Duality based error estimation for electrostatic force computation

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Outline

1. Duality based error estimation
2. Application to electrostatic force computation
3. Conclusion

Duality based error estimation

Duality based error estimation

Primal problem

$$a(u_h, v_h) = \langle f, v_h \rangle \qquad \forall v_h \in V_h$$

Quantity of interest

We are not interested in the solution u directly but in a (linear) functional $F(u)$.

Dual problem

$$a(v, z) = \langle F, v \rangle \qquad \forall v \in V$$

Primal problem + dual problem + Galerkin orthogonality

$$F(e) = a(e,z) = a(e, z - v_h) = \langle f, z - v_h \rangle - a(u_h, z - v_h)$$
$$=: \rho(u_h)(z - v_h) \qquad v_h \in V_h$$

after cell-wise integration by parts (for the Poisson problem $-\Delta u = f$)

$$\rho(u_h)(z - v_h) = \sum_{K \in \mathcal{T}_h} \left\{ \langle f + \Delta u_h, z - v_h \rangle_K + \langle \frac{1}{2}[\partial_n u_h], z - v_h \rangle_{\partial K} \right\}$$

Dual weighted residual method

$$|F(e)| \leq \sum_{K \in \mathcal{T}_h} \rho_K \omega_K$$

ρ_K:	cell residuals	*"smoothness indicators"*
ω_K:	weights	*"influence factors"*

Practical error estimators

Practical error estimators

Starting point

$$F(e) = \sum_{K \in \mathcal{T}_h} \{ \langle R_h, z - v_h \rangle_K + \langle r_h, z - v_h \rangle_{\partial K} \}$$

$$|\, F(e) \,| \leq \eta := \sum_{K \in \mathcal{T}_h} \eta_K$$

- The previous error representations contained the exact solution z of the dual problem which is unkown and cannot be computed.
- derive approximate error representations $\tilde{E}(u_h)$.

Important properties of an error estimator

Sharpness

$\tilde{\eta}$ should be a sharp upper bound for the error in the quantity of interest.

Effectivity

The approximate local error indicators $\tilde{\eta}_K$ should be effective for mesh refinement

Approximation by a higher-order method

EST1

$$F(e) \approx \sum_{K \in \mathcal{T}_h} \left\{ \langle R_h, z_h^{(2)} - I_h z_h^{(2)} \rangle_K + \langle r_h, z_h^{(2)} - I_h z_h^{(2)} \rangle_{\partial K} \right\}$$

$$\eta_K = \left| \langle R_h, z_h^{(2)} - I_h z_h^{(2)} \rangle_K + \langle r_h, z_h^{(2)} - I_h z_h^{(2)} \rangle_{\partial K} \right|$$

- **Expensive**: dual problem is solved with a higher-order method (biquadratic FE)
- estimated error turned out to be close to the true error in most cases.
- *not reliable*: under-estimation can occur.

Approximation by higher-order interpolation

EST2

$$F(e) \approx \sum_{K \in \mathcal{T}_h} \left\{ \langle R_h, I_h^{(2)} z_h - z_h \rangle_K + \langle r_h, I_h^{(2)} z_h - z_h \rangle_{\partial K} \right\}$$

- dual problem is solved with bilinear FE and interpolated to biquadratic FE on each element.
- less computational cost compared to the previous estimator
- error estimate not as accurate as from the the higher-order method.

Approximation by difference quotients

EST3

$$\omega_K^2 = \|z - I_h z\|_K^2 + h_K \|z - I_h z\|_{\partial K}^2 \leq c_I^2 h_K^2 \|\nabla^2 z\|_K^2$$

The second derivatives $\nabla^2 z$ can be replaced by suitable second-order difference quotients.

$$F(e) \leq c_I \sum_{K \in \mathcal{T}_h} h_K^{3/2} \rho_K \|[\partial_n z_h]\|_{\partial K}$$

- usually strong overestimation

Gradient recovery

EST4 The second derivatives $\nabla^2 z$ can be obtained by patchwise gradient recovery.

Convergence property

The error in the output functional is represented by $F(u - u_h) = a(u - u_h, z - z_h)$.

$$a(z - z_h, u - u_h) \leq |\, z - z_h \,|_{1,\Omega} \,|\, u - u_h \,|_{1,\Omega} \leq Ch^2 \,|\, z \,|_{2,\Omega} \,|\, u \,|_{2,\Omega}$$

Provided that the problem is sufficiently regular, i.e. $z, u \in H^2(\Omega)$ the error in the output functional converges with $\mathcal{O}(h^2)$.

Application to electrostatic force computation

Given

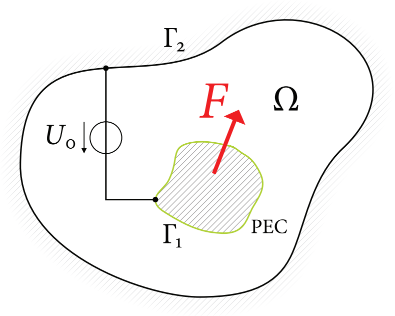
electrostatic BVP

Unkowns

potential u, the **force** acting on the PEC, the **error** in the force

$$\begin{aligned} -\Delta u &= 0 && x \in \Omega \\ u &= U_0 && x \text{ on } \Gamma_1 \\ u &= 0 && x \text{ on } \Gamma_2 \end{aligned}$$

$$E(u) = -\nabla u$$



Force computation

Maxwell stress tensor

$$T(\nabla u) = \nabla u \cdot \nabla u^T - \frac{1}{2}\|\nabla u\|^2 \mathbf{I}$$

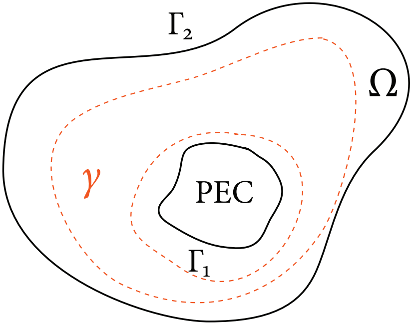
Force

$$F(u) = \int_{\Gamma_1} T \cdot n \,\mathrm{d}\sigma$$

The force is given by integration of the Maxwell stress tensor over the boundary of the object. (not continuous on $H^1(\Omega)$)

By applying Gauss's theorem and inserting a cutoff function Ψ the functional F can be rewritten as an integral over the entire domain Ω. Where Ψ has to be in $H^1(\Omega)$ and $\Psi \equiv 1$ on Γ_1 and $\Psi \equiv 0$ on Γ_2

$$\Rightarrow F(u) = \int_\Omega T(\nabla u) \cdot \nabla \Psi \, \mathrm{d}\mathbf{x}$$



- The domain where the force is computed can be freely choosen as long as it encloses the object of interest.
  "eggshell"-method

Linearization of F

The right hand side of the dual problem must be a linear functional.
$\Rightarrow$ use Gateaux derivative of F.

Dual problems

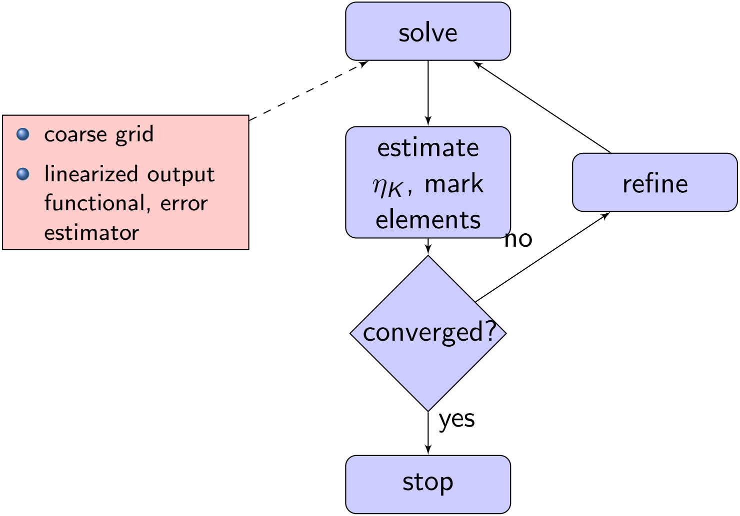
Force in x-direction:

$$a(v^h, z_x^h) = \Big[\mathrm{D}\,F(u^h)(v^h)\Big]_x \qquad \forall v^h \in V_h$$

Force in y-direction:

$$a(v^h, z_y^h) = \Big[\mathrm{D}\,F(u^h)(v^h)\Big]_y \qquad \forall v^h \in V_h$$

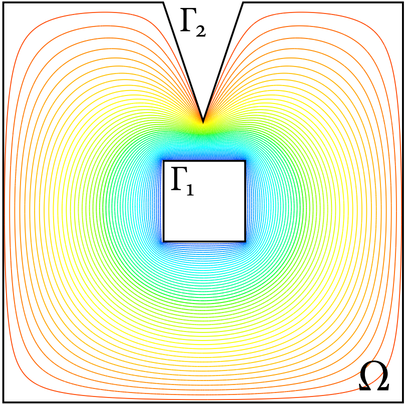
Adaptive mesh refinement



Results

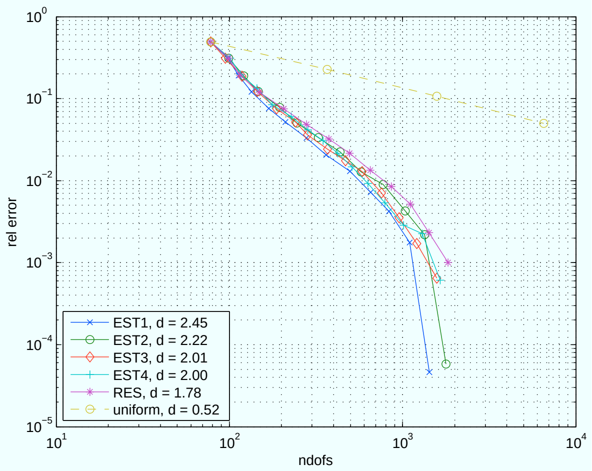
Model problem 1

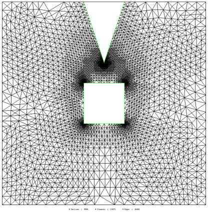
- Error estimation
- Adaptive mesh refinement

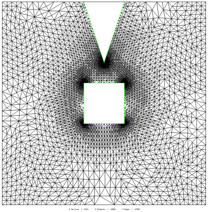


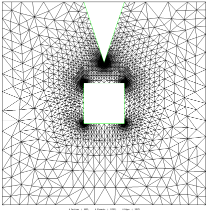
$$u|_{\Gamma_1} \equiv 0, \quad u|_{\Gamma_2} \equiv 1$$

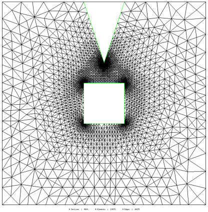
Convergence rates

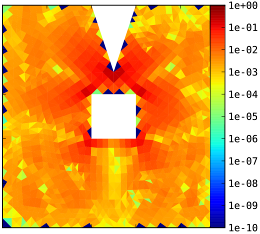



est1

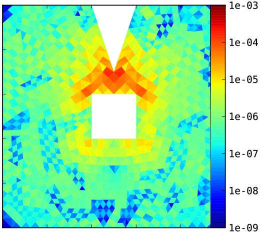

est2


est3

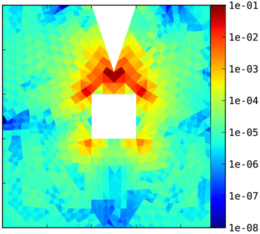

est4



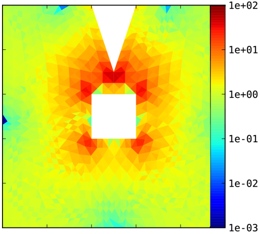
est1: ρ



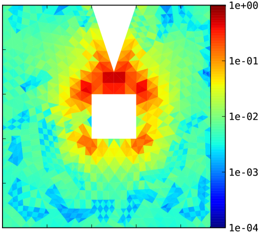
est1: ω



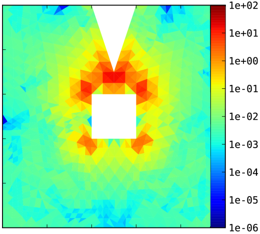
est1: η



est3: ρ



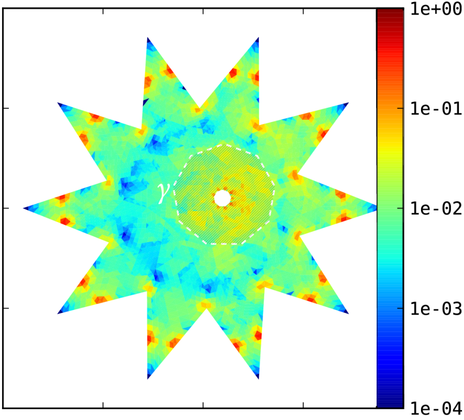
est3: ω



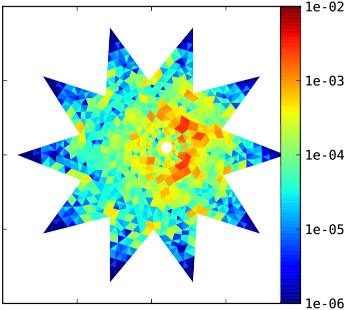
est3: η

Model problem 2

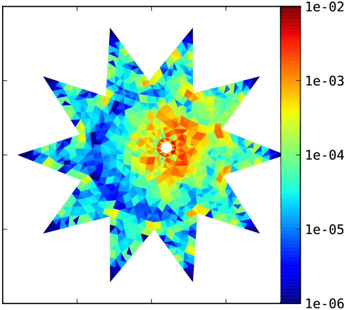
- Example where mesh refinement based on an explicit residual estimator fails.



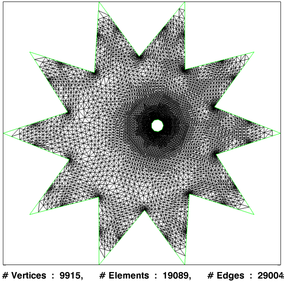
expl. residual η



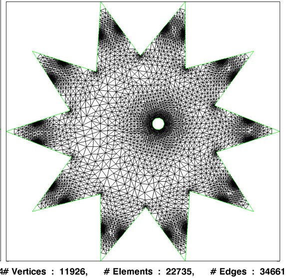
est2: ω



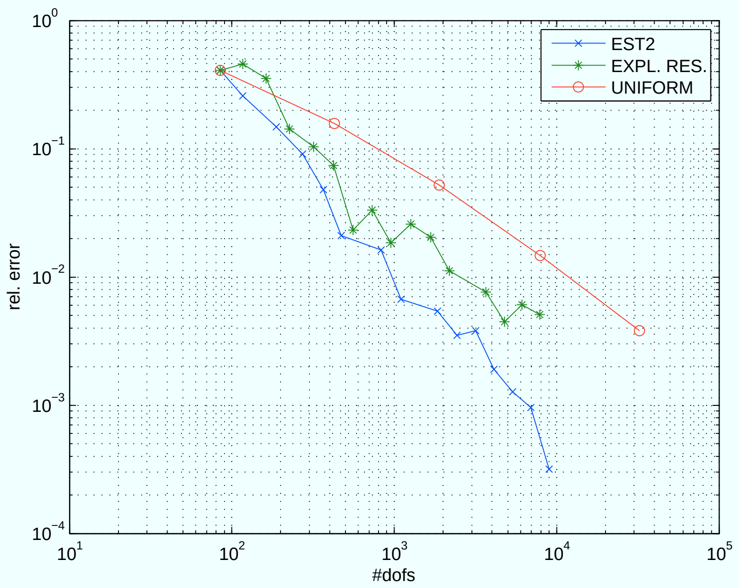
est2: η



est2



explicit residual


EST2
EXPL. RES.
UNIFORM
rel. error
#dofs
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^1
10^2
10^3
10^4
10^5

Effectivity indices

Effectivity indices

$$I_{\mathrm{eff}} \ll 1 \quad \text{(under-estimation)}, \qquad I_{\mathrm{eff}} \gg 1 \quad \text{(over-estimation)}$$

Est1	ndofs	51	103	191	331	591	1040	1781	3082	5334	9026	15151	25256
	I_{eff}	0.721	0.874	0.825	0.842	0.824	0.849	0.859	0.884	0.925	0.994	1.131	1.375
Est2	ndofs	51	102	191	352	640	1198	2242	4126	7617	13958	25591	
	I_{eff}	0.402	2.457	1.547	2.081	1.969	1.679	1.737	2.116	1.740	2.478	2.398	

Table: effectivity indices (M3, compact eggshell)

Est1	ndofs	83	165	293	525	914	1587	2704	4625	7815	13190	21809
	I_{eff}	0.890	1.068	1.010	1.121	1.091	1.259	1.228	1.414	1.376	1.393	1.066
Est2	ndofs	83	167	316	602	1089	2004	3653	6658	11965	21657	
	I_{eff}	0.850	1.204	0.667	0.962	1.440	1.504	2.718	2.538	5.106	3.604	

Table: effectivity indices (M4, force computation on entire domain)

Est1	ndofs	36	74	141	255	462	813	1419	2458	4224	7199	12212
	I_{eff}	0.904	0.996	0.920	0.989	0.905	0.982	0.905	0.990	0.921	1.018	0.964
Est2	ndofs	36	75	153	290	550	1027	1902	3495	6408	11731	
	I_{eff}	0.379	0.460	0.530	0.288	0.892	0.534	1.093	0.881	1.208	1.048	

Conclusion

Conclusion

- EST1 (higher-order method) and EST2 (higher-order interpolation) give effectivity indices close to one. (underestimation can occur)
- unless there are singularities which have no or only a weak effect on the force, a cheap explicit residual estimator will perform equally well in mesh adaption.