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Phase field modeling with IGA and FEM: Error surveillance in the transition zone

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The present contribution compares the solution of a phase field problem by the finite element method (FEM) with isogeometric analysis (IGA). For the sake of simplicity, the coupling to additional fields is neglected. Thus, the phase field variable appears as the only unknown in the boundary value problem. The numerical solutions are compared to the analytical solution, elaborated by Falk, of the Allen-Cahn equation. In this model, the Ginzburg-Landau free energy density combines a free Landau energy of sixth order with a quadratic gradient energy. The benchmark consists of a simple quadrilateral geometry with boundary conditions for the phase field variable which allows to solve static unidirectional phase transitions. For the FEM, the mesh is refined uniformly in space by h- and p-refinement. In IGA, the refinement is realized by the knot insertion and order elevation algorithms from computer aided design (CAD) which is known as k-refinement. Furthermore, IGA allows for a higher continuity between the elements which enhances the gradient of the phase transition variable.

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1 Fundamental equations for a phase field model

The phase field model stems from a Ginzburg-Landau type energy density formulation which is given by

$$\Psi = \Psi_w(\varphi) + \Psi_g(\nabla\varphi), \tag{1}$$

in which φ and $\nabla\varphi$ denote the phase-field variable and its gradient respectively. The first term represents the Landau energy and the second term describes the gradient energy. The local balance of the phase transition problem is given according to

$$\lambda\frac{\partial\varphi}{\partial t} = \nabla\cdot\boldsymbol{\mu} - \eta \qquad \text{with} \qquad \eta = \frac{\partial\Psi_w}{\partial\varphi}, \quad \boldsymbol{\mu} = \frac{\partial\Psi_g}{\partial\nabla(\varphi)}, \tag{2}$$

in which η denotes the internal microforce, $\boldsymbol{\mu}$ is known as the internal microstress and λ is regarded as the inverse mobiliy parameter. The boundary of the phase-field domain is composed by two non-intersecting regions known as Dirichlet $\partial\mathcal{B}_D$ and Neumann $\partial\mathcal{B}_N$ boundary. On these boundaries, the following conditions apply

$$\varphi = \varphi^* \text{ on } \partial\mathcal{B}_D \qquad \text{and} \qquad \boldsymbol{\mu}\cdot\boldsymbol{n} = 0 \text{ on } \partial\mathcal{B}_N. \tag{3}$$

Under the consideration of the boundary condition (3).2, the weak form of balance is defined by

$$G := \int_{\mathcal{B}} \boldsymbol{\mu}\cdot\nabla\delta\varphi + (\eta + \lambda\dot{\varphi})\delta\varphi \,\mathrm{dV} = 0, \tag{4}$$

which has to be solved by the Newton-Raphson scheme. By this means, the linearization of the equation is provided as

$$\mathrm{Lin}G := \overset{*}{G} + \int_{\mathcal{B}} (\frac{\partial\boldsymbol{\mu}}{\partial\nabla\varphi}\cdot\nabla\Delta\varphi)\cdot\nabla\delta\varphi + \frac{\partial\eta}{\partial\varphi}\Delta\varphi\delta\varphi + \lambda\Delta\dot{\varphi}\delta\varphi \,\mathrm{dV}. \tag{5}$$

The numerical implementation in the FEM framework can be reviewed in [1]. In the mentioned work, the focus lies on an enhanced formulation for the phase transition problem. Furthermore, an Euler-backward scheme is considered for the time discretization which is also chosen for the present contribution. In contrast to [1], IGA is considered as the numerical framework. This means that NURBS are used as shape functions for the discretization of the geometry and solution field. In this setting, the discretization is performed in the parametric space of the geometry by a so called knot insertion and order elevation algorithm which is known as k-refinement. A remarkable property of this method is given by the higher continuity of the shape functions between neighboring elements. For a fundamental introduction to IGA, contribution [2] is suggested.

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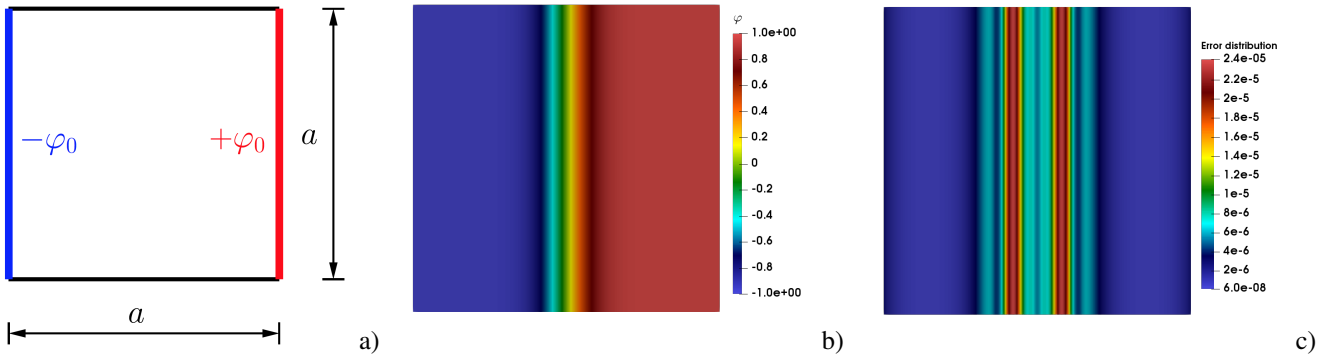

Fig. 1: 2D plate model for phase transition. **a** Geometry and boudary conditions. **b** Numerical solution. **c** Error distribution.

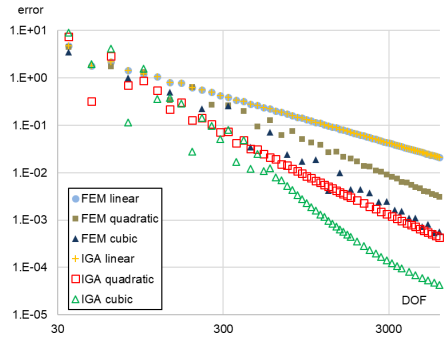

Fig. 2: Error analysis for FEM and IGA.

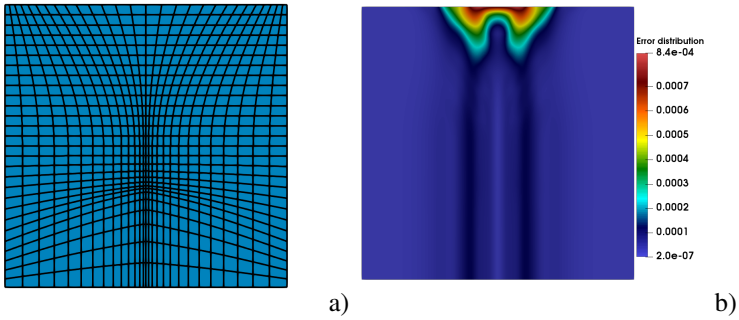

Fig. 3: 2D plate with distorted mesh. **a** Mesh. **b** Error distribution

2 Numerical results

In the present study, the numerical results are compared with an analytical solution of a 1D phase transition which was developed by Falk [3] and revised to the present model in [1]. The Ginzburg-Landau energy of the model is given by

$$\Psi_a = \varphi_a^6 - \varphi_a^4 - \varphi_a^2 + (\nabla\varphi_a)^2. \tag{6}$$

The initial example considers a 2D plate as depicted in Fig. 1.a). The length of the plate is given with $a = 10$ with the Dirichlet boundary condition of $\varphi_0 = 1$ on the left and right hand side. The discretization is performed by means of IGA with 53 x 53 quadratic NURBS elements resulting in 2915 degrees of freedom. The phase field distribution of the numerical result is depicted in Fig. 1.b) in which it can be observed, that the phase transition takes place in a narrow region in the center of the plate. Furthermore, the error distribution, which is given as the absolute difference between the analytical and numerical solution, is shown in Fig. 1.c). Here it can be noted, that the maximal error appears in the region of the highest change of the phase field gradient.

The second example provides a comparison of the IGA formulation with the FEM. For this purpose, the overall solution error is defined by $e := \int_{\mathcal{B}} |\varphi_a - \varphi| \mathrm{d}V / \int_{\mathcal{B}} \mathrm{d}V$. Regarding the interpolation order, linear, quadratic and cubic shape functions are considered for both methods. Furthermore, an increasing mesh refinement is performed. The results of the study are shown in Fig. 2. As expected, the results of linear IGA and FEM coincide since linear NURBS are identical to linear Lagrange polynomials. For higher orders it is observed, that the convergence rates of both methods are similar, but IGA leads to a more precise solution than FEM for a given amount of degrees of freedom.

The last example renders the effects of a mesh distortion, see Fig. 3.a), on the results of the IGA phase field model. To this purpose, the lower part of the mesh is distorted in vertical direction while the upper part is distorted horizontally. Since the phase transition takes place in horizontal direction, the vertical distortion (lower part) has a neglectable influence on the result, while the horizontal distortion (upper part) leads to a deterioration of the numerical analysis, see Fig. 3.b).

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