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VMS ERROR ESTIMATION FOR COMPUTATIONAL FLUID MECHANICS

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Abstract. By decomposing the exact solution into coarse scales (finite element solution) and fine scales (error), the variational multiscale theory has been used to successfully derive a posteriori error estimators for solutions computed with finite element methods. According to the nature of the residuals, the numerial error can be split into two components: element interior residuals and inter-element jumps. A relationship between these residuals (coarse scales) and the error components (fine scales) is established, yielding to a very simple model. In particular, the pointwise error is modeled as a linear combination of bubble functions for the element interior residuals and free-space Green's functions for the inter-element jumps. The numerical error is studied for the standard Galerkin and SUPG methods with application to the convection-diffusion equation.

Keywords: a posteriori error estimation, variational multiscale method, finite element methods.

AMS classification: 65L11,65M60.

§1. Introduction

In this paper, we present recent advances on a posteriori error estimation for finite element methods (FEM) applied to fluid mechanics. When the FEM is employed to solve numerically a differential equation, an inherent error is associated with the computed solution, which can be estimated using various methodologies. Here, the error estimation is driven by the variational multiscale theory (VMS), which consists in splitting the variables of the variational problem in coarse and fine scales. The VMS method has its origin in Hughes et al. works [5, 6] and has been extensively employed to develop the so called stabilized methods. In these methods, a stabilized term is introduced in the variational form that takes into account the influence of the fine scales onto the coarse scales. On the other hand, considering the FEM solution as the coarse scales and the error as the fine scales, the VMS theory can also be used to estimate the committed error by the FEM [3, 4].

A posteriori error estimates [3] may be thought of as emanating from the residuals of the solution. Thus, error estimators address the task of relating these residuals to the error, giving rise to different technologies depending on how this is faced. According to the nature of the residuals, we consider two kinds of residuals: internal residuals, that take into account the non-satisfaction of the differential equation inside the elements; and inter-element residuals, that emerge from the lack of continuity of the numerical solution along the element boundaries. Likewise, the error is decomposed in two components. The first component of the error, called internal residual error, is defined inside each element and has a local character. It is computed with bubble functions. The second component is constructed from a linear combination of free-space Green's functions and models the pollution error, which determines the error inside of an element produced by the residuals of the neighboring elements.

In this work, we estimate the pointwise error applied to the transport equations. The error estimation is based on [9, 8]. Numerical examples are shown that confirm the good behavior of the error estimation.

§2. The variational multiscale framework

Let Ω be a bounded domain in $\mathbb{R}^{n_{sd}}$, where n_{sd} is the number of spatial dimensions, with boundary Γ. In this work, we consider 1D and 2D problems. The boundary is partitioned into two non-overlapping zones Γ_g and Γ_h such that $\Gamma_g \cup \Gamma_h = \Gamma$ and $\Gamma_g \cap \Gamma_h = \emptyset$. We set a general boundary value problem as

$$\left\{ \begin{array}{rll} \mathcal{L}u &= f & \text{in} \quad \Omega, \\ u &= g & \text{on} \quad \Gamma_g, \\ \mathcal{B}u &= h & \text{on} \quad \Gamma_h, \end{array} \right. \tag{1}$$

where $\mathcal{L}$ is a generic differential operator. The $\mathcal{B}$ operator arises from integration by parts of the differential operator, $\mathcal{L}$, and it acts on the Neumann boundary. Let $\mathcal{S}$ and $\mathcal{V}$ be the standard Sobolev spaces for the trial and the test functions, respectively,

$$\mathcal{S} = \{u \in H^1(\Omega) \;\mid\; u = g \quad \text{on} \quad \Gamma_g\}, \tag{2a}$$

$$\mathcal{V} = \{v \in H^1(\Omega) \;\mid\; v = 0 \quad \text{on} \quad \Gamma_g\}. \tag{2b}$$

The variational formulation reads: Find $u \in \mathcal{S}$ such that

$$a(w, u) = (w, f) + (w, h)_{\Gamma_h} \qquad \forall w \in \mathcal{V}, \tag{3}$$

with $a(\cdot, \cdot)$ being the bilinear form, $(\cdot, \cdot)$ the $L^2(\Omega)$ inner product and $(\cdot, \cdot)_{\Gamma_h}$ the $L^2(\Gamma_h)$ inner product on Γ_h. The FEM consists in meshing the domain, Ω, into n_{el} non-overlapping elements with domain Ω^e. Let $\widetilde{\Omega}$ and $\widetilde{\Gamma}$ denote the union of element interiors, Ω^e, and inter-element boundaries, Γ^e, respectively,

$$\widetilde{\Omega} = \bigcup_{e=1}^{n_{\text{el}}} \Omega^e, \qquad \widetilde{\Gamma} = \bigcup_{e=1}^{n_{\text{el}}} \Gamma^e \backslash \Gamma. \tag{4}$$

Taking the elements of the partition, we define the associated finite dimensional spaces $\mathcal{S}^h \subset \mathcal{S}$ and $\mathcal{V}^h \subset \mathcal{V}$ for the trial and weighting functions, respectively,

$$\begin{aligned} \mathcal{S}^h &= \{u_h \in H^1(\Omega) \;\mid\; u_{h|\Omega^e} \in \mathbb{P}_k, u_{h|\Gamma_g} = g, \forall \Omega^e \in \widetilde{\Omega}\}, \\ \mathcal{V}^h &= \{w_h \in H^1(\Omega) \;\mid\; w_{h|\Omega^e} \in \mathbb{P}_k, w_{h|\Gamma_g} = 0, \forall \Omega^e \in \widetilde{\Omega}\}, \end{aligned} \tag{5}$$

where $\mathbb{P}_k$ denotes the space of polynomials of degree k. Thus, the standard Galerkin method reads: Find $u_h \in \mathcal{S}^h$ such that

$$a(w_h, u_h) = (w_h, f) + (w_h, h)_{\Gamma_h} \qquad \forall w_h \in \mathcal{V}^h. \tag{6}$$

In order to stabilize the convection-diffusion equation, a popular method is SUPG, which includes an additional term to the Galerkin method. The SUPG method reads: Find $u_h \in \mathcal{S}^h$ such that

$$a_{\text{SUPG}}(w_h, u_h) = a(w_h, u_h) + a_\tau(w_h; u_h, f) = (w_h, f) + (w_h, h)_{\Gamma_h} \quad \forall w_h \in \mathcal{V}^h. \tag{7}$$

The stabilizing term $a_\tau(\cdot;\cdot,\cdot)$ is

$$a_\tau(w_h; u_h, f) = \sum_{\Omega^e \in \bar{\Omega}} a^e_\tau(w_h; u_h, f), \tag{8}$$

where $a^e_\tau(w_h; u_h, f) = (\boldsymbol{a} \cdot \nabla w_h, \tau^e(\mathcal{L}u_h - f))_{\Omega^e}$ and $\tau^e = \min(\frac{h}{2|\boldsymbol{a}|}, \frac{h^2}{12\kappa})$. The value h is a measure of the element length.

The variational multiscale theory consists on splitting the variational form in a coarse and fine components. We identify the coarse scales, $\bar{u}$, with the finite element solution and the fine scales, u', with the error. Therefore,

$$a(\bar{w}, \bar{u}) + a(\bar{w}, u') = (\bar{w}, f) + (\bar{w}, h)_{\Gamma_h} \qquad \forall \bar{w} \in \bar{\mathcal{V}}, \tag{9a}$$

$$a(w', \bar{u}) + a(w', u') = (w', f) + (w', h)_{\Gamma_h} \qquad \forall w' \in \mathcal{V}'. \tag{9b}$$

The spaces $\bar{\mathcal{V}}$ and $\bar{\mathcal{S}}$ represent the coarse scales and are identified with $\mathcal{V}^h$ and $\mathcal{S}^h$. The fine scales scales are defined such that $\mathcal{S} = \bar{\mathcal{S}} \oplus \mathcal{S}'$ and $\mathcal{V} = \bar{\mathcal{V}} \oplus \mathcal{V}'$.

Observing the variational multiscale form, Eq. (9a) represents the coarse-scale variational form and Eq. (9b), the fine-scale variational form. We focus on this last equation to estimate the error. Integrating by parts Eq. (9b), we establish the relationship between the error and the residuals.

$$a(w', u') = -(w', \mathcal{L}\bar{u} - f)_{\bar{\Omega}} - (w', [\![\mathcal{B}\bar{u}]\!])_{\bar{\Gamma}} - (w', \mathcal{B}\bar{u} - h)_{\Gamma_h}. \tag{10}$$

The LHS of Eq. (10) is the bilinear form applied to the fine scales, where the error u' is projected on the fine scales w'. The RHS of Eq. (10) contains the residuals of the numerical solution. The first term of the RHS is the internal residuals defined inside the elements, the second one considers the jump of the flux on the element boundaries, and finally, the third term represents the Neumann boundary condition residual.

§3. Error estimation framework

Following the nature of the residuals, the error is decomposed in two terms, u'_{bub} and u'_{poll}. Accordingly, the u'_{bub} component is in charge of modeling the error that arises from the internal residuals inside each element, $(w', \mathcal{L}\bar{u} - f)_{\Omega^e}$, and the u'_{poll} component represents the error produced by the residuals on the element boundary, $(w', [\![\mathcal{B}\bar{u}]\!])_{\bar{\Gamma}}$ and $(w', \mathcal{B}\bar{u} - h)_{\Gamma_h}$.

3.1. Internal residual error, u'_{bub}

This kind of error possesses a local character since it is defined inside the element. This error is computed as a combination of bubble functions on each element,

$$u'_{\text{bub},\Omega^e}(\mathbf{x}) = \sum_{i=1}^{n_{\text{bub}}} c_i^{\text{bub}} b_i(\mathbf{x}). \tag{11}$$

There are different ways of defining the bubble functions, $b_i(\mathbf{x})$, depending on whether we consider 1D and 2D problems.

3.1.1. One-dimensional problems

For 1D problems, the internal residual error is modeled by means of residual-free bubbles [1, 5, 6, 2]. In this case, the residual-free bubbles are calculated using fine-scale Green's functions. A relevant article written by Hughes and Sangalli [7], establishes an explicit definition of the fine-scale Green's operator,

$$\mathcal{G}' = \mathcal{G} - \mathcal{G}\mathcal{P}^T(\mathcal{P}\mathcal{G}\mathcal{P}^T)^{-1}\mathcal{P}\mathcal{G}. \tag{12}$$

Eq. (12) shows that the fine-scale Green's operator is computed by the substraction of two terms (see [7, 9] for further details):

- The classical Green's function operator, $\mathcal{G}$, which is the inverse of the differential equation, $\mathcal{G} = \mathcal{L}^{-1}$
- A projection, $\mathcal{P}$, that goes from the space of all scales, $\mathcal{S}$, to the coarse scales, $\bar{\mathcal{S}}$, $\mathcal{P} : \mathcal{S} \to \bar{\mathcal{S}}$. We select a projector induced by the H_0^1-seminorm since it provides fine-scale Green's functions confined in the elements.

Therefore, employing the fine-scale Green's functions, $g'(x, y)$, the internal residual error is computed as

$$u'_{\text{bub},\Omega^e}(x) = -\int_{\Omega^e} g'(x, y)(\mathcal{L}\bar{u} - f)(y)\, \mathrm{d}\Omega_y. \tag{13}$$

In order to compute the error with bubble functions, we consider two cases

- Constant residual:

$$u'_{\text{bub},\Omega^e}(x) = b_0^e(x)(f - \mathcal{L}\bar{u}). \tag{14}$$

- Non-constant residual:

$$u'_{\text{bub},\Omega^e}(x) = b_0^e(x)(f - \mathcal{L}\bar{u})(c_i) + \sum_{k=1}^{\infty} b_k^e(x)\frac{1}{k!}\frac{d^k(f - \mathcal{L}\bar{u})}{dy^k}\bigg|_{y=c_i}, \tag{15}$$

where c_i is the central point of the element and b_k^e is the k-moment order residual-free bubble, defined as

$$b_k^e(x) = \int_{\Omega^e} g'(x, y)(y - c_i)^k\, \mathrm{d}\Omega_y. \tag{16}$$

These bubble functions, which arise from the fine-scale Green's function, are called *residual-free bubbles* since u'_{bub} fulfills

$$\int_{\Omega^e} \mathcal{L}u'_{\text{bub}} w'\, \mathrm{d}\Omega = \int_{\Omega^e} (f - \mathcal{L}\bar{u})w'\, \mathrm{d}\Omega \quad \forall w' \in \mathcal{V}' \cap H_0^1(\Omega^e). \tag{17}$$

That is to say, in each element, u'_{bub} represents the solution that lives in $\mathcal{S}'$ with homogeneous Dirichlet boundary condition, where the source term is $f - \mathcal{L}\bar{u}$.

3.1.2. Multi-dimensional problems

In multidimensional problems, residual-free bubbles are very difficult to obtain. Thus, the error component, $u'_{\text{bub}}(\mathbf{x}) = \sum_{i=1}^{n_{bub}} c_i b_i(\mathbf{x})$ is a linear combination of polynomial bubble functions defined on a finite dimensional space, $\mathcal{S}^h_{\text{bub}}$. For both triangles and quadrilaterals, the first bubble function, $b_1(\mathbf{x})$, is the simplest polynomial that fulfills to be zero on the element boundary. The successive bubbles are built adding the monomials of the Pascal triangle with center at the barycenter of the element. The problem is set on each element as: Find $u'_{\text{bub}} \in \mathcal{S}^h_{\text{bub}}$ such that

$$a(w'_{\text{bub}}, u'_{\text{bub}}) = (w'_{\text{bub}}, f - \mathcal{L}\bar{u}) \qquad \forall w'_{\text{bub}} \in \mathcal{S}^h_{\text{bub}}. \tag{18}$$

3.2. Inter-element error, u'_{poll}

The inter-element error presents a global character and is originated by the lack of continuity of the FEM solution, $\bar{u}$, and the internal residual error, u'_{bub}. This kind of error is in charge of solving the part of the error that u'_{bub} does not consider. Thus, the inter-element error, u'_{poll} represents the solution of the following problem,

$$\begin{cases} \mathcal{L}u'_{\text{poll}} &= 0 & \text{in} \quad \Omega \setminus \widetilde{\Gamma}, \\ \mathcal{L}u'_{\text{poll}} &= -([\![\mathcal{B}\bar{u}]\!] + [\![\mathcal{B}u'_{\text{bub}}]\!])\delta_{\widetilde{\Gamma}} & \text{on} \quad \widetilde{\Gamma}, \\ u'_{\text{poll}} &= 0 & \text{on} \quad \Gamma_g, \\ \mathcal{B}u'_{\text{poll}} &= h - \mathcal{B}\bar{u} - \mathcal{B}u'_{\text{bub}} & \text{on} \quad \Gamma_h. \end{cases} \tag{19}$$

It is assumed that the error component u'_{bub}, defined inside the elements, satisfies $\mathcal{L}u'_{\text{bub}} = f - \mathcal{L}\bar{u}$ enabling to approach $\mathcal{L}u'_{\text{poll}} = 0$ as the first equation in Eq. (19) expresses. Then, the error source is the jump of $\bar{u}$ and u'_{bub} on the element boundaries.

Although it seems that the way of determining the error pollution leads to the solution of a problem in the whole domain, it can be simplified both in 1D and multiD problems.

3.2.1. One-dimensional problems

Here only linear elements are considered (see [9] for the extension to higher-order elements). The error pollution is modeled as a linear combination of free-space Green's functions set at the nodes of the discretization, n_{np},

$$u'_{\text{poll}}(x) = \sum_{A=1}^{n_{np}} c_A^{\text{bnd}} g^F(x, x_A). \tag{20}$$

The coefficients c_A^{bnd} are determined depending on the nodes we are treating:

- Internal nodes
  The coefficients c_A^{bnd} are chosen imposing the Galerkin orthogonality property

$$a(\bar{w}, u') = a(\bar{w}, u'_{\text{bub}}) + a(\bar{w}, u'_{\text{poll}}) = 0 \qquad \forall \bar{w} \in \bar{\mathcal{V}}. \tag{21}$$

  Therefore,

$$a(\bar{w}, u'_{\text{poll}}) = -a(\bar{w}, u'_{\text{bub}}) \qquad \forall \bar{w} \in \bar{\mathcal{V}}. \tag{22}$$

Introducing the definition of u'_{poll} in Eq. (20) and integrating by part the LHS of Eq. (22), for a internal node A

$$(\bar{w}_A, c_A^{\text{bnd}} \mathcal{L} g^F(x, x_A)) = -a(\bar{w}_A, u'_{\text{bub}}), \tag{23}$$

$$(\bar{w}_A, \delta(x, x_A) c_A^{\text{bnd}}) = -a(\bar{w}_A, u'_{\text{bub}}), \tag{24}$$

$$c_A^{\text{bnd}} = -a(\bar{w}_A, u'_{\text{bub}}). \tag{25}$$

- Neumann boundary nodes
  Following the same steps as for the internal nodes, the coefficients c_A^{bnd} at these nodes are computed as

$$c_A^{\text{bnd}} = -a(\bar{w}_A, u'_{\text{bub}}) - \left(\bar{w}_A, \sum_{B=1, B\neq A}^{n_{np}} c_B^{\text{bnd}} \mathcal{B} g^F(x, x_B)\right)_{\Gamma_h}. \tag{26}$$

- Dirichlet boundary nodes
  For the nodes set at the Dirichlet boundaries, we know that the $u' = 0$. Therefore, the c_A^{bnd} coefficients are solved imposing this condition, i.e.,

$$c_A^{\text{bnd}} g^F(x_A, x_A) + \sum_{B=1, B\neq A}^{n_{np}} c_B^{\text{bnd}} g^F(x_A, x_B) = 0. \tag{27}$$

3.2.2. Multi-dimensional problems

Taking problem (19), the second equation is multiplied by the free-space Green's function and integrated by parts twice. Then, we get the expression

$$\begin{aligned} u'_{\text{poll}}(\boldsymbol{x}) = \quad & -\int_{\widetilde{\Gamma}} g^F(\boldsymbol{x}, \boldsymbol{y}) \Big([\![\mathcal{B} \bar{u}]\!](\boldsymbol{y}) + [\![\mathcal{B} u'_{\text{bub}}]\!](\boldsymbol{y}) \Big) \, \mathrm{d}\Gamma_y + \\ & \int_{\partial\Omega} g^F(\boldsymbol{x}, \boldsymbol{y}) \mathcal{B}_y u'_{\text{poll}}(\boldsymbol{y}) \, \mathrm{d}\Gamma_y - \int_{\partial\Omega} u'_{\text{poll}}(\boldsymbol{y}) \mathcal{B}_y g^F(\boldsymbol{x}, \boldsymbol{y}) \, \mathrm{d}\Gamma_y \\ & \text{for all } \boldsymbol{x} \in \Omega. \end{aligned} \tag{28}$$

As can be observed, the calculation of u'_{poll} implies the computation of an integral on the inter-element boundaries, $\widetilde{\Gamma}$, which involves the jumps of $\bar{u}$ and u'_{bub}. The other two integrals are set on the domain boundary and contain both u'_{poll} and its derivative. Hence, the integro-differential equation can be solved via boundary element methods (BEM).

§4. Numerical example: Pointwise error estimation in 1D problems

The convection-diffusion problem is expressed as

$$\begin{cases} -\kappa \dfrac{\mathrm{d}^2 u}{\mathrm{d}x^2} + a \dfrac{\mathrm{d}u}{\mathrm{d}x} = 4x(1-x) & \text{in} \quad \Omega = [0, 1], \\ u = 0 & \text{on} \quad \Gamma_g. \end{cases} \tag{29}$$

The case $\kappa = 0.01$ and $a = 1$ is solved with the standard Galerkin method using a uniform mesh with 5 elements. Fig. 1 represents the exact and the FEM solution, where spurious oscillations can be seen due to the regime being convection-dominated.

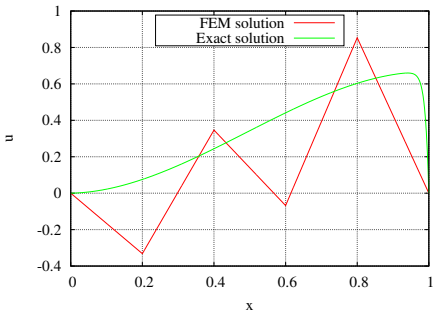
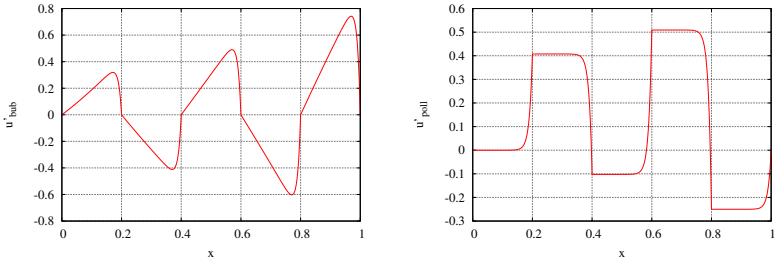


Figure 1: 1D Convection-diffusion problem. Exact and FEM solution.

The error components u'_{bub} and u'_{poll} are depicted in Fig. 2. The internal error is estimated with Eq. (15) and the inter-element error is computed according to Subsection 3.2.1.



(a) u'_{bub} (b) u'_{poll}

Figure 2: 1D Convection-diffusion problem. Error components.

Finally, the estimated error is obtained summing both components, $u = u'_{\text{bub}} + u'_{\text{poll}}$. The estimated and the exact error are shown in Fig. 3. Both are very similar.

§5. Numerical example: Pointwise error estimation in 2D problems

The convection-diffusion problem in 2D is expressed as

$$\begin{cases} -\kappa\Delta u + \boldsymbol{a}\cdot\nabla u &= f & \text{in} & \Omega, \\ u &= g & \text{on} & \Gamma_g, \\ \kappa\nabla u\cdot\boldsymbol{n} &= h & \text{on} & \Gamma_h, \end{cases} \tag{30}$$

where κ and $\boldsymbol{a} = (a_x, a_y)$ are the diffusive and convection coefficients, respectively.

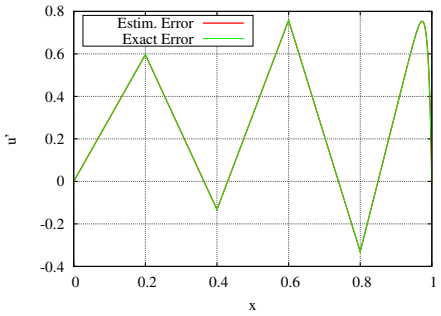
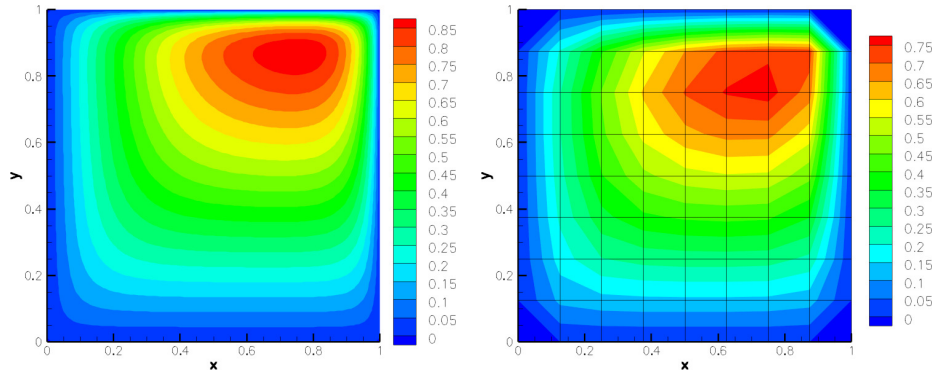


Figure 3: 1D Convection-diffusion problem. Exact and estimated error.

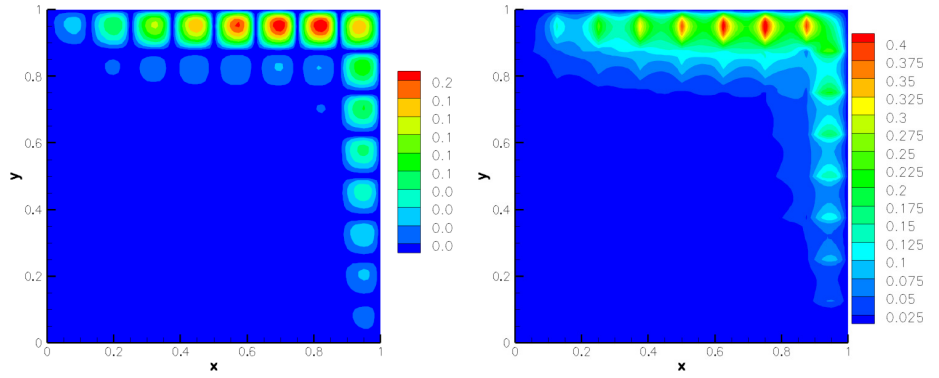
For the example, we select a $(0,1) \times (0,1)$-domain with $\kappa = 0.03$ and $\boldsymbol{a} = (1,2)/\sqrt{5}$ and homogeneous Dirichlet boundary conditions. We take $f = 1$. The numerical solution is obtained via the SUPG method employing a 8×8 mesh with bilinear quadrilaterals. The numerical and the reference solutions are shown in Fig. 4. The reference solution, u_{ref}, has been obtained in a fine mesh (100×100 elements) and is assumed to be similar to the exact solution.



(a) Reference solution (b) FEM solution

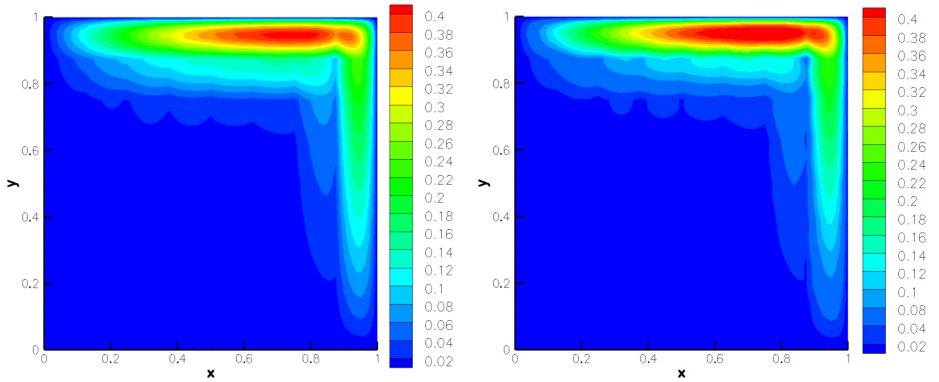
Figure 4: 2D Convection-diffusion equation. Reference and FEM solution.

The internal residual error, u'_{bub}, is depicted in Fig. 5a using six bubble functions per element. On the other hand, the error pollution is computed solving Eq. (28). Fig. 5b shows this error term. Finally, the estimated error is the addition of both components. We can appreciate in Fig. 6 that the reference error, $u'_{\text{ref}} = u_{\text{ref}} - \bar{u}$, and the estimated error are similar. The error is mainly concentrated in the boundary layer where the solution is more abrupt.



(a) u'_{bub} (b) u'_{poll}

Figure 5: 2D Convection-diffusion equation. Internal residual error and inter-element error.



(a) Reference error (b) Estimated error

Figure 6: 2D Convection-diffusion equation. Reference error and estimated error.

§6. Conclusions

In this work, a methodology to estimate a posteriori the pointwise error for fluid dynamics equations is presented. The VMS theory is the framework in which the error is studied. The strategy that is followed is to decompose the error in two components according to the nature of the residuals. The first component is the internal residual error, u'_{bub}, which has a local character, and the second term is the inter-element error, u'_{poll}, with a global character. Numerical examples have been shown for the convection-diffusion equation both in 1D and multiD problems.

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