Meshfree Methods for PDEs

Introduction & Overview

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Meshfree Methods: Motivation

Challenges in mesh-based methods

- Mesh generation for complex geometry very time-consuming and not fully automatic.
- Construction of approximations with high regularity.
- Improvement of approximation by mesh refinement.
- Algorithmic details of *h*-, *p*– and *hp*-adaptive refinement.
- Mesh deformation, entanglement and re-meshing.

- Mesh is approximation of the geometry/domain.
- Mesh cells define supports of approximation functions.
- Constraints accross mesh faces to ensure regularity.
- Mesh cells and faces provide integration sub-domains.

Meshfree Methods must use much different construction of approximation spaces!

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Meshfree Methods: Goals

Historic goals

- Simpler domain approximation than mesh generation.
- Less constraints in adaptive refinement.
- Easy construction of approximations with arbitrary smoothness.
- Allows for large deformations.

Modern (mathematical) goals

- Convergence order independent of regularity of problem/solution.

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Meshfree Methods: Commonalities

The mesh is the problem!

- Mesh defines strict interconnections between nodes.
- Mesh faces imply strict constraints between elements.
- Mesh cells strongly influence quality/stability of approximation.

Approximation must be based on point information only!

The mesh makes life easy!

- Mesh defines discrete domain and boundary.
- Mesh defines approximation functions/space.
- Mesh defines integration rules.

Many details/options not straightforward!

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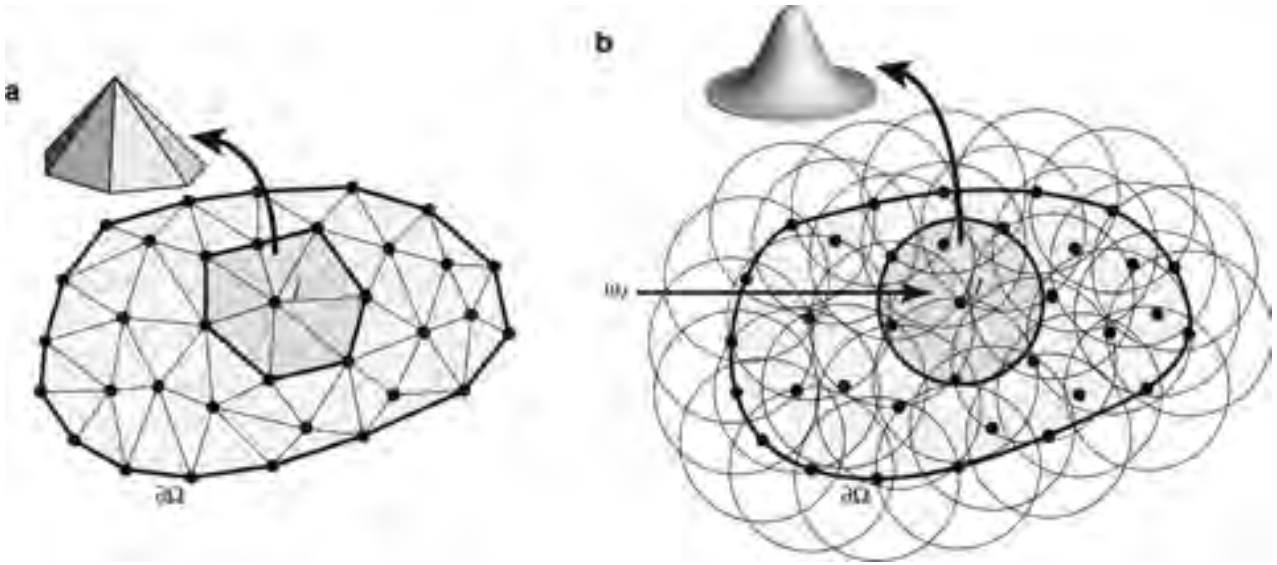
Meshfree Methods: General Procedure



- Generation of point cloud.
- Definition of approximation function/space.
- Discretization of differential operators.
- Discretization of boundary conditions.
- Efficient solvers (implicit & explicit).

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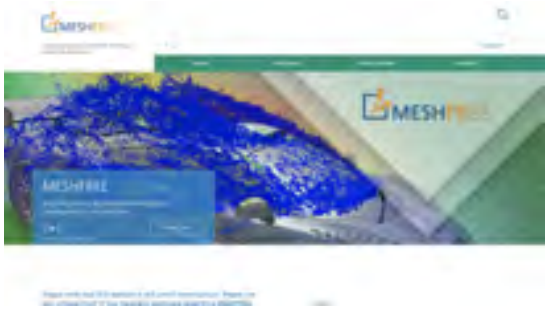
Meshfree Methods: Zoo of Acronyms

Just to name a few:

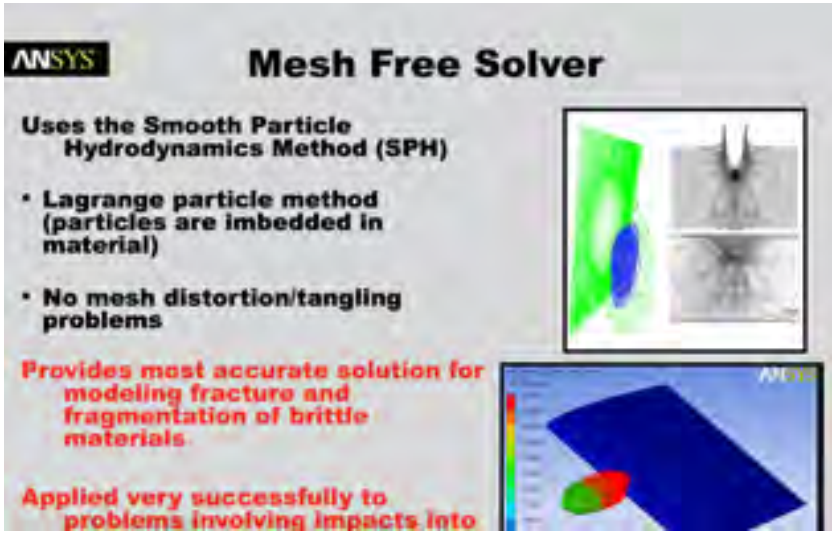
SPH, C-SPH, MLSPH, GFDM, DEM, FPM, FPSM, MLPG, MLS, GIMP, SPG, MaxEnt, DNI, SCNI, VCNI, RBF, RKPM, DEM, EFG, RKEM, MFS, XFEM, GFEM, PUM, HPC, SGFEM, V-GFEM, MS-GFEM, ...

There are many more — not that they are all very different!

Meshfree Methods: Commercial & Research Codes



Meshfree Methods: Commercial & Research Codes



Considerations before Getting into Field

- Solving a stationary problem?
- Eulerian or Lagrangian coordinates suitable?
- Explicit or implicit treatment necessary?
- Expecting smooth or irregular solutions?
- Complex geometry or complex boundary conditions?
- Conservation properties or variational formulation?
- Large scale or proof of concept?
- Numerical analysis or practical problems?
- Why are classical methods not suitable?

Topics Selected for this Course

Construction of Approximation Space

- Least squares based techniques.
- Kernel based techniques.

Discretization of Differential Operators

- Gradients, etc.
- Collocation methods.
- Galerkin approaches.

Discretization of Boundary Conditions

- Conforming vs. non-conforming.
- Weak vs. strong.

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Scattered Data Approximation: Least Squares

The *reconstruction* of an unknown function $u : \Omega \subset \mathbb{R}^D \to \mathbb{R}$ from discrete data pairs $(x_i, f_i = u(x_i)) \in \mathbb{R}^D \times \mathbb{R}$ for $i = 1, \ldots, N$ is probably the most fundamental constructive approximation problem. The goal is the construction of an approximation u_N either such that the data are exactly matched, i.e, $u_N(x_i) = f_i$, then u_N is an *interpolant*, or in some sense approximated, i.e., $u_N(x_i) \approx f_i$. If the data are noisy the latter approach is more appropriate. In both cases the approximation can essentially be written as

$$u_N(x) := \sum_{j=1}^{N} c_j(\{f_i \mid i = 1, \ldots, N\})\ \phi_j(\{x_i \mid i = 1, \ldots, N\}, x)$$

where the coefficients c_j depend on the data values $\{f_i \mid i = 1, \ldots, N\}$ and the basis functions ϕ_j on the data sites $\mathcal{X}_N := \{x_i \mid i = 1, \ldots, N\}$. Note that we do not assume a specific regularity in the distribution of the data sites or sampling points $\mathcal{X}_N$, i.e. the data sites are *scattered* and there is no *given* connectivity pattern among the data sites.

Scattered Data Approximation: Least Squares

Let us consider the vector space $\mathcal{P}^k(\Omega)$ with $d^{\mathcal{P}^k} := \dim(\mathcal{P}^k)$ of all polynomials p with total degree less than or equal to k. Furthermore, let a set of pairs $(x_i, f_i) \in \mathbb{R}^D \times \mathbb{R}$ with sampling points $x_i \in \mathbb{R}^D$ and data values $f_i \in \mathbb{R}$ for $i = 1, \ldots, N$ be given. We obtain the classical *least squares fit* to the data f_i at positions x_i by the minimization of the quadratic energy

$$J_{\mathrm{LS}}(\pi) := \sum_{i=1}^{N} (f_i - \pi(x_i))^2 \tag{1}$$

over all polynomials $\pi \in \mathcal{P}_k(\Omega)$.

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Scattered Data Approximation: Least Squares

Setting the first variation δJ_{LS} to zero and choosing a particular basis $\{p_q \mid q = 1, \ldots, d^{\mathcal{P}^k}\}$ for $\mathcal{P}_k$ we find the solution to the minimization problem by the solution of the linear system

$$G_{\mathrm{LS}}\tilde{u} = \hat{f}_{\mathrm{LS}} \tag{2}$$

where the entries $G_{\mathrm{LS}\,q,r}$ of the system matrix $G_{\mathrm{LS}} \in \mathbb{R}^{d^{\mathcal{P}^k} \times d^{\mathcal{P}^k}}$ are given by

$$G_{\mathrm{LS}\,q,r} := \sum_{i=1}^{N} p_q(x_i) p_r(x_i) \quad \text{for all } q, r = 1, \ldots, d^{\mathcal{P}^k}$$

and the vector $\hat{f}_{\mathrm{LS}} \in \mathbb{R}^{d^{\mathcal{P}^k}}$ on the right-hand side is defined as

$$\hat{f}_{\mathrm{LS}} := \Big(\sum_{i=1}^{N} f_i p_q(x_i) \Big)_{q=1}^{d^{\mathcal{P}^k}}.$$

Scattered Data Approximation: Least Squares

The minimizing polynomial π_{LS} is then simply

$$\pi_{LS}(x) = \sum_{q=1}^{d^{\mathcal{P}^k}} \tilde{u}_q p_q(x).$$

Note that the approximation π_{LS} does in general *not* align with the data, i.e. $\pi_{LS}(x_i) \neq f_i$.
We define the least squares operator A_{LS} which maps a data vector $\tilde{f} = (f_i)_{i=1}^N$ to its associated polynomial $\pi_{LS} \in \mathcal{P}_k$ by $A_{LS}\tilde{f} = \pi_{LS}$. Note that the operator A_{LS} maps elements from a vector space of dimension N to elements of a space of dimension $d^{\mathcal{P}^k}$. To obtain a uniquely solvable linear system (**??**) it is a necessary condition that $d^{\mathcal{P}^k} \leq N$. In fact we attain a unique solution to (**??**) if and only if the set of sampling points $\mathcal{X}_N$ is $\mathcal{P}_k(\Omega)$-unisolvent, see Definition **??** and Theorem **??**.

Definition ($\mathcal{V}$-unisolvent)

A set $Y \subset \mathbb{R}^D$ is called $\mathcal{V}$-unisolvent, if for all $\phi \in \mathcal{V}$ the implication

$$\phi|_Y = 0 \qquad \Rightarrow \qquad \phi \equiv 0$$

holds.

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Scattered Data Approximation: Least Squares

To assess the quality of the least squares approach let us consider the approximation of a smooth function $u \in \mathcal{C}^r(\Omega)$. Given a set of sampling points $\mathcal{X}_N$, we define the data values $f_i = u(x_i)$. Obviously, the error $u(x) - \pi_{\mathrm{LS}}(x)$ with $\pi_{\mathrm{LS}} = A_{\mathrm{LS}}\tilde{f} \in \mathcal{P}_k$ can be bounded with respect to the polynomial degree k. However, increasing the number of sampling points N will provide no further reduction of the error. If we choose the maximal polynomial degree $K = K(N)$ for which the set $\mathcal{X}_N$ is $\mathcal{P}_K$-unisolvent we have a unique solution of **(??)** and the error can be bounded with respect to $K = K(N)$, i.e. with respect to $\min(K, r)$. However, the condition number of G_{LS} will deteriorate rapidly with increasing K and the least squares approach will become instable just like interpolation using global polynomials. Keeping in mind that we approximate a smooth function u we can make use of all available information, i.e. an increasing number of sampling points, by a localization approach. Recall that the value of the least squares approximation π_{LS} at a particular point x involves *all* data pairs $(x_i, f_i = u(x_i))$. However, for a smooth function u it is clear that values $f_i = u(x_i)$ with x_i close to the point of evaluation x provide all relevant information already. Hence, it is very natural to extend the least squares approach in the following way.

Scattered Data Approximation: Moving Least Squares

Consider a locally supported non-negative function $\mathcal{W}$ often referred to as *window function* or *weight function* and the pointwise *moving least squares energy*

$$J_{\mathrm{MLS}}(\pi)(x) := \sum_{i=1}^{N} \mathcal{W}(x - x_i)(f_i - \pi(x_i))^2. \tag{3}$$

Note that **(??)** is defined for all $x \in \Omega$ and formally involves all data pairs (x_i, f_i) for each point of evaluation $x \in \Omega$. Utilizing the fact that the weight function is locally supported we can rewrite **(??)** to obtain

$$J_{\mathrm{MLS}}(\pi)(x) = \sum_{i=1}^{N} \mathcal{W}(x - x_i)(f_i - \pi(x_i))^2 = \sum_{\substack{x_i \in \mathcal{X}_N \\ \mathcal{W}(x - x_i) > 0}} \mathcal{W}(x - x_i)(f_i - \pi(x_i))^2.$$

With the convention $\omega_i := \operatorname{supp}^\circ \mathcal{W}(\cdot - x_i)$ and Definition **??** of a neighborhood $\mathcal{N}(x) \subset \mathcal{X}_N$ of an arbitrary point $x \in \Omega$, compare **(??)**, we attain

$$J_{\mathrm{MLS}}(p)(x) = \sum_{x_i \in \mathcal{N}(x)} \mathcal{W}(x - x_i)(f_i - \pi(x_i))^2. \tag{4}$$

Definition

Let a set of points $\mathcal{X}_N$ and associated patches $C_\Omega := \{\omega_i\}$ be given. Then we refer to the sets

$$\mathcal{N}_i := \{x_k \in \mathcal{X}_N \,|\, x_k \in \omega_i\} \tag{5}$$

and

$$C_i := \{\omega_k \in C_\Omega \,|\, \omega_k \cap \omega_i \neq \emptyset\}. \tag{6}$$

as local neighborhoods of a particular particle x_i or the respective patch ω_i. For an arbitrary point $x \in \overline{\Omega}$ we define its associated neighborhood as

$$\mathcal{N}(x) := \{x_k \in \mathcal{X}_N \,|\, x \in \omega_k\}. \tag{7}$$

The solution $\pi_{\text{MLS}}(x)$ with $\pi_{\text{MLS}} \in \mathcal{P}_k$ to the minimization of **(??)** is obtained by the linear system

$$G_{\text{MLS}}(x)\tilde{u}_x = \hat{f}_{\text{MLS}}(x) \quad \text{with} \quad (G_{\text{MLS}}(x))_{q,r} := \sum_{x_i \in \mathcal{N}(x)} p_q(x_i)\mathcal{W}(x - x_i)p_r(x_i). \tag{8}$$

Scattered Data Approximation: Moving Least Squares

The vector $\hat{f}_{\mathrm{MLS}}(x) \in \mathbb{R}^{d^{\mathcal{P}^k}}$ on the right-hand side is defined as

$$\hat{f}_{\mathrm{MLS}}(x) := \Big(\sum_{x_i \in \mathcal{N}(x)} f_i \mathcal{W}(x - x_i) p_q(x_i) \Big)_{q=1}^{d^{\mathcal{P}^k}}.$$

The linear system (**??**) is uniquely solvable if the neighborhood $\mathcal{N}(x)$ is $\mathcal{P}_k$-unisolvent and we can define the moving least squares operator

$$\left(A_{\mathrm{MLS}} \tilde{f} \right)(x) = \pi_{\mathrm{MLS}}(x) = \sum_{q=1}^{d^{\mathcal{P}^k}} u_{x,q} p_q(x). \tag{9}$$

Note that in the classical least squares approximation we need to solve a *single* linear system (**??**) only to obtain the approximation π_{LS} on the complete domain Ω. The resulting polynomial π_{LS} can then be evaluated directly for all $x \in \Omega$, i.e., the coefficients $\tilde{u}_q$ of π_{LS} are independent of x. In the moving least squares approach, however, we need to solve a linear system for each point of evaluation $x \in \Omega$ to obtain the respective polynomial π_{MLS} which can then be evaluated at x only, i.e., the coefficients $\tilde{u}_x$ of π_{MLS} depend on x, compare (**??**). Let us summarize our findings so-far in the following theorem which generalizes the above setting slightly.

Theorem

Let the set of points $\mathcal{X}_N = \{x_i \mid i = 1, \ldots, N\}$, associated weight functions $W_i \in \mathcal{C}(\mathbb{R}^D, \mathbb{R}_0^+)$ such that $(\mathrm{supp}(W_i))^\circ = \omega_i$ and data $\tilde{f} = (f_i) \in \mathbb{R}^N$ be given. Assume that for $k \in \mathbb{N}_0$ the neighborhood associated with each $x \in \Omega$ defined in (??) is $\mathcal{P}_k$-unisolvent. Then the approximation

$$\left(A_{\mathrm{MLS}} \tilde{f}\right)(x) = \pi_{\mathrm{MLS}}(x)$$

where $\pi_{\mathrm{MLS}} \in \mathcal{P}_k$ and $\pi_{\mathrm{MLS}}(x)$ is the solution of the minimization problem

$$\min_{\pi \in \mathcal{P}_k} J_{\mathrm{MLS}}(\pi)(x) = \min_{\pi \in \mathcal{P}_k} \sum_{x_i \in \mathcal{N}(x)} W_i(x)(f_i - \pi(x_i))^2 \tag{10}$$

is well-defined.

Proof of Theorem ??

Consider an arbitrary but fixed point of evaluation $x^* \in \Omega$ and the respective minimization problem

$$\min_{\pi \in \mathcal{P}_k} J_{\mathrm{MLS}}(\pi)(x^*) = \min_{\pi \in \mathcal{P}_k} \sum_{x_i \in \mathcal{N}(x^*)} W_i(x^*)(f_i - \pi(x_i))^2.$$

The necessary condition $\delta J_{\mathrm{MLS}}(\pi_{\mathrm{MLS}}, \pi) = 0$ for all $\pi \in \mathcal{P}_k$ yields

$$\sum_{x_i \in \mathcal{N}(x^*)} \Big(f_i - \pi_{\mathrm{MLS}}(x_i) \Big) W_i(x^*) \pi(x_i) = 0 \quad \text{for all } \pi \in \mathcal{P}_k.$$

Choosing an arbitrary basis $\{p_q \mid q = 1, \ldots, d^{\mathcal{P}^k}\}$ and setting

$$\pi_{\mathrm{MLS}}(x^*) = \sum_{q=1}^{d^{\mathcal{P}^k}} u_{x^*,q} p_q(x^*) \tag{11}$$

we obtain

$$\sum_{x_i \in \mathcal{N}(x^*)} \Big(f_i - \sum_{q=1}^{d^{\mathcal{P}^k}} u_{x^*,q} p_q(x_i) \Big) W_i(x^*) p_r(x_i) = 0. \quad \text{for all } r = 1, \ldots, d^{\mathcal{P}^k} \tag{12}$$

This is equivalent to the matrix equation

$$G_{\mathrm{MLS}}(x^*)\tilde{u}_{x^*} = \hat{f}_{\mathrm{MLS}}(x^*) \tag{13}$$

with the system matrix $G_{\mathrm{MLS}}(x^*) = (G_{\mathrm{MLS}}(x^*)_{q,r}) \in \mathbb{R}^{d^{\mathcal{P}^k} \times d^{\mathcal{P}^k}}$ and the right-hand side vector $\hat{f}_{\mathrm{MLS}}(x^*) = \left(\hat{f}_{\mathrm{MLS}}(x^*)_q\right) \in \mathbb{R}^{d^{\mathcal{P}^k}}$ defined as

$$G_{\mathrm{MLS}}(x^*)_{q,r} := \sum_{x_i \in \mathcal{N}(x^*)} p_q(x_i) W_i(x^*) p_r(x_i), \quad \text{and} \quad \hat{f}_{\mathrm{MLS}}(x^*)_q := \sum_{x_i \in \mathcal{N}(x)} f_i W_i(x^*) p_q(x_i)$$

Recall that the unique solvability of (**??**) and the minimal property of $\pi_{\mathrm{MLS}}(x^*)$ follow from the positive definiteness of $G_{\mathrm{MLS}}(x^*)$. To this end, we consider for an arbitrary vector $\gamma \in \mathbb{R}^{d^{\mathcal{P}^k}}$ the scalar product

$$\gamma \cdot G_{\mathrm{MLS}}(x^*)\gamma = \sum_{x_i \in \mathcal{N}(x)} W_i(x^*) \Big(\sum_{q=1}^{d^{\mathcal{P}^k}} \gamma_q p_q(x_i) \Big)^2.$$

From the non-negativity of W_i follows $\gamma \cdot G_{\mathrm{MLS}}(x^*)\gamma \geq 0$ and hence G_{MLS} is positive semi-definite. Now let us assume that there is a particular $\gamma \neq 0$ such that $\gamma \cdot G_{\mathrm{MLS}}(x^*)\gamma = 0$. Since $x_i \in \mathcal{N}(x^*)$ we have $x^* \in \omega_i = (\mathrm{supp}(W_i))^\circ$ and due to the smoothness of the weight functions W_i we have $W_i(x^*) > 0$. Therefore, $\gamma_q p_q(x_i) = 0$ for all $q = 1, \ldots, d^{\mathcal{P}^k}$ and $x_i \in \mathcal{N}(x^*)$. The unisolvence of $\mathcal{N}(x^*)$ implies that $\gamma = 0$ which contradicts the assumption $\gamma \neq 0$ and hence we conclude that $G_{\mathrm{MLS}}(x^*)$ is positive definite.

Recall that in the classical least squares approach the minimizer $\pi_{\mathrm{LS}} \in \mathcal{P}^k$ is a global polynomial. It can be represented via the basis $\langle p_q \rangle$ of $\mathcal{P}^k$. In the moving least squares approach however only the value $\pi_{\mathrm{MLS}}(x)$ at the current point of evaluation $x \in \Omega$ can be expressed via $\langle p_q \rangle$. So far we have no representation of π_{MLS} as a function. Hence, the question is if we can construct appropriate basis functions ϕ_i such that $\pi_{\mathrm{MLS}} \in \mathrm{span}\langle \phi_i \rangle$.

Corollary

Let the assumptions of Theorem **??** *be satisfied. Then the representation formula*

$$\left(A_{\mathrm{MLS}}\tilde{f}\right)(x) = \sum_{i=1}^{N} f_i \phi_i(x) \tag{14}$$

holds and the basis functions ϕ_i *are given by*

$$\phi_i(x) := W_i(x) \sum_{q=1}^{d^{\mathcal{P}^k}} \alpha_{x,q} p_q(x_i) \tag{15}$$

where the coefficient vector $\alpha_x = (\alpha_{x,q})$ *is the unique solution of the linear system*

$$G_{\mathrm{MLS}}(x)\alpha_x = p(x) = (p_q(x))_{q=1}^{d_k^{\mathcal{P}}}. \tag{16}$$

Proof of Corollary ??

Again, consider a fixed but arbitrary point of evaluation $x^* \in \Omega$.
According to (**??**) and (**??**) we have

$$\left(A_{\mathrm{MLS}}\tilde{f}\right)(x^*) = \sum_{q=1}^{d^{\mathcal{P}^k}} \tilde{u}_{x^*,q}\, p_q(x^*).$$

With the equivalence (**??**) this yields

$$\left(A_{\mathrm{MLS}}\tilde{f}\right)(x^*) = \tilde{u}(x^*)\cdot G_{\mathrm{MLS}}(x^*)\alpha_{x^*} = \sum_{q=1}^{d^{\mathcal{P}^k}} u_{x^*,q} \sum_{x_i \in \mathcal{N}(x^*)} W_i(x^*) p_q(x_i) \sum_{r=1}^{d^{\mathcal{P}^k}} p_r(x_i)\alpha_{x^*,r}.$$

Rearranging the sums we obtain

$$\left(A_{\mathrm{MLS}}\tilde{f}\right)(x^*) = \sum_{r=1}^{d^{\mathcal{P}^k}} \alpha_{x^*,r} \sum_{x_i \in \mathcal{N}(x^*)} W_i(x^*) \sum_{q=1}^{d^{\mathcal{P}^k}} u_{x^*,q}\, p_q(x_i) p_r(x_i). \qquad (17)$$

Plugging (**??**) into (**??**) gives

$$\left(A_{\mathrm{MLS}}\tilde{f}\right)(x^*) = \sum_{r=1}^{d^{\mathcal{P}^k}} \alpha_{x^*,r} \sum_{x_i \in \mathcal{N}(x^*)} W_i(x^*) f_i p_r(x_i) = \sum_{x_i \in \mathcal{N}(x^*)} f_i W_i(x^*) \sum_{r=1}^{d^{\mathcal{P}^k}} \alpha_{x^*,r} p_r(x_i)$$

and with definition (**??**) this yields the asserted representation (**??**), compare Figures **??** and **??**.

Proof of Corollary ??

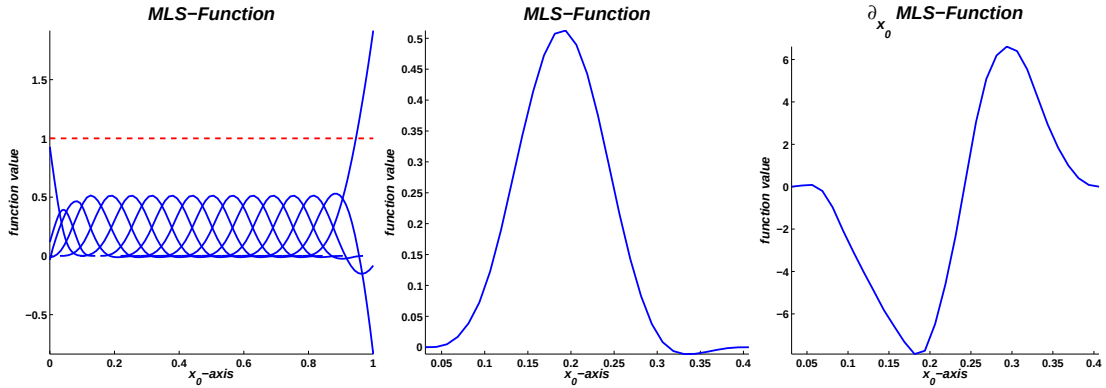

Figure 1: Moving least squares basis functions in one dimension using a cubic spline weight function (left: all basis functions; center: single basis function; right: first derivative).

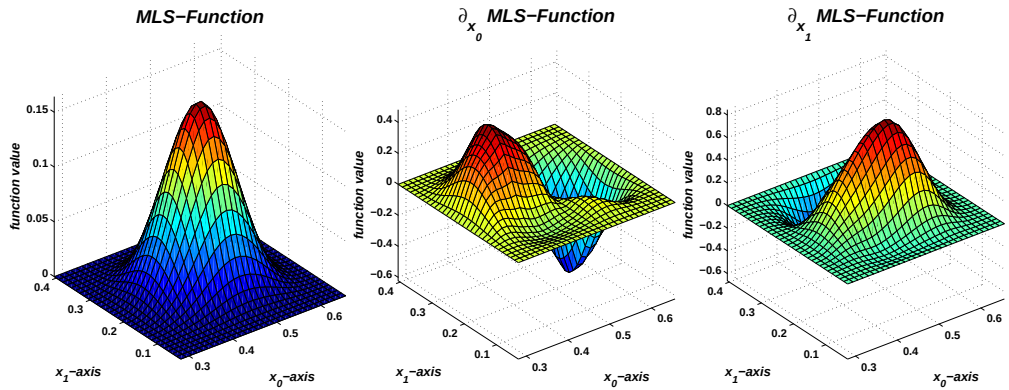

Figure 2: Moving least squares basis function (left) in two dimensions and its partial derivatives (center and right) using a cubic spline weight function.

Remark

Note that the coefficient vector α_x of (**??**) is independent of the particle x_i and hence α_x is *identical* for all particles $x_i \in \mathcal{N}(x)$; i.e. for all respective basis functions ϕ_i. Thus the evaluation of a single basis function ϕ_i at a particular point $x \in \Omega$ is of similar complexity as the simultaneous evaluation of all non-vanishing basis functions ϕ_j in $x \in \Omega$.

Due to (**??**) we can view the moving least squares technique as a constructive approach to obtain compactly supported shape functions ϕ_i with $\text{supp}(\phi_i) = \text{supp}(W_i)$ from scattered independent points $x_i \in \mathcal{X}_N$ only; i.e., an approach for the construction of meshfree shape functions. Since we are ultimately interested in the development of a meshfree Galerkin method for the numerical treatment of partial differential equations we must be concerned with the regularity of the basis functions (**??**).

Lemma

Let the assumptions of Theorem **??** *be satisfied with* $W_i \in \mathcal{C}^r(\mathbb{R}^D)$ *with* $r > 0$ *for all* $i = 1, \ldots, N$*. Then, there holds* $\phi_i \in \mathcal{C}^r(\mathbb{R}^D)$ *for the basis functions* ϕ_i *of* **(??)**.

The second important property we must consider is the consistency of our moving least squares functions **(??)**.

Lemma

Let the assumptions of Theorem **??** *be satisfied. Then, the composed operator*

$$A_{\text{MLS}} E_{\mathcal{X}_N} : \mathcal{C}(\Omega) \to \text{span}\langle \phi_i \mid i = 1, \ldots, N \rangle \subset \mathcal{C}(\Omega)$$

with ϕ_i *defined in* **(??)**, $E_{\mathcal{X}_N} : \mathcal{C}(\Omega) \to \mathbb{R}^N$ *denotes the point evaluation, i.e.* $E_{\mathcal{X}_N}(u) = (u(x_i))_{i=1}^N$*, reproduces all polynomials* $\pi \in \mathcal{P}_k(\Omega)$*, i.e.*

$$A_{\text{MLS}} E_{\mathcal{X}_N}|_{\mathcal{P}_k(\Omega)} = \mathbb{I}, \quad A_{\text{MLS}} E_{\mathcal{X}_N}(\pi) = \pi \quad \text{for all } \pi \in \mathcal{P}_k(\Omega). \tag{18}$$

Recall the representation (**??**)

$$\Big(A_{\mathrm{MLS}} E_{\mathcal{X}_N}(\pi)\Big)(x) = \sum_{i=1}^{N} \pi(x_i)\phi_i(x).$$

The polynomial π has a unique representation in the employed basis for $\mathcal{P}_k(\Omega)$, i.e.

$$\sum_{q=1}^{d^{\mathcal{P}^k}} \gamma_q p_q(x) = \pi(x)$$

for all x. With the representation of the basis (**??**) this yields

$$\Big(A_{\mathrm{MLS}} E_{\mathcal{X}_N}(\pi)\Big)(x) = \sum_{i=1}^{N}\sum_{q=1}^{d^{\mathcal{P}^k}} \gamma_q p_q(x_i)\phi(x) = \sum_{i=1}^{N}\sum_{q=1}^{d^{\mathcal{P}^k}} \gamma_q p_q(x_i) W_i(x) \sum_{r=1}^{d^{\mathcal{P}^k}} \alpha_{x,r} p_r(x_i).$$

Rearranging the sums, we obtain

$$\Big(A_{\mathrm{MLS}} E_{\mathcal{X}_N}(\pi)\Big)(x) = \sum_{q=1}^{d^{\mathcal{P}^k}}\sum_{r=1}^{d^{\mathcal{P}^k}}\sum_{i=1}^{N} \gamma_q p_q(x_i) W_i(x) p_r(x_i) \alpha_{x,r} = \gamma \cdot G_{\mathrm{MLS}}(x)\alpha_x.$$

Since (**??**) holds, we obtain the asserted equivalence

$$\Big(A_{\mathrm{MLS}} E_{\mathcal{X}_N}(\pi)\Big)(x) = \gamma \cdot p(x) = \sum_{q=1}^{d^{\mathcal{P}^k}} \gamma_q p_q(x) = \pi(x) \text{ for all } x \in \Omega.$$

An immediate consequence of this lemma is that the basis functions ϕ_i constructed by the moving least squares approach are a *partition of unity* independent of the employed polynomial degree $k \in \mathbb{N}_0$.

Corollary

Let the assumptions of Theorem **??** *be satisfied. Then, the basis functions defined in* (**??**) *satisfy*

$$\sum_{i=1}^{N} \phi_i(x) = 1 \quad \text{for all } x \in \Omega. \tag{19}$$

Yet, the basis functions ϕ_i in general do *not* satisfy the Kronecker property, i.e.

$$\phi_i(x_j) \neq \delta_{ij} = \begin{cases} 1 & i = j, \\ 0 & i \neq j, \end{cases}$$

compare Figures **??** and **??**.

Note also that the assumption of the $\mathcal{P}_k$-unisolvence of $\mathcal{N}(x)$ for $k \geq 0$ and all $x \in \Omega$ is not trivial to verify for arbitrary point sets $\mathcal{X}_N$, i.e. a specific choice of W_i for $i = 1, \ldots, N$. Thus, the selection of appropriate supports ω_i is in general a somewhat challenging task. Observe though that for the important special case of $k = 0$, i.e. an approximation with the constant function, there holds the equivalence

$$\mathcal{N}(x) \text{ is } \mathcal{P}^0\text{-unisolvent} \quad \Longleftrightarrow \quad \Omega \subset \bigcup_{i=1}^{N} \omega_i.$$

In this case (**??**) reduces to

$$\phi_i(x) = W_i(x)\alpha_{x,0}, \qquad \text{with } G_{\mathrm{MLS}0,0}\alpha_{x,0} = 1 \tag{20}$$

if we choose $p_0 \equiv 1$ as the basis of $\mathcal{P}^0$.

Plugging the definition (**??**) into (**??**) we obtain the *explicit* representation

$$\phi_i(x) = \frac{W_i(x)}{S(x)}, \quad \text{with } S(x) := \sum_{j=1}^{N} W_j(x)$$

whereas in general with $k > 0$ the basis functions ϕ_i of (**??**) are known *implicitly* only via (**??**). Due to the compact support of the weights W_i and the observation that $\mathcal{N}(x) \subset C_i$ for all $x \in \omega_i$, compare (**??**) and Definition **??**, we can rewrite the moving least squares function for $k = 0$ as

$$\phi_i(x) = \frac{W_i(x)}{S_i(x)}, \quad \text{with } S_i(x) := \sum_{\omega_j \in C_i} W_j(x). \tag{21}$$

Observe that these function, the so-called Shepard functions, satisfy Corollary **??**. The Shepard functions are a partition of unity.

Finally, we need to consider the stability of the evaluation of the basis functions (**??**); i.e. the conditioning of the system matrix $G_{\mathrm{MLS}}(x^*)$ for all $x^* \in \Omega$. Note that the choice of the polynomial basis in the proof of Theorem **??** is arbitrary for each point of evaluation x^*. Hence, we can for instance consider linear transformations $T_{x^*} : \mathbb{R}^D \to \mathbb{R}^D$ depending on the point of evaluation x^* of a fixed basis $\{\hat{p}_q \mid q = 1, \ldots, d^{\mathcal{P}^k}\}$, i.e.,

$$T_{x^*} : x \mapsto \frac{x^* - x}{\rho_{x^*}}, \quad p_{x^*,q}(x) = \hat{p}_q \circ T_{x^*}(x) = \hat{p}_q\left(\frac{x^* - x}{\rho_{x^*}}\right). \tag{22}$$

The approximation (**??**) and hence the representation (**??**) and the basis functions (**??**) are unchanged, but the respective linear systems G_{MLS} and right-hand side vectors need to be modified.

Corollary

Consider the choice of basis (??) for the solution of the pointwise minimization problem (??) at a fixed but arbitrary point $x^* \in \Omega$. Then, the solution $\pi_{\mathrm{MLS}}(x^*)$ is obtained by the solution of the linear system (??) with the system matrix

$$G_{\mathrm{MLS}}(x^*) = (G_{\mathrm{MLS}}(x^*)_{q,r}) \in \mathbb{R}^{d^{\mathcal{P}^k} \times d^{\mathcal{P}^k}}$$

$$G_{\mathrm{MLS}}(x^*)_{q,r} := \sum_{x_i \in \mathcal{N}(x^*)} p_{x^*,q}(x_i) W_i(x^*) p_{x^*,r}(x_i) = \sum_{x_i \in \mathcal{N}(x^*)} \hat{p}_q\left(\frac{x^* - x_i}{\rho_{x^*}}\right) W_i(x^*) \hat{p}_r\left(\frac{x^* - x_i}{\rho_{x^*}}\right)$$

and the right-hand side

$$\hat{f}_{\mathrm{MLS}}(x^*)_q := \sum_{x_i \in \mathcal{N}(x^*)} f_i W_i(x^*) p_{x^*,q}(x_i) = \sum_{x_i \in \mathcal{N}(x^*)} f_i W_i(x^*) \hat{p}_q\left(\frac{x^* - x_i}{\rho_{x^*}}\right).$$

The basis functions ϕ_i are given by

$$\phi_i(x^*) := W_i(x^*) \sum_{q=1}^{d^{\mathcal{P}^k}} \alpha_{x^*,q} p_{x^*,q}(x_i) = W_i(x^*) \sum_{q=1}^{d^{\mathcal{P}^k}} \alpha_{x^*,q} \hat{p}_q\left(\frac{x^* - x_i}{\rho_{x^*}}\right) \tag{23}$$

where the coefficient vector $\alpha_{x^*} = (\alpha_{x^*,q})$ is the unique solution of the linear system

$$G_{\mathrm{MLS}}(x^*)\alpha(x^*) = p_{x^*}(x^*) = \hat{p}\left(\frac{x^* - x^*}{\rho_{x^*}}\right) = \hat{p}(0). \tag{24}$$

The advantage of (**??**) over (**??**) in computations is that the condition number of the system matrix $G_{\mathrm{MLS}}(x^*)$ can be controlled via the parameter ρ_{x^*} whereas (**??**) can become unstable when we use more and more points $x_i \in \mathcal{X}_N$. Observe that such a refinement of the point set $\mathcal{X}_N$ does not assume any connectivity among the points x_i. The insertion of new points x_i into $\mathcal{X}_N$ and thereby an *h-adaptive* refinement of the respective meshfree function space $V_{\mathrm{MLS}} := \mathrm{span}\langle \phi_i \rangle$ is straightforward. Unfortunately this is not the case for a local *p-adaptive* refinement.

Recall that the weight functions W_i can be chosen arbitrarily on each ω_i; i.e., they are independent of each other and more importantly independent of the point of evaluation x^*. Hence, we can consider the linear transformations of a window function

$$T_i(x) : x \mapsto \frac{x - x_i}{\rho_i}, \quad W_i(x) := \mathcal{W}\left(\frac{x - x_i}{\rho_i}\right)$$

as weight functions. Then, (**??**) becomes

$$\phi_i(x^*) := \mathcal{W}\left(\frac{x^* - x_i}{\rho_i}\right) \sum_{q=1}^{d^{\mathcal{P}^k}} \alpha_{x^*,q} \hat{p}_q\left(\frac{x^* - x_i}{\rho_{x^*}}\right). \tag{25}$$

Note the difference in the scaling of the window function (using $1/\rho_i$) and the employed polynomial (scaled by $1/\rho_{x^*}$). This is due to the fact that the polynomial basis can be chosen with respect to x^* and is evaluated at x_i, whereas the weight functions can be chosen with respect to x_i and are evaluated at x^*, compare (**??**) and (**??**). From this observation it is clear that the moving least squares approach does not support a p-adaptive approximation, i.e., the variation of the polynomial degree k on each ω_i. We can change the polynomial degree k only with respect to the point of evaluation x^*. Yet, such an approach suggests a disjoint partition of the domain Ω into $\Omega_l = \{x^* \in \Omega \,|\, k(x^*) = k_l\}$ with $k_l \in \mathbb{N}_0$ and it is clear that at the boundaries of these disjoint sub-regions, i.e., $x \in \partial\Omega_{l_1} \cap \partial\Omega_{l_2}$ with $l_1 \neq l_2$, the variation in the polynomial degree may lead to a jump in the resulting approximation $A_{\text{MLS}}(x)\tilde{f}$ and the associated basis functions ϕ_i.

Thus, we can use the moving least squares approach to construct meshfree functions spaces V_{MLS} that support h-adaptive refinement easily but do they not allow for p-adaptive refinement without compromising the regularity of the shape functions. The capability of p-adaptive refinement of our meshfree function space must be provided by an additional construction outside of the moving least squares approach.

Scattered Data Approximation: Kernel Approaches

Meshfree kernel approaches are based on integral convolution

$$u_K(x) := \int_\Omega \phi_a(x-y)u(y)\,dy \tag{26}$$

where ϕ_a is called the kernel function with support size a. The kernel here plays a similar role as the weight function in MLS.
If $\Omega = \mathbb{R}$ and $\phi_a \equiv \delta$ we obviously have

$$u_K(x) = u(x) \quad \text{for all } x.$$

In all other cases (**??**) defines an approximation only, i.e.

$$u_K(x) \approx u(x).$$

Consider the Taylor expansion of a suitable u at y centered in x

$$u(y) = \sum_{i=0}^{\infty} \frac{(y-x)^i}{i!} u^{(i)}(x).$$

Plugging this into (**??**) yields

$$u_K(x) = \int_\Omega \phi_a(x-y)u(y)\,dy = \sum_{i=0}^{\infty} u^{(i)}(x) \int_\Omega \phi_a(x-y)\frac{(y-x)^i}{i!}\,dy.$$

Scattered Data Approximation: Kernel Approaches

Thus, with the definition

$$m_i(x) := \int_\Omega \phi_a(x-y)(x-y)^i \, dy$$

we can write

$$u_K(x) = \sum_{i=0}^{\infty} (-1)^i u^{(i)}(x) \int_\Omega \phi_a(x-y) \frac{(x-y)^i}{i!} \, dy = \sum_{i=0}^{\infty} \frac{(-1)^i}{i!} u^{(i)}(x) m_i(x)$$

and obtain the conditions

$$m_0(x) = 1, \quad m_i(x) = 0 \qquad \text{for all } 0 < i >$$

to achieve $u_K(x) = u(x)$.

Scattered Data Approximation: Kernel Approaches

$$m_i(x) := \int_\Omega \phi_a(x-y)(x-y)^i \, dy$$

These reproducing conditions can e.g. be restricted to

$$m_0(x) = 1, \quad m_i(x) = 0 \qquad \text{for all } 0 < i \leq n$$

to enforce just nth order polynomial completeness.

Kernel selection

Obviously, the reproducing conditions are constraints on the choice of the kernel ϕ_a.

Reproducing Kernel Particle Method

Instead of choosing the right kernel that satisfies the reproducing conditions, the RKP approach assumes a given kernel and then constructs a multiplicative correction function to enforce the reproducing conditions for the corrected kernel. Thus, we define the approximation

$$u_R(x) := \int_\Omega \bar{\phi}_a(x; x-y)u(y)\, dy \tag{27}$$

where the corrected kernel is given by

$$\bar{\phi}_a(x; x-y) := C(x; x-y)\phi_a(x-y) = \sum_{i=0}^{n}(x-y)^i b_i(x)\phi_a(x-y). \tag{28}$$

The correction function is often writen as

$$C(x; x-y) = \langle H(x-y), b(x)\rangle \tag{29}$$

Note that $H(x-y)$ denotes the vector of all monomial basis function $(x-y)^i$ and $b(x)$ is (similarly to MLS) the coefficient vector of the polynomial correction function $C(x; x-y)$ valid at a particular location x only.

Reproducing Kernel Particle Method

The moments for the corrected kernel are defined as

$$\bar{m}_i(x) := \int_\Omega \bar{\phi}_a(x; x-y)(x-y)^i \, dy \tag{30}$$

such that the reproducing conditions again are

$$\bar{m}_0(x) = 1, \quad \bar{m}_i(x) = 0 \qquad \text{for all } 0 < i \leq n.$$

Plugging the explicit form of the corrected kernel into the definition of (**??**) yields

$$\bar{m}_i(x) = \int_\Omega \langle H(x-y), b(x) \rangle \phi_a(x-y)(x-y)^i \, dy = \sum_{k=0}^{n} b_k(x) m_{i+k}(x).$$

Reproducing Kernel Particle Method

With the definition of the moment matrix $M(x)$ for the original kernel

$$M(x) := \begin{pmatrix} m_0(x) & m_1(x) & \cdots & m_n(x) \\ m_1(x) & m_2(x) & \cdots & m_{n+1}(x) \\ \vdots & \vdots & \ddots & \vdots \\ m_n(x) & m_{n+1}(x) & \cdots & m_{2n}(x) \end{pmatrix} \tag{31}$$

we can rewrite the reproducing conditions for the corrected kernel as

$$M(x)b(x) = H(0) \tag{32}$$

such that we have identified formally the coefficient vector $b(x)$ which defines the correction function as

$$b(x) = M^{-1}(x)H(0), \quad \text{i.e.} \quad C(x; x-y) = \langle H(x-y), M^{-1}(x)H(0) \rangle.$$

Reproducing Kernel Particle Method

Moreover, since the vector $H(x-y) = ((x-y)^i))_{i=0}^n$ comprises all monomials of degree $\leq n$ and the matrix $M(x)$ collects all moments of order $\leq 2n$ we can rewrite

$$M(x) = \int_\Omega H(x-y)H^T(x-y)\phi_a(x-y)\,dy. \tag{33}$$

So that we can formally write the RKPM approximant as

$$\begin{aligned} u_R(x) &:= \int_\Omega \bar{\phi}_a(x; x-y)u(y)\,dy \\ &= \int_\Omega \langle H(x-y), M^{-1}(x)H(0)\rangle \phi_a(x-y)u(y)\,dy \\ &= \langle \int_\Omega H(x-y)\phi_a(x-y)u(y)\,dy, \\ &\qquad \big(\int_\Omega H(x-y)H^T(x-y)\phi_a(x-y)\,dy\big)^{-1} H(0)\rangle \end{aligned} \tag{34}$$

using the data function u, the original kernel ϕ_a and the monomial basis functions $(x-y)^i$ only.

Reproducing Kernel Particle Method

The most convenient form however is

$$u_R(x) = \langle M^{-1}(x)H(0), \int_\Omega H(x-y)\phi_a(x-y)u(y)\ dy \rangle$$

especially when we want to "rewrite" a RKPM approximation as a linear combination of respective basis functions

$$u_{R,N}(x) = \sum_{i=0}^{N} \Psi_i(x) f_i.$$

To this end, we simply approximate the integral by a sum over all particles/data sites x_i to define

$$u_{R,N}(x) = \langle M^{-1}(x)H(0), \sum_{i=0}^{N} H(x-x_i)\phi_a(x-x_i)f_i \rangle$$

where $f_i = u(x_i)$ are the given data values.

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Reproducing Kernel Particle Method

Thus, the meshfree basis functions obtained by RKPM are defined as

$$\Psi_i(x) := \langle M^{-1}(x)H(0), H(x - x_i)\phi_a(x - x_i)\rangle$$

where, however, we also approximate the continuous moment matrix $M(x)$ by a respective particle sum

$$M(x) := \sum_{i=0}^{N} H(x - x_i)H^T(x - x_i)\phi_a(x - x_i).$$

Thus, we can view this discrete RKPM as a constructive approach to obtain compactly supported shape functions Ψ_i with $\text{supp}(\Psi_i) = \text{supp}(\phi_a(\cdot - x_i))$ from scattered independent points $x_i \in \mathcal{X}_N$ only.

Meshfree Methods: Generalized Finite Differences

In GFDM we do not construct approximation spaces but rather direct approximations of derivatives and differential operators. Starting point is the truncated Taylor series of a suitable function u centered at x and evaluated at a particle/ data site x_i

$$u(x_i) = f_i := \sum_{|\alpha|=0}^{n} \frac{(-1)^\alpha}{\alpha!}(x - x_i)^\alpha \partial^\alpha u(x).$$

Obviously, this expansion links all derivatives at x to the function value at x_i. Thus, by using m evalutions at neighboring particles/ data sites x_i of this expansion centered at the same x, we obtain a linear system

$$\begin{pmatrix} f_{i_1} \\ \vdots \\ f_{i_m} \end{pmatrix} = \begin{pmatrix} 1 & (x - x_{i_1})^{\alpha_1} & \cdots & (x - x_{i_1})^{\alpha_n} \\ & & & \\ 1 & \vdots & \ddots & \vdots \\ 1 & (x - x_{i_m})^{\alpha_1} & \cdots & (x - x_{i_m})^{\alpha_n} \end{pmatrix} \begin{pmatrix} u(x) \\ \frac{(-1)^{\alpha_1}}{\alpha_1!}\partial^{\alpha_1} u(x) \\ \vdots \\ \frac{(-1)^{\alpha_n}}{\alpha_n!}\partial^{\alpha_n} u(x) \end{pmatrix}. \tag{35}$$

Meshfree Methods: Generalized Finite Differences

Introducing the short-hand notation

$$f = R(x)J_\alpha u_\partial(x) = (H^T(x - x_i))J_\alpha u_\partial(x)$$

for this linear system

$$\begin{pmatrix} f_{i_1} \\ \vdots \\ f_{i_m} \end{pmatrix} = \begin{pmatrix} 1 & (x - x_{i_1})^{\alpha_1} & \cdots & (x - x_{i_1})^{\alpha_n} \\ 1 & \vdots & \ddots & \vdots \\ 1 & (x - x_{i_m})^{\alpha_1} & \cdots & (x - x_{i_m})^{\alpha_n} \end{pmatrix} \begin{pmatrix} u(x) \\ \frac{(-1)^{\alpha_1}}{\alpha_1!}\partial^{\alpha_1}u(x) \\ \vdots \\ \frac{(-1)^{\alpha_n}}{\alpha_n!}\partial^{\alpha_n}u(x) \end{pmatrix}$$

which is in general rectangular with $m \geq n$ to ensure solvability, i.e. the number of particles considered at any location x must be larger than the number of derivatives.
Thus, large neighborhoods have to be consider. To limit the influence of data sites x_i that are further away from the center x than others we introduce a weight function w_a with support size a and consider the normal equations to obtain a uniquely solvable quadratic linear system

$$R^T(x)W(x)f = R^T(x)W(x)R(x)J_\alpha u_\partial(x) =: T(x)J_\alpha u_\partial(x)$$

where $W(x) = \mathrm{diag}(w_a(x - x_i))$.

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Meshfree Methods: Generalized Finite Differences

Solving this linear system

$$R^T(x)W(x)f = R^T(x)W(x)R(x)J_\alpha u_\partial(x) =: T(x)J_\alpha u_\partial(x)$$

for the unknown derivatives $u_\partial(x)$ yields

$$u_\partial(x) = J_\alpha^{-1}T^{-1}(x)R^T(x)W(x)f = \sum_{x_i \in \mathcal{N}(x)} J_\alpha^{-1}T^{-1}(x)H(x-x_i)w_a(x-x_i)f_i.$$

Note that the first entry of the vector $u_\partial(x)$ is in fact the function value $u(x)$ similarly the first entry in J_α is 1 such that we have the scalar equation

$$u(x) = \sum_{x_i \in \mathcal{N}(x)} T^{-1}(x)H(x-x_i)w_a(x-x_i)f_i.$$

which is identical to the MLS approximation of the function value.

Discretization of PDEs

$$\begin{aligned} \nabla \cdot \sigma(u) + b &= 0 && \text{in } \Omega \\ \sigma(u) \cdot n &= h && \text{on } T \subset \partial\Omega \\ u &= g && \text{on } \partial\Omega \setminus T \end{aligned}$$

with $\sigma(u) = C\epsilon(u) = \frac{1}{2} C(\nabla u + (\nabla u)^T)$

Strong Form Collocation

$$\begin{aligned} \nabla \cdot \sigma(u)(x_i) + b(x_i) &= 0 && \text{for all } x_i \in \mathcal{Y}_M \cap \Omega \\ \sigma(u)(x_i) \cdot n(x_i) &= h(x_i) && \text{for all } x_i \in \mathcal{Y}_M \cap T \\ u(x_i) &= g(x_i) && \text{for all } x_i \in \mathcal{Y}_M \cap (\partial\Omega \setminus T) \end{aligned}$$

- Source points $\mathcal{Y}_M$ may be different from data points $\mathcal{X}_N$
- Overdetermined systems, normal equations, conditioning, ...
- Densities of $\mathcal{Y}_M$ and $\mathcal{X}_N$, support size of kernel
- Density of system matrix
- Second order derivatives
- Existance of source points on boundary segments

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