From algebraic flux correction schemes to nonlinear edge diffusion

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Advanced numerical methods:
Recent developments, analysis and applications
Institut Henri Poincaré, Paris
October 3-7, 2016

University of Strathclyde Glasgow

This talk gathers contributions made in collaboration with:

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2. Erik Burman (UCL, UK)
3. Volker John (WIAS, Germany)
4. Fotini Karakatsani (Chester, UK)
5. Petr Knobloch (Charles University, Czech Republic)
6. Richard Rankin (UTFSM, Chile)

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Outline

1. Motivation: From AFC schemes to nonlinear edge diffusion.
2. The edge diffusion method: Main properties.
3. An a posteriori error estimator.
4. Numerical results.
5. Concluding remarks.

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Introduction: The discrete maximum principle

The continuous maximum principle :

Theorem

Let u be the solution of the problem

$$-\varepsilon\Delta u + \boldsymbol{b}\cdot\nabla u + \sigma u = f \quad \text{in}\,\Omega\,,$$

and $u = 0$ on $\partial\Omega$. Then, if $f \geq 0$ in Ω, u can not attain a negative interior minimum in Ω.

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The discrete maximum principle

The DMP :

Theorem

Let $u_h \in \mathbb{P}_1(\Omega)$ be the solution of the problem

$$\varepsilon\,(\nabla u_h, \nabla v_h)_\Omega + (\boldsymbol{b} \cdot \nabla u_h, v_h)_\Omega + (\sigma u_h, v_h)_\Omega = (f, v_h)_\Omega \quad \forall\, v_h \in \mathbb{P}_1(\Omega)\,.$$

Then, if $f \geq 0$ in Ω, the mesh is acute, and $\frac{|\boldsymbol{b}|h + \sigma h^2}{2\varepsilon} < 1$, then u_h does not attain a negative minimum in Ω.

Remark : Under these hypothesis, the matrix

$$[\varepsilon(\nabla \psi_j, \nabla \psi_i)_\Omega + (\boldsymbol{b} \cdot \nabla \psi_j, \psi_i)_\Omega + (\sigma \psi_j, \psi_i)_\Omega]$$

is an M-matrix. This is, it is invertible, all the diagonal elements are positive, and the off-diagonal ones are non-positive.

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Algebraic flux correction schemes

Starting point : A finite element discretisation of our problem of the form:

$$\mathbb{A}\mathrm{U} = \mathrm{G}\,.$$

Define:

$$\mathbb{D} := (d_{ij}) \quad \text{where} \quad d_{ij} := -\max\{a_{ij}, 0, a_{ji}\} \text{ for } i \neq j\,, \quad d_{ii} = -\sum_{j \neq i} d_{ij}\,.$$

Remark: The matrix $\tilde{\mathbb{A}}$ is an M-matrix. Then, it preserves positivity.

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Equivalent system :

$$\tilde{\mathbb{A}}\,\mathrm{U} = \mathrm{G} + \mathbb{D}\mathrm{U}\,.$$

From the properties of $\mathbb{D}$ it follows that

$$\big(\mathbb{D}\mathrm{U}\big)_i = \sum_{j\neq i} f_{ij} \quad \text{where } f_{ij} = d_{ij}(u_j - u_i) \text{ are the fluxes}\,.$$

Goal : To limit the fluxes f_{ij} which are responsible for spurious oscillations.

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The limiters α_{ij} should satisfy the following:

- $\alpha_{ij} \in [0,1]$;
- α_{ij} should be as close to 1 as possible;
- $\alpha_{ij} \approx 1$ where the Galerkin solution is smooth.
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$$(\tilde{\mathbb{A}}\,\mathrm{U})_i = g_i + \sum_{j\neq i} \alpha_{ij}(U) f_{ij}$$

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Algebraic flux correction schemes

Equivalent system :

$$(\mathbb{A}\,\mathrm{U})_i + \sum_{j \neq i} \big(1 - \alpha_{ij}(U)\big) f_{ij} = g_i$$

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The rewriting

A weak formulation : Find $u_h \in \mathbb{P}_1(\Omega)$ such that

$$a(u_h, v_h) + d_h(u_h; u_h, v_h) = (f, v_h)_\Omega \quad \forall\, v_h \in \mathbb{P}_1(\Omega)\,.$$

The stabilisation term $d_h(\cdot;\cdot,\cdot)$ is given by

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$$d_h(u_h; u_h, v_h) = \sum_{i,j=1}^{N} (1 - \alpha_{ij}(u_h))\, d_{ij}(u_h(x_j) - u_h(x_i)) v_h(x_i)$$

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$$d_h(u_h; u_h, v_h) = \text{...a couple of lines using the symmetry of } \alpha_{ij} \text{ and } d_{ij}\text{...}$$

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Remark : Then, AFC schemes achieve a stable result by adding edge-based diffusion to the formulation.

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The nonlinear edge-based diffusion

<u>The method</u> : Find $u_h \in \mathbb{P}_1(\Omega)$ such that

$$\tilde{a}(u_h; v_h) := a(u_h, v_h) + d_h(u_h; u_h, v_h) = (f, v_h)_\Omega \qquad \forall\ v_h \in \mathbb{P}_1(\Omega)\,.$$

The stabilisation term $d_h(\cdot\,;\cdot,\ \cdot)$ is defined by

$$d_h(u_h; u_h, v_h) = \sum_{E \in \mathscr{E}_h} \gamma_0 \alpha_E(u_h) h_E^2 (\partial_{\mathbf{t}} u_h, \partial_{\mathbf{t}} v_h)_E\,.$$

Here, α_E are limiters defined as:

$$\alpha_E(w_h) := \max_{x \in E} \left[\xi_{w_h}(x)\right]^p\,,$$

with $\xi_{w_h} \in \mathbb{P}_1(\Omega)$ given by

$$\xi_{w_h}(x_i) := \begin{cases} \dfrac{\left|\sum_{j \in S_i} w_h(x_i) - w_h(x_j)\right|}{\sum_{j \in S_i} |w_h(x_i) - w_h(x_j)|}, & \text{if } \displaystyle\sum_{j \in S_i} |w_h(x_i) - w_h(x_j)| \neq 0\,, \\ 0, & \text{otherwise}\,, \end{cases}$$

and $p \in \mathbb{N}$.

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Properties of the nonlinear diffusion term

- If the mesh is symmetric with respect to its interior nodes, then the method is linearity preserving, this is,

$$\alpha_E(z) = 0 \qquad \forall\, z \in \mathbb{P}_1(\omega_E)\,.$$

Theorem

The discrete problem has at least one solution. Moreover, if $C_{\text{lip}}\gamma_0\, h < \varepsilon$, where C_{lip} is the Lipschitz constant, then the solution is unique.

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- The nonlinear form $d_h(\cdot;\cdot,\cdot)$ is Lipschitz continuous. More precisely, there exists $C_{\text{lip}} > 0$, independent of h, such that, for all $v_h, w_h, z_h \in \mathbb{P}_1(\Omega)$, the following holds

$$|d_h(v_h; v_h, z_h) - d_h(w_h; w_h, z_h)| \le C_{\text{lip}}\gamma_0 h\, |v_h - w_h|_{1,\Omega}\, |z_h|_{1,\Omega}\,.$$

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The discrete maximum principle

Definition (DMP)

The semilinear form $\tilde{a}(\cdot;\cdot)$ is said to satisfy the *DMP property* if the following holds: If $u_h(x_i)$ is a local negative minimum, then there exist negative quantites $(c_E)_{E\in\mathscr{E}_i}$ such that

$$\tilde{a}(u_h;\psi_i) \leq \sum_{E\in\mathscr{E}_i} c_E \left|\partial_{\mathbf{t}} u_h|_E\right| .$$

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Theorem

- *Let us suppose that the mesh is Delaunay. Then, if* $\gamma_0 > C_0\|\boldsymbol{b}\|_{\infty,E} + C_1\sigma h_E$*, the semilinear form* $\tilde{a}(\cdot;\cdot)$ *satisfies the DMP property.*

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- *Let us suppose that the mesh is Delaunay. Then, if* $\gamma_0 > C_0\|\boldsymbol{b}\|_{\infty,E} + C_1\sigma h_E$, *the semilinear form* $\tilde{a}(\cdot;\cdot)$ *satisfies the DMP property.*
- *For an arbitrary regular mesh, the same result is valid if* $\gamma_0 > C_0\|\boldsymbol{b}\|_{\infty,E} + C_1\sigma h_E + C_2\varepsilon h_E^{-1}$.

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Error estimates

Mesh-dependent norm:

$$\|v_h\|_h^2 := a(v_h, v_h) + d_h(u_h; v_h, v_h)\,.$$

General estimate: There exists $C > 0$, independent of ε such that

$$\|u - u_h\|_h \le C\,\|u - i_h u\|_{1,\Omega} + (d_h(u_h; i_h u, i_h u))^{\frac{1}{2}}\,.$$

Consistency error:

$$d_h(u_h; i_h u, i_h u) \le \gamma_0 \sum_{E \in \mathscr{E}_h} h_E^2 \|\partial_{\mathbf{t}} i_h u\|_{0,E}^2 \le C\,h\,\|u\|_{1,\Omega}^2\,.$$

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There exists a constant $C > 0$, independent of h, such that

$$\|u - u_h\|_h \le C h^{\frac{1}{2}} \|u\|_{2,\Omega}\,.$$

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There exists a constant $C > 0$, independent of h, such that

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An improved error estimate: The role of linearity preservation

$$d_h(i_h u; i_h u, i_h u) = \sum_{E \in \mathscr{E}_h} \gamma_0 \alpha_E(i_h u) h_E^2 \|\partial_{\mathbf{t}} i_h u\|_{0,E}^2$$

Theorem

If the form $d_h(\cdot;\cdot,\cdot)$ is linearity preserving, then there exists a constant $C > 0$, independent of h, such that

$$\|u - u_h\|_h \leq Ch \left(\|u\|_{2,\Omega} + \frac{1}{\sqrt{\varepsilon}} \|u\|_{1,\Omega} \right) .$$

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Error estimates

An improved error estimate: The role of linearity preservation

$$d_h(i_h u; i_h u, i_h u) = \sum_{E \in \mathscr{E}_h} \gamma_0 (\alpha_E(i_h u) - \alpha_E(i_E(u))) h_E^2 \|\partial_{\mathbf{t}} i_h u\|_{0,E}^2$$

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An improved error estimate: The role of linearity preservation

$$d_h(i_h u; i_h u, i_h u) \leq Ch \left\{ \sum_{E \in \mathscr{E}_h} |i_h u - i_E u|^2_{1,\Omega_E} \right\}^{\frac{1}{2}} |i_h u|_{1,\Omega}$$

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If the form $d_h(\cdot;\cdot,\cdot)$ is linearity preserving, then there exists a constant $C > 0$, independent of h, such that

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An improved error estimate: The role of linearity preservation

$$d_h(i_h u; i_h u, i_h u) \le C h^2 |u|_{2,\Omega} |u|_{1,\Omega}\,.$$

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Error estimates

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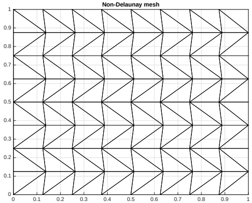
Numerical Results I : Convergence for smooth solutions

Data: $\varepsilon = 1$, $\sigma = 1$, $u(x, y) = \sin(2\pi x)\sin(2\pi y)$.

l	$\|e\|_{0,\Omega}$	ord.	$\|e\|_{1,\Omega}$	ord.	$\|e\|_h$	ord.
3	0.3835	–	3.5299	–	5.5746	–
4	0.1661	1.21	2.0053	0.82	2.4168	1.21
5	0.0451	1.88	0.9808	1.03	1.0317	1.23
6	0.0127	1.82	0.4811	1.03	0.4872	1.08
7	0.0042	1.59	0.2397	1.01	0.2405	1.02
8	0.0016	1.38	0.1198	1.00	0.1199	1.00



Data: $\varepsilon = 10^{-5}$, $\boldsymbol{b} = (-y, x)$, $\sigma = f = 0$.

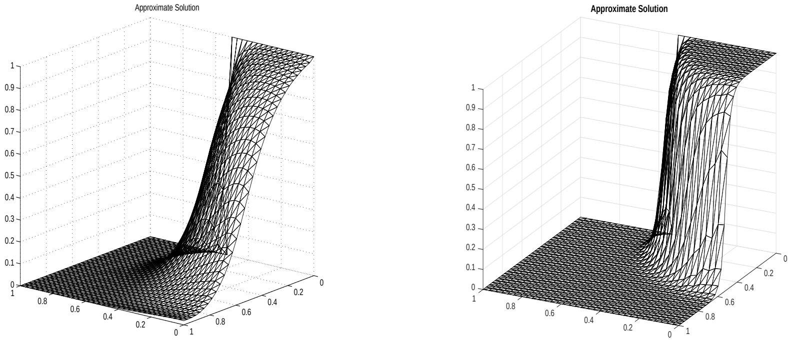


Figure 1 : Discrete solution for $p = 1$ (left) and $p = 8$ (right).

A computable error bound

The residual equation : Defining $e = u - u_h$ one gets, for all $v \in H_0^1(\Omega)$,

$$a(e,v) = \sum_{K\in\mathscr{T}} (f,v)_K - \varepsilon(\nabla u_h, \nabla v)_K - (\boldsymbol{b}\cdot\nabla u_h + \sigma u_h, v)_K$$

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A computable error bound

The residual equation : Defining $e = u - u_h$ one gets, for all $v \in H_0^1(\Omega)$,

$$a(e,v) = \sum_{K \in \mathscr{T}} \left((\mathcal{R}_K, v)_K + \sum_{E \in \mathscr{E}_K \cap \mathscr{E}_I} (-\varepsilon \partial_{\boldsymbol{n}} u_h, v)_E \right)$$

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Equilibrated fluxes: We need a set of *boundary fluxes* $\{g_{E,K} : E \in \mathscr{E}_K, K \in \mathscr{T}\}$ satisfying:

Consistency:

$$g_{E,K} + g_{E,K'} = 0 \quad \text{if } E \in \mathscr{E}_K \cap \mathscr{E}_{K'},$$

Full first order equilibration: For all $n \in \mathcal{V}_K$ and all $K \in \mathscr{T}$,

$$0 = (f, \lambda_n)_K - a_K(u_h, \lambda_n) - d_h^K(u_h; u_h, \lambda_n) + \sum_{E\in\mathscr{E}_K} (g_{E,K}, \lambda_n)_E ,$$

for all basis function λ_n of $\mathbb{P}_1(\Omega)$.

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A computable error bound

The residual equation : Defining $e = u - u_h$ one gets, for all $v \in H^1_0(\Omega)$,

$$a(e,v) = \sum_{K\in\mathscr{T}}\Bigg((\underbrace{\mathcal{R}_K}_{=-\nabla\cdot\boldsymbol{\sigma}_K}, v)_K + \sum_{E\in\mathscr{E}_K} (\underbrace{g_{E,K} - \varepsilon\partial_{\boldsymbol{n}} u_h}_{=\boldsymbol{\sigma}_K\cdot\boldsymbol{n}}, v)_E \Bigg)$$

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A computable error bound

The residual equation : Defining $e = u - u_h$ one gets, for all $v \in H_0^1(\Omega)$,

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A computable error bound

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$$\begin{aligned} a(e,v) &= \sum_{K\in\mathscr{T}} (\boldsymbol{\sigma}_K, \nabla v)_K \\ &\leq \sum_{K\in\mathscr{T}} \|\boldsymbol{\sigma}_K\|_{0,K} \|\nabla v\|_{0,K} \end{aligned}$$

The computable error bound

Theorem

For each element $K \in \mathscr{T}$, define a local error indicator by the rule

$$\eta_K = \frac{1}{\sqrt{\varepsilon}} \|\boldsymbol{\sigma}_K\|_{0,K} \,.$$

Then

$$\|e\|_\Omega^2 \leq \eta^2 := \sum_{K \in \mathscr{T}} \eta_K^2 .$$

Remark : $\|\boldsymbol{\sigma}_K\|_{0,K}$ can be computed analytically.

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The computable error bound: efficiency

Using known/familiar arguments :

$$\eta_K \leq C \sum_{K' \in \Omega_K} \left(\mathsf{C}_{K'} \|u - u_{\mathscr{T}}\|_{K'} + |d_h^{K'}(u_{\mathscr{T}}; u_{\mathscr{T}}, \lambda_n)| \right).$$

where

$$\mathsf{C}_K := \max \left\{ 1, Pe_K, \sqrt{\sigma} \frac{h_K}{\sqrt{\varepsilon}} \right\} .$$

Using the linearity preservation and Lipschitz continuity (as before):

$$d_h^{K'}(u_{\mathscr{T}}; u_{\mathscr{T}}, \lambda_n) \leq C \left(\frac{h_{K'}}{\varepsilon} \|u - u_{\mathscr{T}}\|_{\Omega_{K'}} + \frac{h_{K'}}{\sqrt{\varepsilon}} |u - \tilde{u}_{K'}|_{1,\Omega_{K'}} \right),$$

where $\tilde{u}_{K'}$ is the projection of u in $\mathbb{P}_1(\Omega_{K'})$.

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where $\tilde{u}_{K'}$ is the projection of u in $\mathbb{P}_1(\Omega_{K'})$.

The computable error bound: effciency

Theorem

There exists $C > 0$, independent of the size of the elements in the mesh $\mathscr{T}$, such that, for every $K \in \mathscr{T}$, the following local lower bound holds

$$\eta_K \le C \sum_{K' \in \Omega_K} \left(\left(\mathsf{C}_{K'} + \frac{h_{K'}}{\varepsilon} \right) |||u - u_{\mathscr{T}}|||_{K'} + \frac{h_{K'}}{\sqrt{\varepsilon}} |u - \tilde{u}_{K'}|_{1,K'} \right).$$

Numerical results

Data: $\varepsilon = 10^{-3}$, $\sigma = 1$, $u(x,y,z) = yz(1-y)(1-z)\left(x - \frac{e^{\frac{-(1-x)}{\varepsilon}} - e^{-\frac{1}{\varepsilon}}}{1-e^{-\frac{1}{\varepsilon}}}\right)$.

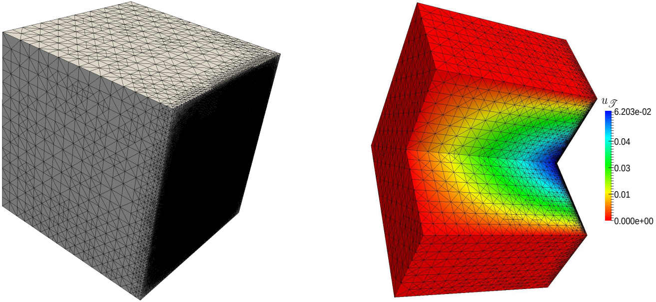

Figure 2 : 3D Example: Adapted mesh and isovalues of the solution.

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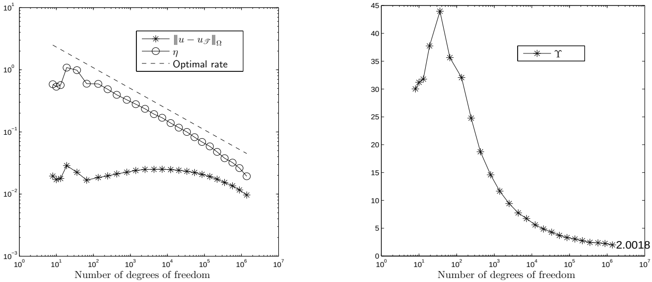

Figure 2 : 3D Example: Error estimator and effectivity indices.

Numerical results

Data: $\varepsilon = 10^{-4}$, $\sigma = 0$, $\boldsymbol{b} = (-y, x)$, $f = 0$.

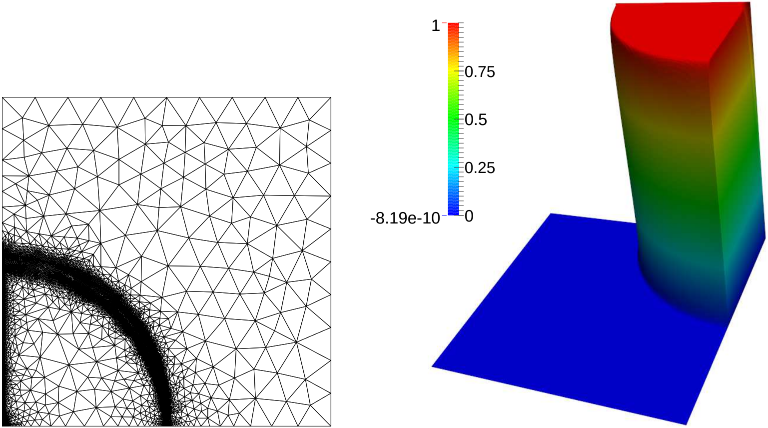

Figure 3 : Rotating converction field: adapted mesh, and discrete solution.

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Conclusions and perspectives

1. AFC schemes can be rewritten as edge diffusion methods.
2. A new definition of the limiters: convergence in any regular mesh.
3. Linearity preservation and Lipschitz continuity provide:
    1. an improved error estimate;
    2. a computable error bound which can be proven to be locally efficient.

Future extensions:

- General meshes.
- Time-dependent problems.
- Nonlinear problems.
- ......

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