20. Bounds for Linear-Functional Outputs of Coercive Problems in Three Space Dimensions

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Introduction

A domain decomposition finite element technique for efficiently generating lower and upper bounds to outputs which are linear functionals of the solution to the convection-diffusion equation is presented. The bound method is particularly useful to investigate characteristic quantities of a physical system. These quantities, which we term "outputs", must be expressed as functionals of the field solution obtained from numerical simulations. Large computational gains can be obtained if a fast and accurate method can provide the output value without accurately calculating the expensive field solution. For the past few years, the bound method has been developed [PPP97, Par97, PP98] to calculate, instead of the output value, upper and lower quantitative bounds to this output. The advantages of this approach are the reduced computational time by calculating an approximation of the field solution and the mathematical proof that the bounds are rigorous.

The bound method has been extended to address outputs of the Helmholtz equation, the Burgers equation and the incompressible Navier–Stokes equations in two space dimensions [PP99, MPP00]. Initial work has been performed to address sensitivity derivatives as well as reduced-order approximations to solve design optimization problems [LPP00, MMO+00]. However, two key extensions are still desired: application to compressible flows and extension to three space dimensions. In this paper, we address the latter. The Ladeveze procedure used to approximate the hybrid flux between sub-domains in two space dimensions does not extend to three space dimensions. Therefore a new procedure is needed. We investigate the finite element tearing and interconnecting (FETI) procedure which is independent of dimensionality. This iterative method is ideal to approximate the hybrid flux in the bound method, i.e. the inter-sub-domain connectivity.

The FETI procedure is well established both in the literature as well as in commercial softwares [Far91, FR92, FCM95, FCRR98]. It was shown that, for structural problems, the FETI procedure outperforms direct and iterative algorithms. For parallel processing the FETI procedure becomes even more attractive; it provides parallel scalability. Furthermore, the application of the FETI procedure in the bound method permits simple modifications which drastically reduce the computational time and memory. To be more precise, all the inverse problems do not need to be solved exactly, only an order of magnitude reduction in the residual error suffice. Similarly, the FETI global iterations can also be limited to only a few iterations because only an approximation of the hybrid fluxes is needed. The contribution of this paper is the description of an inexpensive procedure to calculate the inter-sub-domain connectivity

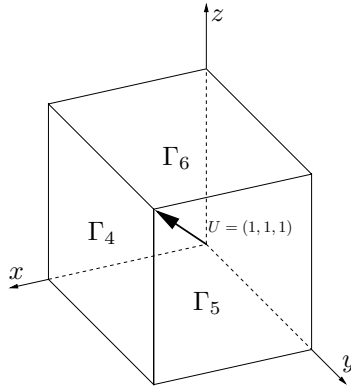[1]Department of Mechanical and Industrial Engineering, University of Toronto, marius@mie.utoronto.ca

Figure 1: Convection-diffusion Geometry.

by exploiting simplifications made to the FETI method.

The convection-diffusion problem

The convection-diffusion problem is formulated in three space dimensions. This problem provides an example of a scalar non-symmetric problem,

$$-(\nu u_{,i})_{,i} + U_i u_{,i} = f \ \ \text{in } \Omega, \ i = 1, ..., 3 \ , \tag{1}$$

with inhomogeneous Dirichlet boundary conditions

$$u = g_D, \quad \text{on } \Gamma_D, \tag{2}$$

where ν is the positive viscosity and Ω is a bounded domain in $\mathbb{R}^3$.

The computational domain, Ω, is the unit cube, the six sides of which are denoted Γ^j, $j = 1, ..., 6$, as shown in Figure 1. We impose the boundary data on $g_D|_{\Gamma^4} = x_2 \times x_3$, $g_D|_{\Gamma^5} = x_1 \times x_3$, $g_D|_{\Gamma^6} = x_1 \times x_2$; and on $g_D|_{\Gamma^1} = g_D|_{\Gamma^2} = g_D|_{\Gamma^3} = 0$. The velocity is prescribed as $U = (1, 1, 1)$, and $f = 0$ to avoid any quadrature issues. Note that, for $U = (0, 0, 0)$ we recover the Poisson problem.

Bounds formulation

The bound method is based upon the construction of an augmented Lagrangian, in which the objective is a quadratic reformulation of the desired output, and the constraints are the finite element equilibrium equations and the inter-sub-domain continuity requirements. In the context of the bound method, computations are focused on evaluating a design quantity, i.e. an output. For simplicity, the particular linear functional investigated here is the average value of the field solution. Many engineering relevant linear functionals can be constructed, including the value at one point or the flux over a domain boundary [MPP99, Par97, PPP97].

For the discrete problems, we introduce a partition of the computational domain Ω into a set of N_k tetrahedra, $\mathcal{T}_H$. We also decompose each tetrahedron, $\Omega^{(k)}$, of $\mathcal{T}_H$, into a uniform refinement of tetrahedra $\mathcal{T}_h$ with characteristic diameter h.

Our discrete functional is constructed from the multiplication of the unit vector with the finite element mass matrix M, discretized on $\mathcal{T}_h$, $\ell = M\ \mathbf{1}$. The output of interest becomes $s = \ell^T u$, where u is an n-long vectors representing the discrete field solution to the Equations (1) and (2). Note that n is the number of nodes associated with the finite element discretization of u. For discretization, we exploit the finite element dimensional vector space X consisting of continuous piecewise linear functions on $\mathcal{T}_h$. For the convection-diffusion problem, the unknown nodal values of u, i.e. $\tilde{u}$, are obtained by solving the algebraic system

$$\tilde{L}\tilde{u} = \tilde{f} - b, \tag{3}$$

where $\tilde{L}$ is $r \times r$ non-symmetric positive-definite sparse matrix arising from the finite element discretization of the problem, and $\tilde{f}$ is a right-hand side r-long vector representing a prescribed force. The vector b contains the known data of u multiplied by L and transported to the right-hand side, i.e. the inhomogeneity. Clearly, the interior degrees-of-freedom r is less than n.

To avoid the expensive calculation of the system in (3), we introduce a discontinuous space $\hat{X}$ with jumps across the elements $\Omega^{(k)}$ and calculate bounds to s, i.e. $s_{LB} \leq s \leq s_{UB}$. Rigorous bounds are obtained by application of quadratic–linear duality theory [Str86], in which the candidate Lagrange multipliers are obtained from inexpensive calculations. The lower bound value is obtained from the Lagrangian, $\mathcal{L}(\hat{u}^{(k)}, \hat{\mu}, \hat{\lambda})$, where $\hat{\mu}$ and $\hat{\lambda}$ are approximations of the Lagrange multipliers. The lower bound to the output of interest, s, is

$$s_{LB} = \sum_{k=1}^{N_k} \left(\hat{u}^{(k)^T} A^{(k)} \hat{u}^{(k)} - f^{(k)^T} \hat{u}^{(k)} + \ell^{(k)^T} \hat{u}^{(k)} \right) + C_u \tag{4}$$

$$- \hat{\mu}^T \sum_{k=1}^{N_k} \left(L^{(k)} \hat{u}^{(k)} - f^{(k)} \right) - \hat{\lambda}^T \sum_{k=1}^{N_k} B^{(k)} \hat{u}^{(k)}, \tag{5}$$

where the superscript (k) is the restriction of the operator or the vector to the domain k. After simplifications we obtain

$$s_{LB} = -\sum_{k=1}^{N_k} \hat{u}^{(k)^T} A^{(k)} \hat{u}^{(k)} + C_u + f^{(k)^T} \hat{\mu}^{(k)}, \tag{6}$$

where all $\hat{u}^{(k)}$ are solutions of the decoupled local problems

$$2A^{(k)} \hat{u}^{(k)} = f^{(k)} - \ell^{(k)} + L^{(k)^T} \hat{\mu}^{(k)} - B^{(k)^T} \hat{\lambda}, \tag{7}$$

and $A^{(k)}$ is the finite element discretization of the symmetric term of $L^{(k)}$ and $B^{(k)}$ is the sign Boolean matrix which localizes the "jumps" at the interface. C_u is a boundary data value given by $C_u = G^T (L - A)\, G$, where G is a discrete function containing the Dirichlet boundary values and zero values elsewhere. In solving each Equation (7),

care has to be taken to include the boundary condition for the elements lying on the boundary.

To guarantee solvability of each Equation (7), the candidate Lagrange multipliers must satisfy

$$(f^{(k)} - \ell^{(k)} + L^{(k)^T}\hat{\mu}^{(k)} - B^{(k)^T}\hat{\lambda}) \perp \text{Ker}(A^{(k)}), \quad k = 1, ..., N_f, \tag{8}$$

where N_f is the number of pure Neumann problems.

The calculation of $\hat{\mu}$ has to be inexpensive such that the cost of calculating s_{LB} is considerably less than the cost of calculating s. Hence, a coarse discretization $\mathcal{T}_H$ is exploited. We denote by X_H the corresponding conforming space of finite element functions, i.e. piecewise linear continuous functions in $\mathcal{T}_H$ including the Dirichlet boundary data. Following the bound method [Par97, PPP97], we solve

$$\tilde{L}_H\tilde{u}_H = \tilde{f}_H - b_H, \tag{9}$$

followed by

$$\tilde{L}_H^T\tilde{\mu}_H = 2\tilde{A}_H\tilde{u}_H - \tilde{f}_H + \tilde{\ell}_H + b_H, \tag{10}$$

where $\tilde{u}_H$ and $\tilde{\mu}_H$ are both in X_H. Note that there is no jump across the interface because of this continuous space. Afterward, $\hat{\mu}$ is interpolated on $\mathcal{T}_h$ to obtain $\hat{\mu} \in X$.

The FETI approach is employed to calculate the inter-sub-domain problems, i.e. calculation of $\hat{\lambda}$. Reformulating the FETI interface problem for the bounds gives

$$\begin{bmatrix} 2F_I & -G_I \\ -G_I^T & 0 \end{bmatrix} \begin{bmatrix} \hat{\lambda} \\ \alpha \end{bmatrix} = \begin{bmatrix} 2d \\ -e \end{bmatrix}, \tag{11}$$

where each of these terms is given by

$$F_I = \sum_{k=1}^{N_k} B^{(k)}A^{(k)^+}B^{(k)^T}, \tag{12}$$

$$G_I = \begin{bmatrix} B^{(1)}R^{(1)} & ... & B^{(N_f)}R^{(N_f)} \end{bmatrix}, \tag{13}$$

$$\alpha = \begin{bmatrix} \alpha^{(1)} & ... & \alpha^{(N_f)} \end{bmatrix}, \tag{14}$$

$$d = \sum_{k=1}^{N_k} B^{(k)}A^{(k)^+}(f^{(k)} - \ell^{(k)} + L^{(k)^T}\hat{\mu}^{(k)}), \tag{15}$$

$$e = \begin{bmatrix} R^{(1)^T}f^{(1)} \end{bmatrix} & ... & \begin{bmatrix} R^{(N_f)^T}f^{(N_f)} \end{bmatrix}, \tag{16}$$

where $A^{(k)^+}$ is a generalized inverse of $A^{(k)}$ when the latter is singular. For sub-domains with Dirichlet nodes, $A^{(k)^{-1}}$ is calculated. This domain decomposition based algorithm can be viewed as a two-step preconditioned conjugate gradient method to solve the interface problem [FCRR98]. The solution algorithm can be found abundantly in the literature [Far91, FR91, FR92, FCRR98, FM98, FCM95, Rix97]. Hence, it is not reviewed here.

We make several remarks regarding the computational simplifications in the context of the bound method. First, the inverse or the generalized inverse of $A^{(k)}$ is not calculated exactly, an iterative conjugate gradient solver is used. Note that this operation is need at each FETI iteration and such an approach may seem expensive. However, because we only require an approximation $\hat{\lambda}$, the conjugate gradient iterative procedure is terminated after the residual error is reduced by one order of magnitude. This approach requires less storage and fewer arithmetic operations than the Cholesky factorization used in the standard FETI approach. Note that this simplification is restricted to the bound method [FR91]. Second, we know that the null space, $R^{(k)}$, of the singular matrix $A^{(k)}$ is the unit vector avoiding the computational cost of its calculation. Third, the global FETI iterations can be stopped at any step and still provide rigorous bounds. Indeed, the constraint in the FETI interface problem (Equation 11) guarantees that the pure Neumann sub-domains are equilibrated. Numerical results will show that the sharpness of the bounds improves with the FETI iterations, however over solving the interface problem is not necessary as we will report in the numerical results Section.

Once $\hat{\mu}$ and $\hat{\lambda}$ are calculated, Equation (7) is solved for each subdomain to give $\hat{u}^{(k)}$ and finally s_{LB} is calculated from Equation (6). Similarly, the upper bound is obtained by taking the sign inverse of the lower bound of $-s$.

Numerical results

The convection-diffusion problem is investigated for the case where $f = 0$ and $\nu = 1/5$. The output of interest is the average of the solution on the fine discretization $\mathcal{T}_h$. This "triangulation" consists of 82,944 tetrahedron elements and 15,625 degrees-of-freedom. Three different coarse subdivisions are considered. The following notation, $\mathcal{T}_{(H,N)}$, is used to identify the coarse discretizations where N is the number of sub-domains per edge, i.e. $N \times N \times N \times 6$ sub-domains. Figure 2 presents, on the left, a coarse subdivision $\mathcal{T}_{(H,6)}$ and, on the right, the fine refinement $\mathcal{T}_h = \mathcal{T}_{(H,24)}$. A slice, at $z = 0.5$, of the finite element solution on $\mathcal{T}_{(H,6)}$ and of the reconstructed solution, $\mathcal{T}_{(H,N)}$, are presented in Figure 3.

To analyze the behavior of this method, we first report the values of the bounds and their convergence for different $\mathcal{T}_H$ meshes, Figure 4. The FETI iterations' stopping criterion is $\|r^n\|_2/\|r^0\|_2 < 10^{-2}$ where the numerator and the denominator are the n-th and the initial residual errors respectively. Obviously, for a given stopping criterion, the sharpness of the bounds depend on the richness of the coarse mesh. Recall that, the bound method guarantees that the output is within these values. Indeed, the expensive calculation on the fine mesh field solution is not required any longer as sufficient rigorous information is obtained for design.

Discussion of the computational cost of calculating the upper and lower bounds may be found in [Par00]. In this paper, we only pointout that the cost is related to the number of FETI iterations. As we have discussed previously, these iterations can be interrupted at any step and rigorous bounds can be calculated. The sharpness of the bounds depends on the number of iterations, or more precisely on the residual reached, as reported in Figure 5. The convergence curves show that the difference between of each bound and the fine mesh output value is considerably decreased in
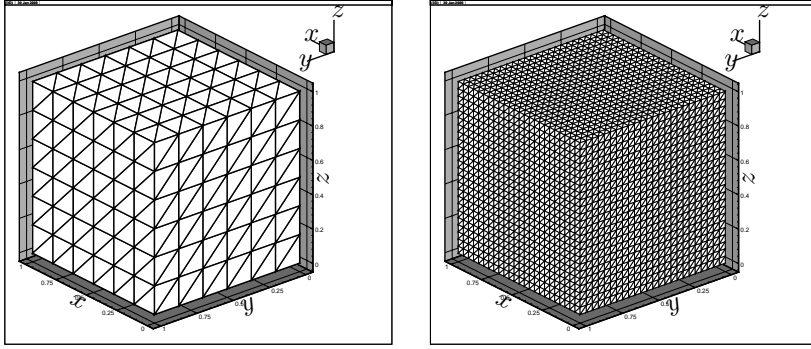
Figure 2: Two examples of meshes: (left) coarse mesh, $\mathcal{T}_{(H,6)}$; (right) fine mesh, $\mathcal{T}_h = \mathcal{T}_{(H,24)}$.
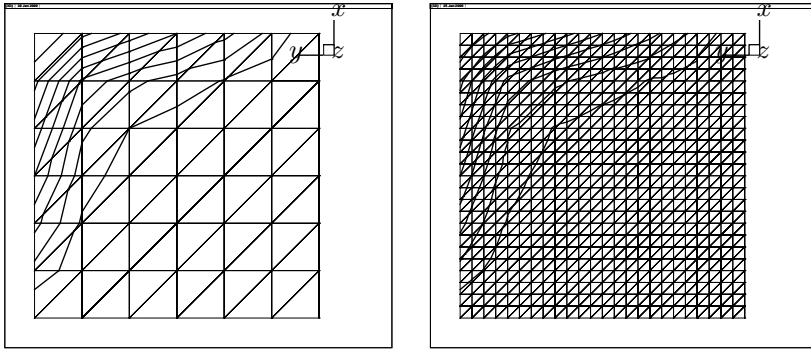

Figure 3: Isocontours (0 to 0.5 at intervals of 0.05) of (left) u_H on $\mathcal{T}_{H,6}$, and (right) $\hat{u}^{(k)}$, $k = 1, ..., N_k$
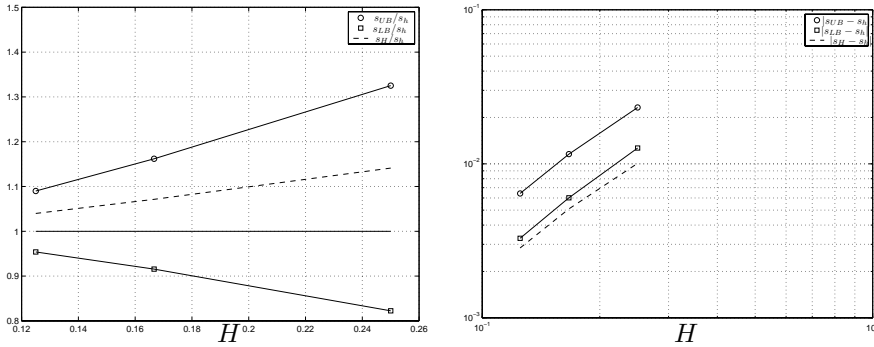

Figure 4: (left) Plots of s_{LB}/s_h, s_{UB}/s_h, and s_H/s_h as a function of the coarse mesh characteristic diameter H; (right) Log plots $|s_{LB} - s_h|$, $|s_{UB} - s_h|$ and $|s_H - s_h|$ as a function of H.
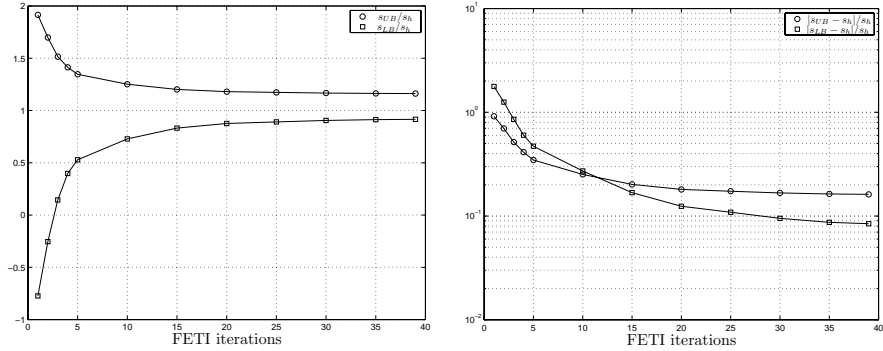
Figure 5: (left) Plots of s_{LB}/s_h and s_{UB}/s_h as a function of FETI iterations; (right) Log plots of $|s_{LB} - s_h|/s_h$ and $|s_{UB} - s_h|/s_h$ as a function of FETI iterations.

the first iterations. This indicates that an optimal number of iterations may exist. Both the hybrid flux and the adjoint approximations contribute to the bound gap. During the initial iterations, the bound gap is sensitive to the hybrid flux calculations. During later iterations, the adjoint interpolation dominates the bound gap. Clearly, resolving the interface problem more accurately will not improve the bounds because it does not improve the adjoint approximation. For improving the adjoint, there exists an adaptive approach to refine the coarse mesh in order to obtain the desired bound gap [PP97].

Acknowledgements

References

[Far91] Charbel Farhat. A Lagrange multiplier based on divide and conquer finite element algorithm. *J. Comput. System Engng*, 2:149–156, 1991.

[FCM95] Charbel Farhat, Po-Shu Chen, and Jan Mandel. A scalable Lagrange multiplier based domain decomposition method for time-dependent problems. *Int. J. Numer. Meth. Eng.*, 38:3831–3853, 1995.

[FCRR98] C. Farhat, P.-S. Chen, F. Risler, and F.-X. Roux. A unified framework for accelerating the convergence of iterative substructuring methods with Lagrange multipliers. *Int. J. Numer. Meth. Engng.*, 42:257–288, 1998.

[FM98] C. Farhat and J. Mandel. The two-level feti method for static and dynamic plate problems - part i: an optimal iterative solver for biharmonic systems. *Computer Methods in Applied Mechanics and Engineering*, 155:129–152, 1998.

[FR91]Charbel Farhat and Francois-Xavier Roux. A Method of Finite Element Tearing and Interconnecting and its Parallel Solution Algorithm. *Int. J. Numer. Meth. Engng.*, 32:1205–1227, 1991.

[FR92]C. Farhat and F.X. Roux. An unconventional domain decomposition method for an efficient parallel solution of large-scale finite element systems. *SIAM J. Sc. Stat. Comput.*, 13:379–396, 1992.

[LPP00]R. M. Lewis, A. T. Patera, and J. Peraire. *A Posteriori* finite element bounds for sensitivity derivatives of partial-differential-equation outputs. *Finite Element Analysis & Design*, 34(3-4):271–290, 2000.

[MMO+00]L. Machiels, Y. Maday, I. B. Oliveira, A. T. Patera, and D. V. Rovas. Output bounds for reduced-basis approximations of symmetric positive definite eigenvalue problems. *C. R. Acad. Sci. Paris, Série I*, 2000.

[MPP99]Y. Maday, A.T. Patera, and J. Peraire. A general formulation for *a posteriori* bounds for output functionals of partial differential equations; application to the eigenvalue problem. *C.R. Acad. Sci. I-Math.*, 328(9):823–828, 1999.

[MPP00]L. Machiels, J. Peraire, and A.T. Patera. *A Posteriori* finite element output bounds for incompressible Navier-Stokes equations; application to a natural convection problem. *Journal of Computational Physics*, 2000.

[Par97]M. Paraschivoiu. *A Posteriori finite element bounds for linear-functional outputs of coersive partial differential equations and of the Stokes problem.* PhD thesis, Massachusetts Institute of Technology, 1997.

[Par00]M. Paraschivoiu. A posteriori finite element output bounds in three space dimensions using the FETI method. *submitted to Comp. Meth. Appl. Mech. Engrg.*, 2000.

[PP97]J. Peraire and A.T. Patera. Bounds for linear-functional outputs of coercive partial differential equations: Local indicators and adaptive refinement. In P.Ladeveze and J.T. Oden, editors, *Workshop On New Advances in Adaptive Computational Methods in Mechanics.* Elsevier, 1997.

[PP98]M. Paraschivoiu and A. T. Patera. A hierarchical duality approach to bounds for the outputs of partial differential equations. *Comp. Meth. Appl. Mech. Engrg.*, 158:389–407, 1998.

[PP99]J. Peraire and A. T. Patera. Asymptotic *a posteriori* finite element bounds for the outputs of noncoercive problems: the Helmholtz and Burgers equations. *Comp. Meth. Appl. Mech. Engrg.*, 171:77–86, 1999.

[PPP97]M. Paraschivoiu, J. Peraire, and A. T. Patera. *A Posteriori* finite element bounds for linear–functional outputs of elliptic Partial Differential Equations. *Comput Methods Appl. Mech. Engrg.*, 150:289–312, 1997.

[Rix97]D. Rixen. *Substructuring and dual methods in structural analysis.* PhD thesis, University of Liège, Belgium, 1997.

[Str86]G. Strang. *Introduction to Applied Mathematics.* Wellesley-Cambridge Press, Wellesley, Massachusetts, 1986.