathbf{n}$  denotes the outward unit normal. The fracture field  $s$  is governed by an nonlocal evolution equation, which is driven by the variational derivative of the free energy with respect to  $s$ . In the terminology of phase field models this evolution equation is also referred to as the time dependent Ginzburg-Landau equation:

$$\dot{s} = -M \frac{\delta \Psi}{\delta s} = M \left[ 2\mathcal{G}_c \epsilon \Delta s - 2s W(\boldsymbol{\varepsilon}) + \frac{\mathcal{G}_c}{2\epsilon} (1-s) \right], \quad (3.7)$$

where  $\dot{s}$  is the rate of  $s$  with respect to time  $t$ , and " $\Delta$ " denotes the Laplace operator. The mobility constant  $M$  has to chosen sufficiently large to approximate quasi-static crack growth conditions. The fracture field is also associated with either Dirichlet conditions

$$s = s^* \quad \text{on } \partial\mathcal{B}_s \quad (3.8)$$

with prescribed fracture field  $s^*$  on the Dirichlet boundary  $\mathcal{B}_s$ , or Neumann conditions

$$\partial s_n = \nabla s \cdot \mathbf{n} = q^* \quad \text{on } \partial\mathcal{B}_q \quad (3.9)$$

with prescribed flux  $q^*$  on the flux boundary  $\partial\mathcal{B}_q$ . Frequently, homogeneous Neumann boundary conditions are set on the fracture field  $s$  and  $s$  is set to zero at certain locations to model initial cracks. Additionally, the fracture field  $s(\mathbf{x}, t)$  has to be supplied by initial conditions, as (3.7) is a first order differential equation in time  $t$ . Thus, we must provide:

$$s(\mathbf{x}, 0) = s_0(\mathbf{x}). \quad (3.10)$$

If the material is unbroken and no preexisting cracks are treated,  $s_0(\mathbf{x}) = 1$  everywhere.

To conclude the presentation of the mathematical model some remarks are given:

- the fracture field  $s$  is bounded  $s \in [0, 1]$
- different evolution strategies are possible, see Kuhn [2012]
  - damage-like behavior:  $\dot{s} \leq 0$
  - indicator-like behavior:  $\dot{s} = 0$  if  $s = 0$
- different solution strategies are possible
  - monolithic solution of (3.4) and (3.7)
  - staggered solution of (3.4) and (3.7)

using the stress from (3.3) and strain energy density from (3.2) in both strategies.

### 3.2 3D setup

In Fig. 3.1 a 3D initial-boundary value problem is defined on a block-like geometry. The block is loaded on a part of its top surface by a linearly increasing displacement load, while being fixed on the lower surface.

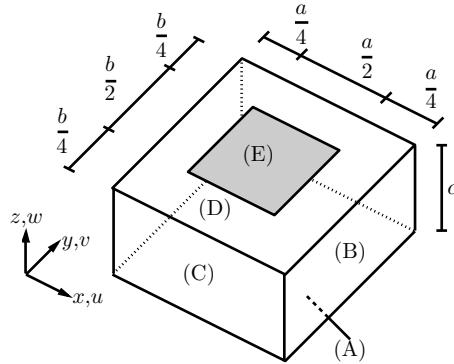


Figure 3.1: Geometry of the 3D benchmark problem

The following dimensionless parameters are used:

$$\text{Geometry parameters: } a = 2, b = 2, c = 1 \quad (3.11)$$

Material and model parameters:

$$\lambda = 100000, \mu = 100000, \epsilon = 0.1, \eta = 0.0001, \mathcal{G}_c = 1, M = 10 \quad (3.12)$$

$$\text{Initial conditions at } t = 0: \quad s_0 = 1 \quad (3.13)$$

Boundary conditions on the surfaces (A)-(E):

$$\begin{aligned} (\text{A}) : \quad & u = 0, v = 0, w = 0, \quad \partial_n s = 0 \\ (\text{B}) : \quad & \sigma_{xx} = 0, \sigma_{xy} = 0, \sigma_{xz} = 0, \quad \partial_n s = 0 \\ (\text{C}) : \quad & \sigma_{yy} = 0, \sigma_{xy} = 0, \sigma_{yz} = 0, \quad \partial_n s = 0 \\ (\text{D}) : \quad & \sigma_{zz} = 0, \sigma_{xz} = 0, \sigma_{yz} = 0, \quad \partial_n s = 0 \\ (\text{E}) : \quad & u = 0, v = 0, w = 0.01t, \quad s = 1 \end{aligned} \quad (3.14)$$

This setup leads to a crack initiation in the bulk. The crack then propagates to the top surface resulting in a shell like fracture surface. Intermediate steps of the computation are reported in Fig. 3.2. The finest mesh of Tab. 3.1 is used for the plots in Fig. 3.2.

The results are obtained by standard 8-node finite elements with tri-linear shape functions. The same spatial interpolation is used for  $u$ ,  $v$ ,  $w$  and  $s$ . The time integration of (3.7) is done by an implicit/backward Euler scheme using adaptive time step control. The initial time step is set to  $\Delta t = 0.01$ . The time step  $\Delta t$  is halved if the Newton method for the increments does not converge in 8 iterations. This time step halving is repeated at most 10 times. The time step  $\Delta t$  is increased to twice its value if 4 or less Newton iterations are required. Using  $n$  elements along the edges  $a$ ,  $b$  and  $c$ , the number of degrees of freedom (d.o.f.) is reported in Tab. 3.1. The monolithic solution strategy was used. As a quantitative result, the reaction force  $F$  in  $z$ -direction on the segment (E)

$$F = \int_{A(\text{E})} \sigma_{zz} dA \quad (3.15)$$

is reported with respect to the prescribed displacement  $w$  in Fig. 3.3.

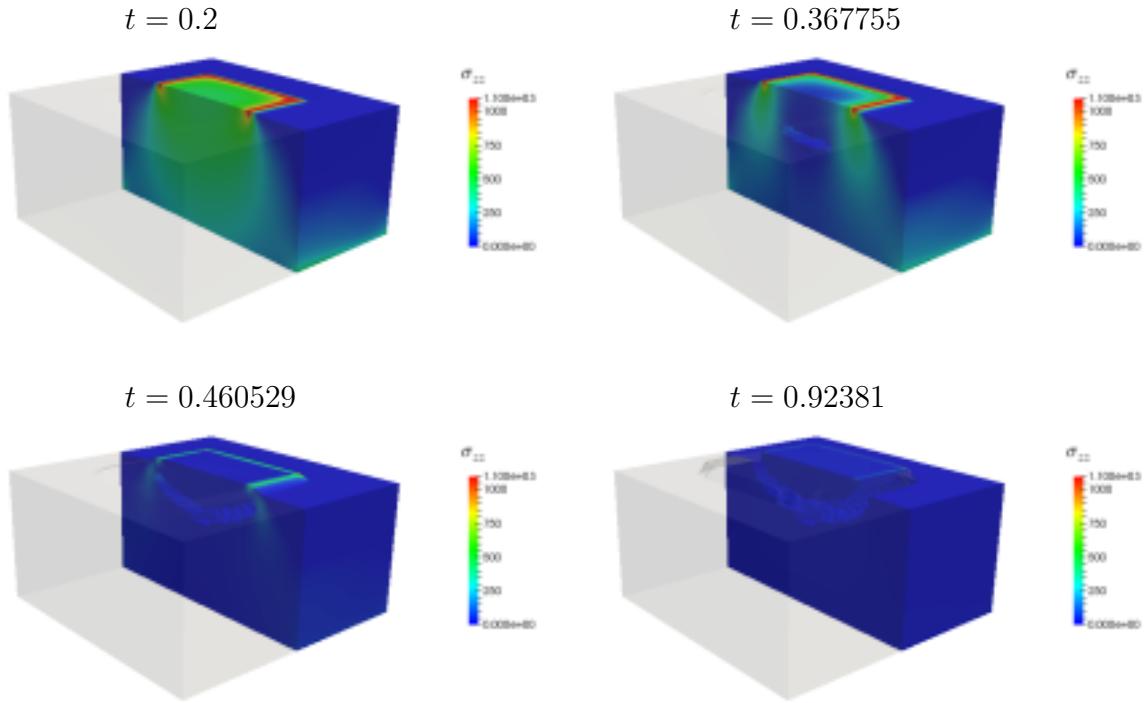


Figure 3.2: Evolution of crack configuration and normal stress  $\sigma_{zz}$  at four time steps ( $t = 0.2 / 0.367755 / 0.460529 / 0.92381$ ). Elements with  $s < 0.05$  are suppressed in the plots to indicate fracture.

Table 3.1: Number of degrees of freedom for different spatial discretisations

$n$	10	20	30	40	50	60
d.o.f.	4,861	35,237	115,381	268,877	520,301	892,917

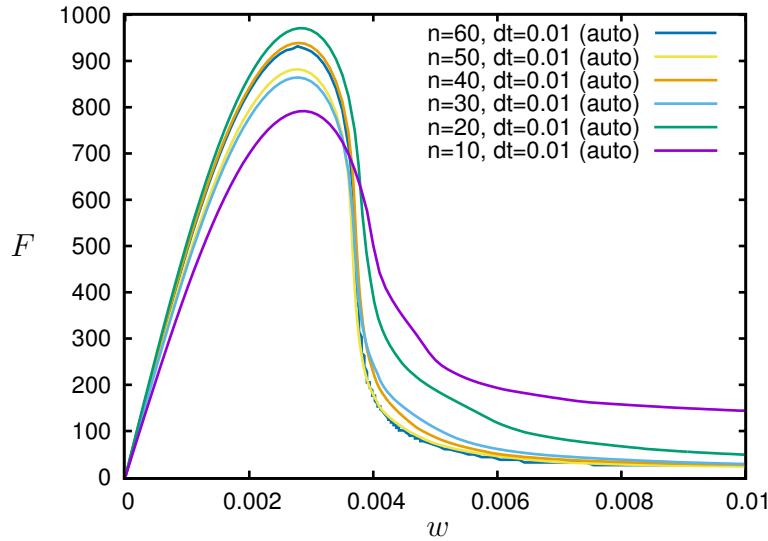


Figure 3.3: Displacement-reaction force curve for different spatial discretisations

### 3.3 2D setup

In Fig. 3.4 a 2D initial-boundary value problem is defined on a block geometry. The block is loaded on a half of its top surface by a linearly increasing displacement load, while being fixed on the lower surface.

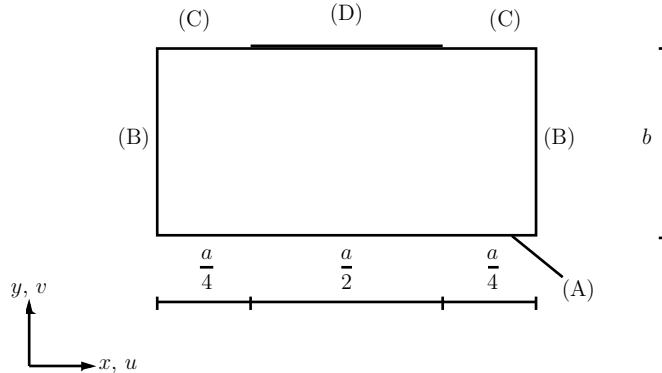


Figure 3.4: Geometry of the 2D benchmark problem

The following dimensionless parameters are used:

$$\text{Geometry parameters: } a = 2, b = 1 \quad (3.16)$$

Material and model parameters:

$$\lambda = 100000, \mu = 100000, \epsilon = 0.1, \eta = 0.0001, \mathcal{G}_c = 1, M = 10 \quad (3.17)$$

$$\text{Initial conditions at } t = 0: \quad s_0 = 1 \quad (3.18)$$

Boundary conditions on the surfaces (A)-(D):

$$\begin{aligned} (\text{A}) : \quad & u = 0, v = 0, \quad \partial_n s = 0 \\ (\text{B}) : \quad & \sigma_{xx} = 0, \sigma_{xy} = 0, \quad \partial_n s = 0 \\ (\text{C}) : \quad & \sigma_{yy} = 0, \sigma_{xy} = 0, \quad \partial_n s = 0 \\ (\text{D}) : \quad & u = 0, v = 0.01t, \quad s = 1 \end{aligned} \quad (3.19)$$

This setup leads to a crack initiation in the bulk. The crack then propagates to the top surface resulting in an arch like fracture line. Intermediate steps of the computation are reported in Fig. 3.5. The plots in Fig. 3.5 are computed by a discretization of  $100 \times 100$  elements. The results are obtained by standard 4-node finite elements with bi-linear shape functions. The same spatial interpolation is used for  $u$ ,  $v$  and  $s$ . The time integration of (3.7) is done by an implicit/backward Euler scheme using adaptive time step control. The initial time step is set to  $\Delta t = 0.01$ . The time step  $\Delta t$  is halved if the Newton method for the increments does not converge in 8 iterations. This time step halving is repeated at most 10 times. The time step  $\Delta t$  is increased to twice its value if 4 or less Newton iterations are required. Using  $n$  elements along the edges  $a$  and  $b$ , the number of degrees of freedom (d.o.f.) is reported in Tab. 3.2. The monolithic solution strategy was used. As a quantitative result the overall reaction force  $F$  in  $y$ -direction on the segment (D)

$$F = \int_{A(\text{D})} \sigma_{yy} dA \quad (3.20)$$

is reported with respect to the displacement  $v$  in Fig. 3.6.

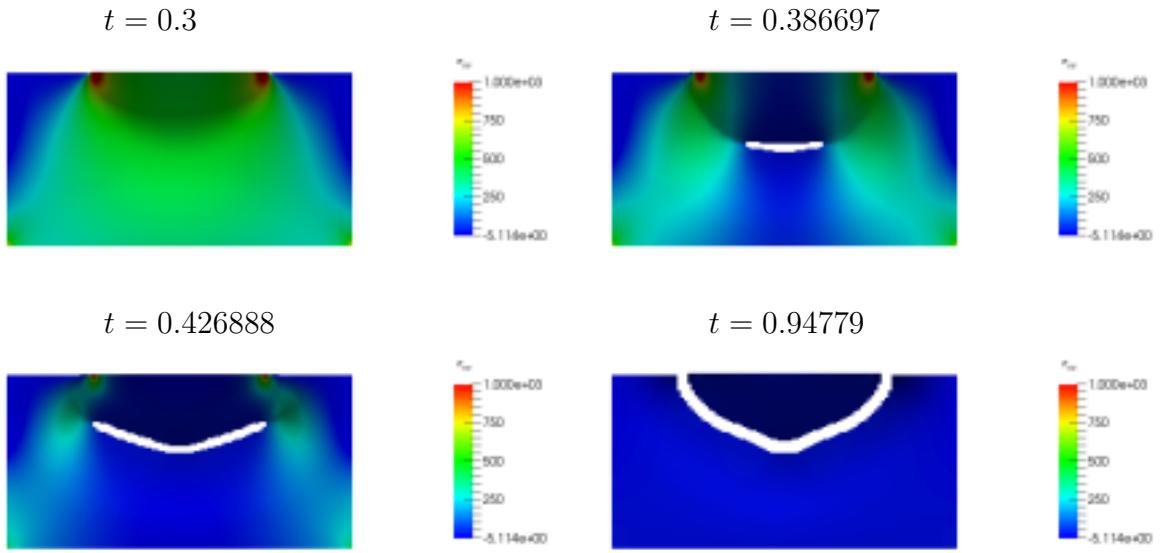


Figure 3.5: Evolution of crack configuration and normal stress  $\sigma_{zz}$  at four time steps ( $t = 0.3 / 0.386697 / 0.426888 / 0.94779$ ). Elements with  $s < 0.05$  are suppressed in the plots to indicate fracture.

Table 3.2: Number of degrees of freedom for different plane discretizations

$n$	25	50	75	100	125	150
d.o.f.	1,940	7,626	17,061	30,248	47,190	67,876

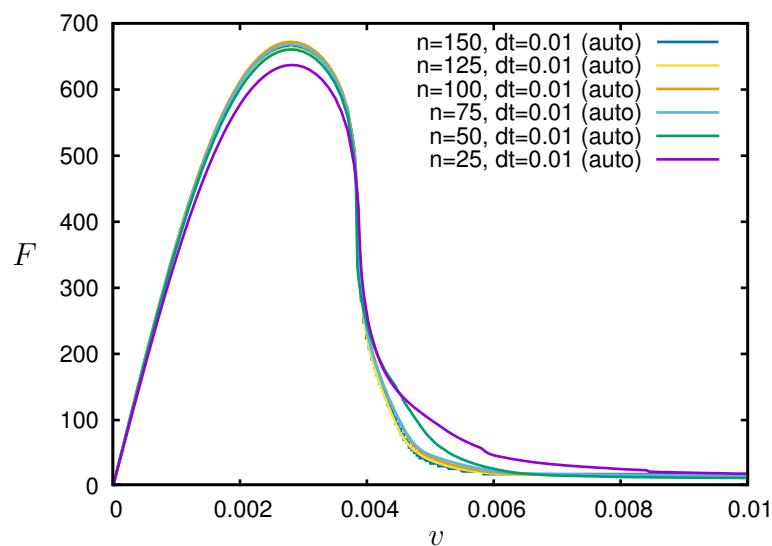


Figure 3.6: Displacement-reaction force curve for different plane discretizations

## 4 Quasi-static pressure-driven cavity

### 4.1 Introduction

In this benchmark, we consider a lower-dimensional fracture in a  $d$ -dimensional domain. For the time being we restrict ourselves to  $d = 2$ . This fracture has a constant length and varying width (also known in the literature as aperture, crack opening displacement or COD). The driving force is a given constant pressure prescribed in the fracture. The setting is motivated by the book of Sneddon and Lowengrub [Sneddon and Lowengrub 1969] and therefore known as ‘Sneddon’ benchmark or ‘pressure-driven cavity’. Analytical solutions are derived in Sneddon and Lowengrub [1969] and are also discussed in [Bourdin et al. 2012]. Subsequently, [Wheeler et al. 2014, Heister et al. 2015] coin the proposed benchmark, and provide numerical results.

### 4.2 Equations

In this section, we introduce the used notation and state the governing equations. In the following, the  $L^2$  product is denoted as  $(\cdot, \cdot)$ :

$$(x, y) := \int_{\Omega} x \cdot y \, d\Omega,$$

and for vector-valued quantities by

$$(X, Y) := \int_{\Omega} X : Y \, d\Omega.$$

The domain  $\Omega \subset \mathbb{R}^d$  ( $d = 2$  for the 2D benchmark problem) is an open, connected and bounded set. The crack  $C$  is a one-dimensional set contained in  $\Omega$ .

**4.2.1 The energy formulation** The Francfort-Marigo functional [Francfort and Marigo 1998] describes the energy of a crack in an elastic medium as

$$E(u, C) = \frac{1}{2}(\sigma, e(u)) - \int_C \tau \cdot u \, ds + G_C \mathcal{H}^1(C), \quad (4.1)$$

where  $u : \Omega \rightarrow \mathbb{R}^d$  is the vector-valued displacement function and  $\sigma = \sigma(u)$  the classical stress tensor of linearized elasticity defined as

$$\sigma(u) := 2\mu e(u) + \lambda \operatorname{tr}(e(u))I,$$

with the Lamé parameters  $\mu, \lambda > 0$ . The symmetric strain tensor  $e(u)$  is defined as

$$e(u) := \frac{1}{2}(\nabla u + \nabla u^T).$$

The energy functional  $E$  consists of three terms: a bulk energy term, a traction energy, and a crack energy contribution. Specifically, traction forces are denoted by  $\tau$ . The critical

energy release rate is denoted by  $G_C > 0$ . The term  $\mathcal{H}^1(C)$  stands for the Hausdorff measure denoting the length of the crack.

Combining this notation with the poro-elastic stress  $\sigma_{\text{poro}} = \sigma - \alpha p I$  with the Biot coefficient  $\alpha \in [0, 1]$  and including the phase-field variable  $\varphi$ , we get the following energy functional Mikelić et al. [2019]:

$$E(u, C) = \frac{1}{2}(\sigma, e(u)) - (\alpha - 1)(\varphi^2 p, \text{Div } u) + (\varphi^2 \nabla p, u) + G_C \mathcal{H}^1(C),$$

where  $p : \Omega \rightarrow \mathbb{R}$  is a given pressure.

**Remark 1** *The considered benchmark setting in this study is posed in an elastic medium. For this reason, we set  $\alpha = 0$ . Moreover, a constant pressure is applied, and therefore the pressure gradient is zero, i.e.,  $\nabla p = 0$ . This yields the simplified energy functional*

$$E(u, C) = \frac{1}{2}(\sigma, e(u)) + (\varphi^2 p, \text{Div } u) + G_C \mathcal{H}^1(C),$$

*which is used in the following.*

Following Bourdin et al. [2000], the crack  $C$  is approximated by a continuous phase-field variable  $\varphi : \Omega \rightarrow [0, 1]$ , which is zero in the crack and one in the unbroken solid with a transition zone with size  $\epsilon > 0$ . The regularization parameter  $\epsilon > 0$  allows control of the diffusive transition zone. So the crack surface energy  $G_C \mathcal{H}^1(C)$  in equation (4.1) can be reformulated to an elliptic Ambrosio-Tortorelli functional, which yields:

### Formulation 1 (Regularized energy functional for pressurized fractures)

$$\begin{aligned} E_\epsilon(u, \varphi) &= \frac{1}{2} \left( ((1 - \kappa)\varphi^2 + \kappa) \sigma(u), e(u) \right) + (\varphi^2 p, \text{Div } u) \\ &\quad + G_C \left( \frac{1}{2\epsilon} \|1 - \varphi\|^2 + \frac{\epsilon}{2} \|\nabla \varphi\|^2 \right), \end{aligned}$$

*where  $\kappa$  is a positive regularization parameter for the elastic energy with  $\kappa \ll \epsilon$ .*

**Formulation 2 (Fracture energy minimization under constraint)** *Find functions  $u$  and  $\varphi$  for almost all times  $t$  with*

$$\min E_\epsilon(u, \varphi) \quad s. t. \quad \partial_t \varphi \leq 0. \quad (4.2)$$

*The constraint realizes the crack irreversibility. Physically-speaking: the crack cannot heal. To derive an incremental version, the constraint is discretized in time via:*

$$\frac{\varphi(t^{n+1}) - \varphi(t^n)}{t^{n+1} - t^n} \leq 0.$$

**Remark 2** *We notice that this benchmark setting is a stationary test case. Due to the crack irreversibility constraint, we compute a few time step solutions in order to converge to this stationary limit.*

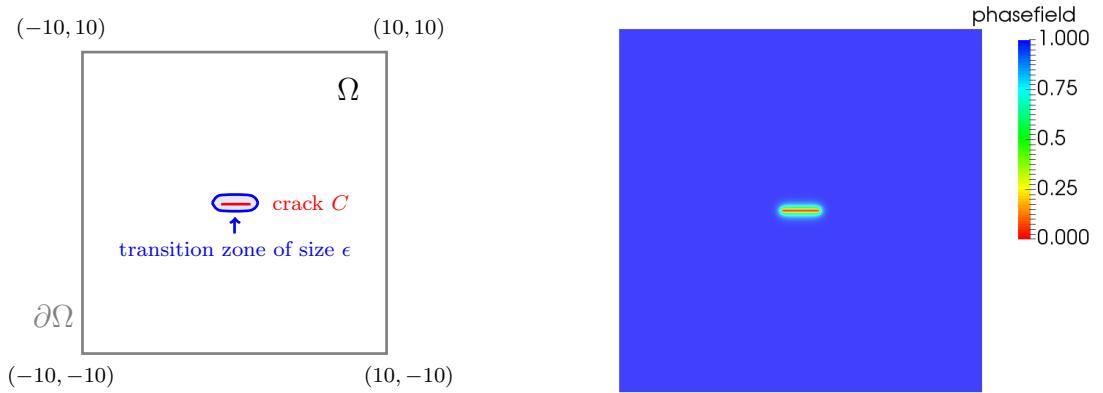


Figure 4.1: Domain  $\Omega$  (in 2D) with Dirichlet boundaries  $\partial\Omega$ , an initial crack  $C$  of length  $2l_0$  and a zone of width  $\epsilon$ , where the phase-field function  $\varphi$  is defined.

**4.2.2 The weak formulation** Our weak formulation is based on [Heister et al. 2015]. With

$$V := H_0^1(\Omega), \quad W_{\text{in}} := \{w \in H^1(\Omega) | w \leq \varphi^{n-1} \leq 1 \text{ a.e. on } \Omega\}, \quad \text{and} \quad W := H^1(\Omega),$$

we obtain the following weak formulation of equation (4.2).

**Formulation 3 (Euler-Lagrange System of Formulation 2)** Find  $(u, \varphi) \in V \times W$  with

$$((((1 - \kappa)\varphi^2 + \kappa)\sigma(u), e(w)) + (\varphi^2 p, \text{Div } w) = 0 \quad \forall w \in V,$$

and

$$(1 - \kappa)(\varphi\sigma(u) : e(u), \psi - \varphi) + 2(\varphi p \text{Div } u, \psi - \varphi) + G_C \left( -\frac{1}{\epsilon}(1 - \varphi, \psi - \varphi) + \epsilon(\nabla\varphi, \nabla(\psi - \varphi)) \right) \geq 0 \quad \forall \psi \in W_{\text{in}} \cap L^\infty(\Omega).$$

### 4.3 A 2D pressurized fracture

The theoretical calculations of Sneddon [Sneddon 1946] and Sneddon and Lowengrub [Sneddon and Lowengrub 1969] form the basis of this example. All settings to simulate the benchmark of the given pressurized fracture problem are listed in the following sections.

#### 4.3.1 Setup

**4.3.1.1 Domain definition** The two-dimensional domain  $\Omega = (-10, 10)^2$  is sketched in Figure 4.1.

**4.3.1.2 Initial conditions** An initial crack with length  $2l_0 = 2.0$  and thickness  $d$  of two cells on  $\Omega_c = [-1, 1] \times [-d, d] \subset \Omega$  is prescribed by help of the phase-field function  $\varphi$ , i.e.,  $\varphi = 0$  in  $\Omega_c$  and  $\varphi = 1$  in  $\Omega \setminus \Omega_c$ . Note that the thickness of  $2d$  corresponds to  $2h/\sqrt{2}$ .

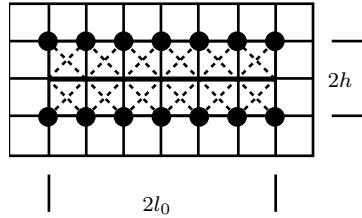


Figure 4.2: Zoom-in to the center of the domain  $\Omega$ . The lower-dimensional crack with length  $2l_0 = 2.0$  (middle line in black) is approximated as a volume by extending it by one cell in normal up and down direction.

**4.3.1.3 Boundary conditions** As boundary conditions, the displacements  $u$  are set to zero on  $\partial\Omega$ . For the phase-field variable, we use homogeneous Neumann conditions (traction free), i.e.,  $\epsilon\partial_n\varphi = 0$  on  $\partial\Omega$ .

**4.3.1.4 Parameter settings** The determined parameter values are listed in Table 4.1.

Table 4.1: Setting of the benchmark and numerical parameters in 2D.

Parameter	Definition	Value
$\Omega$	Domain	$(-10, 10)^2$
$h$	cell diameter (diagonal)	
$l_0$	Half crack length	1.0
$G_c$	Fracture toughness	1.0
$E$	Young's modulus	1.0
$\nu$	Poisson's ratio	0.2
$p$	Injected pressure	$10^{-3}$
$TOL_t$	Tolerance time step loop	$10^{-5}$
$\epsilon$	Bandwidth of the crack	$4h$
$\kappa$	Regularization parameter	0

If it is of interest to compute the exact values of the Lamé coefficients  $\lambda$  and  $\mu$ , the converting formulae are:  $\lambda = \frac{\nu E}{(1+\nu)(1-2\nu)}$  and  $\mu = \frac{E}{2(1+\nu)}$ .

**4.3.2 Quantities of interest** As benchmark comparisons, we propose the following quantities of interest:

1. Section 4.3.2.1: Crack opening displacement (COD) as a function of the  $x$  coordinate;
2. Section 4.3.2.2: The maximal COD<sub>max</sub> in the middle of the fracture;
3. Section 4.3.2.3: Total volume of the crack (TCV);
4. Section 4.3.2.4: Bulk energy;

### 5. Section 4.3.2.5: Crack energy.

For the COD, COD<sub>max</sub> and TCV, manufactured reference values can be computed for a infinite domain from the formulae presented in [Sneddon and Lowengrub 1969][Section 2.4]. We restate the corresponding formulae below and provide the reference values for our proposed material, and model parameters. In our comparisons, the reference values on an infinite domain are denoted by **reference Sneddon**. Additionally, we provide values based on fine computations on adaptively refined meshes for the finite domain. See Heister and Wick [2018]for more details about the used method. These reference values are denoted by **reference adaptive**. Here, we also calculate the errors between the **reference adaptive** solution and our numerical results. These errors are ‘relative’ errors computed via

$$\frac{|\text{numerical result} - \text{reference adaptive}|}{|\text{reference adaptive}|}.$$

**4.3.2.1 Crack opening displacement** The width or crack opening displacement (COD) under spatial mesh refinement can be measured in the numerical tests. The width is defined as

$$\text{COD}(x) := [u \cdot n](x) \approx \int_{-\infty}^{\infty} u(x, y) \cdot \nabla \varphi(x, y) \, dy, \quad (4.3)$$

where  $x \in [-1, 1]$  the  $x$ -coordinate along the integral in  $y$  direction. The reference value for a infinite domain (cf. Sneddon and Lowengrub [Sneddon and Lowengrub 1969]) is given by:

$$\text{COD}_{\text{ref}}(x) = 2 \frac{p l_0}{E'} \left(1 - \frac{x^2}{l_0^2}\right)^{1/2} = 1.92 \times 10^{-3} \left(1 - \frac{x^2}{l_0^2}\right)^{1/2}, \quad (4.4)$$

where  $p$  is the applied pressure,  $l_0$  is the half crack length and  $E' := \frac{E}{1-\nu^2}$ .

**4.3.2.2 Maximum crack opening displacement** We evaluate the COD in the middle of the fracture (due to symmetry the maximum is attained at  $x = 0$ ):

$$\text{COD}_{\text{max}} := [u \cdot n](0) \approx \int_{-\infty}^{\infty} u(0, y) \cdot \nabla \varphi(0, y) \, dy.$$

**4.3.2.3 Total crack volume** The total crack volume (TCV) can be computed numerically using

$$\text{TCV}_{h,\epsilon} = \int_{\Omega} u(x, y) \cdot \nabla \varphi(x, y) \, d(x, y). \quad (4.5)$$

A formula for the limit can be obtained using Sneddon and Lowengrub [1969]. Using symmetry of the configuration, i.e.,  $u_y(x, 0^+) = -u_y(x, 0^-)$ , and the known crack location  $[-1, 1] \times \{0\}$ , one obtains

$$\text{TCV}_{2D} = 2 \int_{-\infty}^{\infty} u_y(x, 0^+) \, dx,$$

where  $0^\pm$  denotes the respective limit from above or below, and  $u_y$  denotes the second ( $y$ ) component of the displacement.

Using the exact representation of  $u_y$  (cf. Sneddon and Lowengrub [1969], page 29)

$$u_y(x, 0^+) = \frac{pl_0}{E'} \left(1 - \frac{x^2}{l_0^2}\right)^{1/2}$$

we obtain:

$$\text{TCV}_{2D} = \int_{-\infty}^{\infty} 2u_y(x, 0^+) \, dx = \frac{2\pi pl_0^2}{E'}. \quad (4.6)$$

Applied to our parameter settings, we consequently obtain the reference value for an infinite domain as:

$$\text{TCV}_{2D} \approx 6.03186 \times 10^{-3}.$$

In the following, the formula to compute bulk and crack energy as two further numerical quantities of interest are given.

**4.3.2.4 Bulk energy** Next, we compute the bulk energy  $E_B$  given by

$$E_B = \int_{\Omega} ((1 - \kappa)\varphi^2 + \kappa)\psi(e) \, d(x, y). \quad (4.7)$$

The strain energy functional  $\psi(e)$  in equation (4.7) is defined as

$$\psi(e) := \mu \operatorname{tr}(e(u)^2) + \frac{1}{2}\lambda \operatorname{tr}(e(u))^2.$$

Here, no manufactured reference values are provided and we only present values computed numerically.

**4.3.2.5 Crack energy** Finally, we compute the crack energy

$$E_C = \frac{G_C}{2} \int_{\Omega} \left( \frac{(\varphi - 1)^2}{\epsilon} + \epsilon |\nabla \varphi|^2 \right) \, d(x, y). \quad (4.8)$$

Again, no manufactured reference values are provided and we only present values computed numerically.

## 4.4 Numerical Results for the 2D Benchmark

**4.4.1 Solution approaches** We use  $H^1$  conforming finite elements on quadrilaterals (2D). Specifically, we use bilinear elements  $Q_1^c$  Ciarlet [2002] for both, the displacements and the phase-field variable. In accordance with Heister et al. [Heister et al. 2015], a monolithic approach with an extrapolation of the phase-field variable in the displacement equation is used.

To treat the variational inequality, we employ a primal-dual active set method (again following [Heister et al. 2015]) with the recent open-source code published in Heister and Wick [2018] based on deal.II Arndt et al. [2019]. Furthermore, we emphasize that in this benchmark setting we exclusively use uniform mesh refinement.

The benchmark is sensitive to how the phase field variable is initialized from the given initial condition in 4.3.1.2. We use nodal interpolation<sup>1</sup> of the piecewise bi-linear finite element variable as shown in Figure 4.2. Using an  $L^2$  projection (or any other form of projection) instead, yields slightly different benchmark results.

The overall nonlinear discrete problem is then solved with a Newton method in which (when necessary), globalization is achieved with a simple backtracking line search method.

The code for the benchmarks performed here, again based on the Finite Element library deal.II Arndt et al. [2019], is available at [https://github.com/tjhei/cracks/tree/sneddon\\_spp\\_benchmark](https://github.com/tjhei/cracks/tree/sneddon_spp_benchmark) including all necessary parameter files.

**4.4.2 Numerical results** In the following sections all numerical results for the determined quantities of interest are given and compared to reference values.

We start the computation with a structured mesh of 10 by 10 cells, where each cell has an extent of 2 by 2 units and a diameter  $h = \sqrt{8} \approx 2.828$ . From there, we refine the mesh globally, cutting the size of each cell by a factor of 2 in each step.

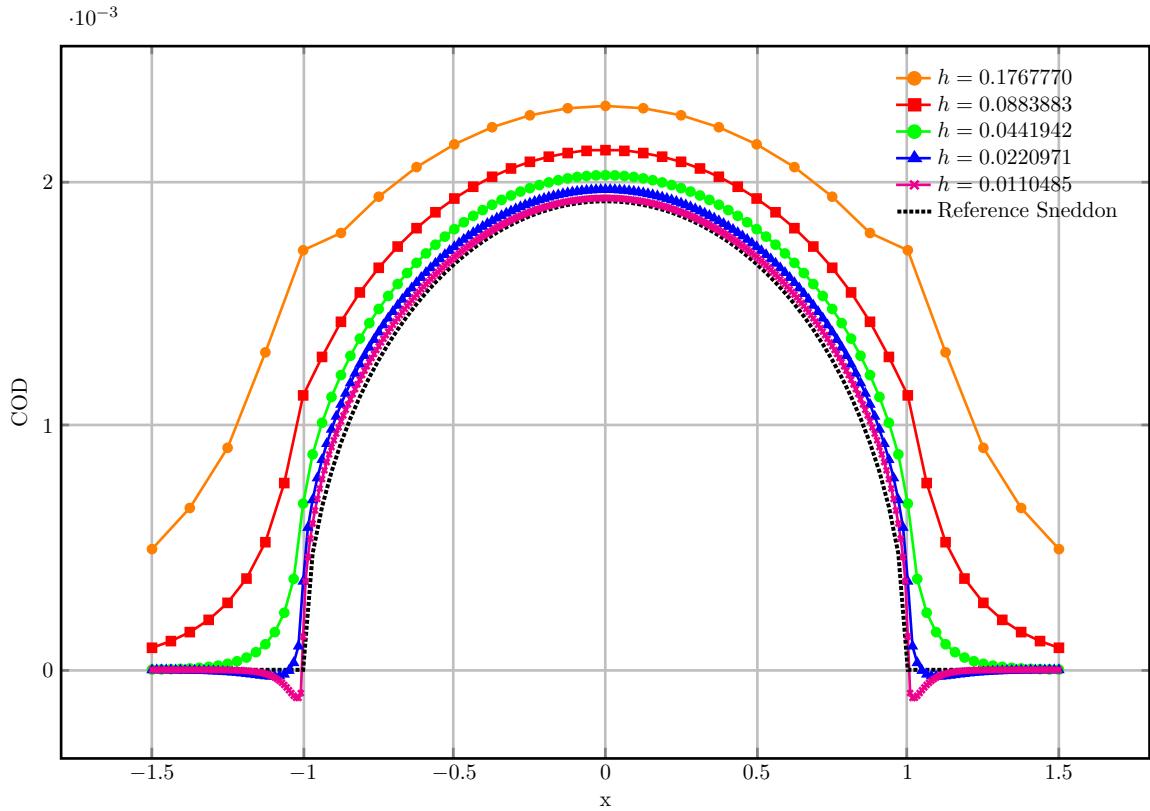
**Remark 3** *Keep in mind that the reference values of COD and TCV in the previous section are valid for  $\epsilon = 0$  and for an infinite domain  $\Omega_\infty$ . While we can expect convergence of the results presented here against the reference values with  $\epsilon \rightarrow 0$ , the problem is still given on a finite domain. Therefore, convergence against these reference values can not be expected.. Instead, we compare with numerical results on the same finite domain but on very fine, adaptively refined meshes from Heister and Wick [2018]. The reference values from Sneddon/Lowengrub are denoted as Reference Sneddon, while the numerical reference values are denoted as Reference adaptive.*

**4.4.2.1 COD (quantity of interest No. 1)** Figure 4.3 shows the crack opening displacements (COD), computed with equation (4.3), over the width of the crack for several tests with different sizes of the mesh size parameter  $h$ . The computations correspond to 4 to 8 global refinements of the initial mesh. The dotted black line gives the exact COD values from equation (4.4).

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<sup>1</sup>In deal.II done using VectorTools::interpolate().

Figure 4.3: Benchmark 3: Crack opening displacements (COD) for various refinement levels.



**4.4.2.2 Maximum COD (quantity of interest No. 2)** To compare the COD values at one fixed point, in Table 4.2 the values of  $\text{COD}_{\max}$  using equation (4.3) are listed and the (relative) error of the numerical COD value in comparison to the computed value on a adaptively refined mesh (Reference adaptive) are given.

Table 4.2: Benchmark 3: Numerical  $\text{COD}_{\max}$  values for five refinement levels in 2D and respectively the error to reference values based on an adaptively refined mesh Heister and Wick [2018]. For comparison, the exact  $\text{COD}_{\max}$  given by Sneddon and Lowengrub (Reference Sneddon) for an infinite domain is listed.

	DoF	$h$	$\text{COD}_{\max}$	Rel. error to adapt.
	77,763	0.1767770	$2.31073 \times 10^{-3}$	0.22166
	309,123	0.0883883	$2.12944 \times 10^{-3}$	0.12581
	1,232,643	0.0441942	$2.02688 \times 10^{-3}$	0.07159
	4,922,883	0.0220971	$1.96789 \times 10^{-3}$	0.04040
	19,676,163	0.0110485	$1.93355 \times 10^{-3}$	0.02225
Reference adaptive Heister and Wick [2018]	-	-	$1.89147 \times 10^{-3}$	-
Reference Sneddon on $\Omega_\infty$	-	-	$1.92000 \times 10^{-3}$	-

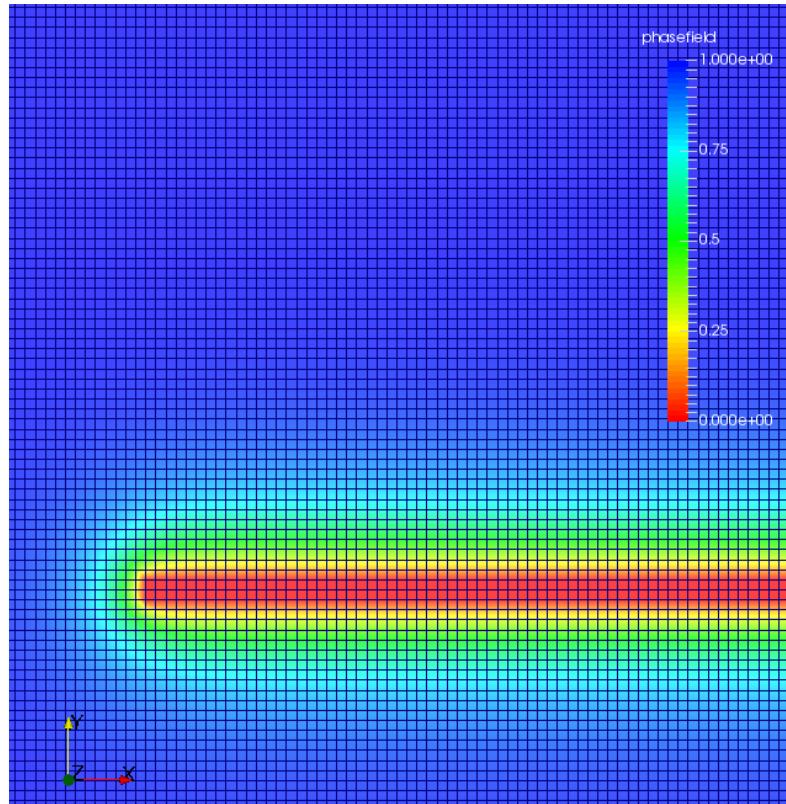


Figure 4.4: Benchmark 3: A zoom of the left half of the pressurized fracture based on the setup in 2D with 7 refinements: 4,922,883 degrees of freedom,  $h = 0.0220971$ .

**4.4.2.3 Total crack volume (quantity of interest No. 3)** In Table 4.3, the computed values of the total crack volume equation (4.5) are provided for five mesh refinement levels and compared to the exact TCV value equation (4.6).

Table 4.3: Benchmark 3: Total crack volume for five refinement levels in 2D and respectively the error to reference values based on an adaptively refined mesh (Reference adaptive) Heister and Wick [2018]. For comparison we include the exact TCV given by Sneddon and Lowengrub for an infinite domain.

	DoF	$h$	TCV	Rel. error to adapt.
	77,763	0.1767770	$11.31650 \times 10^{-3}$	0.90536
	309,123	0.0883883	$8.18239 \times 10^{-3}$	0.37767
	1,232,643	0.0441942	$6.91774 \times 10^{-3}$	0.16474
	4,922,883	0.0220971	$6.39662 \times 10^{-3}$	0.07699
	19,676,163	0.0110485	$6.16564 \times 10^{-3}$	0.03810
Reference adaptive Heister and Wick [2018]		-	$5.93930 \times 10^{-3}$	-
Reference Sneddon on $\Omega_\infty$		-	$6.03186 \times 10^{-3}$	-

**4.4.2.4 Bulk and crack energies (quantity of interest No. 4 and No. 5)** For the bulk and crack energy no reference values are provided. Here, in Table 4.4, the bulk and crack energy values are shown for five mesh refinement levels using the definitions of equation (4.7) and equation (4.8), respectively.

Table 4.4: Benchmark 3: Bulk and crack energy for five refinement levels in 2D. Relative error with respect to adaptively refined mesh (Reference adaptive) Heister and Wick [2018].

DoF	$h$	Bulk energy	Rel error	Crack energy	Rel. error
77,763	0.1767770	$5.86652 \times 10^{-6}$	0.9746	3.43192	0.4566
309,123	0.0883883	$4.06538 \times 10^{-6}$	0.3684	2.89463	0.2285
1,232,643	0.0441942	$3.38745 \times 10^{-6}$	0.1402	2.62540	0.1143
4,922,883	0.0220971	$3.13916 \times 10^{-6}$	0.0566	2.49078	0.0571
19,676,163	0.0110485	$3.04430 \times 10^{-6}$	0.0247	2.42347	0.0286
Reference adaptive Heister and Wick [2018]	-	$2.97093 \times 10^{-6}$	-	2.35616	-

## 5 Conclusions

In this second part of the SPP 1748 benchmark collection, we proposed three studies. In the first benchmark, material interfaces were considered. Therein, two discretization methods, finite elements and isogeometric analysis are compared, which show very good agreements for various inclusion configurations. In the second benchmark, a phase-field fracture method was applied to two settings. First a three dimensional configuration and then a two-dimensional setting. As quantity of interest, displacement-reaction curves were adopted. In the last benchmark, a pressurized fracture in elasticity was considered for which numerical and manufactured reference values were generated. Moreover, some codes are open-source to reproduce the presented findings. All benchmarks shall serve as future reference for other discretization methods and other numerical solution algorithms.

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