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Why does MLPG work?

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Why Does MLPG Work?

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Abstract

This is a short summary of recent mathematical results on error bounds and convergence of certain unsymmetric methods, including variations of Kansa's collocation technique and Atluri's MLPG method. The presentation is kept as simple as possible in order to address a larger community working on applications in Science and Engineering.

Introduction and Summary

The Meshless Local Petrov-Galerkin method (MLPG) of S.N. Atluri and T.L. Zhu [3] [4] of 1998 has been applied widely and very successfully in recent years, and it led already to various surveys and two books [1] [2]. However, its rigorous mathematical analysis lagged far behind its success in Science and Engineering. The same holds for the unsymmetric collocation technique introduced as early as 1986 by E. Kansa [7], which is confined to problems in strong form and uses collocation for trial spaces generated by multiquadrics, a special kind of radial kernel. It can be viewed as a special case of the MLPG, and it was called MLPG2 in [1] [2]. Its mathematical analysis was attempted by the author and others for several years, but was finally bound to fail because of a counterexample [5] given in 2001, showing that solvability of the final linear system cannot be guaranteed in general. Changes of the original method are necessary, avoiding solvability problems. This argument applies also to the more general situation of the MLPG, but the easier case of strong collocation was tackled first. A non-quantitative convergence result for a variation of Kansa's unsymmetric collocation method was given in [9], while [10] contained a general convergence theory for a class of unsymmetric methods in *strong* form. The paper [6] by Hu, Li, and Cheng deals with the important special case of solving elliptic problems with analytic solutions by unsymmetric collocation based on analytic radial basis functions, leading to exponential convergence rates. Handling unsymmetric problems in weak form turned out to be more complicated, because there was no satisfactory theory of weak testing, so far. After investigating weak approximation problems [11] without differential equations, it was finally possible [12] to deal with a large class of unsymmetric methods solving partial differential equations in weak form, including a variation of the MLPG.

The cited papers [10] [12] contain the mathematical core of a general framework built for analysis of computational methods solving general linear operator equations by unsymmetric methods in strong or weak form. However, the presentation and the results are necessarily in a rigorous and abstract mathematical style, and they require a solid background in mathematics, including regularity theory of PDEs and nonstandard results of approximation theory.

To address a wider audience interested in computational methods in Science and Engineering, this paper summarizes these results in a somewhat more application-oriented

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language, and taking a Poisson problem

$$\begin{array}{rcl}
-\Delta u &=& f_{\Omega} & \text{in } \Omega \subset \mathbf{R}^{d} \\
\frac{\partial u}{\partial \mathbf{n}} &=& f_{N} & \text{in } \Gamma_{N} \subset \partial \Omega \\
u &=& f_{D} & \text{in } \Gamma_{D} \subseteq \partial \Omega
\end{array} \tag{1}$$

as a running example for explanation.

The final result is that unsymmetric computational methods can be rigorously proven to converge at certain rates, if

- 1. the underlying problem can be written as a *solvable well-posed linear operator equation* which need *not* be elliptic,
- 2. the chosen scale of trial spaces can approximate the solution well,
- 3. differential equations and boundary conditions are *tested* via *separated* local weak or strong forms, leading to sufficiently many well-formulated linear *test* equations satisfying a *stability condition*,
- 4. the final overdetermined non-square linear system of test equations for trial functions is solved approximately by minimization of the discrete residuals.

Note that Atluri's MLPG method and Kansa's collocation technique are special cases, and they can be proven to converge, if they are set up properly along the above lines. Furthermore, the framework allows very general trial spaces and test strategies. This is in line with the many variations of the MLPG method induced by different test and trial strategies (see pages 140-143 of [1]), but the paper [12] does not cover all variations, since it only shows how *kernel-based* trial and test strategies fit into the framework. This leaves plenty of leeway for future research.

However, readers should be aware that items 3 and 4 above contain two major differences to the standard setting of the MLPG variants. Problems like (1) are viewed here as *systems* whose equations are always tested *separately*. This is standard for strong testing, but for weak testing it means that *we do not use a single weak form combining the three equations*. We rather stay with separate local weak forms to be tested separately.

Item 3 leads to non-square linear systems consisting of linear weak or strong test equations whose number must be expected to be much larger than the number of unknowns on the trial side, i.e. the number of columns in the system matrix. This calls for solution methods like least-squares which keep the residuals of the equations small. The framework of [12] proves that good approximate solutions to these systems exist, and reasonable numerical methods will not overlook them.

Convergence rates are mainly dependent on item 2. They cannot be positively influenced by testing, since they are a matter of the trial side. Testing cares for safety, while the trial side determines the attainable accuracy. If trial functions are chosen via translates of smooth kernels, convergence rates increase with the smoothness of the kernel and the solution. The rest of the paper will explain the above items one by one, adding more details.

Well-Posedness

The MLPG method and Kansa's collocation can be used for very general equations and boundary conditions. Ellipticity is not required, and the standard local weak form of the MLPG does not in general describe a variational equation arising as a necessary condition for a minimum of some functional in the sense of the Calculus of Variations. This makes mathematical analysis hard, because standard properties like positive definiteness and symmetry of stiffness matrices are not valid, and there is no "energy" minimization built into the method. Thus the mathematical analysis of the MLPG cannot mimic the theory of finite elements, as several other meshless methods based on more general trial spaces do.

But this is a feature, not a bug of unsymmetric methods. They allow a much wider scope of applicability at the expense of a more difficult mathematical background theory. The crucial property replacing ellipticity is *well-posedness* of the problem, or *continuous dependence* of the *solution* on the *data*. For this, we view equations like Poisson's (1) as a system L(u) = f with a solution u and *data* f which will usually consist of several different kinds of "data", e.g. a forcing term f_{Ω} , a Dirichlet boundary data function f_D and a Neumann data function f_N . Viewing (1) as a system of equations will also be crucial for our presentation of item 3 of the introduction. Furthermore, it paves the way for treating systems of differential equations.

Continuous dependence of the solution u on the aggregated data f must be formulated rigorously as $||u||_U \leq C||f||_F$ in terms of certain normed linear spaces U and F whose choice usually is a mathematically hazardous problem in itself. We do not describe details here, but we remind the application-oriented reader that the problem should have the property that small perturbations of the data lead only to small perturbations of the solution. Any nonlinear blow-up effect will spoil continuous dependence. Note further that this is independent of trial functions, testing, and numerical methods. If problems are ill-posed, special techniques are necessary [10] and deserve future attention.

Trial Spaces

The choice of trial spaces can be rather arbitrary, provided that the solution u can be well approximated by some function \tilde{u} from the trial space. This "comparison" function \tilde{u} is not calculated directly, but our subsequent analysis depends on the fact that any numerical method should not produce an approximate solution u^* from the trial space which is much worse than \tilde{u} . This type of argument also occurs in the mathematical foundation of the finite element method: the FEM solution u^* has an error which is comparable to the error of the best approximation \tilde{u} to u in the energy norm.

For users, this freedom of choosing trial functions implies that they can add very spe-

cial application-dependent functions, e.g. to model cracks, discontinuities, or singularities at incoming vertices.

Testing

The previous section showed that the dimension of the trial space can be kept low, if the user is sure that the solution will be well "captured" by the span of functions from the trial space. It is a major advantage of unsymmetric methods to be able to avoid a fine space discretization on the trial side, if the solution can be well approximated by a few nicely chosen trial functions. This keeps the *trial* space small, while *testing* will always require a fine space granularity in order to make sure that the approximate solution actually satisfies the requirements everywhere. But we allow unsymmetric overdetermined systems here, and if the final linear system of equations is able to reproduce the right-hand side well, we do not care too much about the number of equations required for careful testing.

In general, *testing* works on linear combinations of trial functions and should come up with a number of equations for the coefficients of an approximate solution. *Strong* testing is synonymous for *collocation*, because it is based on plain evaluations of trial functions and their derivatives at certain "test points". If an operator equation like (1) is viewed as a *system*, each equation is tested separately, using different test points for the differential equation and each boundary condition. The link between these different tests is provided only by the common trial function which is tested. Users should note that collocation completely avoids all the hassles of numerical integration. If data and solutions are smooth enough to allow evaluation of function values and derivatives, it does not make much sense to make a detour via weak forms at all.

Here, we use a similar strategy for *weak* testing. Instead of merging several equations like (1) into a single weak form with several localized domain and boundary integrals, we look at each equation separately and test each equation with a possibly different test strategy. Users may, for instance, even choose strong testing for boundary values and weak testing for the differential equation, or vice versa. Like in strong testing, the common link is via the trial functions only. For a weak treatment of the Poisson problem (1), we can use three possibly different kinds of test functions v_{Ω} , v_D , v_N on Ω , Γ_D , and Γ_N , respectively, and set up test equations of the form

where we do not care if the first inner product is transformed via integration by parts or not.

The mathematical analysis of testing is a major challenge. For both kinds of testing, one only has a *finite* number of test equations to make sure that the approximate solution is close to the true solution *everywhere* or in norm. To overcome this *discretization* effect, the mathematical framework of [10], [12] requires a *stability condition* of the following simplified form:

If a trial function satisfies the test equations with a small residual, it must be globally small.

This can be satisfied in most applications by using sufficiently many well-defined test equations for a given trial space, and it implies that the final non-square overdetermined system must have maximal rank and thus no nonzero homogeneous solution. But in our mathematical background theory, we need the above stability *uniformly* with respect to refinement of discretizations on both the trial and the test side, and this is hard to prove. As an aside, we note that popular *patch tests* and *consistency conditions* have absolutely no significance for the mathematical analysis we present here.

Up to this point, there is no difference between strong and weak testing. But weak testing has a serious complication: it contains a *hidden convolution*. This can be easily seen when test functions are provided by translates of compactly supported bell-shaped kernels like the "shape functions" of moving least squares, or by Wendland-type [13] radial basis functions. Each weak test equation as in (2) compares the convolution of the *solution* with the kernel to the convolution of the *data* with the kernel, and it is satisfied if the results of these convolutions coincide. Thus weak testing solves an equation by first convolving both sides and then solving the convolved equation strongly. This means that *weak* testing acts like convolution followed by *strong* testing, and it will always have a smoothing effect.

Consequently, any mathematical analysis of weak testing has to fight with the hidden convolution. This is a challenging research topic. To overcome these problems, the paper [12] makes use of convolution instead of fighting it. Testing is done there exclusively via convolution with smooth compactly supported positive definite kernels. Then the paper uses results on convolution operators to shift the smoothness requirements of the underlying spaces accordingly, and it arrives at error bounds and convergence rates in weak norms, i.e. in norms taken after convolution. This seems to be a serious drawback at first sight, but a closer inspection reveals that it is rather a feature than a bug. For instance, our background theory [12] allows weak problems with distributional data whose solutions u are only in L_2 , and then it is quite normal that convergence rates can only be obtained in negative Sobolev norms. On the other hand, this again confirms that weak formulations only make sense in cases where there is not enough smoothness to allow strong function evaluations, and then our theory provides quite appropriate results.

Numerical Methods

The previous section explained item 3 of the introduction, and we finally deal with item 4. Our analysis sets up a non-square unsymmetric linear system of N weak or strong test equations for $m \ll N$ coefficients of trial functions. If the trial space is chosen well along the lines of item 2, there will be a good candidate \tilde{u} for a solution. Furthermore, a good testing strategy observing item 3 will ensure that the rank of the system matrix is m, employing the stability condition we described in the previous section.

Now any numerical method which solves overdetermined full-rank systems will do, if it picks an approximate solution which is not much worse than \tilde{u} . Any least-squares

solver will suffice, and in cases of bad condition one can use projections to subspaces of the trial space, provided that they still contain a good approximation to the solution. This explains why many ill-conditioned systems arising in weak or strong discretizations still can produce satisfactory solutions if SVD or careful pivoting techniques are applied. It does not make sense to go for an exact solution. Instead, the task is not to miss an existing good *approximate* solution. It is possible [8] to extend all of this to *adaptive* numerical techniques.

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