

Lean complementarity for Poisson problems

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We introduce a novel technique—*lean complementarity*—that eliminates any waste of computational resources occurring during the pursuing of complementarity. First, it requires the solution of the scalar potential formulation only, since flux equilibration is performed explicitly, i.e. without solving any linear system. Second, the systems arising during adaptive mesh refinement are solved inexactly on purpose, by stopping the iterations of the iterative solver when the algebraic error gets negligible with respect to the estimated discretization error. Discretization error is estimated with complementarity, whereas the algebraic error is computed very accurately with a novel and cheap technique.

Index Terms—Poisson problem, finite elements (FEM), finite integration technique (FIT), fully computable error bounds, hypercircle method, one stroke complementarity, explicit flux equilibration, adaptive stopping criterion

I. INTRODUCTION

COMPLEMENTARITY provides, at least for Poisson-like problems, rigorous error bounds for system energy [1] and a robust error estimator [2] for mesh adaptivity. Yet, exploiting complementarity is costly as it requires to solve the problem two times, for example with the scalar potential Finite Element formulation and any of its complementary or complementary-dual [3] counterparts. *One stroke* complementarity [4] shows that the irrotational electric field and the solenoidal current density of a stationary conduction paradigm problem not necessarily have to be the ones produced by a pair of complementary formulations. Those ones yield optimal bounds, but sub-optimal bounds may be found by solving least squares problems in each dual element [3] starting from a solenoidal current. Still, a solenoidal current is obtained by complementary formulations which are quite costly.

One aim of this paper is to devise lean techniques to achieve one-stroke complementarity also with the scalar potential formulation \mathcal{V} . This formulation provides an irrotational electric field, whereas the current $\tilde{\mathbf{I}}$ is defined on the dual complex $\tilde{\mathcal{K}}$ and is there conservative [5], i.e. $\tilde{\mathbf{D}}\tilde{\mathbf{I}} = \mathbf{0}$, where $\tilde{\mathbf{D}} = -\mathbf{G}^T$ and \mathbf{G} is the edge-node incidence matrix. The question is whether it is possible to construct, by *local manipulations* only, a solenoidal current \mathbf{I} defined on the primal complex that represents a current density as close as possible to the one computed by the \mathcal{V} formulation. We remark that methods based on (Galerkin or least squares) projections or discrete Hodge decomposition are not suitable as they require the solution of a global system.

A technique to construct \mathbf{I} is called *flux equilibration* by numerical analysts. Tight bounds are obtained in [6], [7] by solving non-linear programming problems and local systems. The implementation is complicated, that is why less accurate techniques based on spanning trees [8] have been proposed instead. An original technique introduced in [9] exploits the conservativity of $\tilde{\mathbf{I}}$. Each dual volume is tessellated with a new (finer) simplicial mesh and the local corrections are found by trying to “interpolate inside such cells while enforcing current conservation” [9].

II. LEAN COMPLEMENTARITY

Let us call v the potential which is the exact solution of the problem, \mathbf{V} the exact solution of the discrete problem and $\mathbf{V}^{(k)}$ the solution of the discrete problem after the k th iteration of the linear iterative solver. The *total error* $\mathbf{e} = v - \mathbf{V}^{(k)}$ can be clearly written as the sum of the *discretization error* $\mathbf{e}_d = v - \mathbf{V}$ and the *algebraic error at the k th iteration* $\mathbf{e}_a^{(k)} = \mathbf{V} - \mathbf{V}^{(k)}$, which vanishes if the system is solved exactly. We have neglected the so-called oscillation error term by assuming sources and boundary conditions piecewise uniform in each element. The stopping criterion for iterative solvers used in lean complementarity is $\|\mathbf{e}_a^{(k)}\| < d \|\mathbf{e}_d\|$, where we set $d = 0.01$, $\|\mathbf{e}\| = \sqrt{\mathbf{e}^T \mathbf{K} \mathbf{e}}$ is the standard energy norm and \mathbf{K} is the stiffness matrix. The proposed stopping criterion attempts to balance the two sources of error, as insisting in reducing $\|\mathbf{e}_a^{(k)}\|$ down to zero would not improve the total error significantly.

Lean complementarity requires to face two challenges. First, one has to devise a fast and accurate technique to evaluate the algebraic error. Second, conservativity of $\tilde{\mathbf{I}}$ does not hold at a given iteration of the linear solver, which means that one has to develop a novel flux equilibration technique since state of the art methods rely on current conservation.

A. Effective evaluation of the algebraic error

The stopping criterion shouldn’t be defined—as happens in the usual practice—with the Euclidean norm of the residual $\mathbf{r}^{(k)} = \mathbf{b} - \mathbf{K} \mathbf{V}^{(k)}$, where \mathbf{b} is the right-hand side of the system, or the relative residual $\|\mathbf{r}^{(k)}\|/\|\mathbf{r}^{(0)}\|$. The reason is clear after looking at the relationship between $\mathbf{e}_a^{(k)}$ and $\mathbf{r}^{(k)}$

$$\mathbf{e}_a^{(k)} = \mathbf{V} - \mathbf{V}^{(k)} = \mathbf{K}^{-1}(\mathbf{b} - \mathbf{K} \mathbf{V}^{(k)}) = \mathbf{K}^{-1} \mathbf{r}^{(k)}. \quad (1)$$

This paper introduces a computationally inexpensive technique to obtain a remarkably precise estimation of $\mathbf{e}_a^{(k)}$. Let us run the iterative solver for additional ν iterations obtaining $\mathbf{V}^{(k+\nu)}$, where ν is such that $\mathbf{r}^{(k+\nu)} < c \mathbf{r}^{(k)}$ and $c \ll 1$ (we set $c = 0.05$). Then, let us consider the difference of the systems $\mathbf{K}(\mathbf{V}^{(k+\nu)} - \mathbf{V}^{(k)}) = \mathbf{r}^{(k)} - \mathbf{r}^{(k+\nu)}$ at these two stages. Comparing this result with (1), $\mathbf{e}_a^{(k)} \approx \mathbf{V}^{(k+\nu)} - \mathbf{V}^{(k)}$ holds.

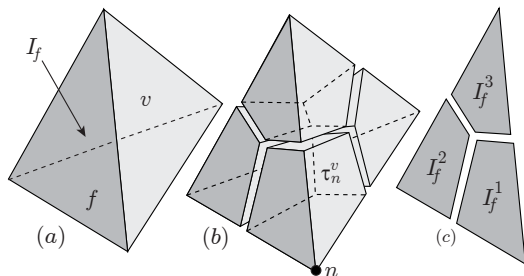


Fig. 1. (a) Tetrahedron v . Current I_f associated with face f (highlighted in the picture). (b) v is partitioned in four dual volume portions. (c) I_f over face f is obtained as $I_f^1 + I_f^2 + I_f^3$.

B. Explicit flux equilibration

We use complementarity to estimate $|||e|||$ through a novel and fast flux equilibration technique. Let us consider an element v of the mesh, see Fig. 1a. Let us also define the portion τ_n^v of dual volume \tilde{v} (dual to node n) inside the element v as $\tau_n^v = v \cap \tilde{v}$, see Fig. 1b.

The idea is to construct a current that is solenoidal in each portion of dual volume. If so, it is solenoidal also in the initial tetrahedral mesh, as the current continuity law on v is a linear combination of continuity laws on its four dual volume portions. Then \mathbf{I} is constructed by assembling exactly three contributions for each face, see Fig. 1c.

To obtain a solenoidal current in dual volume portions one may solve a Neumann problem in \tilde{v} with a current conservative formulation with obvious advantages w.r.t. [6], [7] and [9]. Local systems are small (30×30 on average) and may be solved in parallel. Yet, their solution requires an unacceptable amount of time for 3d problems. Moreover, one needs to construct globally edges, faces and their incidences, which are not needed in the \mathcal{V} formulation.

We introduce in this paper an explicit technique for flux equilibration that does not require any system solution, even local ones. The key idea is that \tilde{v} is a polyhedron whose (flat) faces are the portions of dual faces $\tilde{f}_e^v = \tilde{f} \cap v$, where \tilde{f} is the dual face dual to the primal edge e . Then, a uniform current density \mathbf{J} inside \tilde{v} is found by using face basis functions devised for star-shaped polyhedral elements [10]. What is also remarkable is that \mathbf{J} can be found by assembling contributions element-wise. Finally, the current on one thirds of primal faces is found by integrating \mathbf{J} over them. How to treat nodes that lie on the boundary or that are surrounded by more than one material will be described in detail in the full paper.

III. NUMERICAL EXPERIMENTS

Lean complementarity has been implemented in the CDICE code [3] and the novel stopping criterion in the AGMG algebraic multigrid solver [11]. We present the results on a benchmark consisting of a square resistor, see [3]. The effectiveness of lean complementarity is striking. Both algebraic and total errors are estimated very accurately, as Fig. 2 shows. Moreover, the iterative solver is stopped at iteration 4, whereas the classical stopping criterion (relative residual set to $1e-8$) performs 12 iterations. It turns out that lean complementarity

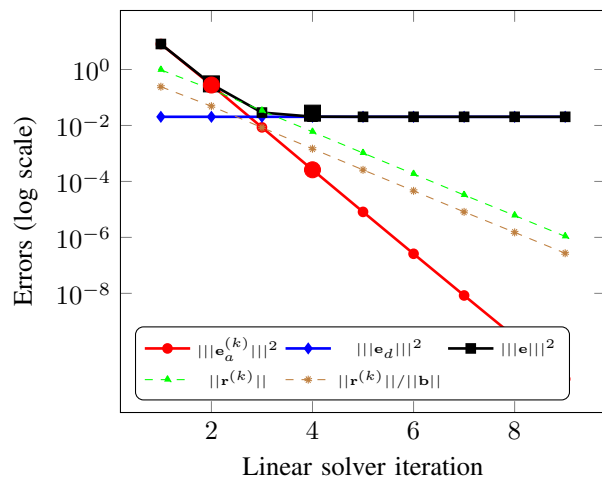


Fig. 2. Continuous lines represent the exact values of $|||e_a^{(k)}|||^2$, $|||e_d|||^2$ and $|||e|||^2$ in logarithmic scale. Bigger marks represents the same quantities estimated by lean complementarity at iterations 2 and 4. The residuals $||r^{(k)}||$ and the relative ones are also shown. The mesh consists of 889,350 tetrahedra and 157,239 nodes.

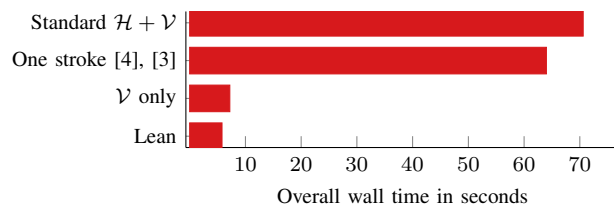


Fig. 3. $\mathcal{H} + \mathcal{V}$ exploits complementarity in the standard way, i.e. by solving with both \mathcal{V} and mixed-hybrid \mathcal{H} formulations. One stroke complementarity [4], [3] saves the \mathcal{V} solution. Lean complementarity is even faster than the \mathcal{V} formulation alone even though it exploits complementarity.

is even faster w.r.t. the \mathcal{V} formulation, see Fig. 3, even though the latter cannot exploit complementarity.

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