A posteriori error estimators for high-order FEM applied to 1D reaction-diffusion equations

Ded. to Michal Křižek on his 60th birthday

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Introduction

Model problem

$$\mathcal{L}u := -\varepsilon^2 u'' + cu = f \quad \text{in} \quad (0,1), \quad u(0) = u(1) = 0.$$

$0 < \varepsilon \ll 1$, $c \geq \gamma^2$ on $[0,1]$, $\gamma > 0$

- boundary/interiour layers

Goal: *maximum-norm a posteriori error estimators*

$$\|(u - u_h)\|_\infty \leq \eta(\text{data}, u_h)$$

of interpolation type

$$\eta(\text{data}, u_h) = C_r h_i^\kappa \, \|D^\kappa u_h\|_{[x_{i-1},x_i]} + \text{osc}$$

Introduction

Renewed motivation: FEM for parabolic problems

$$u_t - \varepsilon^2 u_{xx} + cu = f \quad \text{in} \;\; (0,1) \times (0,T].$$

- general framework:
  elliptic reconstruction
  - Nochetto, Makridakis, Akrivis, Lakkis
  - Kopteva, Linß
- elliptic estimators (for stationary problems)
- estimators for temporal discretisation
  - Euler
  - Crank-Nicolson
  - dG(r)

Outline

- variational formulation
- Green's functions
- FE-discretisation
- a posteriori error analysis
- numerical results

Variational formulation

Boundary value problem:

$$\mathcal{L}u := -\varepsilon^2 u'' + cu = f \text{ in } (0,1), \quad u(0) = u(1) = 0$$

Variational formulation: Find $u \in V := H_0^1(0,1)$ such that

$$a(u,v) = f(v) \quad \forall\, v \in V$$

with

$$a(u,v) := \varepsilon^2 (u', v') + (cu, v), \quad f(v) := (f,v) := \int_0^1 fv$$

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Green's function

$\mathcal{G} : [0,1] \times [0,1] \to$ with

$$v(x) = a\big(v, \mathcal{G}(x,\cdot)\big) \quad \forall\, v \in V \;\text{ and }\; x \in (0,1)$$

"$\Longleftrightarrow$" $\qquad [v \to u - u_\Delta]$

$$v(x) = \int_0^1 (\mathcal{L}v)(\xi)\mathcal{G}(x,\xi)\, d\xi$$

Characterisation:

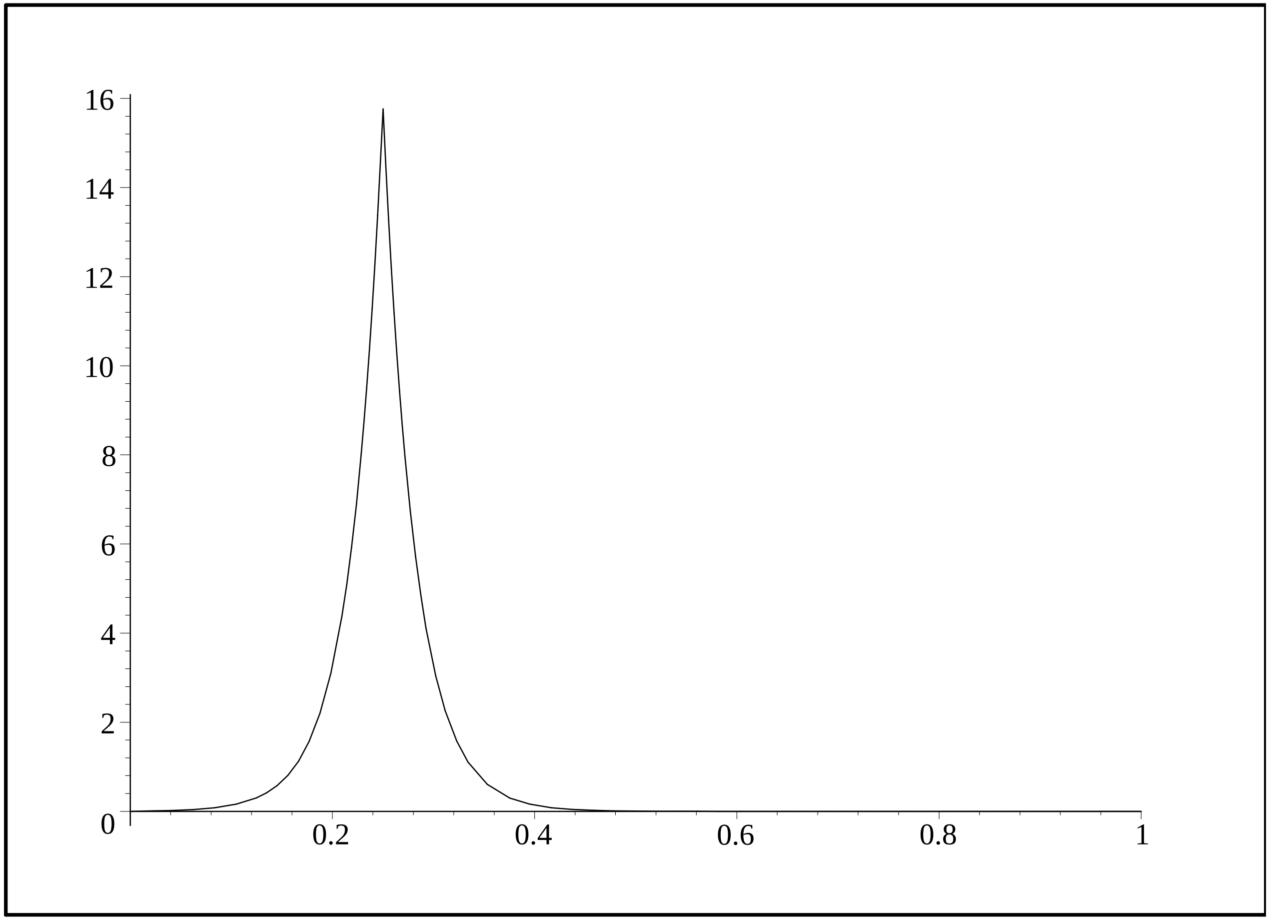
$$\left(\mathcal{L}\mathcal{G}(\cdot,\xi)\right)(x) = \delta(x-\xi) \;\; x \in (0,1), \quad \mathcal{G}(0,\xi) = \mathcal{G}(1,\xi) = 0$$

$$\boxed{\left(\mathcal{L}^*\mathcal{G}(x,\cdot)\right)(\xi) = \delta(\xi - x), \;\; \xi \in (0,1), \quad \mathcal{G}(x,0) = \mathcal{G}(x,1) = 0}$$

$$\ldots\; \mathcal{L} = \mathcal{L}^* \quad \Longrightarrow \quad \mathcal{G}(x,\xi) = \mathcal{G}(\xi,x)$$

Green's function

$\mathcal{G}(x,\cdot)$, $\varepsilon^2 = 10^{-3}$



Green's function

Pointwise bounds:

$$0 \le \mathcal{G}(x,\xi) \le \frac{\mathrm{e}^{-\gamma|x-\xi|/\varepsilon}}{2\varepsilon\gamma}$$

and

$$\mathcal{G}_\xi(x,\xi) \ge 0 \quad \text{for} \;\; \xi < x,$$
$$\mathcal{G}_\xi(x,\xi) \le 0 \quad \text{for} \;\; x < \xi.$$

Green's function

L_1-bounds:

$$\int_0^1 c(\xi)\mathcal{G}(x,\xi)\,d\xi \le 1,$$

$$\int_0^1 \left|\mathcal{G}_\xi(x,\xi)\right|\,d\xi = 2\mathcal{G}(x,x) \le \frac{1}{\varepsilon\gamma}$$

and

$$\varepsilon^2 \int_0^1 \left|\mathcal{G}_{\xi\xi}(x,\xi)\right|\,d\xi \le 2.$$

FEM discretisation

Mesh: $\Delta : 0 = x_0 < x_1 < \cdots < x_N = 1$,
$J_i := [x_{i-1}, x_i]$, $h_i := x_i - x_{i-1}$.

FE: piecewise Π_r, C^0, bc's

$$\mathcal{S}^0_{r,0}(\Delta) := \left\{ v \in H^1_0(0,1) : v|_{J_i} \in \Pi_r,\ i = 1, \dots, N \right\}$$

Galerkin FEM: Find $u_\Delta \in V_r = \mathcal{S}^0_{r,0}(\Delta)$ such that

$$a\big(u_\Delta, v\big) = f\big(v\big) \quad \forall\, v \in V_r.$$

$\longrightarrow$ quadrature is essential

FEM discretisation

Lagrange Interpolation: sub mesh on $[0,1] \to J_i$

$$0 \le t_0 < t_1 < \cdots < t_r \le 1.$$

$I_r^L : v \in C_0[0,1] \mapsto I_r^L v \in \mathcal{S}_r^0(\Delta)$ with

$$I_r^L v(x_i + t_j h_i) = v(x_i + t_j h_i), \quad i = 1, \ldots, N, \;\; j = 0, \ldots, r.$$

Then $(w,v) \approx \big(w,v\big)_\Delta := \big(I_r^L w, v\big)$,

FEM with quadrature: Find $u_\Delta \in V_r$ such that

$$\boxed{a_\Delta(u_\Delta, v) := \varepsilon^2 \big(u_h', v'\big) + \big(c u_\Delta, v\big)_\Delta = (f,v)_\Delta \quad \forall v \in V_r,}$$

FEM, a posteriori analysis

Error in point $x \in (0,1)$**,** $\Gamma := \mathcal{G}(x,\cdot)$**:**

$$
\begin{aligned}
(u - u_\Delta)(x) &= a(u - u_\Delta, \Gamma) = (f,\Gamma) - a(u_\Delta,\Gamma) \\
&= (f,\Gamma) - (f, I_r^M\Gamma)_\Delta - a(u_\Delta,\Gamma) + a_\Delta(u_\Delta, I_r^M\Gamma)
\end{aligned}
$$

Special interpolant: $I_r^M : v \in C_0[0,1] \mapsto I_r^M v \in V_r$ with

$$I_r^M v(x_i) = v(x_i), \quad i = 0,\ldots,N,$$

and

$$\int_{J_i} \big(I_r^M v - v\big)(\xi)\pi(\xi)\, d\xi = 0 \quad \forall \pi \in \Pi_{r-2},\ i = 1,\ldots,N.$$

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FEM, a posteriori analysis

Then

$$(u - u_\Delta)(x) = (\underbrace{f - cu_\Delta}_{=:\, q}, \Gamma) - \underbrace{(f - cu_\Delta, I_r^M \Gamma)_\Delta}_{= (I_r^L q, I_r^M \Gamma)}$$

Error representation:

$$\boxed{(u - u_\Delta)(x_k) = \left(q - I_r^L q, \Gamma\right) - \left(I_r^L q, \Gamma - I_r^M \Gamma\right)}$$

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FEM, a posteriori analysis

Then

$$\left(u-u_\Delta\right)(x) = (\underbrace{f-cu_\Delta}_{=:\,q},\Gamma) - \underbrace{(f-cu_\Delta, I_r^M\Gamma)_\Delta}_{=(I_r^L q, I_r^M\Gamma)}$$

Error representation:

$$\boxed{\left(u-u_\Delta\right)(x_k) = \Big(q - I_r^L q, \Gamma\Big) - \Big(I_r^L q, \Gamma - I_r^M\Gamma\Big)}$$

First term: interpolation error/data oscillations

$$\left|\Big(q - I_r^L q, \Gamma\Big)\right| \le \left\|\frac{q - I_r^L q}{c}\right\|_\infty \quad \Rightarrow \quad \textit{sampling}$$

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FEM, a posteriori analysis

Then

$$(u - u_\Delta)(x) = (\underbrace{f - cu_\Delta}_{=: q}, \Gamma) - \underbrace{(f - cu_\Delta, I_r^M \Gamma)_\Delta}_{= (I_r^L q, I_r^M \Gamma)}$$

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FEM, a posteriori analysis

Taylor:

$$\left(I_r^L q\right)(\xi) = \sum_{j=0}^{r} \frac{\left(I_r^L q\right)_{i-1/2}^{(j)}}{j!} \left(\xi - x_{i-1/2}\right)^j$$

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FEM, a posteriori analysis

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$$(-1)^{r+1} \int_{J_i} \left(I_r^L q\right)(\xi) \left(\Gamma - I_r^M \Gamma\right)(\xi)\, d\xi$$

$$= \frac{\left(I_r^L q\right)_{i-1/2}^{(r)}}{(2r+1)!} \int_{J_i} \frac{d^{r-1}}{d\xi^{r-1}} \Big(p_{r,i}(\xi)(\xi - x_{i-1/2})\Big) \Gamma''(\xi)\, d\xi$$

$$+ \frac{\left(I_r^L q\right)_{i-1/2}^{(r-1)}}{(2r)!} \int_{J_i} \frac{d^{r-1}}{d\xi^{r-1}} p_{r,i}(\xi) \Gamma''(\xi)\, d\xi,$$

$$p_{r,i}(\xi) := (\xi - x_i)^r \,(\xi - x_{i-1})^r$$

FEM, a posteriori analysis

Constants

$$\alpha_r := \max_{\xi\in[0,1]} \left| \frac{d^{r-1}}{d\xi^{r-1}} \Big(\xi^r (\xi-1)^r \Big) \right|$$

$$\beta_r := \max_{\xi\in[0,1]} \left| \frac{d^{r-1}}{d\xi^{r-1}} \Big(\xi^r (\xi-1)^r (\xi-1/2) \Big) \right|$$

Then,

$$\left\| \frac{d^{r-1}}{d\xi^{r-1}} \Big(p_{r,i}(\xi)(\xi - x_{i-1/2}) \Big) \right\|_{\infty,J_i} \leq \beta_i h_i^{r+2}$$

$$\left\| \frac{d^{r-1}}{d\xi^{r-1}} p_{r,i}(\xi) \right\|_{\infty,J_i} \leq \alpha_i h_i^{r+1}$$

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FEM, a posteriori analysis

Constants

	α_r	β_r
$r=1$	$\frac{1}{4}$	$\frac{\sqrt{3}}{36}$
$r=2$	$\frac{\sqrt{3}}{9}$	$\frac{1}{16}$
$r=3$	$\frac{3}{8}$	$\frac{\left(3\sqrt{30}+9\right)\sqrt{525-70\sqrt{3}}}{2450}$
$r=4$	$\frac{\left(12\sqrt{30}+36\right)\sqrt{525-70\sqrt{3}}}{1225}$	$\frac{3}{8}$
$r=5$	$\frac{15}{4}$	≈ 1.434081520

FEM, a posteriori analysis

$(I_r^L q)_{i-1/2}^{(r-1)}$, $(I_r^L q)_{i-1/2}^{(r)}$: $\quad q_{i-(r+\ell)/r} := q\left(x_{i-1} + t_\ell h_i\right), \; t_\ell = \ell/r$

$$D_-^{r-1} q_i := \left(\frac{r}{h_i}\right)^{r-1} \sum_{j=0}^{r-1} \binom{r-1}{j} (-1)^j q_{i-(1+j)/r}$$

$$D_+^{r-1} q_i := \left(\frac{r}{h_i}\right)^{r-1} \sum_{j=0}^{r-1} \binom{r-1}{j} (-1)^j q_{i-j/r}.$$

$$\boxed{\begin{aligned} (I_r^L q)_{i-1/2}^{(r-1)} &= \frac{D_+^{r-1} q_i + D_-^{r-1} q_i}{2} \\ (I_r^L q)_{i-1/2}^{(r)} &= \frac{r\left(D_+^{r-1} q_i - D_-^{r-1} q_i\right)}{h_i} \end{aligned}}$$

FEM, a posteriori analysis

Theorem 1.

$$\|u - u_\Delta\|_\infty \le \left\| \frac{q - I_r^L q}{c} \right\|_\infty + \max_{i=1,\dots,N} \left\{ \frac{h_i^{r+1}}{\varepsilon^2} \left(\frac{\alpha_r}{(2r)!} \left| D_+^{r-1} q_i + D_-^{r-1} q_i \right| + \frac{2r\beta_r}{(2r+1)!} \left| D_+^{r-1} q_i - D_-^{r-1} q_i \right| \right) \right\}.$$

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FEM, a posteriori analysis

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Remark: If c and f smooth, then

$$\lim_{h_i \to 0} \left| D_+^{r-1} q_i - D_-^{r-1} q_i \right| = 0$$

FEM, a posteriori analysis

Theorem 1.

$$\|u - u_\Delta\|_\infty \le \left\|\frac{q - I_r^L q}{c}\right\|_\infty + \max_{i=1,\dots,N}\left\{\frac{h_i^{r+1}}{\varepsilon^2}\left(\frac{\alpha_r}{(2r)!}\left|D_+^{r-1}q_i + D_-^{r-1}q_i\right| + \frac{2r\beta_r}{(2r+1)!}\left|D_+^{r-1}q_i - D_-^{r-1}q_i\right|\right)\right\}.$$

Remark: $q \mathrel{\widehat{=}} \varepsilon^2 u_\Delta'' \implies D_+^{r-1}q, D_-^{r-1}q \mathrel{\widehat{=}} \varepsilon^2 D^{r+1}u_\Delta$

Interpolation:

$$\left\|u - I_r^L u\right\|_{J_i} \le C h_i^{r+1}\left\|u^{(r+1)}\right\|_{J_i}$$

FEM, a posteriori analysis

Theorem 1.

$$\|u - u_\Delta\|_\infty \le \left\| \frac{q - I_r^L q}{c} \right\|_\infty + \max_{i=1,\dots,N} \left\{ \frac{h_i^{r+1}}{\varepsilon^2} \left(\frac{\alpha_r}{(2r)!} \left| D_+^{r-1} q_i + D_-^{r-1} q_i \right| + \frac{2r\beta_r}{(2r+1)!} \left| D_+^{r-1} q_i - D_-^{r-1} q_i \right| \right) \right\}.$$

Remark: On a badly adapted mesh: $\eta \sim \varepsilon^{-2}$,
but $\|u - u_\Delta\|_\infty \le C$

FEM, a posteriori analysis

alternative estimate: trade h_i for ε^{-1}

$$\left(I_r^L q\right)_{i-1/2}^{(r)} \int_{J_i} \frac{d^{r-1}}{d\xi^{r-1}} \Big(p_{r,i}(\xi)(\xi - x_{i-1/2})\Big) \Gamma''(\xi)\, d\xi$$
$$= -\left(I_r^L q\right)_{i-1/2}^{(r)} \int_{J_i} \frac{d^{r}}{d\xi^{r}} \Big(p_{r,i}(\xi)(\xi - x_{i-1/2})\Big) \Gamma'(\xi)\, d\xi,$$

$$\left(I_r^L q\right)_{i-1/2}^{(r-1)} \int_{J_i} \frac{d^{r-1}}{d\xi^{r-1}} p_{r,i}(\xi) \Gamma''(\xi)\, d\xi$$
$$= -\left(I_r^L q\right)_{i-1/2}^{(r-1)} \int_{J_i} \frac{d^{r}}{d\xi^{r}} p_{r,i}(\xi) \Gamma'(\xi)\, d\xi$$

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FEM, a posteriori analysis

Theorem 1′.

$$\|u - u_\Delta\|_\infty \le \left\| \frac{q - I_r^L q}{c} \right\|_\infty + \frac{2}{(2r)!} \max_{i=1,\dots,N} h_i^{r+1} \left[\bar\alpha_r \left| D_+^{r-1} q_i + D_-^{r-1} q_i \right| + \frac{r}{2r+1} \bar\beta_r \left| D_+^{r-1} q_i - D_-^{r-1} q_i \right| \right].$$

with

$$\bar\alpha_r := \min\left\{ \frac{2\alpha_r}{\varepsilon^2}, \frac{r!}{h_i \varepsilon \gamma} \right\}, \quad \bar\beta_r := \min\left\{ \frac{2\beta_r}{\varepsilon^2}, \frac{r!}{2h_i \varepsilon \gamma} \right\}$$

Numerical results

$$-\varepsilon^2 u''(x) + (1 + x^2 + \cos x)\, u(x) = \mathrm{e}^{-x}, \quad u(0) = u(1) = 0.$$

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Numerical results

$$-\varepsilon^2 u''(x) + (1 + x^2 + \cos x)\, u(x) = \mathrm{e}^{-x}, \quad u(0) = u(1) = 0.$$

Bakhvalov mesh, $r = 5$, $\varepsilon = 10^{-8}$:

N	$\|u - u_\Delta\|_\infty$	rate	η_I	η_D	η	eff
2^8	2.753e-12	5.99	8.512e-19	1.104e-11	1.104e-11	4.012
2^9	4.344e-14	5.99	1.331e-20	8.824e-14	8.824e-14	2.031
2^{10}	6.820e-16	6.00	2.081e-22	1.375e-15	1.375e-15	2.015
2^{11}	1.068e-17	6.00	3.252e-24	2.144e-17	2.144e-17	2.007
2^{12}	1.671e-19	6.00	5.082e-26	3.348e-19	3.348e-19	2.003
2^{13}	2.613e-21	6.00	7.941e-28	5.229e-21	5.229e-21	2.001
2^{14}	4.084e-23	6.00	1.241e-29	8.169e-23	8.169e-23	2.001
2^{15}	6.382e-25	6.00	1.939e-31	1.276e-24	1.276e-24	2.000
2^{16}	9.972e-27	—	3.029e-33	1.994e-26	1.994e-26	2.000

Numerical results

$$-\varepsilon^2 u''(x) + (1 + x^2 + \cos x)\, u(x) = \mathrm{e}^{-x}, \quad u(0) = u(1) = 0.$$

Bakhvalov mesh, $r = 10$, $\varepsilon = 10^{-8}$:

N	$\|u - u_\Delta\|_\infty$	rate	η_I	η_D	η	eff
2^8	1.566e-21	10.96	2.918e-28	1.493e-20	1.493e-20	9.538
2^9	7.840e-25	10.98	1.462e-31	7.469e-24	7.469e-24	9.527
2^{10}	3.877e-28	10.99	7.228e-35	3.691e-27	3.691e-27	9.522
2^{11}	1.905e-31	11.00	3.552e-38	1.813e-30	1.813e-30	9.520
2^{12}	9.330e-35	11.00	1.740e-41	8.881e-34	8.881e-34	9.518
2^{13}	4.563e-38	11.00	8.509e-45	4.343e-37	4.343e-37	9.518
2^{14}	2.230e-41	11.00	4.158e-48	2.122e-40	2.122e-40	9.517
2^{15}	1.089e-44	11.00	2.031e-51	1.037e-43	1.037e-43	9.517
2^{16}	5.319e-48	—	9.920e-55	5.062e-47	5.062e-47	9.517

Numerical results

$$-\varepsilon^2 u''(x) + \left(1 + x^2 + \cos x\right) u(x) = x^{3/2} + \mathrm{e}^{-x}, \quad u(0) = u(1) = 0.$$

Numerical results

$$-\varepsilon^2 u''(x) + (1 + x^2 + \cos x)\, u(x) = x^{3/2} + \mathrm{e}^{-x}, \quad u(0) = u(1) = 0.$$

Bakhvalov mesh, $r = 7$, $\varepsilon = 10^{-8}$:

N	$\|u - u_\Delta\|_\infty$	rate	η_I	η_D	η	eff
2^8	2.943e-07	1.52	2.943e-07	6.343e-06	6.637e-06	22.548
2^9	1.028e-07	1.53	1.028e-07	2.115e-06	2.218e-06	21.569
2^{10}	3.555e-08	1.56	3.555e-08	6.881e-07	7.236e-07	20.357
2^{11}	1.205e-08	1.61	1.205e-08	2.160e-07	2.280e-07	18.920
2^{12}	3.949e-09	1.69	3.949e-09	6.438e-08	6.833e-08	17.304
2^{13}	1.220e-09	1.84	1.220e-09	1.780e-08	1.902e-08	15.594
2^{14}	3.418e-10	2.06	3.418e-10	4.411e-09	4.752e-09	13.903
2^{15}	8.203e-11	2.40	8.203e-11	9.300e-10	1.012e-09	12.338
2^{16}	1.555e-11	—	1.555e-11	1.549e-10	1.704e-10	10.959

Numerical results

$$-\varepsilon^2 u''(x) + (1 + x^2 + \cos x)\, u(x) = x^{3/2} + e^{-x}, \quad u(0) = u(1) = 0.$$

Adaptive algorithm, $r = 7$, $\varepsilon = 10^{-8}$:

N	$\|u - u_\Delta\|_\infty$	rate	η_I	η_D	η	eff	K
2^8	9.130e-16	5.91	1.467e-16	4.606e-15	4.753e-15	5.2	16
2^9	1.522e-17	11.41	4.000e-18	1.076e-16	1.116e-16	7.3	7
2^{10}	5.587e-21	8.77	1.031e-19	2.827e-20	1.314e-19	23.5	8
2^{11}	1.279e-23	8.05	2.273e-21	5.604e-23	2.329e-21	182.2	8
2^{12}	4.816e-26	4.98	1.769e-23	6.188e-25	1.831e-23	380.1	9
2^{13}	1.528e-27	10.60	8.918e-27	9.763e-27	1.868e-26	12.2	12
2^{14}	9.817e-31	7.03	1.398e-28	9.326e-30	1.491e-28	151.9	11
2^{15}	7.537e-33	9.43	1.230e-30	1.178e-31	1.347e-30	178.8	11
2^{16}	1.094e-35	—	3.463e-33	7.680e-35	3.540e-33	323.5	12
		8.27	7.32	8.21	7.53		

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Outlook

- reaction-diffusion in 1D,
  theoretical results & numerical experiments ☺
- adaptivity, mesh equidistribution (preliminary results)
- reaction-convection-diffusion

$$-\varepsilon u'' + \nu b u' + c u = f$$

  (SD)FEM ☺
- time-dependent problems
  - theory: ☺ (with Natalia Kopteva)
  - numerical validation: in progress

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Thank you.