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SYMMETRIZATION OF DIFFUSION-ADVECTION-REACTION PROBLEM AND *HP*-ADAPTIVE FINITE ELEMENT APPROXIMATIONS

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In this paper we use scaling of the independent variable to introduce similarity criteria of Péclet and Strouhal as indicators of singular perturbations of considered diffusion-advection-reaction equation with Robin boundary conditions. In the terms of these criteria, we analyze the corresponding variational problem for well posedness and establish sufficient conditions for this. Finally we transform the original problem to the equivalent problem of minimization for quadratic functional. Furthermore we introduce hp-adaptive finite element scheme for solving the considered problem. Constructed scheme combines classic explicit and implicit error estimators for selecting elements for refinement and making decision for each selected element about its bisection or incrementing of polynomial order on it respectively. In the end we present some numerical examples and comparison with the results, obtained using reference solution algorithm.

Ключові слова: diffusion-advection-reaction boundary value problem, Péclet criteria, Strouhal criteria, well-posedness of variational problem, symmetrization, minimization of quadratic functional, finite element method, condensation of internal degrees of freedom, a posteriori error estimator, *hp*-adaptive scheme, reference solution.

1. INTRODUCTION

Finite element method is an universal tool for solving boundary value problems for partial differential equations (see [1]). It is applicable for problems on very complex domains in 2- and 3-dimensional spaces. During last years the main focus is on the adaptive algorithms for FEM. The main idea is to adapt mesh (*h*-adaptivity), element polynomial order (*p*-adaptivity) or both mesh and order (*hp*-adaptivity) to minimize computational cost needed for solving the given problem. Such algorithms are implemented using local a posteriori error estimators. It's naturally to interpret *hp*-schemes as most advanced as they give us most wide approximation capabilities. Theoretically it is proven that they can produce exponentially convergent sequences of approximations to original solution of boundary value problem [2].

In this work we construct *hp*-adaptive algorithm for solving the diffusion-advection-reaction boundary value problems with self-adjoint operators. We prove the optimality in some sense of refinement selection step used in algorithm. Also we introduce symmetrization procedure which can be used to transform given nonsymmetrical variational problem to equivalent symmetric problem, therefore making possible application of constructed algorithm to nonsymmetrical problems too.

To drive adaptation process we introduce two a posteriori error estimators. For element selection for refinement procedure we use explicit estimator, i.e. explicit formula which gives upper bound of actual error on finite element. After elements for refinement were selected we need to choose on each element refinement pattern: bisection with original element order preservation or increment of polynomial degree on element by one.

Also we studied precisely conditions which problem data needs to satisfy to make boundary value problem to be well-posed.

The paper is structured according to the following order: in section 2 we define model problem; in section 3 we provide some specific problem transformations; in section 4 we construct variational formulation; in section 5 we study conditions of well posedness of variational problem; in section 6 we introduce transformation of initial variational problem to bring its symmetric equivalent; in section 7 we make review of general finite element method schemes; section 8 is devoted to finite element optimality investigation; in section 9 we provide error estimators which will be used in adaptation algorithm; in section 10 *hp*-adaptation algorithm is described. In section 11 we demonstrate some numerical results.

2. MODEL PROBLEM

We consider the following boundary value problem for diffusion-advection-reaction equation

$$\begin{cases} \textit{given diffusion coefficient } \bar{\mu} = \bar{\mu}(x), \ \textit{convection } \bar{\beta} = \bar{\beta}(x), \\ \qquad \textit{reaction } \bar{\sigma} = \bar{\sigma}(x), \ \textit{sources } \ \bar{f} = \bar{f}(x) \\ \qquad \textit{and } \bar{\alpha}, \bar{\gamma}, \bar{g}_0, \bar{g}_L \in \mathbb{R}; \\ \textit{find function } \ u = u(x) \ \ \textit{such that} \\ \quad -\dfrac{d}{dx}\left(\bar{\mu}\dfrac{d}{dx}u\right) + \bar{\beta}\dfrac{d}{dx}u + \bar{\sigma}u = \bar{f} \quad \text{in } \ G = (0, L), \\ \quad \left(\bar{\mu}\dfrac{d}{dx}u - \bar{\alpha}u\right)\Big|_{x=0} = \bar{g}_0, \ \ \left(-\bar{\mu}\dfrac{d}{dx}u - \bar{\gamma}u\right)\Big|_{x=L} = \bar{g}_L. \end{cases} \tag{1}$$

3. SCALING OF VARIABLES

In order to show specific of the boundary value problem (1) we introduce a scaled variable $t \in [0,1]$, in such way that $x := Lt$, transforming dependent variables

$$\begin{cases} \mu := \bar{\mu} \, \| \bar{\mu} \|_{\infty,G}^{-1}, \ \ \beta := \bar{\beta} \, \| \bar{\beta} \|_{\infty,G}^{-1}, \ \ \sigma := \bar{\sigma} \, \| \bar{\sigma} \|_{\infty,G}^{-1}, \ \ f := L^2 \, \| \bar{\mu} \|_{\infty,G}^{-1} \, f, \\ \alpha := \bar{\alpha} L \, \| \bar{\mu} \|_{\infty,G}^{-1}, \ \ \gamma := \bar{\gamma} L \, \| \bar{\mu} \|_{\infty,G}^{-1}, \ \ g_0 := L \, \| \bar{\mu} \|_{\infty,G}^{-1} \, \bar{g}_0, \ \ g_1 := L \, \| \bar{\mu} \|_{\infty,G}^{-1} \, \bar{g}_L. \end{cases}$$

and after small algebra we rewrite problem (1) in the following form

$$\begin{cases} \textit{find function } \ u = u(t) \ \ \textit{such that} \\ -(\mu \, u')' + Pe\left[\, \beta u' + Sh \, \sigma u \right] = f \quad \text{in } \ \ \Omega = (0,1), \\ (\mu u' - \alpha u)\,|_{t=0} = g_0, \ \ (-\mu u' - \gamma u)\,|_{t=1} = g_1. \end{cases} \tag{2}$$

where $v' := \dfrac{dv}{dt}$ and dimensionless numbers

$$\mathrm{Pe} := \frac{\| \bar{\beta} \|_{\infty,G} \, L}{\| \bar{\mu} \|_{\infty,G}}, \qquad \mathrm{St} := \frac{\| \bar{\sigma} \|_{\infty,G} \, L}{\| \bar{\beta} \|_{\infty,G}} \tag{3}$$

are well-known Péclet criteria and Strouhal criteria respectively.

4. VARIATIONAL FORMULATION

The boundary value problem (2) admits the following variational formulation

$$\begin{cases} \text{find} \quad u \in V := H^1(\Omega) \ \text{ such that} \\ \quad c_\Omega(u,v) = < l_\Omega, v > \quad \forall v \in V, \end{cases} \tag{4}$$

where

$$c_\Omega(u,v) := (\mu u', v') + \mathrm{Pe}\cdot[(\beta u', v) + \mathrm{St}\cdot(\sigma u, v)] \\ + \alpha uv|_{t=0} + \gamma uv|_{t=1} \quad \forall u, v \in V, \tag{5}$$

$$< l_\Omega, v > := (f, v) + \alpha g_0 v(0) + \gamma g_1 v(1) \qquad \forall v \in V. \tag{6}$$

5. WELL-POSEDNESS OF VARIATIONAL PROBLEM

We are able to prove the well-posedness of variational problem (4).

Proposition 5.1. Let data of the problem (1) satisfies the following conditions

$$\begin{cases} \mu \in L^\infty(\Omega), \\ \mu(x) \ge \mu_0 = const > 0 \quad a.e. \ in \ \ \Omega \ , \end{cases} \tag{7}$$

$$\begin{cases} \beta, \sigma \in L^\infty(\Omega) \\ \sigma(x) - \tfrac{1}{2}\mathrm{Pe}\,\beta'(x) \ge c_0 = const > 0 \quad a.e. \ in \ \ \Omega, \end{cases} \tag{8}$$

$$\alpha - \tfrac{1}{2}\mathrm{Pe}\,\beta(0) > 0, \ \ \gamma + \tfrac{1}{2}\mathrm{Pe}\,\beta(1) > 0, \tag{9}$$

$$f \in L^2(\Omega)\,. \tag{10}$$

Then

(i) bilinear form $c_\Omega(\,.\,,\,.\,) : V \times V \to R$ is continuous, and the following inequality holds

$$|c_\Omega(u,v)| \le 4\max\{1, \mathrm{Pe}, \mathrm{Pe}\cdot\mathrm{St}, |\alpha|, |\gamma|, |\alpha+\gamma|\}\, \|u\|_V \|v\|_V \quad \forall u, v \in V\,; \tag{11}$$

(ii) bilinear form $c_\Omega(\,.\,,\,.\,) : V \times V \to R$ is $V-$elliptical, and defines energy norm

$$\|v\|_\Omega := \sqrt{c_\Omega(v,v)} \qquad\qquad \forall v \in V = H^1(\Omega)\,, \tag{12}$$

moreover

$$c_0 \|v\|_V^2 \le \|v\|_\Omega^2 \qquad \forall v \in V, \tag{13}$$

where $c_0 = \min\{\tfrac{1}{2}\mu_0, \mathrm{Pe}(\mathrm{St}\,\sigma - \tfrac{1}{2}\beta' + C_F \min\{\tfrac{1}{2}\mu_0, C_D\})\}$;

(iii) linear functional $l_\Omega : V \to R$ is continuous and

$$|< l_\Omega, v >| \le (\|f\|_{0,\Omega} + \\ + 2\max\{|\alpha|, |\gamma|, |\alpha+\gamma|\}\, \|(g_1 - g_0)x + g_0\|_{1,\Omega})\, \|v\|_V \quad \forall v \in V; \tag{14}$$

(iv) there exists one and only one solution $u \in V$ of problem (4), and

$$\|u\|_V \le \frac{1}{c_0} \|l_\Omega\|_* \quad \forall v \in V. \tag{15}$$

Proof. Let us define the linear function $\rho = \rho(x)$ such that $\rho(x) := (\gamma + \alpha)x - \alpha.$ Then

$$\begin{aligned}\alpha uv|_{t=0} + \gamma uv|_{t=1} = \rho uv|_0^1 &= \int_0^1 [\{(\gamma+\alpha)x-\alpha\}uv]' dx \\ &= \int_0^1 [(\gamma+\alpha)uv + \rho u'v + \rho uv']dx \\ &\le \max\{\|\rho\|_{\infty,\Omega}, |\gamma+\alpha|\}\int_0^1 (|uv| + |u'v| + |uv'|)dx \\ &\le 2\max\{|\alpha|,|\gamma|,|\alpha+\gamma|\}\|u\|_{1,\Omega}, \|v\|_{1,\Omega} \qquad \forall u,v\in V.\end{aligned} \tag{16}$$

(i) Using this estimation we obtain

$$\begin{aligned}|c_\Omega(u,v)| &\le |(\mu u', v')| + \mathrm{Pe}[|(\beta u', v)| + \mathrm{St}\cdot|(\sigma u, v)|] + |(\rho uv)|_0^1| \\ &\le \|u'\|_{0,\Omega}\|v'\|_{0,\Omega} + \mathrm{Pe}[\|u'\|_{0,\Omega} + \mathrm{St}\|u\|_{0,\Omega}]\|v\|_{0,\Omega} + |(\rho uv)|_0^1| \\ &\le 2\max\{1,\mathrm{Pe},\mathrm{Pe}\cdot\mathrm{St}\}\|u\|_V\|v\|_V \\ &\quad + 2\max\{|\alpha|,|\gamma|,|\alpha+\gamma|\}\|u\|_V, \|v\|_V \\ &\le 4\max\{1,\mathrm{Pe},\mathrm{Pe}\cdot\mathrm{St},|\alpha|,|\gamma|,|\alpha+\gamma|\}\|u\|_V\|v\|_V \qquad \forall u,v\in V.\end{aligned} \tag{17}$$

To obtain (13) we start from the following estimation

$$\begin{aligned}c_\Omega(v,v) &= \int_0^1 [\mu(v')^2 + \mathrm{Pe}(\mathrm{St}\,\sigma - \tfrac{1}{2}\beta')v^2]dx \\ &\quad + (\alpha - \tfrac{1}{2}\mathrm{Pe}\,\beta)v^2(0) + (\gamma + \tfrac{1}{2}\mathrm{Pe}\,\beta)v^2(1) \\ &\ge \int_0^1 [\mu_0(v')^2 + \mathrm{Pe}(\mathrm{St}\,\sigma - \tfrac{1}{2}\beta')v^2]dx + C_D[v^2(0)+v^2(1)] \\ &\ge \int_0^1 [\tfrac{1}{2}\mu_0(v')^2 + \mathrm{Pe}(\mathrm{St}\,\sigma - \tfrac{1}{2}\beta')v^2]dx \\ &\quad + \min\{\tfrac{1}{2}\mu_0, C_D\}[\int_0^1 (v')^2 dx + v^2(0) + v^2(1)] \qquad \forall v\in V,\end{aligned}$$

where $C_D := \min\{(\alpha - \frac{1}{2}\mathrm{Pe}\,\beta), (\gamma + \frac{1}{2}\mathrm{Pe}\,\beta)\} > 0.$ Using Friedrichs inequality [10]

$$\int_0^1 (v')^2 dx + [v^2(0) + v^2(1)] \ge C_F \int_0^1 v^2 dx \quad C_F = const > 0 \quad \forall v \in H^1(\Omega),$$

we obtain declared in (13) estimation

$$\begin{aligned}c_\Omega(v,v) &\ge \int_0^1 [\tfrac{1}{2}\mu_0(v')^2 + \mathrm{Pe}(\mathrm{St}\,\sigma - \tfrac{1}{2}\beta')v^2]dx + C_F\min\{\tfrac{1}{2}\mu_0, C_D\}\int_0^1 v^2 dx \\ &= \int_0^1 [\tfrac{1}{2}\mu_0(v')^2 + \mathrm{Pe}(\mathrm{St}\,\sigma - \tfrac{1}{2}\beta' + C_F\min\{\tfrac{1}{2}\mu_0, C_D\})v^2]dx \\ &\ge c_0\|v\|_V^2 \quad \forall v\in V, \quad c_0 = \min\{\tfrac{1}{2}\mu_0, \mathrm{Pe}(\mathrm{St}\,\sigma - \tfrac{1}{2}\beta' + C_F\min\{\tfrac{1}{2}\mu_0, C_D\})\}.\end{aligned}$$

(ii) To prove the continuity of the linear functional we apply the used technique, a namely

$$\begin{aligned}|\langle l_\Omega, v\rangle| &\le |(f,v)| + |\alpha g_0 v(0) + \gamma g_1 v(1)| \\ &\le \|f\|_{0,\Omega}\|v\|_{0,\Omega} + |\rho[(g_1-g_0)x + g_0]v|_0^1| \\ &\le \|f\|_{0,\Omega}\|v\|_{0,\Omega} + 2\max\{|\alpha|,|\gamma|,|\alpha+\gamma|\}\|\|(g_1-g_0)x+g_0\|_{1,\Omega}\|v\|_{1,\Omega} \\ &\le (\|f\|_{0,\Omega} + 2\max\{|\alpha|,|\gamma|,|\alpha+\gamma|\}\|(g_1-g_0)x+g_0\|_{1,\Omega})\|v\|_V \quad \forall v\in V.\end{aligned}$$

(iii) Taking into account Lax-Milgram-Vyshyk lemma [8], we can simply prove that the variational problem (2) has unique solution.

6. SYMMETRIZED VARIATIONAL PROBLEM

For further needs we consider now the procedure of changing problem with nonsymmetric bilinear form $c_\Omega(\,\cdot\,,\,\cdot\,):V\times V\to\mathbb{R}$ to identical problem with symmetric form. It can be achieved using some decomposition of an admissible functions [7].

To demonstrate the possibility of construction of an alternative variational formulation for the boundary value problem (1) we prove the following

Proposition 6.1. Let $z=z(x)$ be the function

$$z(x):=\exp[-\mathrm{Pe}\int_0^x \mu^{-1}\beta dt] \qquad \forall x\in[0,1]\,. \tag{18}$$

Then

(i) the variational problem (4) is equivalent to the following minimization problem of a quadratic functional

$$\begin{cases}\text{find}\quad u\in V:=H^1(\Omega)\ \text{ such that}\\ \quad J(u)\ \le \mathrm{J}(w)\quad \forall w\in V,\end{cases} \tag{19}$$

where

$$\mathrm{J}(w):=s_\Omega(\mathrm{z};w,w)-2<l_\Omega,\mathrm{z}\,w> \qquad \forall w\in V, \tag{20}$$

$$\begin{aligned} s_\Omega(z;u,w):=&(\mu z\,u',w')+\mathrm{Pe}\cdot\mathrm{St}\cdot(\sigma z\,u,w)\\ &+\alpha zuw\,|_{t=0}+\gamma zuw\,|_{t=1}\quad \forall u,w\in V;\end{aligned} \tag{21}$$

(ii) there is the unique solution $u\in V$ of the problem (19).

Proof. In order to see relation between bilinear forms (5) and (21) we obtain

$$\begin{aligned} c_\Omega(u,zw)=&(\mu u',(zw)')+\mathrm{Pe}\cdot[(\beta u',zw)+\mathrm{St}\cdot(\sigma u,zw)]\\ &+\alpha uzw\,|_{t=0}+\gamma uzw\,|_{t=1}\\ =&(\mu u',zw')+(\mu z'+\mathrm{Pe}\beta z)u',w)+\mathrm{Pe}\cdot\mathrm{St}\cdot(\sigma u,zw)\\ &+\alpha uzw\,|_{t=0}+\gamma uzw\,|_{t=1}\qquad \forall u,v\in V,\end{aligned} \tag{22}$$

and note that function $z=z(x)$ satisfies equation $\mu z'+\mathrm{Pe}\beta z=0.$ Hence,

$$s_\Omega(z;u,w):=c_\Omega(u,zw)\qquad \forall u,w\in V. \tag{23}$$

Moreover, to take into account definition (21) we have

$$s_\Omega(z;u,w):=s_\Omega(z;w,u)\qquad\qquad \forall u,w\in V\ ,$$

and thus, statement of the problem (19) is a classical approach of variational analysis. Taking into account that $c_\Omega(\mathrm{z};\,.\,,.\,):V\times V\to\mathbb{R}$ is a new scalar product on V we can define the energy norm

$$\|\,u\,\|_E:=\sqrt{c_\Omega(\mathrm{z};u,u)}\qquad\qquad \forall u\in V \tag{24}$$

and rewrite the quadratic functional $J=J(w)$ in the following form

$$J(w)=\|\,w-u\,\|_E^2-\|\,u\,\|_E^2=\|\,w-u\,\|_E^2+J(u)\qquad \forall v\in V\ , \tag{25}$$

where $u\in V$ is the solution of variational problem (19) or it equivalently (4).

Hence, at that moment we have two equivalent variational formulations (4) and (19) for the boundary value problem (1). Then we have possibility to use a finite element approximations for solving of (1) by the Petrov-Galerkin method or Ritz method.

7. FINITE ELEMENT METHOD

Let $\{V_h\}_{h>0}$ be a family of finite element approximation subspaces $V_h \subset V$, $\dim V_h = N_h < +\infty$, $\cup_{h>0} V_h$ is dense in V, moreover, for each $v \in V$ there is $v_h \in V_h$ such that

$$\| v - v_h \|_{H^1(\Omega)} \le Ch^k \| v \|_{H^{k+1}(\Omega)}, \; C = const > 0. \tag{26}$$

7.1. RITZ-GALERKIN FINITE ELEMENT SCHEME

In general case Ritz-Galerkin finite element scheme deal with following minimization problem

$$\begin{cases} \textit{given subspace } V_h \subset V, \dim V_h = N_h < +\infty, \\ \text{find } \; u_h \in V_h \; \text{ such that} \\ \quad J(u_h) \le \mathrm{J}(w) \;\; \forall w \in V_h, \end{cases} \tag{27}$$

Let us denote by $\{\varphi_k\}_{k=1}^N$ a fixed basis of the space V_h. Consequently sought solution of (26) will take form of the linear combination

$$u_h(x) := \sum_{k=1}^N q_k \varphi_k(x) \tag{28}$$

with unknown coefficients $q_1, \dots, q_N$. Substituting (28) into (27), and then applying a conditions of minimum to resulting quadratic function of variables $q_1, \dots, q_N$ we get algebraic problem

$$\begin{cases} \text{find } \; \mathrm{q}=(q_1, \dots, q_N) \in \mathbb{R}^N \; \text{ such that} \\ \sum_{k=1}^N s_\Omega(z; \varphi_k, \varphi_i) q_k = < l_\Omega, z\varphi_i > i = 1, \dots, N. \end{cases} \tag{29}$$

Matrix $S_\Omega = \{s_\Omega(\mathrm{z}; \varphi_k, \varphi_i)\}_{i,k=1}^N$ is symmetric positively defined. Therefore, there is a unique solution $\mathrm{q}=(q_1, \dots, q_N) \in \mathbb{R}^N$ to the system of the linear algebraic equations, and problem (27) is uniquely solvable.

7.2. PETROV-GALERKIN FINITE ELEMENT SCHEME

As an alternative the classic Ritz method we demonstrate the additional possibilities of Petrov-Galerkin method, which generates following discrete problem:

$$\begin{cases} \textit{given subspaces } V_h \subset V \textit{ and } W_h \subset V, \\ \qquad \dim V_h = \dim W_h = N_h < +\infty, \\ \text{find } \; u_h \in V_h \; \text{ such that} \\ \quad c_\Omega(u_h, v) = < l_\Omega, v > \qquad \forall v \in Y_h. \end{cases} \tag{30}$$

Let $\{\varphi_j\}_{j=1}^N$ and $\{w_m\}_{m=1}^N$ be basis of V_h and Y_h spaces respectively. Then problem (30) results to system of linear algebraic equations

$$\begin{cases} \textit{given subspaces } V_h \subset V \textit{ and } W_h \subset V, \\ \qquad \dim V_h = \dim W_h = N_h < +\infty, \\ \text{find } \; u_h = \sum_{k=1}^N q_k \varphi_k \in V_h \; \text{ such that} \\ \quad \sum_{k=1}^N c_\Omega(\varphi_k, w_i) q_k = < l_\Omega, w_i > \qquad i = 1, \dots N. \end{cases} \tag{31}$$

This is a main relation between systems of linear algebraic equations (29) and (31) which shows as we may symmetrize the algebraic problem (31). Taking $w_i := z\varphi_i$ into (31) we lead to (29).

8. OPTIMALITY OF FINITE ELEMENT APPROXIMATIONS

Now we are interested in the error of a finite element approximation $u_h \in V_h$, i.e. $e_h := u - u_h \in V$.

Let approximation $u_h \in V_h$ is obtained as the solution of the minimization problem (27). Than it is well-known that

(i) $c_\Omega(z; e_h, w) = 0 \quad \forall w \in V_h$ (errror orthogonality);

(ii) $e_h \in V_h^\perp,\ V = V_h \oplus V_h^\perp$;

(iii) $\| e_h \|_E = \inf_{w \in V_h} \| u - w \|_E$ (error optimality);

(iv) $\| e_h \|_E^2 = \| u \|_E^2 - \| u_h \|_E^2 \qquad \forall h > 0.$

If $\Delta < h$, $V_h \subset V_\Delta$, $u_h \in V_h$ and $u_\Delta \in V_\Delta$ are the finite element approximations of the solution $u \in V$ of problem (19). Then we have the decompositions $u = u_h + e_h \in V_h \oplus V_h^\perp$ and $u = u_\Delta + e_\Delta \in V_\Delta \oplus V_\Delta^\perp$ respectively, and

$$\| e_h \|_E^2 = \| u \|_E^2 - \| u_h \|_E^2, \quad \| e_\Delta \|_E^2 = \| u \|_E^2 - \| u_\Delta \|_E^2,$$
$$\| u_\Delta - u_h \|_E^2 = \| u_\Delta \|_E^2 - \| u_h \|_E^2,$$

implies inequality

$$\| u_h \|_E \le \| u_\Delta \|_E \le \| u \|_E \qquad \forall \Delta < h, \tag{32}$$
$$\| e_h \|_E^2 - \| e_\Delta \|_E^2 = \| u_\Delta \|_E^2 - \| u_h \|_E^2 \ge 0$$

and

$$\| e_\Delta \|_E \le \| e_h \|_E \qquad \forall \Delta < h. \tag{33}$$

Therefore if the sequence finite element spaces $\{V_h\}$ is inclusive sequence of finite element spaces then for finite element approximations sequence $\{u_h\}$ corresponding errors $\{e_h\}$ are monotonically convergent to 0 as $h \to 0$. On the other hand the error $e_h := u - u_h \in V_h^\perp$ is the solution of the minimization problem

$$\begin{cases} given\ \ u_h \in V_h \subset V, \dim V_h = N_h < +\infty, \\ \text{find} \quad e_h \in V_h^\perp \quad \text{such that} \\ \qquad R(e_h) \le \mathrm{R}(w) \qquad\qquad \forall w \in V_h^\perp, \end{cases} \tag{34}$$

where

$$R(w) := s_\Omega(z; w, w) - 2 < \rho_\Omega(u_h), w > \qquad\qquad \forall w \in V_h^\perp, \tag{35}$$
$$< \rho_\Omega(u_h), w > := < l_\Omega, \mathrm{z}\, w > - s_\Omega(z; u_h, w) \qquad\qquad \forall w \in V_h^\perp \tag{36}$$

Let $\bar{e}_h$ be a posteriori error estimator of the finite element approximation $u_h \in V_h$ i. e. the solution of discrete problem

$$\begin{cases} given\ subspace\ W_h \subset V_h^\perp, \dim W_h < +\infty, \\ \text{find} \quad \bar{e}_h \in W_h \quad \text{such that} \\ \qquad R(\bar{e}_h) \le \mathrm{R}(w) \forall w \in W_h. \end{cases} \tag{37}$$

Since

$$\| e_h \|_E^2 = \| e_h - \bar{e}_h \|_E^2 + \| \bar{e}_h \|_E^2 \qquad \forall h > 0. \tag{38}$$

We define

$$\bar{u}_h := u_h + \bar{e}_h \in \bar{V}_h := V_h \oplus W_h ,$$

and rewrite the last equations in the following form

$$\| u - \bar{u}_h \|_E^2 = \| e_h \|_E^2 - \| \bar{e}_h \|_E^2 \qquad \forall h > 0. \tag{39}$$

As a conclusion of (39) we have the estimation

$$\| \bar{e}_h \|_E \le \| e_h \|_E \qquad \forall h > 0. \tag{40}$$

Proposition 8.1. Given finite element approximation $u_h \in V_h$ for the solution $u \in V$ of the variational problem (19), then a posteriori error estimator $\bar{e}_h \in W_h \subset V_h^{\perp}$, $\dim W_h < +\infty$, obtained as the solution of problem (37), generates the improved approximation

$$\bar{u}_h := u_h + \bar{e}_h \in \bar{V}_h = V_h \oplus W_h$$

$$\| u - \bar{u}_h \|_E^2 = \| u - u_h \|_E^2 - \| \bar{e}_h \|_E^2 \qquad \forall h > 0 \tag{41}$$

9. A POSTERIORI ERROR ESTIMATORS OF FINITE ELEMENT APPROXIMATIONS

Let us describe two different ways for obtaining error level on each finite element. Explicit estimator is an explicit formula which gives us upper bound of error estimate as one number. Implicit estimator is obtained as function which approximates actual error of finite element discretization. To obtain it we solve auxiliary variational problem.

9.1. EXPLICIT ERROR ESTIMATOR FOR 1D

To estimate error level we will use explicit error estimator i.e. explicit formula which gives us upper bound to approximation error on each finite element. Let us define the *approximation error* $e = u - u_h \in V = V$, the residual

$$R[u_h] := f + (\mu\, u_h')' - \beta \mathrm{Pe}\; u_h' - \sigma \mathrm{Pe}\, \mathrm{St}\; u_h , \tag{42}$$

and bubble function

$$\omega_K(x) := (x_k - x)(x - x_{k-1}), \;\; \mathrm{supp}\, \omega_K := K \qquad \forall K \in \Im_h. \tag{43}$$

Proposition 9.1. The following global estimate holds

$$\|e\|_{H^1(\Omega)}^2 \le 4\left[\min\{\mu_0, c_0\}\right]^{-1} \sum_{K \in \Im} [\, p_K(p_K + 1)]^{-1} \left\| \sqrt{\omega_K}\, R[u_h] \right\|_{L^2(K)}^2 , \tag{44}$$

where $p_K = \deg(u_h|_K)$.

Proof see in [11].

The terms of sum in (44) can be used as error estimates on each element.

9.3. IMPLICIT ERROR ESTIMATOR

Described estimator gives us only one number per finite element which we interpret as error level. To combine *h*- and *p*- refinements of elements we need to construct some type of estimator which:

- will give us distinct error estimate for each of available refinement patterns of element;
- will be simply computable on each element.

For this purposes we will solve auxiliary variational problem like described by (34) on each element, using finite element method for different finite element spaces.
Let us define $X^p(a,b)$ as a space of all polynomials of order p on closed interval $[a,b]$.

For all refinement patterns we may define corresponding approximation spaces. We will use only two refinements: division of the element into two elements with the same polynomial orders and increasing element order by one. Corresponding spaces are the following:

$$\begin{gathered} V_{hp}^1(K) = \{v \in C(K) \mid v \in X^{p_K}(x_{k-1},[x_{k-1}+x_k]/2), \\ v \in X^{p_K}([x_{k-1}+x_k]/2, x_k), v|_{\partial K} = 0\}, \\ V_{hp}^2(K) = \{v \in X^{p_K+1}(K) \mid v|_{\partial K} = 0\}. \end{gathered} \tag{45}$$

To obtain error estimate as a single number for finite element error approximation on each space for $m = 1,2$ we solve the next problems:

$$\begin{cases} find \;\; e_h^m \in V_{hp}^m(K) \;\; such \;\; that \\ c_\Omega(e_h^m, v_h) = \int\limits_K R[u_h^k] v_h dx \quad \forall v_h \in V_{hp}^m(K), \end{cases} \tag{46}$$

then error estimates for given two refinements are defined as $r_m = \|e_h^m\|_E$, $m = 1,2$.

10. ADAPTATION ALGORITHM

The main idea in our adaptation algorithm is to use implicit error indicator to select proper refinement pattern on each element and explicit to select elements for refinement. So the question is, why we need to use another explicit error estimator? Let us observe mechanics of implicit estimator under the hood. So 1) we obtain actually some error estimate as function, and 2) this approximation depends on used approximation space. At least, order of this space should be larger than order of space, used on element to obtain global solution. As we will have in general case different degrees on all elements so it is problematic to compare error values between two different elements because for example the larger value will just say that the error estimate was obtained with larger accuracy. So there is no any sense to compare different values of using implicit estimates. Also we need to note than from (41) we can conclude that we should use refinement which gives approximation to error with larger norm.

Let us define: *TOL* - acceptable relative error level in percent, $p_{\max}$ – maximum element order (polynomial degree),

$$C := 2\left[\min\{\mu_0, c_0\}\right]^{-1/2}.$$

Step 1: Find FEM solution on the current mesh – u_h.

Step 2: *Stop condition check.* For all elements K compute

$$\eta_K = C[p_K(p_K+1)]^{-1/2} \left\| \sqrt{\omega_K}\, R[u_h^K] \right\|_{L^2(K)}. \tag{47}$$

Define

$$\eta := \left(\sum\nolimits_{K\in\Im} \eta_K^2\right)^{1/2}.$$

Then if

$$\eta \|u_h\|_E^{-1} \times 100\% < TOL$$

we stop the algorithm (TOL is an acceptable relative error level in percent), else

Step 3: *Choose elements for refinement*. Compute $\eta_{\max} = \max_K \eta_K$ .We will change those elements K , for which

$$\eta_K > (1-\theta)\eta_{\max}, \ \theta \in (0,1)$$

is fixed value. The set of all selected elements we name as A_θ .

Step 4: *Mesh modification*. For all selected elements $K = [x_{k-1}, x_k]$ ($p_K := \deg(u_h|_K)$) choose between bisection and increasing of polynomial degree on it by one.

If $p_K = p_{\max}$ then we divide element into two with orders (p_K, p_K) , otherwise: Let us compute values

$$r_m = \left\| e_h^m \right\|_E, \ m = 1,2$$

by solving problems (46).

Consider the difference

$$\Delta = r_2 - r_1 .$$

If $\Delta > \delta$, where δ is predefined value, then we increase element order by 1, otherwise we bisect it into two elements with approximation polynomial orders (p_K, p_K) .

Step 5: *Go to* Step 1.

Remark 10.1. From the theoretical point of view we should set $\delta = 0$ but in practice, according to errors in numerical quadratures and round-off errors, furthermore the maximum order of approximating polynomial is bounded – so it's logically to use bisection in case when Δ is very small. For this purposes we choose small number $\delta > 0$.

Remark 10.2. Parameters δ and θ need to be set manually for each iteration as "optimal" in some sense. There is unsolved problem of automation of selection δ and θ on all iterations. Parameters δ and θ have the following meanings:

δ set the priority between element bisection and order increasing;

θ is a percent of elements need to be refined.

11. NUMERICAL RESULTS

In this chapter we present results of our algorithm in comparison with reference solution one [3] for singular perturbed problems. Parameters δ and θ are equal for all iterations and are selected using search from several values to provide "optimal" values which minimize final number of iterations and final count of degrees of freedom.

Problem 1. We consider boundary value problem (1) with the following data

$$\mu = 1, \beta = 0, \sigma = 10^5 e^x, \ f = 10^5, \alpha = \gamma = 10^8, \bar{u}_0 = \bar{u}_L = 0, L = 1.$$

Fig. 1 and Table 1 demonstrate numerical results which we obtained using algorithm with the following parameters: TOL = 5%, $p_{\max} = 9$, $\delta = 2, \ \theta = 0.6$.

Fig. 2 and Fig. 4 show relation between error indicator and number of degrees of freedom for constructed algorithm and algorithm based on reference solution.

Fig. 3 and Table 2 shows corresponding results obtained using reference solution algorithm.

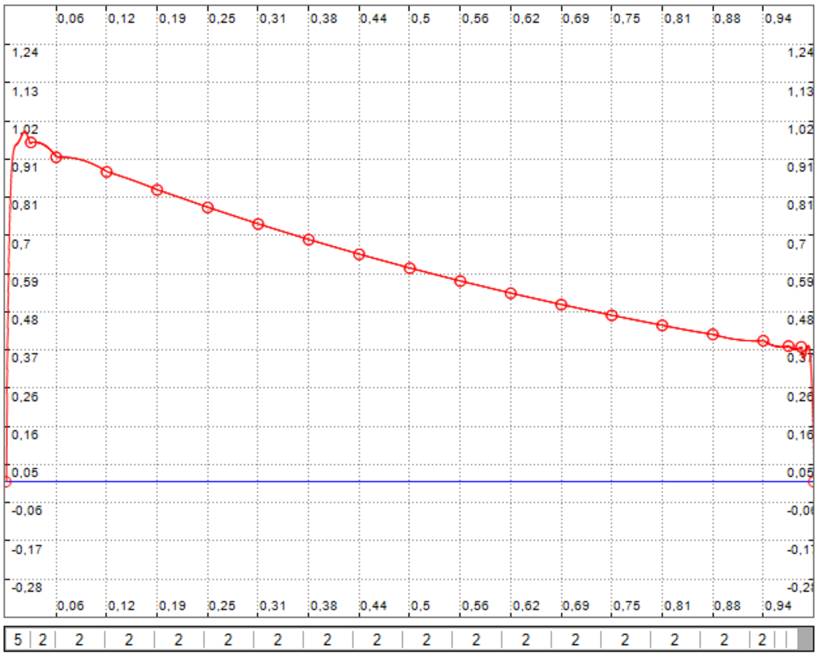

Fig. 1. Approximation to solution of Problem 1, obtained on final iteration of algorithm described in Section 9. The row below the table shows corresponding polynomial degrees on finite elements. The solid horizontal line represents x-axis

Table 1

Convergence history for Problem 1: n is an iteration number, $N_{dof}^{(n)}$ count of degrees of freedom, $\varepsilon_n^{\Omega} = \eta$ absolute error indicator, $r_n^{\Omega} = \eta \| u_h \|_E^{-1} \times 100\%$ relative error,

$$p_n = -\frac{\ln \varepsilon_n^{\Omega} - \ln \varepsilon_{n-1}^{\Omega}}{\ln N_{dof}^{(n)} - \ln N_{dof}^{(n-1)}}$$ rate of convergence.

n	$N_{dof}^{(n)}$	ε_n^{Ω}	r_n^{Ω}	p_n
0	3	12579,37	6045	–
1	5	3998,07	1695	2.24
2	9	1457,71	599	1.72
… … …				
7	34	25,53	10,19	1.49
8	39	24,94	9,95	0.16
9	43	7,59	3,03	12.19

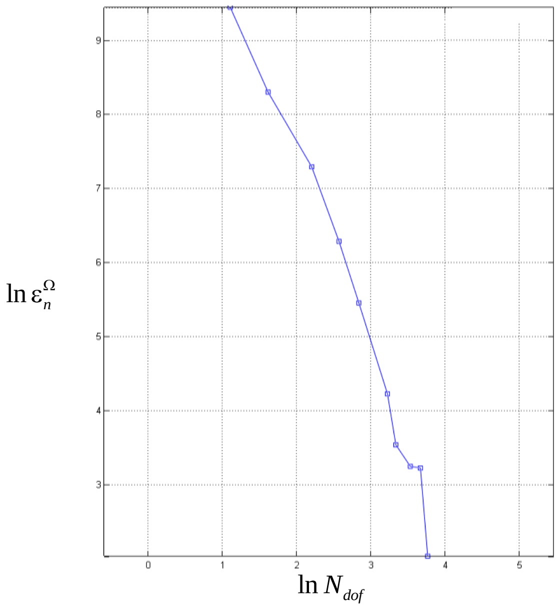

Fig. 2. Plot of dependency between absolute error indicator ε_n^{Ω} and number of degrees of freedom N_{dof} in logarithmic scale for Problem 1 for algorithm from Section 9

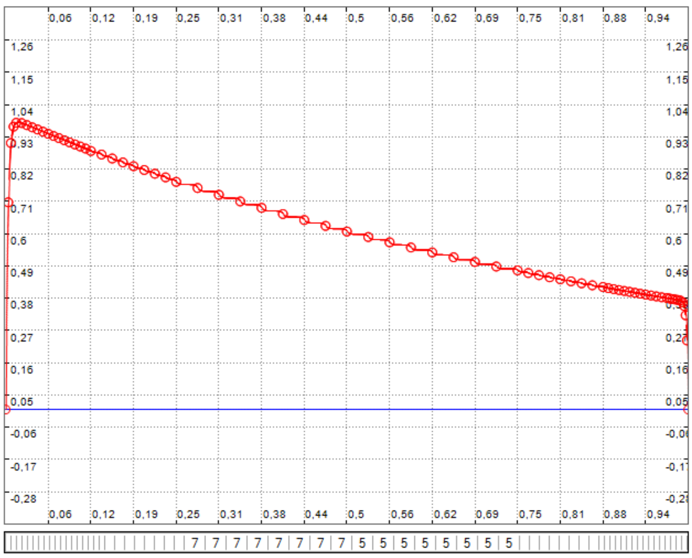

Fig. 3. Approximation to solution of Problem 1, obtained on final iteration, using reference solution algorithm (see [3,4]). The row below the table shows corresponding polynomial degrees on finite elements. The solid horizontal line represents x-axis

Table 2

Reference solution algorithm convergence history for Problem 1.

n	N_{dof}	ε_n^{Ω}	r_n^{Ω}	p_n
… … …				
12	32	3,60	28,08	-1.05
13	35	3,14	23,81	1.53
… … …				
30	333	0,77	5,52	1.14
31	379	0,70	5,04	0.70
32	437	0,58	4,19	1.32

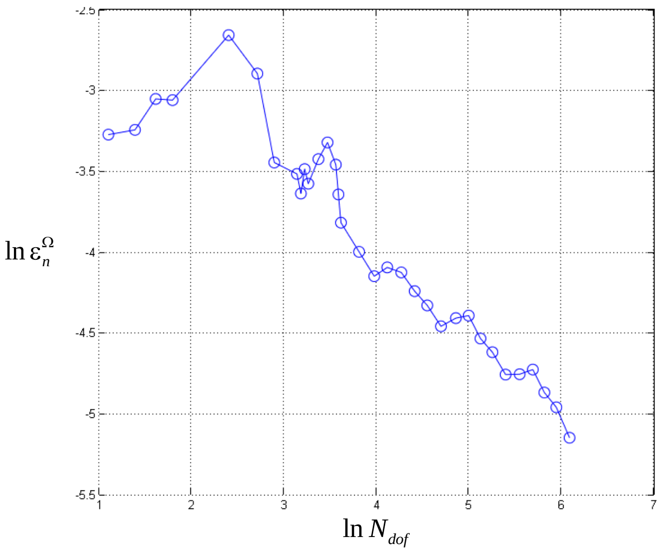

Fig. 4. Plot of dependency between absolute error indicator ε_n^{Ω} and number of degrees of freedom N_{dof} in logarithmic scale for Problem 2 for reference solution algorithm

Comparing tables 1 and 2 shows than constructed algorithm obtain up to 3 time less iterations and 10 times less final system of linear equations in comparing to reference solution algorithm.

Problem 2. We consider boundary value problem (1) with following data

$$\mu = 1, \beta = e^{2x} - 200,\ \sigma = 100(\cos x + 2),$$

$$f = 1000e^{-100(x-0.5)^2},\ \alpha = \gamma = 10^8,\ \bar{u}_0 = \bar{u}_L = 0,\ L = 1.$$

Fig. 5 and Table 3 demonstrate numerical results which we obtained using algorithm with the following parameters: TOL = 5%, $p_{\max} = 9$, $\delta = 0,\ \theta = 0.6$. We should note, that in this example algorithm is applied to the problem without using symmetrization, demonstrating the capability of handling nonsymmetric problems by algorithm itself.

Fig. 6 and Fig. 8 show relation between error indicator and number of degrees of freedom for constructed algorithm and algorithm based on reference solution.
Fig. 7 and Table 4 shows corresponding results obtained using reference solution algorithm.

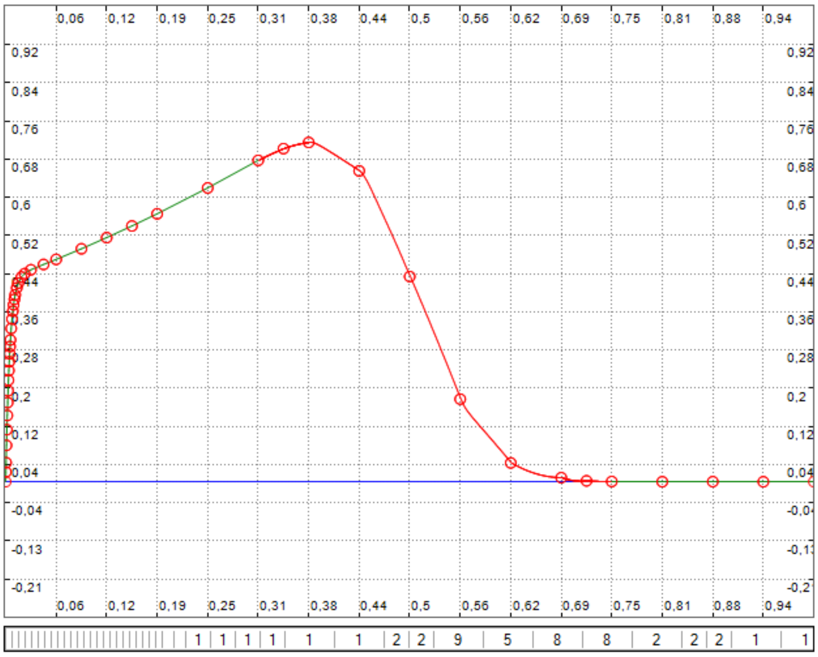

Fig. 5. Approximation to solution of Problem 2, obtained on final iteration of algorithm described in Section 9. The row below the table shows corresponding polynomial degrees on finite elements. The solid horizontal line represents x-axis

Table 3

Convergence history for Problem 2.

n	N_{dof}	ε_n^{Ω}	r_n^{Ω}	p_n
0	3	65,86	47675	–
1	5	56,51	580	0.2
2	9	54,02	296	1.4
… … …				
13	68	0,55	5,72	0.07
14	72	0,49	5,07	2.13
15	77	0,43	4,51	1.75

On Fig. 5 algorithm constructed mesh with many low-order elements near boundary layer and few high-order at smooth solution part. It's a good example of "well" mesh according to theoretical investigations [2].

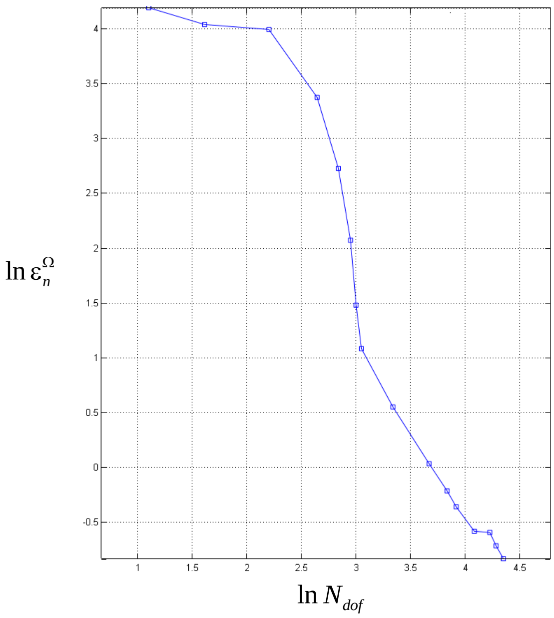

Fig. 6. Plot of dependency between absolute error indicator ε_n^{Ω} and number of degrees of freedom N_{dof} in logarithmic scale for Problem 2 for algorithm from Section 9

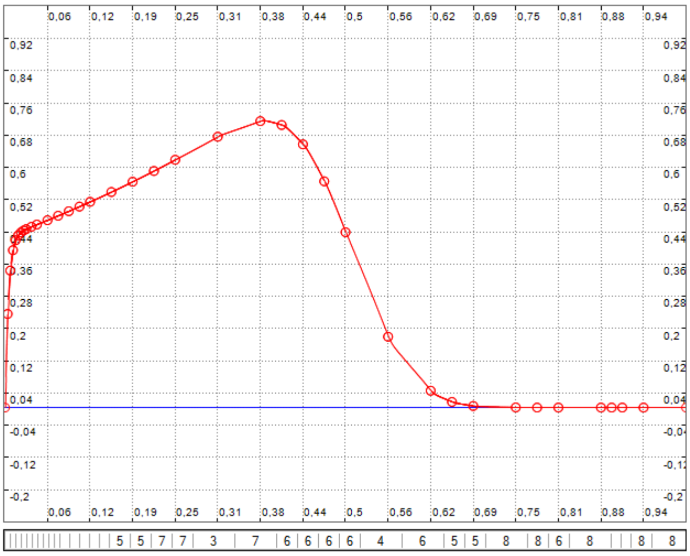

Fig. 7. Approximation to solution of Problem 2, obtained on final iteration, using reference solution algorithm (See. [3,4]). The row below the table shows corresponding polynomial degrees on finite elements. The solid horizontal line represents x-axis

Table 4

Reference solution algorithm convergence history for Problem 2.

n	N_{dof}	ε_n^{Ω}	r_n^{Ω}	p_n
… … …				
14	39	2,11	131,42	-0.02
15	46	2,10	130,70	0.01
… … …				
31	171	0,45	9,92	-0.002
32	196	0,43	9,43	0.4
33	224	0,18	3,85	6.6

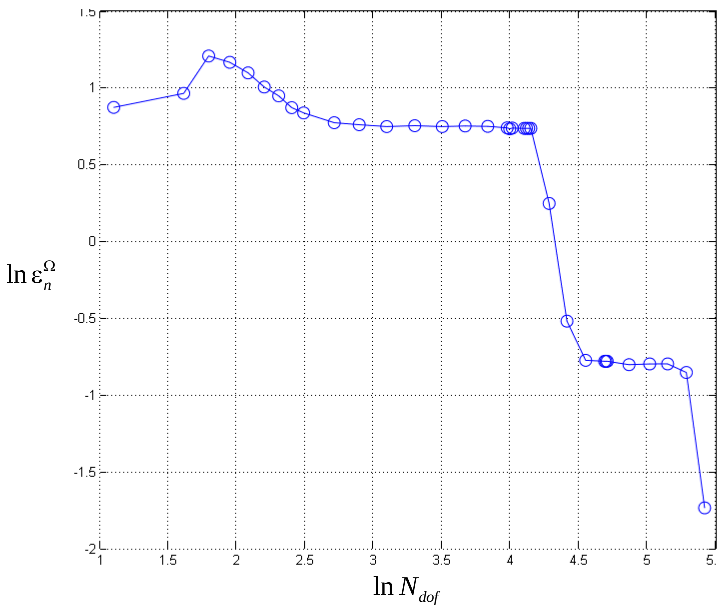

Fig. 8. Plot of dependency between absolute error indicator ε_n^{Ω} and number of degrees of freedom N_{dof} in logarithmic scale for Problem 2 for reference solution algorithm

12. CONCLUSIONS

In this work we constructed *hp*-adaptive algorithm for solving the diffusion-advection-reaction boundary value problems with self-adjoint operators. We proved the optimality in some sense of refinement selection step used in algorithm. Also we introduced symmetrization procedure which can be used to transform given nonsymmetrical variational problem to equivalent symmetric problem, therefore making possible application of constructed algorithm to nonsymmetrical problems too. Also we studied precisely conditions which problem data needs to satisfy to make boundary problem well-posed.

To drive adaptation process we introduce two a posteriori error estimators. For element selection for refinement procedure we use explicit estimator, i.e. explicit formula which gives upper bound of actual error on finite element. After elements for refinement were selected we need to choose on each element refinement pattern: bisection with original element order preservation or increment of polynomial degree on element by one. For this purpose we use classic implicit error estimator (i.e. in the form auxiliary variational problem for error function). Using explicit estimator gives us way of homogeneous computation of per-element error, needed for proper selection elements for refinement. Respectively, using auxiliary error problem gives us elegant way to choose between different types of elements refinement.

In the end we provide the results of some numerical experiments comparing them to the corresponding results, obtained using reference solution algorithm.

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СИМЕТРИЗАЦІЯ КРАЙОВОЇ ЗАДАЧІ ДИФУЗІЇ-АДВЕКЦІЇ-РЕАКЦІЇ ТА *HP*-АДАПТИВНІ АПРОКСИМАЦІЇ МЕТОДУ СКІНЧЕННИХ ЕЛЕМЕНТІВ

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За допомогою масштабування незалежної змінної вводяться критерії подібності Пекле і Струхаля, які сигналізують про сингулярну збуреність розглядуваної крайової задачі дифузії-адвекції-реакції з крайовими умовами Робена. В термінах цих критеріїв проаналізовано відповідну варіаційну задачу щодо коректності її формулювання, визначено достатні для цього умови на ці задачі. Ми симетризуємо останню задачу і подаємо еквівалентну їй задачу мінімізації квадратичного функціонала.

На цій підставі далі будується *hp*–адаптивний алгоритм методу скінченних елементів для відшукання оптимальних апроксимацій розв'язку розглядуваної задачі. Пропонована схема використовує явний і неявний критерії адаптування схеми , які дають змогу на кожній ітерації оптимізувати прийняття рішення стосовно локального згущення сітки чи підвищення порядку апроксимації на скінченному елементі.

Подано результати розв'язування деяких модельних задач і порівняння їх із результатами, які отримали за допомогою алгоритму методу взірцевого розв'язку (reference solution).

Key words: крайова задача дифузії-адвекції-реакції, критерій Пекле, критерій Струхаля, коректність варіаційної задачі, симетризація, мінімізація квадратичного функціонала, метод скінченних елементів, конденсація внутрішніх параметрів, апостеріорний оцінювач похибки, *hp*-адаптивна схема, взірцевий розв'язок.