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 across mesh faces to ensure regularity.
- Mesh cells and faces provide integration sub-domains.

Meshfree Methods must use much different construction of approximation spaces!
## 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.
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!
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).
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

Mesh Free Solver

Uses the Smooth Particle Hydrodynamics Method (SPH)

- Lagrange particle method (particles are imbedded in material)
- No mesh distortion/tangling problems

Provides most accurate solution for modeling fracture and fragmentation of brittle materials

Applied very successfully to problems involving impacts into...

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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.
Scattered Data Approximation: Least Squares

The reconstruction of an unknown function $u : \Omega \subset \mathbb{R}^D \rightarrow \mathbb{R}$ 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 $\phi_j$ 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

\[
J_{\text{LS}}(\pi) := \sum_{i=1}^{N} (f_i - \pi(x_i))^2
\]

over all polynomials \( \pi \in \mathcal{P}_k(\Omega) \).
Scattered Data Approximation: Least Squares

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

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

(2)

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

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

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

$$\hat{f}_{LS} := \left(\sum_{i=1}^{N} f_i p_q(x_i)\right)_{q=1}^{d^\mathcal{P}_k}.$$
Scattered Data Approximation: Least Squares

The minimizing polynomial $\pi_{\text{LS}}$ is then simply

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

Note that the approximation $\pi_{\text{LS}}$ does in general not align with the data, i.e. $\pi_{\text{LS}}(x_i) \neq f_i$.

We define the least squares operator $A_{\text{LS}}$ which maps a data vector $\tilde{f} = (f_i)_{i=1}^N$ to its associated polynomial $\pi_{\text{LS}} \in \mathcal{P}_k$ by $A_{\text{LS}} \tilde{f} = \pi_{\text{LS}}$. Note that the operator $A_{\text{LS}}$ 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

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

holds.
Scattered Data Approximation: Least Squares

To assess the quality of the least squares approach let us consider the approximation of a smooth function \( u \in C^r(\Omega) \). Given a set of sampling points \( \mathcal{X}_N \), we define the data values \( f_i = u(x_i) \). Obviously, the error \( u(x) - \pi_{LS}(x) \) with \( \pi_{LS} = A_{LS} \tilde{f} \in \mathcal{P}_k \) 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 \( \pi_{LS} \) 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 $W$ often referred to as window function or weight function and the pointwise moving least squares energy

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

Note that (3) 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 (3) to obtain

$$J_{\text{MLS}}(\pi)(x) = \sum_{i=1}^{N} W(x - x_i)(f_i - \pi(x_i))^2 = \sum_{x_i \in \mathcal{N}(x), W(x-x_i) > 0} W(x - x_i)(f_i - \pi(x_i))^2. \quad (4)$$

With the convention $\omega_i := \text{supp}^\circ W(\cdot - x_i)$ and Definition ?? of a neighborhood $\mathcal{N}(x) \subset \mathcal{X}_N$ of an arbitrary point $x \in \Omega$, compare (3), we attain

$$J_{\text{MLS}}(\pi)(x) = \sum_{x_i \in \mathcal{N}(x)} W(x - x_i)(f_i - \pi(x_i))^2. \quad (4)$$
Definition

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

$$N_i := \{x_k \in \mathcal{X}_N | x_k \in \omega_i\}$$

and

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

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

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

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

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

(8)
Scattered Data Approximation: Moving Least Squares

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

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

The linear system (9) is uniquely solvable if the neighborhood $\mathcal{N}(x)$ is $\mathcal{P}_k$-unisolvent and we can define the moving least squares operator

$$\left( A_{\text{MLS}} \hat{f} \right)(x) = \pi_{\text{MLS}}(x) = \sum_{q=1}^{d_{\mathcal{P}^k}} u_{x,q} p_q(x). \quad (9)$$

Note that in the classical least squares approximation we need to solve a single linear system (9) only to obtain the approximation $\pi_{\text{LS}}$ on the complete domain $\Omega$. The resulting polynomial $\pi_{\text{LS}}$ can then be evaluated directly for all $x \in \Omega$, i.e., the coefficients $\tilde{u}_q$ of $\pi_{\text{LS}}$ 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 $\pi_{\text{MLS}}$ which can then be evaluated at $x$ only, i.e., the coefficients $\tilde{u}_x$ of $\pi_{\text{MLS}}$ depend on $x$, compare (9). Let us summarize our findings so-far in the following theorem which generalizes the above setting slightly.
Let the set of points $\mathcal{X}_N = \{x_i \mid i = 1, \ldots, N\}$, associated weight functions $W_i \in C(\mathbb{R}^D, \mathbb{R}_0^+)$ such that $(\text{supp}(W_i))^\circ = \omega_i$ 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

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

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

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

(10)

is well-defined.
Proof of Theorem ??

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

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

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

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

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

$$\pi_{\text{MLS}}(x^*) = \sum_{q=1}^{d^{\mathcal{P}_k}} u_{x^*,q} p_q(x^*) \quad (11)$$

we obtain

$$\sum_{x_i \in \mathcal{N}(x^*)} \left( f_i - \sum_{q=1}^{d^{\mathcal{P}_k}} u_{x^*,q} p_q(x_i) \right) W_i(x^*)p_r(x_i) = 0. \quad \text{for all } r = 1, \ldots, d^{\mathcal{P}_k} \quad (12)$$
This is equivalent to the matrix equation

\[ G_{\text{MLS}}(x^*) \tilde{u}_{x^*} = \hat{f}_{\text{MLS}}(x^*) \]  

(13)

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

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

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

\[
\gamma \cdot G_{\text{MLS}}(x^*) \gamma = \sum_{x_i \in \mathcal{N}(x)} W_i(x^*) \left( \sum_{q=1}^{d^P_k} \gamma_q p_q(x_i) \right)^2.
\]
From the non-negativity of $W_i$ follows $\gamma \cdot G_{\text{MLS}}(x^\ast)\gamma \geq 0$ and hence $G_{\text{MLS}}$ is positive semi-definite. Now let us assume that there is a particular $\gamma \neq 0$ such that $\gamma \cdot G_{\text{MLS}}(x^\ast)\gamma = 0$. Since $x_i \in \mathcal{N}(x^\ast)$ we have $x^\ast \in \omega_i = (\text{supp}(W_i))^\circ$ and due to the smoothness of the weight functions $W_i$ we have $W_i(x^\ast) > 0$. Therefore, $\gamma_qp_q(x_i) = 0$ for all $q = 1, \ldots, d\mathcal{P}^k$ and $x_i \in \mathcal{N}(x^\ast)$. The unisolvence of $\mathcal{N}(x^\ast)$ implies that $\gamma = 0$ which contradicts the assumption $\gamma \neq 0$ and hence we conclude that $G_{\text{MLS}}(x^\ast)$ is positive definite.

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

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

\[
\left( A_{\text{MLS}} \tilde{f} \right)(x) = \sum_{i=1}^{N} f_i \phi_i(x)
\]  \hspace{1cm} (14)

holds and the basis functions \( \phi_i \) are given by

\[
\phi_i(x) := W_i(x) \sum_{q=1}^{d_P^k} \alpha_{x,q} p_q(x_i)
\]  \hspace{1cm} (15)

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

\[
G_{\text{MLS}}(x) \alpha_x = p(x) = \left( p_q(x) \right)_{q=1}^{d_P^k}.
\]  \hspace{1cm} (16)
Proof of Corollary ??

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

\[
\left( A_{\text{MLS}} \tilde{f} \right)(x^*) = \sum_{q=1}^{d^P} \tilde{u}_{x^*,q} p_q(x^*).
\]

With the equivalence (??) this yields

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

Rearranging the sums we obtain

\[
\left( A_{\text{MLS}} \tilde{f} \right)(x^*) = \sum_{r=1}^{d^P} \alpha_{x^*,r} \sum_{x_i \in \mathcal{N}(x^*)} W_i(x^*) \sum_{q=1}^{d^P} u_{x^*,q} p_q(x_i) p_r(x_i). \quad (17)
\]
Plugging (??) into (??) gives

\[
\left( A_{\text{MLS}} \hat{f} \right)(x^*) = \sum_{r=1}^{d_P^k} \alpha_{x^*,r} \sum_{x_i \in \mathcal{N}(x^*)} W_i(x^*) f_i p_r(x_i) = \sum_{x_i \in \mathcal{N}(x^*)} f_i W_i(x^*) \sum_{r=1}^{d_P^k} \alpha_{x^*,r} p_r(x_i)
\]

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 \( \alpha_x \) of (??) is independent of the particle \( x_i \) and hence \( \alpha_x \) is identical for all particles \( x_i \in \mathcal{N}(x) \); i.e., for all respective basis functions \( \phi_i \). Thus the evaluation of a single basis function \( \phi_i \) at a particular point \( x \in \Omega \) is of similar complexity as the simultaneous evaluation of all non-vanishing basis functions \( \phi_j \) in \( x \in \Omega \).

Due to (??) we can view the moving least squares technique as a constructive approach to obtain compactly supported shape functions \( \phi_i \) 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 $W_i \in C^r(\mathbb{R}^D)$ with $r > 0$ for all $i = 1, \ldots, N$. Then, there holds $\phi_i \in C^r(\mathbb{R}^D)$ for the basis functions $\phi_i$ 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

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

with $\phi_i$ defined in (??), $E_{\chi_N} : C(\Omega) \to \mathbb{R}^N$ denotes the point evaluation, i.e. $E_{\chi_N}(u) = (u(x_i))_{i=1}^N$, reproduces all polynomials $\pi \in P_k(\Omega)$, i.e.

$$A_{\text{MLS}} E_{\chi_N} |_{P_k(\Omega)} = I, \quad A_{\text{MLS}} E_{\chi_N}(\pi) = \pi \quad \text{for all} \ \pi \in P_k(\Omega). \quad (18)$$
Recall the representation (??)

$$\left( \text{AMLS}\, E_{\chi_N}(\pi) \right)(x) = \sum_{i=1}^{N} \pi(x_i) \phi_i(x).$$

The polynomial $\pi$ 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

$$\left( \text{AMLS}\, E_{\chi_N}(\pi) \right)(x) = \sum_{i=1}^{N} \sum_{q=1}^{d_{\mathcal{P}_k}} \gamma_q p_q(x_i) \phi(x) = \sum_{i=1}^{N} \sum_{q=1}^{d_{\mathcal{P}_k}} \gamma_q p_q(x_i) W_i(x) \sum_{r=1}^{d_{\mathcal{P}_k}} \alpha_{x,r} p_r(x_i).$$

Rearranging the sums, we obtain

$$\left( \text{AMLS}\, E_{\chi_N}(\pi) \right)(x) = \sum_{q=1}^{d_{\mathcal{P}_k}} \sum_{r=1}^{d_{\mathcal{P}_k}} \sum_{i=1}^{N} \gamma_q p_q(x_i) W_i(x) p_r(x_i) \alpha_{x,r} = \gamma \cdot G_{\text{MLS}}(x) \alpha_x.$$

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

$$\left( \text{AMLS}\, E_{\chi_N}(\pi) \right)(x) = \gamma \cdot p(x) = \sum_{q=1}^{d_{\mathcal{P}_k}} \gamma_q p_q(x) = \pi(x) \text{ for all } x \in \Omega.$$
An immediate consequence of this lemma is that the basis functions $\phi_i$ 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

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

Yet, the basis functions $\phi_i$ 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 $\mathcal{W}_i$ for $i = 1, \ldots, N$. Thus, the selection of appropriate supports $\omega_i$ 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

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

In this case (??) reduces to

$$\phi_i(x) = W_i(x)\alpha_{x,0}, \quad \text{with } G_{\text{MLS}0,0}\alpha_{x,0} = 1$$  \hspace{1cm} (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 \( \phi_i \) of (??) are known implicitly only via (??). Due to the compact support of the weights \( W_i \) and the observation that \( N(x) \subset C_i \) for all \( x \in \omega_i \), compare (??) and Definition ??, we can rewrite the moving least squares function for \( k = 0 \) as

\[ \phi_i(x) = \frac{W_i(x)}{S_i(x)}, \quad \text{with } S_i(x) := \sum_{\omega_j \in C_i} W_j(x). \] (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 $G_{\text{MLS}}(x^*)$ 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 $T_{x^*} : \mathbb{R}^D \rightarrow \mathbb{R}^D$ depending on the point of evaluation $x^*$ of a fixed basis $\{\hat{p}_q | q = 1, \ldots, d^P_k\}$, i.e.,

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

The approximation (??) and hence the representation (??) and the basis functions (??) are unchanged, but the respective linear systems $G_{\text{MLS}}$ 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 $\pi_{\text{MLS}}(x^*)$ is obtained by the solution of the linear system (??) with the system matrix

$$G_{\text{MLS}}(x^*) = (G_{\text{MLS}}(x^*))_{q,r} \in \mathbb{R}^{dP_k \times dP_k}$$

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

and the right-hand side

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

The basis functions $\phi_i$ are given by

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

(23)

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

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

(24)
The advantage of (??) over (??) in computations is that the condition number of the system matrix $G_{\text{MLS}}(x^*)$ can be controlled via the parameter $\rho_{x^*}$ 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 $V_{\text{MLS}} := \text{span}\langle \phi_i \rangle$ 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 $\omega_i$; 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

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

as weight functions. Then, (25) becomes

$$\phi_i(x^*) := \mathcal{W}\left(\frac{x^* - x_i}{\rho_i}\right) \sum_{q=1}^{q \in \mathcal{P}^k} \alpha_{x^*,q} \hat{p}_q\left(\frac{x^* - x_i}{\rho_{x^*}}\right).$$  \hspace{1cm} (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 $\omega_i$. 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 $\Omega$ into $\Omega_l = \{x^* \in \Omega \mid k(x^*) = k_l\}$ 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 $\phi_i$. 

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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.
Meshfree kernel approaches are based on integral convolution

\[ u_K(x) := \int_{\Omega} \phi_a(x - y)u(y) \, dy \]  \hspace{1cm} (26)

where \( \phi_a \) 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

\[ u_K(x) = u(x) \hspace{1cm} \text{for all } x. \]

In all other cases \((\Omega)\) 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 \((26)\) yields

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

\[ m_0(x) = 1, \quad m_i(x) = 0 \quad \text{for all } 0 < i \]

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

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

to enforce just \( n \)th order polynomial completeness.

**Kernel selection**

Obviously, the reproducing conditions are constraints on the choice of the kernel \( \phi_a \).
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

\[ u_R(x) := \int_{\Omega} \phi_a(x; x - y) u(y) \, dy \]  \hspace{1cm} (27)

where the corrected kernel is given by

\[ \bar{\phi}_a(x; x - y) := C(x; x - y) \phi_a(x - y) = \sum_{i=0}^{n} (x - y)^i b_i(x) \phi_a(x - y). \]  \hspace{1cm} (28)

The correction function is often written as

\[ C(x; x - y) = \langle H(x - y), b(x) \rangle \]  \hspace{1cm} (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

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

such that the reproducing conditions again are

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

Plugging the explicit form of the corrected kernel into the definition of (30) 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

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

we can rewrite the reproducing conditions for the corrected kernel as

$$M(x)b(x) = H(0) \quad (32)$$

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

\[
u_R(x) := \int_{\Omega} \tilde{\phi}_a(x; x - y) u(y) \, dy
= \int_{\Omega} \langle H(x - y), M^{-1}(x)H(0) \rangle \phi_a(x - y) u(y) \, dy
= \langle \int_{\Omega} H(x - y) \phi_a(x - y) u(y) \, dy, \big( \int_{\Omega} H(x - y) H^T(x - y) \phi_a(x - y) \, dy \big)^{-1} H(0) \rangle \tag{34}
\]

using the data function \( u \), the original kernel \( \phi_a \) 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.
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 $\psi_i$ with $\text{supp}(\psi_i) = \text{supp}(\phi_a(\cdot - x_i))$ from scattered independent points $x_i \in \mathcal{X}_N$ only.

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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 $m$ evaluations at neighboring particles/data sites $x_i$ of this expansion centered at the same $x$, we obtain a linear system

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

(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

\[
\begin{pmatrix}
  f_{i1} \\
  \vdots \\
  f_{im}
\end{pmatrix} =
\begin{pmatrix}
  1 & (x - x_{i1})^{\alpha_1} & \cdots & (x - x_{i1})^{\alpha_n} \\
  1 & \vdots & \ddots & \vdots \\
  1 & (x - x_{im})^{\alpha_1} & \cdots & (x - x_{im})^{\alpha_n}
\end{pmatrix}
\begin{pmatrix}
  \frac{u(x)}{\alpha_1!} \partial^{\alpha_1} u(x) \\
  \vdots \\
  \frac{(-1)^{\alpha_n}}{\alpha_n!} \partial^{\alpha_n} u(x)
\end{pmatrix}
\]

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 considered. 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 \( W(x) = \text{diag}(w_a(x - x_i)) \).
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

\[ u_\partial(x) = J^{-1}_\alpha T^{-1}(x) R^T(x) W(x) f = \sum_{x_i \in N(x)} J^{-1}_\alpha T^{-1}(x) H(x - x_i) w_a(x - x_i) f_i. \]

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

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

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

\[ \nabla \cdot \sigma(u) + b = 0 \quad \text{in } \Omega \]
\[ \sigma(u) \cdot n = h \quad \text{on } T \subset \partial \Omega \]
\[ u = g \quad \text{on } \partial \Omega \setminus T \]

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

**Strong Form Collocation**

\[ \nabla \cdot \sigma(u)(x_i) + b(x_i) = 0 \quad \text{for all } x_i \in \mathcal{Y}_M \cap \Omega \]
\[ \sigma(u)(x_i) \cdot n(x_i) = h(x_i) \quad \text{for all } x_i \in \mathcal{Y}_M \cap T \]
\[ u(x_i) = g(x_i) \quad \text{for all } x_i \in \mathcal{Y}_M \cap (\partial \Omega \setminus T) \]

- 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
- Existence of source points on boundary segments