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Final Report for "Least-Squares Approaches for the Time-Dependent Maxwell Equations"

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Final Report

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Final Progress Report

Zhiqiang Cai *

When I was at CASC in LLNL during the period between July and December of last year, I was working on two research topics: (1) least-squares approachs for elasticity and Maxwell equations and (2) high-accuracy approximations for non-smooth problems. Below is the description.

1 First-order system least squares for linear and nonlinear elasticity equations

Basic equations of elasticity are generally in self-adjoint form, so they lend themselves naturally to an energy minimization principle, cast in terms of the primitive displacement variables. Unfortunately, this direct approach seems to have many practical difficulties (e.g., degrading approximation properties of the discretization and convergence properties of the solution process) as the material tends to become incompressible (i.e., the Lamé constant λ tends to infinity for fixed Lamé constant μ, or, more precisely, the Poisson ratio ν tends to 0.5^-). There have been several attempts to develop alternate approaches that are robust in the incompressible limit. Compounding these difficulties is the fact that what is often needed in practice are the stress tensor. These variables can be obtained by differentiating displacements, but this weakens the *order* and *strength* of the approximation.

The practical need of the stress tensor motivated extensive studies of mixed finite element methods in the stress-displacement formulation. Unlike mixed methods for second-order scalar elliptic boundary value problems, stress-displacement finite elements are extremely difficult to construct. This is due to the fact that the stress tensor is symmetric. A beautiful finite element space has not been constructed until a few months ago by Arnold and Winther. Their space is a natural extension of the Raviart-Thomas space of $H(\text{div})$. Previous works impose the symmetry condition weakly via a Lagrange multiplier. The minimum degree of freedom on each triangle of Arnold-Winther space for the symmetric stress tensor in two dimensions is twenty-four, which is very expensive. Like scalar elliptic problems, mixed methods lead to saddle-point problems and mixed finite elements are subject to the inf-sup condition. Many solution methods which work well for symmetric positive problems cannot be applied directly.

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Although substantial progress in solution methods for saddle-point problems has been achieved, these problems may still be difficult and expensive to solve.

In the recent years there has been a serious interest in least-squares methods. A number of least-squares formulations have been proposed, analyzed, and implemented. In particular, the least-squares method by Cai, Manteuffel, and McCormick aims to compute the stress tensor directly and, hence, accurately, and it is robust in the incompressible limit. This method is a two-stage algorithm that first solves for the gradients of displacement (which immediately yield stress tensor), then for the displacement itself (if desired). Under certain H^2 regularity assumptions, it admits optimal H^1-like performance for standard finite element discretization and standard multigrid and domain decomposition solution methods that is uniform in the Poisson ratio for all variables. A limitation of this approach is the requirement of sufficient smoothness of the original problem. Also, the gradient of displacement is not an immediate physical quantity and it is hard to extend this approach to nonlinear elasticity.

With goals of the accurate approximation to the stress, robustness in the incompressible limit, efficient solvers, and applicability to nonlinear elasticity, we developed a least-squares finite element method based on the stress-displacement formulation. As we mentioned before, a major numerical difficulty is how to handle the symmetry of the stress tensor in the stress-displacement formulation. To circumvent such a difficulty, we impose the symmetry condition in the first-order system and then apply the least-squares principle to this over-determinant, but consistent system. The least-squares functional uses the L^2 norm and it is shown that the homogeneous functional is equivalent to the energy norm involving the Lamé constant for the displacement and the standard $H(\mathrm{div})$ norm for the stress. This implies that our least-squares finite element method using the respective Crouzeix-Raviart and Raviart-Thomas spaces for the displacement and stress yields optimal error estimates uniform in the incompressible limit. The total degree of freedoms is twelve per triangle in two dimensions and eighteen per tetrahedron in three dimensions. This work has been written as a research article which has been submitted for possible publication in *SIAM Journal on Numerical Analysis.* The algebraic system resulting in this discretization may be efficiently solved by multigrid methods which is the topic of our current study. We will also continue our effort by the important extension of this approach to nonlinear elasticity and possible applications in the ALE3D project in LLNL.

2 High-accuracy approximations for non-smooth problems

It is common knowledge from approximation theory that the order of accuracy for almost all numerical methods is limited by order of the highest derivative of the approximated function. It is also well known that solutions of many differential equations are not smooth. Hence, almost all current numerical methods for non-smooth problems are low order.

In the beginning of the last century, Richardson proposed the so-called extrapolation technique (or the *deferred approach to the limit*) for an approximate sequence $\lim_{h \to 0} u(h) = u$ parameterized by h (the discretization step), in order to increase the accuracy of discretization methods. Richardson extrapolation is a simple, but ingenious technique, and it is called "a method for turning straw into gold" by authors of *Numerical Recipes*. This technique has been widely used in numerical calculations involving numerical differentiation, integration, ordinary and partial differential equations, algebraic equations, and integral equations. In particular, its application to ordinary differential equations with sufficiently smooth solutions, i.e., the Bullirsch-Stoer method, is the best known approach to obtain high-accuracy approximations with minimal computational effort.

The theoretical foundation of extrapolation methods is the asymptotic expansion of the error $u - u(h)$ in terms of powers of the parameter h:

$$u(h) = u + \tau_1 h^{\alpha_1} + \cdots + \tau_{n-1} h^{\alpha_{n-1}} + h^{\alpha_n} \gamma_n(h). \tag{1}$$

Here, the exponents $0 < \alpha_1 < \alpha_2 < \cdots < \alpha_n$ need not be integers, the coefficients $\tau_i \neq 0$ is independent of h, and the function $\gamma_n(h)$ is bounded as $h \to 0$. For a very limited number of problems with certain types of singularities, expansion (1) has been derived for numerical integration and differential equations. But the derivation of (1) is usually tedious, hard, or impossible. In many applications, solutions of the underlying differential equations are not smooth and their singular behavior are unknown, and, hence, the asymptotic expansion in (1) cannot be established using the existing mathematical mechanism. With unknown exponents α_i, Richardson extrapolation cannot be used.

Based on approximation theory, the order of accuracy of the current approximation, i.e., the exponent α_1, depends on the smoothness of the underlying approximated function. When it is not smooth, then α_1 can be very small in many applications. For example, for simple Poisson equations on polygonal domains, standard finite element approximations on a quasi-uniform mesh obtain only $\mathcal{O}(h^{\alpha_1})$ accuracy with α_1 between half and one. The value of α_1 depends on the interior angle of the re-entrance corner. Therefore, it is necessary and important to obtain approximations that are more accurate than $\mathcal{O}(h^{\alpha_1})$. To do so, extrapolation seems to be a feasible, almost universal, and effective approach. However, the unavailability of asymptotic expansions prevents the use of extrapolation. When $u(h)$ is sufficiently smooth, the exponents α_i for $i \geq 2$ are determined by its higher order derivatives. Currently, there are no known quantities characterizing these exponents when $u(h)$ is not smooth.

To quantify these exponents or, equivalently, determine the order of accuracy without expansions, we introduce the rate of corrections:

$$\delta_1 = \lim_{h \to 0} \frac{u(h/2) - u(h)}{u(h/4) - u(h/2)}, \tag{2}$$

which is computationally feasible. It is been shown that $\delta_1 = 2^{\alpha_1}$. Hence, the order of accuracy is increased by using Richardson extrapolation with $\alpha_1 = \log_2 \delta_1$:

$$u_1(h) = u(h/2) + \omega_1(u(h/2) - u(h)) \tag{3}$$

where $\omega_1 = 1/(2^{\alpha_1} - 1) = 1/(\delta_1 - 1)$. The exponents α_i for $i = 2, ..., n-1$ can be calculated recursively in a similar fashion. For example,

$$2^{\alpha_2} = \delta_2 = \lim_{h \to 0} \frac{u_1(h/2) - u_1(h)}{u_1(h/4) - u_1(h/2)}.$$

One step of our method consists of computing an approximation to δ_1 based on (2) and then computing the extrapolation $u_1(h)$ based on (3). The order of accuracy for $u_1(h)$ is then $\mathcal{O}(h^{\alpha_2})$. This procedure can be repeatedly used to compute higher order approximations. It is important to recognize that this method is a recursive procedure and that it does not use any extra information other than the sequence itself. Basically, our approach can be applied to any convergent sequence $\{u(h)\}$ whose rate of corrections exists. We performed preliminary numerical experiments for numerical differentiation, integration, and ordinary differential equations with non-smooth data. In these examples, we are able to compute higher order approximations. For example, a 6^{th}-order approximation to the derivative of $f(x) = x^{1.01} - \sin(10x)/10$ at $x = 0$ is calculated with the rate relaxation method based on the forward difference approximation sequence. Note that the $f(x)$ is differentiable at $x = 0$ only up to the 1.01^{th} order. We are writing a research article on this work, which will be submitted for possible journal publication. Topics of our current study is to (1) combine this procedure with the Bullirsch-Stoer method for ordinary differential equations with non-smooth data and (2) apply this method to partial differential equations. We will also continue our effort by identifying possible applications in LLNL program.