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Received July 2005
Revised January 2006
Accepted October 2006

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Abstract

Purpose – This paper aims to show that simple geometry-based *hp*-algorithms using an explicit *a posteriori* error estimator are efficient in wave propagation computation of complex structures containing geometric singularities.

Design/methodology/approach – Four different *hp*-algorithms are compared with common *h*- and *p*-adaptation in electrostatic and time-harmonic problems regarding efficiency in number of degrees of freedom and runtime. An explicit *a posteriori* error estimator in energy norm is used for adaptive algorithms.

Findings – Residual-based error estimation is sufficient to control the adaptation process. A geometry-based *hp*-algorithm produces the smallest number of degrees of freedom and results in shortest runtime. Predicted error algorithms may choose inappropriate kind of refinement method depending on *p*-enrichment threshold value. Achieving exponential error convergence is sensitive to the element-wise decision on *h*-refinement or *p*-enrichment.

Research limitations/implications – Initial mesh size must be sufficiently small to confine influence of phase lag error.

Practical implications – Information on implementation of *hp*-algorithm and use of explicit error estimator in electromagnetic wave propagation is provided.

Originality/value – The paper is a resource for developing efficient finite element software for high-frequency electromagnetic field computation providing guaranteed error bound.

Keywords Electromagnetic fields, Finite element analysis, Algorithmic languages

Paper type Research paper

Introduction

It is natural to perform simulations in frequency domain, when structures are designed for a specific operation frequency or a frequency band. The FE-FD method is well suited for this task. Literature is vast about this method. The mathematical side of finite element method (FEM) is well explained (Brenner and Ridgway Scott, 2002). See Salazar-Palma *et al.* (1998), Jin (2002) and Monk (2003) for FEM application in electromagnetics.

Any discretisation method suffers from discretisation error (Salazar-Palma *et al.*, 1998), thus mesh adaptation and self adaptivity are appealing issues for simulation algorithms. Adaptation methods have to rely on some local (element-wise) *a posteriori*

COMPEL: The International Journal for Computation and Mathematics in Electrical and Electronic Engineering
Vol. 26 No. 2, 2007
pp. 431-446

0332-1649
DOI 10.1108/03321640710727782

error estimate. Different estimators are in use (Verfürth, 1996; John, 2000; Babuška and Strouboulis, 2001; Melenk and Wohlmuth, 2001; Verfürth, 2005). There are explicit and implicit residual estimators as well as the method of patch recovery, which was originally proposed by Zienkiewicz and Zhu (1987) (ZZ estimator). During adaptation, the number of degrees of freedom (DOF) in an element with error greater than a given tolerance is increased in order to obtain the largest possible error reduction. There are two possible means for increasing the number of DOF. The first widely used type is the *h*-refinement (with h being the mesh size), where an element is split up into sub-elements. Neighbouring elements need to be subdivided to retain mesh conformity, when not using hanging nodes. Earlier approaches (Ratnajeevan and Hoole, 1990; Fernandez *et al.*, 1993; Golias *et al.*, 1994; Díaz-Morcillo *et al.*, 2000; Tsuji and Koshiba, 2000) concentrate on *h*-adaptivity by introducing error estimates and criteria whether to refine a mesh cell or not. *h*-refinement is needed in case of singularities or phase lag at high wave numbers (Ihlenburg and Babuška, 1997; Babuška and Strouboulis, 2001; Monk, 2003; Ainsworth, 2004) and results in polynomial convergence. The second method to reduce error is to increase polynomial order p of the shape functions. This method is called *p*-enrichment and results in exponential error convergence $\mathcal{O}(h^p)$ if the solution is smooth and phase lag error can be neglected (Salazar-Palma *et al.*, 1998; Monk, 2003; Ainsworth, 2004). Thus, we favour local *p*-enrichment whenever possible. The *hp*-version combines both methods as an up-to-date but less common adaptation method in engineering. New algorithms are still evolving in the mathematic and engineering community using different approaches (Melenk and Wohlmuth, 2001; Bangerth and Rannacher, 2003; Heuveline and Rannacher, 2003; Eibner and Melenk, 2004; Rachowicz *et al.*, 2004). *hp*-algorithms are often tested for functionality on standard examples like the unit square, slit or L-shaped domain. Their practical use in wave propagation is not well established due to difficulties in implementation and the decision whether to use local *h*-refinement or *p*-enrichment.

We compare four different fully *hp*-adaptive algorithms for 2D computations of wave propagation problems showing that simple algorithms using an explicit error estimate in energy norm are sufficient for electromagnetic wave propagation. The finite element software PolyDE, which is currently developed at the Institute of Micro Systems Technology (Hamburg University of Technology), is used as the simulation platform. It facilitates solving different scalar partial differential equations in lossy, anisotropic, inhomogeneous media using shape function polynomial order of up to $p = 20$. Besides the *hp*-adaptive algorithm, the program offers pure *h*- and *p*-adaptation.

Subsequently, we first introduce the wave propagation problem and notations. Then, we examine the error estimator used by the software and present selected *hp*-adaptation strategies. The performance of algorithms is studied on four examples, comparing error convergence and numerical efficiency in terms of number of DOF and runtime.

Electromagnetic wave propagation problem and notation

The scalar wave equation for the electric or magnetic field strength is used for computing 2D electromagnetic wave propagation. We solve for the z-component of the field, which is continuous in the xy-plane.

There are two types of scalar wave equations, defined on the domain Ω which is polygonally bounded by Dirichlet boundary conditions on $\partial\Omega_D$ and Neumann or mixed boundary conditions on $\partial\Omega_N$. The first is the transverse electric (TE) wave equation solved for the electric field strength E_z:

$$\nabla \cdot (\boldsymbol{\mu}_{r;x,y}^{-1} \nabla E_z) + k_0^2 \varepsilon_{r;z} E_z = j\omega\mu_0 J_z \tag{1}$$

with boundary conditions defined by:

$$E_z = E_D \quad \text{on } \partial\Omega_D \tag{2}$$

$$[\boldsymbol{\mu}_{r;x,y}^{-1} \nabla E_z]|_n = p_N + q_N E_z \quad \text{on } \partial\Omega_N \tag{3}$$

and $\boldsymbol{\mu}_{r;x,y}^{-1}$ being the inverse of relative permeability rank two tensor to take anisotropic materials into account, relative dielectric permittivity $\varepsilon_{r;z}$, current density J_z as a scalar source term and free space wave number $k_0 = \omega\sqrt{\mu_0\varepsilon_0}$ with angular frequency ω. E_D, p_N and q_N are scalar values used for setting the boundary conditions. Material data are considered to be complex valued in order to allow for lossy media.

The transverse magnetic (TM) wave equation is solved for the magnetic field strength H_z. It is similar to the TE-wave – only terms for permittivity and permeability are interchanged and source terms need a slightly different treatment (change $j\omega\mu_0 J_z \rightarrow \nabla \times (\varepsilon_{r;x,y}^{-1} \mathbf{J})$).

Error estimation is presented for the case of TE-waves. The derivation of an estimator for a TM-wave is analogous.

Error estimator

Explicit error estimators compute an error indicator directly from the residual for each element K in the mesh, while the implicit method solves a local problem on a patch of elements with higher computational cost compared to the explicit one. Being a method of recovered gradients, the ZZ estimator is widely used although it is possible to construct a simple problem where it fails completely. It might happen that this estimator computes an error estimate of nearly zero while the real error may be arbitrarily large. See Ainsworth and Oden (2000) for a deeper explanation. Implicit methods are more reliable in presence of pollution, however, they are costly especially in the case of high order methods. Explicit methods are known to be reliable as long as the solution has high regularity but do not result in guaranteed error bounds at corner singularities or in the case of phase lag. Recovery methods may not be reliable for high order methods and likewise are not able to treat pollution effects (Babuška and Strouboulis, 2001). We restrict our analysis to explicit residual error estimates due to the fact that implicit estimators are excessive in run time. However, we are faced with potentially non-reliable error prediction in the case of pollution because the error estimator does not recognize numerical phase lag. Recent error estimators had been derived only for the case of convection-diffusion or reaction-diffusion equations (Melenk and Wohlmuth, 2001; Verfürth, 2005) and thus may fail in the case of the wave equation. One of the aims of this paper is to test whether explicit estimators are at least sufficient to serve as an error indicator in the adaptation process for wave propagation problems.

John (2000) numerically compares various error estimators concerning their efficiency and behaviour in the mesh *h*-adaptation process. Although, explicit residual

estimators in H^1-semi norm and L^2-norm produce well refined meshes, he concludes that none of the estimators worked satisfactory in all examples. The explicit error estimator of Melenk and Wohlmuth (2001) incorporates the polynomial degree in local error estimation contrarily to John (2000), Ainsworth and Oden (2000) and Verfürth (2005). This indicator does not underestimate the error for the Poisson equation. The refinement procedure leads to graded meshes at singularities of reentrant corners. For this reason, an explicit residual error estimator seems to be suited for practical use.

Error estimation delivers local error indicators η_K^2 in energy norm for all elements K in a discretisation $\mathscr{T}$ and a relative error estimate e_r for the whole solution. The common approach is to sum up internal contribution $\eta_{\mathrm{i}_K}^2$ and boundary contribution $\eta_{\mathrm{b}_K}^2$.

The interior error indicator $\eta_{\mathrm{i}_K}^2$ depends on element size $h_K = \mathrm{diam}(K)$ and polynomial order p_K:

$$\left\|\eta_{\mathrm{i}_K}\right\|_{\mathrm{eng},K}^2 = \frac{h_K^2}{p_K^2}\left\|\mu_{r;x,y}^{-1}\right\| \cdot \int_K |j\omega\mu_0 J_z - \nabla\cdot(\mu_{r;x,y}^{-1}\nabla E_{z;h}) - k_0^2\varepsilon_{r;z}E_{z;h}|^2 \mathrm{d}A_K \quad (4)$$

with element area A_K and the norm of inverse permeability tensor computed by $\|\boldsymbol{\mu}_{r;x,y}^{-1}\| = \max|\boldsymbol{\mu}_{r;x,y}^{-1}|$.

The second contribution to the local error indicator $\eta_{\mathrm{b}_K}^2$ consists of the field gradient jump $[\boldsymbol{\mu}_{x,y}^{-1}\nabla E_{z;h}]_{\mathbf{n}_K}$ with respect to the unit outward normal vector $\mathbf{n}_K \perp \partial K$:

$$\begin{aligned}\left\|\eta_{\mathrm{b}_K}\right\|_{\mathrm{eng},K}^2 = \left\|\bar{\boldsymbol{\mu}}_{r;x,y}\right\| \Bigg(& \sum_{\gamma\in\partial K\neq\partial\Omega} \frac{h_{\gamma_K}}{h_{\gamma_K}+h_{\gamma_{K'}}} \frac{l_\gamma}{2p_\gamma} \cdot \int_\gamma \left|[\boldsymbol{\mu}_{x,y}^{-1}\nabla E_{z;h}]_{\mathbf{n}_K}\right|^2 \mathrm{d}l_\gamma \\ & + \sum_{\gamma\in\partial K\cap\partial\Omega_N} \frac{l_\gamma}{2p_\gamma}\int_{\partial K\cap\Gamma_N} |p_N + q_N E_{z;h} - \mathrm{n}_K\cdot(\mu_{x,y}^{-1}\nabla E_{z;h})|^2 \mathrm{d}l_\gamma \Bigg)\end{aligned} \quad (5)$$

with shared edge polynomial degree $p_\gamma = \min(p_K, p_{K'})$, $h_{\gamma_K}, h_{\gamma_{K'}}$ being the heights over common edge γ with length l_γ of element K and its neighbour K' and permeability mean value $\bar{\boldsymbol{\mu}}_{r;x,y}$ of K and K'. A weighting factor depending on $h_{\gamma_K}, h_{\gamma_{K'}}$ is included to distribute the error between neighbouring elements.

The global error η composed of element contributions is defined by:

$$\|\eta\| := \left(\sum_{K\in\mathrm{T}}\|\eta_K\|^2\right)^{1/2} = \left[\sum_{K\in\mathrm{T}}(\|\eta_{\mathrm{i}_K}\|^2 + \|\eta_{\mathrm{b}_K}\|^2)\right]^{1/2} \quad (6)$$

In measuring the error, we use the energy norm similar to Verfürth (1996, 2005) as reference:

$$\|E_z\|_{\mathrm{eng},\Omega}^2 := \int_\Omega |\mu_{r;x,y}^{-1}\nabla E_z\cdot\nabla E_z| + |k_0^2\varepsilon_{r;z}E_z\cdot E_z|\mathrm{d}\Omega \quad (7)$$

Relative error estimate e_r can be expressed as a dimensionless quantity by:

$$\|e_r\|_{eng} = 100\,\text{percent}\left(\frac{\|\eta\|^2_{eng}}{\|E_z\|^2_{eng}}\right)^{1/2} \tag{8}$$

The relative error e_r is used as a stopping criterion in the adaptation process, while the local error η_K for each element K controls the local refinement of DOF.

Usually, initial values for mesh size h and polynomial degree p are chosen in order to control pollution error related to phase lag. Ainsworth (2004) distinguishes between oscillatory, transition and exponential zone. For optimum convergence, it is desirable to stay in the exponential zone. In approaching this zone, h-refinement is more economically, while error reduction is larger with p-enrichment in the exponential zone. Dispersion error decreases at an exponential rate at $kh < 2p + 1$. Thus, mesh size and polynomial order have to be chosen such that the following condition is fulfilled:

$$\kappa kh < 2p + 1 \Rightarrow h < \kappa^{-1}\frac{2p+1}{2\pi}\,\frac{\lambda_0}{n} \tag{9}$$

with constant $\kappa > 1$, free space wavelength $\lambda_0 = c_0/f$ and refractive index n of the material. This criterion is sharp – meaning if not fulfilled, the error oscillates despite increasing polynomial order. In first order FE or FD methods, it is a common practice to use mesh size $h \approx \lambda_0/(10 \cdot n)$ (Monk, 2003), leading to highly refined meshes.

It had been shown by Babuška and Sauter (1997) that it is possible to modify the usual FEM procedure in a way that the effect of pollution is eliminated in one dimension. In two dimensions, it is possible to substantially reduce but not avoid pollution with an appropriate modification. However, the construction of such a method seems not to be straightforward. If the error of an element exceeds the error criterion, an additional check for the mesh-size and polynomial order according to equation (9) could be included in the *hp*-adaptive algorithm to reduce phase lag for initially coarse meshes. The element requires h-refinement, if the actual element diameter h_K is larger than the required mesh-size.

hp-algorithms

In the course of adaptation, we aim to achieve exponential convergence of the error and reach a prescribed error tolerance TOL in energy norm for the whole solution. The paradigm of adaptive meshing is equipartition of error in the mesh. It had been shown, that numerical efficiency and convergence speed of h-adaptation are not very sensitive to mesh topology as long as the criterion of error equilibration is fulfilled (Babuška and Strouboulis, 2001). At corner singularities, the optimal mesh should have a geometric density distribution of mesh size h and linearly decreasing polynomial order p in approaching the singularity. Singularities are caused by adjacent Dirichlet and Neumann boundary conditions, reentrant or material interface corners and interfaces between perfectly matched layers (PMLs) of different directions.

Two decisions based on error estimation are to be made in *hp*-adaptation – whether the element should be refined and which kind of refinement (either h or p) should be used. Typically, p-enrichment is preferred due to the higher convergence rate in regions of a smooth solution. If material coefficients are smooth or element-wise constant, it is guaranteed that singularities demanding h-refinement only appear at material

interfaces or at the boundary. An approach preferred by Rachowicz *et al.* (2004) is to test both refinement strategies on a local patch of elements and to choose the remedy, which leads to the larger error reduction. Simpler explicit residual error estimators only give one information requiring some additional criterion, which can be extracted from geometry, error distribution or adaptation history.

There are different strategies for choosing *h*-refinement or *p*-enrichment. A simple adaptation strategy is to use *p*-enrichment and to switch to *h*-refinement if this is not successful. For instance, we may use *h*-refinement only for the few elements, whose error is significantly larger than the mean error. This strategy is simple, robust and only uses information, which is easily available. However, it may not be optimal in the number of DOF, since it possibly produces more *h*-refined elements than are needed even in the case of a smooth solution. Thus, a further criterion, which excludes *h*-refinement in regions of high regularity, would be beneficial.

In the following, we present four algorithms. The first is a simple algorithm that bases the kind of refinement on a sorted list of element error, the second is a geometry based algorithm, the third is based on articles from Melenk and Wohlmuth (2001) and Eibner and Melenk (2004) and the last is a mixture of the algorithms presented by Heuveline and Rannacher (2003) and Eibner and Melenk (2004).

Top 5 percent h-*refine and keypoint-based strategy*

The simplest *hp*-algorithm always refines the top 5 percent of the sorted local element error list if η_K^2 is greater than a prescribed value. All other elements, having an error larger than the tolerance, are *p*-refined. The algorithm assumes that singularities possess the highest local error and thus have to be *h*-refined. In this way, singularities should always be sufficiently resolved independently of geometry while other elements are *p*-refined. The percentage of elements, which have to be *h*-refined depends on the geometry and can be estimated in advance. An empirical value of 5 percent has proved its usefulness on the average of various examples. This algorithm is denoted by *T5*.

The keypoint-based algorithm depends on structure. Corner singularities which require *h*-refinement are assumed to be located at intersection points of two or more geometry objects, which we refer to as keypoints. Further, it is assumed that corner singularities possess the largest errors. While this algorithm is well suited for corner singularities, it might fail for singularities located in the domain caused by inhomogeneous material distributions. Narrow arcs or circles, as in the case of photonic crystals, have to be well refined initially to suppress singularities caused by polygonal approximation of arcs when not using isoparametric elements. This algorithm is denoted by *KP*. Both strategies are included in the algorithm below:

(1) Sort error vector η_K^2 by decreasing error.

(2) For the worst 5 percent elements, check whether $\eta_K^2 \leq \sigma[\mathrm{TOL}/(\#K \cdot 100\,\mathrm{percent})]^2 \|E_z\|_{\mathrm{eng}}^2$.
   - If YES, exit loop.
   - ELSE, decide by algorithm:
     - for top 5 percent strategy, mark element K for *h*-refinement and set polynomial degree to $p_K/2$ if $p_K \geq 2$.
     - for keypoint strategy, check if at least one element node is a keypoint.

- If YES, mark element K for h-refinement and set polynomial degree to $p_K/2$.
- ELSE, raise p_K to $p_K + 1$ and leave element unchanged.

- For the worst 5-50 percent elements, check whether $\eta_K^2 \leq \sigma[\mathrm{TOL}/(\#K \cdot 100\,\mathrm{percent})]^2 \|E_z\|_{\mathrm{eng}}^2$.
  - If YES, exit loop.
  - ELSE, raise p_K to $p_K + 1$.

Parameter σ can be used to set the stopping criterion of element adaptation. The polynomial degree is decreased for the worst 5 percent elements when starting at a polynomial degree of $p_{\mathrm{init}} \geq 2$. This leads to an optimal polynomial order distribution at corner singularities. At the end of the adaptation the polynomial order at the singularity should be one.

Predicted error strategy by Melenk and Wohlmuth

This adaptation process uses error prediction for the subsequent refinement cycle. During the actual cycle, it is assumed that the solution is smooth and a predicted error η_K^{pred} based on the current solution is computed for the next adaptation cycle. If the computed error in the next cycle is higher than the predicted error from the preceding cycle, the assumption of a smooth solution must have been wrong. Now h-refinement is used. Otherwise the algorithm proceeds with p-enrichment, assuming a smooth solution. Variables γ_h and γ_p (Melenk and Wohlmuth, 2001) are introduced as a threshold for controlling the amount of h-refinement or p-enrichment. Increasing one or both variables leads to increased p-enrichment, while decreasing leads to increased h-refinement. The initial value for the predicted error determines refinement in the first adaptation step. A value of $\eta_{K;\mathrm{init}}^{\mathrm{pred}} = 0$ leads to h-, while setting $\eta_{K;\mathrm{init}}^{\mathrm{pred}} \to \infty$ leads to p-enrichment for all elements. The algorithm is denoted by *M07* and *M04* for $\gamma_p = 0.7$ and $\gamma_p = 0.4$, respectively. γ_h was chosen to be 4 in both algorithms.

The article from Melenk and Wohlmuth (2001) describes the algorithm in detail. Error prediction is modified for green h-refinement corresponding to Eibner and Melenk (2004) and for the case of restoring polynomial order conformity.

Refinement history with predicted error strategy

A refinement history for the last step is used for the algorithm based on the proposal from Heuveline and Rannacher (2003), which is similar to the one proposed by Melenk and Wohlmuth (2001). Error prediction based on the kind of refinement of the preceding adaptation step is used for all elements. Since, the algorithm by Heuveline uses a different error estimator, error prediction based on the earlier type of refinement had been modified according to Melenk and Wohlmuth.

The kind of refinement is chosen according to the predicted error. Refinement information is stored for the next step, which is the major difference to Melenk and Wohlmuth (2001). p-enrichment is used for elements which have not been refined before and is generally preferred for elements which have been refined earlier.

Initially, p-enrichment is used for marked elements in the first cycle, since there was no previous refinement. Variables γ_h and γ_p control the adaptation process similar to

Melenk and Wohlmuth (2001). They were set to $\gamma_h = 4$ and $\gamma_p = 0.7$. The algorithm is denoted by *RH*.

Comparison of algorithms

The algorithms of the previous section are compared with respect to their use in microphotonics using four examples. The results are given as estimated relative error over number of DOF.

Computations were done on an Athlon 64 X2 Dual Core 4200 + and 4 GB RAM running Windows XP. The vacuum wavelength was fixed at $\lambda_0 = 1.55\,\mu$m for wave propagation examples, being common in optical communication. This leads to $\lambda = \lambda_0/n$ in material with isotropic refractive index n. All structures were computed for TE waves with excitation given by Dirichlet boundary $E_z = \sin(\pi/w)$ for waveguide width w. Initial mesh size h_{init} was chosen, such that equation (9) is fulfilled with $\kappa = 2$ and $p_{\text{init}} = 1$ staying in the superexponential decay zone.

Adaptation was stopped after 20 steps or if relative errors of 0.01 percent for sharp bend and etalon example and 0.1 percent for sphere-cone and photonic crystal example were reached. These relative errors seem to be large compared to errors reached when solving the Laplace or Poisson equation on the unit square. Hence, it is indeed a demanding criterion to reach for wave propagation in complex structures, because of the moderate number of singularities that might occur. Results for *p*- and *h*-adaptation algorithms are added for comparison with the *hp*-versions.

Sphere-cone example

We chose the electrostatic sphere-cone example (Solin *et al.*, 2005) as a structure containing one singularity at the tip of the cone (width $w = 200$ mm, height $h = 500$ mm) located 100 mm above the sphere (radius $r = 200$ mm). The potentials are set to 0 V at the cone and 100 kV at the sphere in the geometry center. Top and bottom boundaries are set to homogeneous Dirichlet, left and right to homogeneous Neumann boundary conditions. We chose this example to compare *hp*-algorithms with respect to resolving singularities located at reentrant corners.

The structure was triangulated with mesh as coarse as possible and sphere approximated by 30 nodes per 90°. SSOR-conjugate gradient solver with linear solver error of 10^{-16} was used for solving system matrices. Observed field is smooth except for the singularity located at the cone tip.

Error convergence of relative estimated error in energy norm over number of DOF for *h*-, *p*- and different *hp*-adaptation algorithms is shown in Figure 1. *h*-adaptation shows algebraic convergence as expected stopping after 20 steps with an error of 2.42 percent. *p*-adaptation was not able to reduce error lower than 10.8 percent despite raising polynomial order, indicating that the singularity cannot be refined by *p*-enrichment. *hp*-algorithms *M04*, *M07* and *RH* approximately show the same slope as *h*-adaptation while needing more DOF. The best *hp*-algorithm in this example is *KP* followed by *T5*. *KP* was able to reach the desired tolerance in 19 steps needing approximately 80,000 DOF. *T5* was able to reach TOL = 0.0761 percent with 225,527 DOF using one step less.

Sharp bend example

The second structure is a $w = 0.2\,\mu$m wide waveguide with a sharp bend using a square resonator with a side length of $0.7\,\mu$m and a chamfer at the main reflection

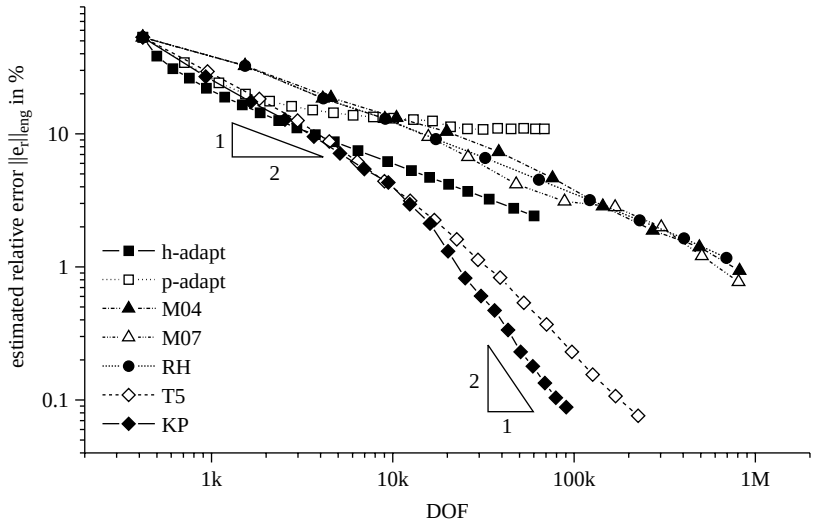

Figure 1.
Error convergence based on estimated error in energy norm for sphere cone example (TOL = 0.1 percent)

corner. It is intended for silicon with a refractive index of $n = 3.2$ surrounded by air demonstrating wave propagation. See Pollock and Lipson (2003) and continuative reference for further details. The structure is surrounded by PML with thickness $\lambda_0/2$ and truncated by homogeneous Dirichlet boundaries. The geometry was initially meshed with $h_{\text{init;Si}} = 0.115\,\mu$m and $h_{\text{init;air}} = 0.37\,\mu$m. Resulting field pattern for phase $\phi = 0°$ is shown in Figure 2.

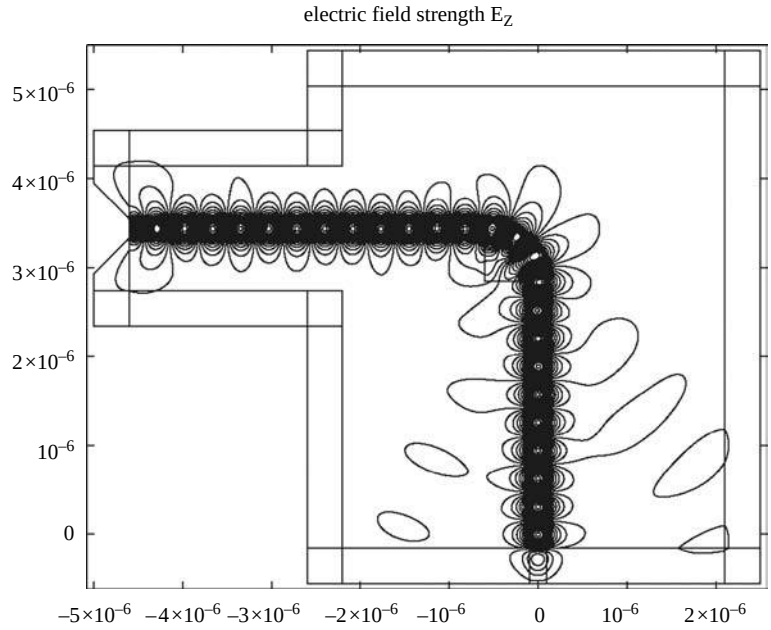

Figure 2.
Equipotentials of electric field strength E_z for phase $\phi = 0°$ showing scattering at sharp bend

Strongest singularities are supposed to reside at the input port at the left and interfaces between perfectly matched layers of different direction. Weaker singularities appear at the corners of the resonator. These areas are expected to be *h*-refined while the rest of the geometry is anticipated to be *p*-enriched.

Figure 3 shows the results of the estimated relative error in dependence of number of DOF. Pure *p*-adaptation reduces error successfully up to tenth adaptation step. After the second adaptation step, all *hp*-algorithms show better – almost exponential – error convergence (Figure 3) than *h*-adaptation with the most effective algorithm being the *KP*. It needs 100,000 DOF less than the second best algorithm *M04*. Algorithms *KP*, *M04* and *T5* show almost the same slope with different number of DOF. Graphs for *M07* and *RH* bend up during adaptation, which indicates higher amount of *p*-enrichment when comparing to *p*-adaptation graph. The algorithm first proposed by Melenk and Wohlmuth (2001) requires a careful choice of γ_h and γ_p, which have a strong effect on the number of elements generated. The polynomial degree for this algorithm is always higher than one, which deviates from the optimal polynomial degree distribution at corner singularities, while the mesh grading is good.

It is interesting to observe the connection between relative error $\|e_r\|_{\text{eng}}$ and physical quantities in electromagnetics like the relative phase connected to propagation speed. Relative phase plays an important role for designing optical components like Mach-Zehnder interferometers. Figure 4 shows the dependence of phase ϕ on relative error, which can be seen as an indicator for phase lag. A value of $\varphi = \arctan\ (\text{Im}(E_z)/\text{Re}(E_z)) = -3.080466278°$ with a relative error estimate of $\|e_r\|_{\text{eng}} = 0.00482$ at coordinates (0, 0) (Figure 2) using the *KP* algorithm was taken as the reference value for $\Delta\varphi$. The graph can be linearly fitted in double-logarithmic scale by $\log \Delta\varphi = -3.42 + 1.87 \cdot \log\|e_r\|_{\text{eng}}$.

All algorithms except *M07* were able to decrease the error at corners of the bend by *h*-refinement. The *KP*-algorithm decreases the polynomial degree at corners which leads to a polynomial degree of $p = 1$ at stronger singularities. Together with *T5*, it is

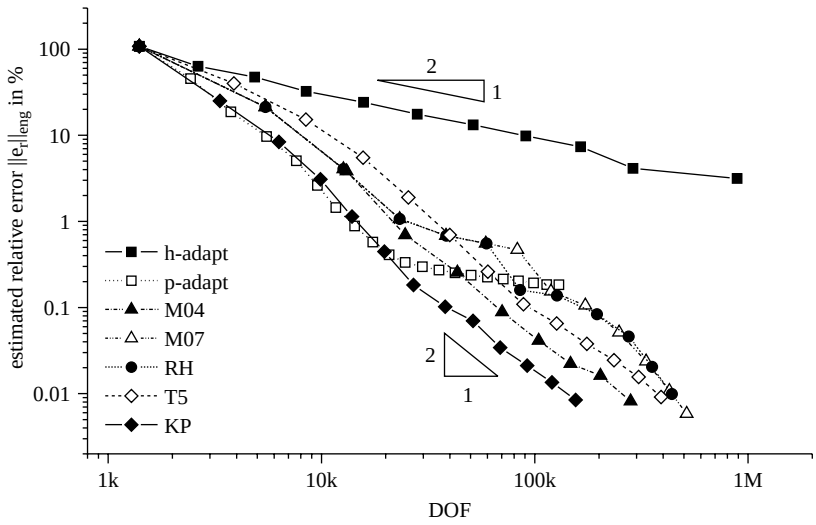

Figure 3.
Error convergence based on estimated error in energy norm for sharp bend (TOL = 0.01 percent)

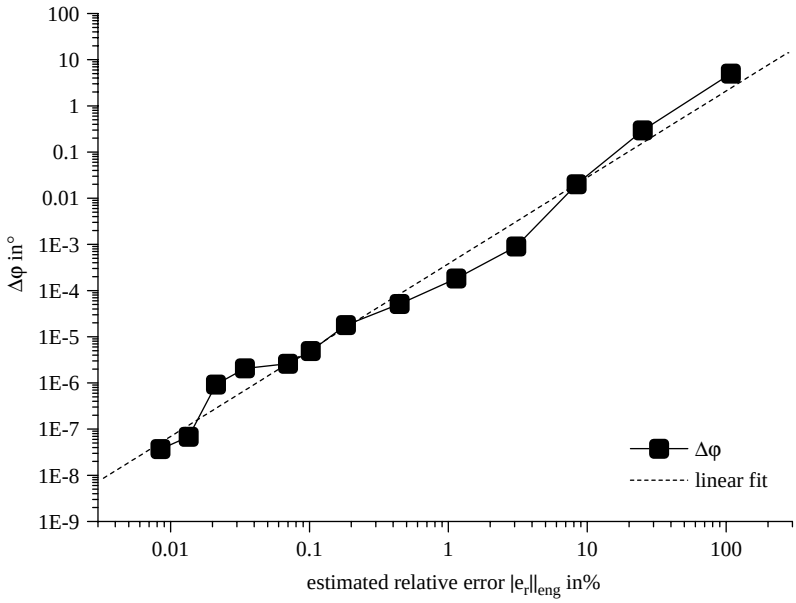

Figure 4.
Dependence of phase $\Delta\phi$ on relative error estimate $\|e_r\|_{eng}$ using *KP* algorithm for sharp bend

the only algorithm that shows a linear increase of polynomial degree away from the singularity together with a geometric mesh (Figure 5).

Etalon

An etalon in terms of a resonant cavity in a $w = 0.4\,\mu$m wide waveguide ($n = 3.45$) truncated by air spacings was chosen as the third example. The resonator has length $l = 2.246\,\mu$m with adjacent air spacing ($d_{air} = 387.5$ nm). Perfectly matched layers of thickness $\lambda_0/2$ with bordering homogeneous Dirichlet boundaries were used for domain truncation. The geometry was initially meshed with $h_{init;wg} = 0.1\,\mu$m and

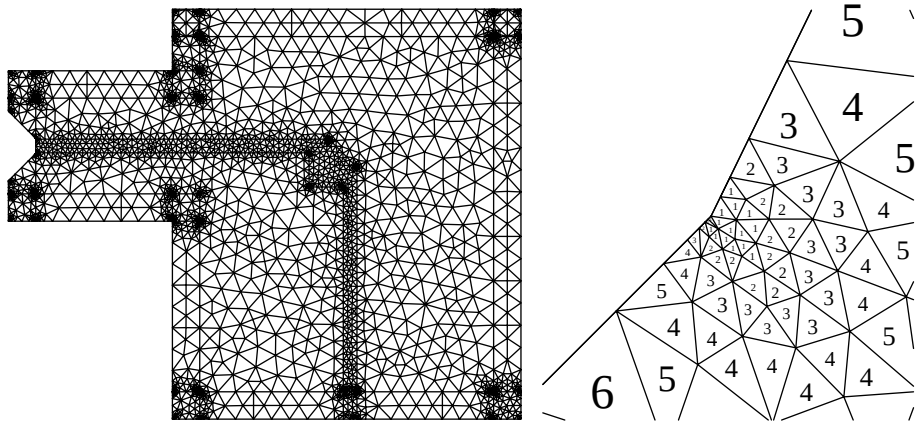

Figure 5.
Meshing of sharp bend using *KP* algorithm: (a) final mesh showing refined geometric singularities at TOL = 0.01 percent; and, (b) magnification of lower input port singularity with polynomial order

$h_{\text{init;air}} = 0.37\ \mu$m. UMF direct solver was used for computation. Weaker singularities are located at waveguide or resonator vertices at the air spacing (Figure 7(b)). This example was chosen to show a drawback of all *hp*-algorithms except from *KP* with respect to resonator refinement.

Results for error convergence are shown in Figure 6. Like in the preceding example, *KP* is the most efficient algorithm with respect to number of DOF followed by *M04*, *M07* and *RH*. These algorithms need 100,000 to 150,000 DOF more than *KP*, with *RH* spending 295,852 to reach $\|e_r\|_{\text{eng}} = 0$, 00424 percent. Except for a small upward bend in graph of *M07*, they show similar curvature. Although needing 394,111 DOF, *T5* shows exponential convergence up to an error of 0.1 percent and comparable computation time to *M07* and *RH* (Table I).

The drawback addressed earlier occurs during adaptation in the resonator region. Predicted error algorithms show local *h*-refinement in immediate vicinity of standing wave nodes (Figure 7(a)) inside the resonator, where field gradient is large (Figure 7(c)). *M04* additionally shows *h*-refinement in scattering region near the output. As the field is still smooth in these regions, a mesh as generated by the *KP* algorithm (Figure 7(b)) – only using *h*-refinement at corner singularities – is expected. *T5* produces a mesh with improper local agglomerations of *h*-refinements (Figure 7(d)).

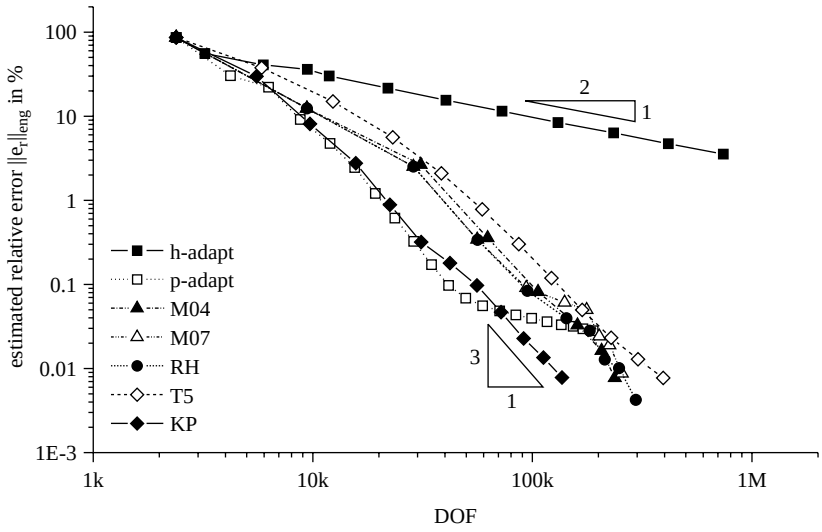

Figure 6.
Error convergence based on estimated error $\|e_r\|_{\text{eng}}$ for etalon (TOL = 0.01 percent)

Example	*M04*	*M07*	*RH*	*T5*	*KP*	$\|e_r\|_{\text{eng}}$ (percent)
Sphere-cone	21.33	28.73	18.67	1.33	1.00	1.00
Sharp bend	1.30	5.52	3.05	2.45	1.00	0.01
Etalon	1.67	2.70	2.63	2.52	1.00	0.01
Photonic crystal	6.25	2.87	2.88	2.08	1.00	0.30

Table I.
Comparison of CPU time for presented examples

Photonic crystal bend

The fourth example is a 90° bend in a dielectric rod ($\varepsilon_z = 11.4$) photonic crystal with a square lattice (lattice parameter $a = 620$ nm) of 14 × 16 rods with radius $r = 124$ nm. Domain is truncated by absorbing boundary conditions (ABC) of the first kind. The problem was solved using SSORCG solver accuracy 10^{-9}. The example was chosen to demonstrate a drawback of the keypoint-based algorithm, which can be shown in Figure 8. Photonic crystals consist of rods of or holes in high refractive material, which are defined by keypoints in our program. Usually, circles are approximated by polygons whose corners result in weak singularities. Consequently, the initial mesh has

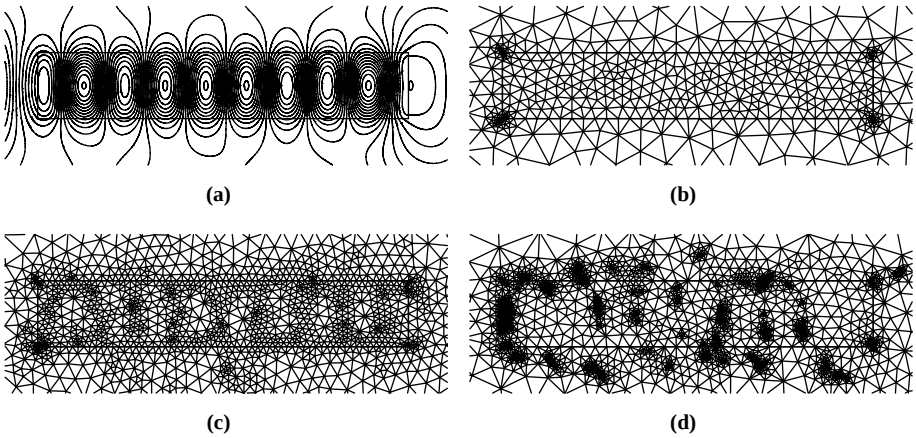

Figure 7.
Comparison of meshing results for etalon resonator display detail: (a) equipotentials of electric field strength E_z at $\varphi = 0°$; (b) *KP* algorithm showing homogeneous mesh inside resonator; (c) *M07* algorithm showing *h*-refinement in vicinity of standing wave nodes; and, (d) *T5* algorithm showing local mesh agglomerations

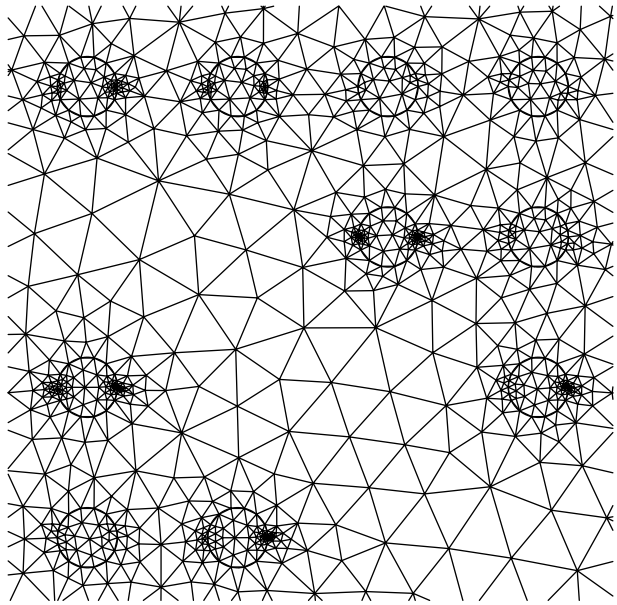

Figure 8.
Display detail of final mesh for keypoint algorithm at photonic crystal bend

to be sufficiently refined at circles. If the error is still high at these polygons, the algorithm only splits elements at keypoints, which is not appropriate for properly approximated circles.

Despite this drawback, the *KP*-algorithm shows its practical usefulness in Figure 9 with the least number of DOF used to reach the required error bound in nine steps. *p*-adaptation works efficiently up to a relative error of 0.8 percent due to low number of singularities and well refined circles. *T5* needs approx. 300,000 DOF more than KP to reach an error of 0.121 percent showing exponential, although slow, error convergence in parts of the graph. Algorithms *M07* and *RH* need additional 150,000-200,000 DOF to reach an error of 0.103 percent.

Algorithm run time

Another requirement for adaptation is efficiency in terms of run time. Table I shows CPU times to reach $\|e_r\|_{eng}$ for given examples. Timing is given relative to KP algorithm.

Considering the number of adaptation steps needed to reach the error bound for the sharp bend example (Figure 3), *M04*-algorithm needs three steps less than the other *hp*-algorithms. This cannot be strictly set in comparison to CPU time, as shown in Table I. Although *M04* needs less steps, *KP* is 23 percent faster. Long runtime for *M04* in the photonic crystal example is caused by poor solver convergence. *KP* is the fastest algorithm in all examples.

Conclusion

Different *hp*-algorithms were tested for efficiency and practical use on various examples. Although theoretically not being safe in the case of wave propagation problems and singularities at reentrant corners, results show that explicit residual error estimation is sufficient for guiding the adaptation process. Considering the computational effort of explicit error estimators, they are a reasonable choice in practice.

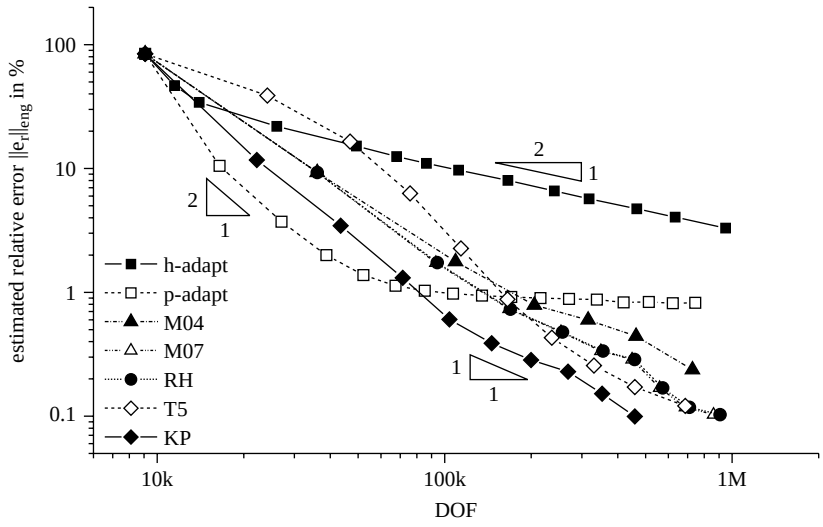

Figure 9.
Error convergence based on estimated relative error $\|e_r\|_{eng}$ for photonic crystal bend (TOL = 0.1 percent)

As expected, all *hp*-algorithms are superior to *h*- or *p*-adaptation with respect to the treatment of wave propagation problems in presence of geometric singularities. Comparing results of the tested algorithms, the geometry-based algorithm performs best and in some cases results in error being smaller by a factor of ten for the same number of DOF. According to expectations, we observed an increase in convergence order in the course of adaptation. However, convergence behaviour seems not to have overall exponential characteristic for any of the algorithms. This probably is attributed to wrong decisions in the kind of refinement leading to an unnecessary increase in the number of DOF. Mesh generation was not optimal in all examples. Unnecessary *h*-refinement occurred for predicted error and top 5 percent algorithms in etalon example and keypoint algorithm at curved interfaces. It should be noted that instead of using hanging nodes, the FEM code modifies the mesh in order to maintain mesh quality in successive steps. This could be the source of inappropriate decisions in predicted error algorithms.

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