

Mesh-hardened finite element analysis through a Generalized Moving Least-Squares approximation of variational problems

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Abstract. In most finite element methods the mesh is used to both represent the domain and to define the finite element basis. As a result the quality of resulting discretizations is tied to the quality of the mesh and may suffer when the latter deteriorates. This paper formulates an alternative approach, which separates the discretization of the domain, i.e., the meshing, from the discretization of the PDE. The latter is accomplished by extending the Generalized Moving Least-Squares (GMLS) regression technique to approximation of bilinear forms and using the mesh only for the integration of the GMLS polynomial basis. Our approach yields a non-conforming discretization of the weak equations that can be handled by standard discontinuous Galerkin or interior penalty terms.

Keywords: Galerkin methods · Generalized Moving Least Squares · Nonconforming Finite Elements.

1 Introduction

The vast majority of finite element methods uses the mesh to both approximate the computational domain and to define the shape functions necessary to discretize the weak forms of the governing PDEs. These dual roles of the mesh are often in conflict. On the one hand, the properties of the discrete equations depend strongly on the quality of the underlying mesh and may deteriorate to the point of insolvability on poor quality grids. For example, high-aspect or “sliver” elements lead to nearly singular shape functions, which result in ill-conditioned or even singular discrete equations [4, 13]. On the other hand, automatic generation of high-quality grids remains a challenge. Currently, hexahedral grids can deliver robust results but require prohibitive manual efforts. Conversely, tetrahedral grids can be constructed more efficiently but their quality may be insufficient

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for traditional Finite Element Analysis (FEA) due to poor aspect ratios. Summarily, meshing can consume significant resources, creating a computational bottleneck in the finite element workflow [9]. Moreover, in some circumstances such as Lagrangian simulations of large-deformation mechanics [12], distorted grids are unavoidable. As a result, hardening finite element methods for substandard grids can have significant impacts towards enabling automated CAD-to-solution capabilities by reducing or even removing the performance barriers created by the mesh-quality requirements of conventional FEA.

Attaining these goals requires either reducing or altogether eliminating the dependency of the finite element shape functions on the underlying mesh. In this paper we aim for the latter by extending Generalized Moving Least Squares (GMLS) [15] regression techniques to approximate the weak variational forms of the PDE problems, that are at the core of FEA.

In so doing our approach limits the role of the underlying mesh to performing numerical integration and enables generation of well-conditioned discrete problems that are independent of its quality. These problems are obtained by (i) solving a small local quadratic program on each element; (ii) substituting the test and trial functions by the polynomial basis of the GMLS reproduction space, and (iii) integrating the resulting products of polynomials, which can be accomplished with relatively few quadrature points. The approximate weak forms generated by this process fall into the category of non-conforming FEM, which are supported by a mature and rigorous stability theory and error analysis. This allows us to borrow classical “off-the-shelf” stabilization techniques from, e.g., Discontinuous Galerkin [2, 8] or Interior Penalty [16, 1] methods.

These traits, i.e., formulations that require only integration of polynomials and can be stabilized by standard non-conforming FEM terms, set our approach apart from other techniques, such as meshfree Galerkin methods [5, 11, 3, 10] that also aim to alleviate mesh quality issues. These methods use GMLS, or similar regression techniques, to define *meshfree shape functions* which replace the standard mesh-based finite element bases in the weak forms. However, the meshfree shape functions are not known in closed form and are non-polynomial. As a result, their integration requires a relatively large number of quadrature points, which increases the computational cost of such schemes, as every shape function evaluation involves a solution of a small linear algebra problem. This has prompted consideration of reduced order integration [7, 6]; however, such integration leads to numerical instabilities due to underintegration and requires application-specific stabilizations.

2 Generalized Moving Least Squares (GMLS) regression

GMLS is a non-parametric regression technique for the approximation of bounded linear functionals from scattered data [15, Section 4.3]. A typical GMLS setting includes (i) a function space U with a dual U^* ; (ii) a finite dimensional space $\Phi \subset U$ with basis $\phi = \{\phi_1, \dots, \phi_q\}$; (iii) a Φ -unisolvent¹ set of sam-

¹ We recall that Φ -unisolvency implies $\{\phi \in \Phi \mid u'_i(\phi) = 0, i = 1, \dots, n\} = \{0\}$.

pling functionals $S' = \{u'_1, \dots, u'_n\} \subset U^*$; and (iv) a locally supported kernel $w : U^* \times U^* \mapsto \mathbb{R}^+ \cup \{0\}$.

GMLS seeks an approximation $\tilde{\tau}(u)$ of the *target* $\tau(u) \in U^*$ in terms of the sample vector $\mathbf{u} := (u'_1(u), \dots, u'_n(u)) \in \mathbb{R}^n$, such that $\tilde{\tau}(\phi) = \tau(\phi)$ for all $\phi \in \Phi$, i.e., the approximation is Φ -reproducing. To define $\tilde{\tau}(u)$ we need the vector $\boldsymbol{\tau}(\phi) \in \mathbb{R}^q$ with elements $(\boldsymbol{\tau}(\phi))_i = \tau(\phi_i)$, $i = 1, \dots, q$, the diagonal weight matrix $W(\tau) \in \mathbb{R}^{n \times n}$ with element $W_{ii}(\tau) = w(\tau; u'_i)$, and the basis sample matrix $B \in \mathbb{R}^{n \times q}$ with element $B_{ij} = u'_i(\phi_j)$; $i = 1, \dots, n$; $j = 1, \dots, q$. Let $|\cdot|_{W(\tau)}$ denote the Euclidean norm on \mathbb{R}^n weighted by $W(\tau)$, i.e.,

$$|\mathbf{b}|_{W(\tau)}^2 = \mathbf{b}^\top W(\tau) \mathbf{b} \quad \forall \mathbf{b} \in \mathbb{R}^n.$$

The GMLS approximant of the target is then given by

$$\tilde{\tau}(u) := \mathbf{c}(\mathbf{u}; \tau) \cdot \boldsymbol{\tau}(\phi), \quad (1)$$

where the GMLS coefficients $\mathbf{c}(\mathbf{u}; \tau) \in \mathbb{R}^q$ solve

$$\mathbf{c}(\mathbf{u}; \tau) = \underset{\mathbf{c} \in \mathbb{R}^q}{\operatorname{argmin}} \frac{1}{2} |B\mathbf{c} - \mathbf{u}|_{W(\tau)}^2. \quad (2)$$

It is straightforward to check that $\mathbf{c}(\mathbf{u}; \tau) = (B^\top W(\tau) B)^{-1} (B^\top W(\tau)) \mathbf{u}'(u)$. We refer to [14] for information about the efficient and stable solution of (2). Lastly, let $\mathbf{e}_i \in \mathbb{R}^n$ be the i th Cartesian unit vector and let $u_i^\tau := \mathbf{c}(\mathbf{e}_i; \tau) \cdot \boldsymbol{\tau}(\phi) \in \Phi$. We call the set $S^\tau = \{u_1^\tau, \dots, u_n^\tau\} \subset \Phi$ a *GMLS reciprocal of S' relative to τ* .

3 GMLS approximation of variational equations

To motivate the approach we first formulate a GMLS approximation of an abstract variational equation. Let U and V denote Hilbert spaces with duals U^* and V^* , respectively. We consider the following abstract variational equation: *given $f \in V^*$ find $u \in U$ such that*

$$a(u, v) = f(v) \quad \forall v \in V, \quad (3)$$

where $a(\cdot, \cdot) : U \times V \rightarrow \mathbb{R}$ is a given bilinear form. We refer to U and V as the trial and the test space, respectively. To approximate (3) we will use two separate instances of the GMLS regression for the test and trial spaces, respectively. To differentiate between these instances we tag their entities with a sub/superscript indicating the underlying space, e.g., S'_U and $\mathbf{c}^U(u)$ denote a sampling set and a coefficient vector, respectively, for the *trial space*. One exception to this rule will be the dual GMLS functions u_i^τ and v_i^τ .

We obtain the GMLS approximation of (3) in two steps. For any fixed $u \in U$ the form $a(u, \cdot)$ defines a bounded linear functional on V , i.e., $a(u, \cdot) \in V^*$. We shall assume that the kernel w is such that $W(a(u, \cdot)) = W(f)$. For this reason we retain the generic label τ to indicate dependence of various GMLS entities

on their respective target functionals. Then, the GMLS approximants of $a(u, \cdot)$ and f can be written in terms of the same GMLS coefficient vector as

$$\tilde{a}(u, v) := \mathbf{c}^V(v; \tau) \cdot a(u, \phi^V) \quad \text{and} \quad \tilde{f}(v) = \mathbf{c}^V(v; \tau) \cdot f(\phi^V) \quad \forall v \in V,$$

respectively. Combining these representations yields the following approximation of (3): *find* $u \in U$ *such that* $\tilde{a}(u, v) = \tilde{f}(v)$ for all $v \in V$, or equivalently,

$$\mathbf{c}^V(v; \tau) \cdot a(u, \phi^V) = \mathbf{c}^V(v; \tau) \cdot f(\phi^V) \quad \forall v \in V. \quad (4)$$

The weak problem (4) has infinitely many “equations” and “variables”. To reduce the number of equations we restrict the test space in (4) to the GMLS reciprocal set S_V^τ to obtain the following problem: *find* $u \in U$ *such that* $\tilde{a}(u, v_i^\tau) = \tilde{f}(v_i^\tau)$ for all $v_i^\tau \in S_V^\tau$ or, which is the same,

$$\mathbf{c}^V(\mathbf{e}_i; \tau) \cdot a(u, \phi^V) = \mathbf{c}^V(\mathbf{e}_i; \tau) \cdot f(\phi^V) \quad i = 1, \dots, n^V. \quad (5)$$

This completes the first step. The second step discretizes the trial space by restricting the search for a solution to the reciprocal GMLS space S_U^τ , i.e., we consider the problem: *find* $u^\tau \in S_U^\tau$ *such that*

$$\tilde{a}(u^\tau, v_i^\tau) = \tilde{f}(v_i^\tau) \quad \forall v_i^\tau \in S_V^\tau. \quad (6)$$

where $u^\tau := \sum_{j=1}^{n^U} a_j u_j^\tau$. Using (5) and $u_j^\tau := \mathbf{c}^U(\mathbf{e}_j; \tau) \cdot \phi$ one can write (6) as

$$\sum_{j=1}^{n^U} (\mathbf{c}^V(\mathbf{e}_i; \tau) \cdot a(\phi^U, \phi^V) \cdot \mathbf{c}^U(\mathbf{e}_j; \tau)) a_j = \mathbf{c}^V(\mathbf{e}_i; \tau) \cdot f(\phi^V) \quad i = 1, \dots, n^V. \quad (7)$$

It is easy to see that this problem is equivalent to the following $n^V \times n^U$ system of linear algebraic equations for the GMLS degrees-of-freedom (DoF) $\mathbf{a} = \{a_1, \dots, a_{n^U}\}$

$$K\mathbf{a} = F \quad (8)$$

where $K \in \mathbb{R}^{n^V \times n^U}$ and $F \in \mathbb{R}^{n^V}$ have elements

$$K_{ij} = \mathbf{c}^V(\mathbf{e}_i; \tau) \cdot a(\phi^U, \phi^V) \cdot \mathbf{c}^U(\mathbf{e}_j; \tau) \quad \text{and} \quad F_i = \mathbf{c}^V(\mathbf{e}_i; \tau) \cdot f(\phi^V)$$

respectively. Problems (6) and (8) can be viewed as GMLS analogues of a conforming Petrov-Galerkin discretization of (3) and its equivalent linear algebraic form. In this context, the reciprocal fields u_j^τ and v_i^τ are analogues of modal bases for the trial and test spaces. Just as in the finite element case “assembling” (8) amounts to computing the action of the bilinear form $a(\cdot, \cdot)$ and the right hand side functional f on the polynomial basis functions ϕ^U and ϕ^V .

However, application of (8) for the numerical solution of PDEs is subject to additional considerations, if one wishes to obtain a computationally effective scheme. This has to do with the fact that in the PDE context $a(\cdot, \cdot)$ and f usually involve integration over a domain Ω . In such a case one would have to

consider a GMLS regression with a kernel w whose support contains the entire problem domain. Unfortunately, this renders (8) dense, making the discretization impractical for all but small academic problems.

The key to obtaining computationally efficient discretizations from (6), resp. (8) is to apply this formulation *locally*. In the following section we demonstrate one possible application of the approach to generate a non-conforming scheme for a model PDE.

3.1 Application to a model PDE

Consider the advection-diffusion equation with homogeneous Dirichlet boundary conditions

$$-\varepsilon \Delta u + \mathbf{b} \cdot \nabla u = f \quad \text{in } \Omega \quad \text{and} \quad u = 0 \quad \text{on } \Gamma, \quad (9)$$

where $\Omega \subset \mathbb{R}^d$, $d = 1, 2, 3$ is a bounded region with Lipschitz continuous boundary Γ , \mathbf{b} is a solenoidal vector field, and f is a given function. The weak form of (9) is given by the abstract problem (3) with $U = V = H_0^1(\Omega)$,

$$a(u, v) = \int_{\Omega} \varepsilon \nabla u \cdot \nabla v + (\mathbf{b} \cdot \nabla u) v dx \quad \text{and} \quad f(v) = \int_{\Omega} f v dx.$$

Let Ω^h and $X^\eta \subset \Omega$ denote a conforming partition of the computational domain into finite elements $\{\mathcal{K}_k\}_{k=1}^{N_e}$ and a point cloud comprising points $\{\mathbf{x}_i\}_{i=1}^{N_p}$, respectively. We seek approximation of u on the point cloud, i.e., the DoF are associated with X^η rather than the underlying mesh. Furthermore, no relationship is assumed between Ω^h and X^η , in practice though one may define X^η using mesh entities such as element vertices, element centroids, etc..

Using the additive property of the integral $a(u, v) = \sum_{k=1}^{N_e} a_k(u, v)$ and $f(v) = \sum_{k=1}^{N_e} f_k(v)$, where $a_k(\cdot, \cdot)$ and $f_k(\cdot)$ are restrictions of $a(\cdot, \cdot)$ and $f(\cdot)$ to element \mathcal{K}_k . To discretize (9) we will apply GMLS *locally* to approximate $a_k(\cdot, \cdot)$ and $f_k(\cdot)$. Since $U = V$ we can use the same regression process for the trial and test spaces and drop the sub/superscripts used earlier to distinguish between them. We define the local GMLS kernel as $w(\mathcal{K}_k, \mathbf{x}_j) := \rho(|\mathbf{b}_k - \mathbf{x}_j|)$, where \mathbf{b}_k is the centroid of \mathcal{K}_k and $\rho(\cdot)$ is a radially symmetric function with $\text{supp } \rho = O(h)$. This kernel satisfies the assumption $W(a_k(u, \cdot)) = W(f_k)$. The GMLS approximants of $a_k(\cdot, \cdot)$ and $f_k(\cdot)$ will be constructed from point samples close to \mathbf{b}_k using the local sampling set $S'_k = \{\delta_{\mathbf{x}_j} \mid w(\mathcal{K}_k, \mathbf{x}_j) > 0\}$ with cardinality n_k . We assume that the support of ρ is large enough to ensure that S'_k is P^m -unisolvant. We also have the GMLS reciprocal set $S^k = \{u_1^k, \dots, u_{n_k}^k\}$ with $u_i^k := \mathbf{c}(\mathbf{e}_i^k; \mathbf{b}_k) \cdot \boldsymbol{\phi}$ and $\mathbf{e}_i^k \in \mathbb{R}^{n_k}$. Eq.(7) implies that the local GMLS approximations of $a_k(\cdot, \cdot)$ is given by

$$\tilde{a}_k(u_j^k, u_i^k) = \mathbf{c}(\mathbf{e}_i^k; \mathbf{b}_k) \cdot a_k(\boldsymbol{\phi}, \boldsymbol{\phi}) \cdot \mathbf{c}(\mathbf{e}_j^k; \mathbf{b}_k)$$

where $a_k(\boldsymbol{\phi}, \boldsymbol{\phi}) \in \mathbb{R}^{n_q \times n_q}$ has element

$$(a_k(\boldsymbol{\phi}, \boldsymbol{\phi}))_{st} = \int_{\mathcal{K}_k} \nabla \phi_s \cdot \nabla \phi_t dx$$

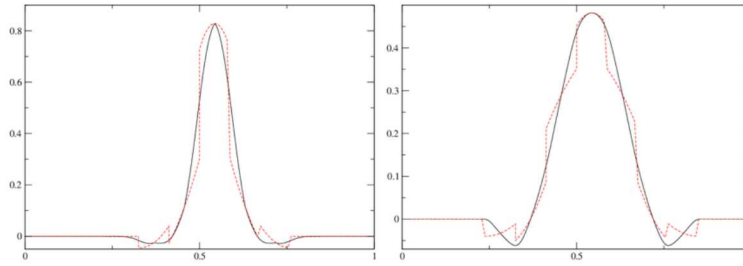


Fig. 1. Comparison of a Moving Least Squares basis function (black) and a composite reciprocal basis function $[u]_i$ (red) in one-dimensions for $\Phi = P^2$ and two different kernels.

Likewise, we have that $\tilde{f}_k(u_i^k) = \mathbf{c}(\mathbf{e}_i^k; \mathbf{b}_k) \cdot f_k(\phi)$ where $f_k(\phi) \in \mathbb{R}^{n_q}$ with

$$(f_k(\phi))_s = \int_{\mathcal{K}_k} f \phi_s dx.$$

The local approximations $\tilde{a}_k(\cdot, \cdot)$ and $\tilde{f}_k(\cdot)$ give rise to a local matrix $K_{ij}^k = \mathbf{c}(\mathbf{e}_i^k; \mathbf{b}_k) \cdot a_k(\phi, \phi) \cdot \mathbf{c}(\mathbf{e}_j^k; \mathbf{b}_k)$ and a local vector $F_i^k = \mathbf{c}^V(\mathbf{e}_i; \tau) \cdot f(\phi)$, respectively, which are analogues of the element stiffness matrix and load vector in FEA.

To define the global approximants of $a(\cdot, \cdot)$ and $f(\cdot)$ from the local ones we first need to define a global discrete space to supply the global test and trial functions. We construct this space as $[S] = \cup_{\mathcal{K}_k \in \Omega^h} S^k$ and denote its elements by $[u]$. Stacking all local DoF in a single vector $[a] := \{\mathbf{a}^1, \dots, \mathbf{a}^{N_e}\}$ produces the global DoF set for $[u]$. We now define the global approximants by summing over all elements, i.e.,

$$\tilde{a}([u], [v]) := \sum_{\mathcal{K}_k \in \Omega^h} \tilde{a}_k(u^k, v^k) \quad \text{and} \quad \tilde{f}([v]) := \sum_{\mathcal{K}_k \in \Omega^h} \tilde{f}_k(v^k),$$

where $u^k, v^k \in S^k$. In general, a sampling functional $\delta_{\mathbf{x}_j}$ can belong to multiple local sampling sets S'_k , which means that $[u]$ will be multivalued at \mathbf{x}_j . In fact, one can show that the global approximants $\tilde{a}(\cdot, \cdot)$ and $\tilde{f}(\cdot)$ can be generated by using a composite “basis” of the global space $[S]$ assembled from the local reciprocal bases as

$$[u]_i := \sum_{\mathcal{K}_k \in \Omega^h} \chi_k u_i^k,$$

where χ_k is the characteristic function of element \mathcal{K}_k . Figure 1 shows an example of a composite global basis function in one dimension and compares it to a Moving Least Squares basis function used in many meshfree Galerkin methods; see, e.g., [5, 11].

The multivalued character of the global approximation space $[S]$ means that $\tilde{a}(\cdot, \cdot)$ and $\tilde{f}(\cdot)$ are *non-conforming* approximations of $a(\cdot, \cdot)$ and $f(\cdot)$, resembling the type of “broken” forms one sees in Discontinuous Galerkin (DG) and interior penalty methods. The similarity between $\tilde{a}(\cdot, \cdot)$ and a broken DG form indicates

that the former may not be stable without any additional modifications. At the same time, this similarity also suggests that standard DG terms could be used to stabilize $\tilde{a}(\cdot, \cdot)$. Below we describe one possible scheme that results from this approach, focusing on the handling of the local bilinear forms and skipping for brevity the modifications to $f_k(\cdot)$

Following [8] we integrate the advective term in the element forms $a_k(\cdot, \cdot)$ and use the upwind trace \bar{u} on each boundary facet to obtain the upwind element form

$$\bar{a}_k(u, v) = \sum_{\mathcal{K}_k \in \Omega^h} \int_{\mathcal{K}_k} \nabla u \cdot \nabla v dx - \int_{\mathcal{K}_k} u \mathbf{b} \cdot \nabla v dx + \int_{\partial \mathcal{K}_k} \bar{u} v \mathbf{b} \cdot \mathbf{n}_k dS$$

To stabilize the diffusive term we use the interior penalty method [1]. These steps transform the element forms into the following stabilized, ‘‘DG’’ versions

$$a_k^{DG}(u, v) = \bar{a}_k(u, v) - \sum_{\mathcal{F}} \int_{\mathcal{F}} \{ \{ \nabla u \} \} \cdot \llbracket v \rrbracket dS + \int_{\mathcal{F}} v \cdot \llbracket u \rrbracket dS - \frac{\delta}{h} \int_{\mathcal{F}} \llbracket u \rrbracket \cdot \llbracket v \rrbracket dS,$$

where the sum is over all element facets in the mesh, $\{ \{ \cdot \} \}$ is the average operator, $\llbracket \cdot \rrbracket$ is the jump operator, and δ is stabilization parameter; see [8, p.1261].

Formulation of the method proceeds by using the local GMLS regression to obtain approximations $\tilde{a}_k^{DG}(\cdot, \cdot)$ of the local ‘‘DG’’ form followed by summation of these form over all elements to obtain the global DG form $\tilde{a}^{DG}(\cdot, \cdot)$.

4 Numerical examples

To demonstrate the approach we implemented the ‘‘DG’’ scheme described above in one-dimension using the element centroids to define the point cloud X^n . The left plot in Fig. 2 highlights the importance of the stabilization for the scheme. The dashed lines in this plot show error plots obtained with the ‘‘raw’’ unstabilized global form $\tilde{a}(\cdot, \cdot)$. We can clearly see that convergence stagnates and is well below the best approximation-theoretic rate for the polynomial spaces used in the local GMLS regression. On the other hand, $\tilde{a}^{DG}(\cdot, \cdot)$ achieves the optimal rates.

The right plot in Fig. 2 demonstrates the scheme for increasing Péclet numbers. Solution plots in this figure reveal that the simple upwind strategy adopted in our implementation is inadequate for high Péclet numbers. Future work will consider improved upwinding, alternatives to the interior penalty stabilization, and extension to higher dimensions.

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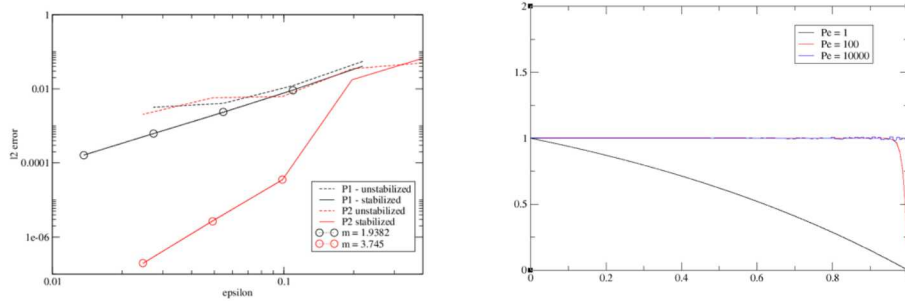


Fig. 2. Left: convergence of the nonconforming scheme with and without stabilization. Right: solution of one-dimensional advection-diffusion problem for increasing Péclet numbers.

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