

Computational Hydraulics
Professor Anirban Dhar
Department of Civil Engineering
Indian Institute of Technology Kharagpur
Lecture 22
Mesh - Free Method: Moving Least Squares Method

Welcome to lecture number 22 of the course computational hydraulics. We are in module 2, numerical methods. And this is unit 18, mesh free method, moving least squares method. Learning objective, to discretize ordinary differential equation using moving least squares method.

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Moving Least Squares Method
Problem Definition
Discretization
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Learning Objective

- To discretize ODE using [Moving Least Squares Method](#).

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What is this moving least squares? In our polynomial interpolation we have represented our function in terms of $P^T A$. And depending on the basis we have different kind of approximations. And we can utilize the A values which we can get from the inversion of the polynomial matrix based on available function values for construction of weight functions.

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Moving Least Squares Method

Function $\phi(x)$ at a point (x) can be approximated as,

$$\phi^h(x) = \sum_{j=0}^m p_j(x)a_j(x) = \mathbf{p}^T(x)\mathbf{a}(x)$$

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Now we can use this first step and then again we can use our basis for moving least squares.

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Moving Least Squares Method

Function $\phi(x)$ at a point (x) can be approximated as,

$$\phi^h(x) = \sum_{j=0}^m p_j(x)a_j(x) = \mathbf{p}^T(x)\mathbf{a}(x)$$

The complete polynomial basis of order m can be written in a general form (Liu and Gu, 2005).

$$\mathbf{p}^T(x) = \{1 \ x \ x^2 \ \dots \ x^m\}$$
$$\mathbf{p}^T(x, y) = \{1 \ x \ y \ x^2 \ xy \ y^2 \ \dots \ x^m \ \dots \ y^m\}$$

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Now in local domain for arbitrary point x , we can have this $\phi(x)$, x_i where x_i is for this polynomial and Ax is our original vector, A vector. Now in this case MLS approximation or moving least squares method approximation is based on minimization of weighted residual for variable Ax . So Ax is variable. Previously we have got the Ax value based on inversion of matrix. Now we can represent it as minimization problem.

So in this case we have a definite structure for this ω or weight function for minimization. This h is the approximated value based on polynomial approximation. And x_i

is the original value for that point. So if we consider any arbitrary point, so obviously if this is our original function value and this is constructed polynomial, so obviously we will try to reduce the difference between these two values.

Now in this minimization problem the first condition is that if we differentiate this J which is the objective function for this minimization problem with respect to variables, the first order derivative should be zero.

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Moving Least Squares Method

Weighted Residual

In local domain for arbitrary point x ,

$$\phi^h(x, x_i) = \mathbf{p}^T(x_i)\mathbf{a}(x)$$

MLS approximation is based on minimization of weighted residual for variable $\mathbf{a}(x)$. (Liu and Gu, 2005)

Weighted Residual can be calculated as,

$$J = \sum_{i=1}^{N_n} \omega(x - x_i) [\phi^h(x, x_i) - \phi(x_i)]^2$$

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So in this case if we replace our original form from this equation then we can write this equation as $\mathbf{P}^T \mathbf{x}_i \mathbf{A} \mathbf{x}$. And this is our again function value for $\phi^h(x_i)$. And given this $\omega(x - x_i)$ which is given function for this particular problem.

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Weighted Residual

In local domain for arbitrary point \mathbf{x} ,

$$\phi^h(\mathbf{x}, \mathbf{x}_i) = \mathbf{p}^T(\mathbf{x}_i)\mathbf{a}(\mathbf{x})$$

MLS approximation is based on minimization of weighted residual for variable $\mathbf{a}(\mathbf{x})$. (Liu and Gu, 2005)
Weighted Residual can be calculated as,

$$J = \sum_{i=1}^{N_n} \omega(\mathbf{x} - \mathbf{x}_i) [\phi^h(\mathbf{x}, \mathbf{x}_i) - \phi(\mathbf{x}_i)]^2$$

or,

$$J = \sum_{i=1}^{N_n} \omega(\mathbf{x} - \mathbf{x}_i) \underbrace{[\mathbf{p}^T(\mathbf{x}_i)\mathbf{a}(\mathbf{x}) - \phi(\mathbf{x}_i)]^2}$$

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Now minimization condition, J should be differentiated with respect to \mathbf{A} . \mathbf{A} means for all \mathbf{A} values. Now in this case if we differentiate with respect to A_1, A_2 , then we will get system of equations. Because individually if we equate with zero so we will get number of terms for this particular derivative.

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Weighted Residual

Minimization condition requires,

$$\frac{\partial J}{\partial \mathbf{a}} = 0$$

Thus, linear system of equations can be written as,

$$\mathbf{A}(\mathbf{x})\mathbf{a}(\mathbf{x}) = \mathbf{B}(\mathbf{x})\phi_n$$

$\frac{\partial J}{\partial a_1} = 0$
 $\frac{\partial J}{\partial a_2} = 0$

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So this linear system is $\mathbf{A}\mathbf{x} = \mathbf{B}$ where your \mathbf{A} is again represented in terms of $\omega(\mathbf{x} - \mathbf{x}_i)\mathbf{p}^T(\mathbf{x}_i)$ and \mathbf{B} on the right hand side, this is B_1, B_2 to B_N . N is again number of points in the support domain. And B_i is our $\omega(\mathbf{x} - \mathbf{x}_i)\phi(\mathbf{x}_i)$. So this is for a one particular \mathbf{B} . That means B_i if we write B_1 , so

obviously in this case this is first point x_1 , P_1 , like that. But P is again vector in this case.

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Now in this case this ϕ is column vector. So we have ϕ_1, ϕ_2 to ϕ_{N_s} in this case.

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So with this we can calculate A . So we can take inverse of A into B . And ϕ_s is the value which is available in the neighborhood of the given point. So in this case we can represent this ω_i . This is x into ϕ_i number of points in the support domain. And ω_i , this can be represented as $P^T A B_i$. Because we are considering only one i in this case. So the matrix form in this case is our $W^T x, \phi_s, w_1$ to w_{N_s} .

That means weight for all the points available in the support domain. So we can utilize this concept in case of our one dimensional problem.

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Discretization

Weight Calculation

$\mathbf{a}(\mathbf{x})$ can be calculated as,

$$\mathbf{a}(\mathbf{x}) = \mathbf{A}^{-1}(\mathbf{x})\mathbf{B}(\mathbf{x})\phi_s$$

$$\phi^h(\mathbf{x}) = \sum_{i=1}^{N_n} w_i(\mathbf{x})\phi_i$$

The shape functions can be represented as

$$w_i(\mathbf{x}) = \sum_{j=0}^m p_j(\mathbf{x})(\mathbf{A}^{-1}(\mathbf{x})\mathbf{B}(\mathbf{x}))_{ji} = \mathbf{p}^T(\mathbf{x})\mathbf{A}^{-1}(\mathbf{x})\mathbf{B}_i$$

The matrix form can be written as,

$$\phi^h(\mathbf{x}) = \mathbf{W}^T(\mathbf{x})\phi_s$$

$$\mathbf{W}^T(\mathbf{x}) = \{w_1(\mathbf{x}) \ w_2(\mathbf{x}) \ \dots \ w_{N_n}(\mathbf{x})\}$$

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But one problem is there. The problem is associated with the derivative calculation of \mathbf{W} . In previous case of polynomial interpolation, the calculation of derivative is simple. But in this case this is somewhat different. So let us represent this \mathbf{W} transpose comma \mathbf{x} , \mathbf{P} transpose \mathbf{x} , \mathbf{A} inverse \mathbf{B} . And we need to differentiate this whole thing with respect to \mathbf{x} .

So let us reduce this full expression into two parts. That is first term, let us write it as γ transpose. That means γ transpose equals to \mathbf{P} transpose \mathbf{A} inverse. Now if we take transpose of this one, so obviously this will be \mathbf{A} inverse and this is \mathbf{P} .

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Discretization

Derivative Computation

Derivative of the function can be computed as,

$$\underline{W}_{,x}^T = \left[\underline{p}^T(x) \underline{A}^{-1} \underline{B} \right]_{,x}$$

$$= [\underline{\gamma}^T \underline{B}(x)]_{,x}$$

$\gamma^T = p^T A^{-1}$
 $\gamma^T = A^{-1} p$

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In this case we will have gamma and there will be change of side. So we can write this A gamma equals to P. So this is our form.

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Discretization

Derivative Computation

Derivative of the function can be computed as,

$$\underline{W}_{,x}^T = \left[\underline{p}^T(x) \underline{A}^{-1} \underline{B} \right]_{,x}$$

$$= [\underline{\gamma}^T \underline{B}(x)]_{,x}$$

where

$$\underline{\gamma}^T = \underline{p}^T \underline{A}^{-1}$$

Applying transpose and differentiating w.r.t. x

$$\underline{A} \underline{\gamma} = \underline{p}$$

$$\underline{A} \underline{\gamma}_{,x} = \underline{p}_{,x} - \underline{A}_{,x} \underline{\gamma}$$

$$\underline{\gamma}_{,x} = \underline{A}^{-1} (\underline{p}_{,x} - \underline{A}_{,x} \underline{\gamma})$$

$\gamma^T = p^T A^{-1}$
 $\gamma = A^{-1} p$
 $A\gamma = p$

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Now we know that how to calculate derivative of this. So first part this is A gamma x and this is p comma x. This is represented as A comma x gamma y. So this is nothing but full derivative. And we can write it in two parts. Plus A comma x into gamma. And we can directly equate it with P comma x and we can get this expression.

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Discretization

Derivative Computation

Derivative of the function can be computed as,

$$\underline{W}_{,x}^T = \left[\underline{p}^T(x) \underline{A}^{-1} \underline{B} \right]_{,x}$$

$$= [\underline{\gamma}^T \underline{B}(x)]_{,x}$$

where

$$\underline{\gamma}^T = \underline{p}^T \underline{A}^{-1}$$

Applying transpose and differentiating w.r.t. x

$$\underline{A} \underline{\gamma} = \underline{p}$$

$$\underline{A} \underline{\gamma}_{,x} = \underline{p}_{,x} - \underline{A}_{,x} \underline{\gamma}$$

$$\underline{\gamma}_{,x} = \underline{A}^{-1} (\underline{p}_{,x} - \underline{A}_{,x} \underline{\gamma})$$

Handwritten notes:

$$\underline{\gamma}^T = \underline{p}^T \underline{A}^{-1}$$

$$\underline{\gamma} = \underline{A}^{-1} \underline{p}$$

$$\underline{A} \underline{\gamma} = \underline{p}$$

$$\underline{A} \underline{\gamma}_{,x} = \underline{p}_{,x} - \underline{A}_{,x} \underline{\gamma}$$

$$(\underline{A} \underline{\gamma})_{,x}$$

$$\Rightarrow \underline{A} \underline{\gamma}_{,x} + \underline{A}_{,x} \underline{\gamma} = \underline{p}_{,x}$$

Now gamma x or first derivative of gamma can be directly calculated with A inverse, this whole thing, P comma x minus A comma x into gamma. So this is all about first order derivative of gamma, that is gamma comma x.

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Discretization

Derivative Computation

Derivative of the function can be computed as,

$$\underline{W}_{,x}^T = \left[\underline{p}^T(x) \underline{A}^{-1} \underline{B} \right]_{,x}$$

$$= [\underline{\gamma}^T \underline{B}(x)]_{,x}$$

where

$$\underline{\gamma}^T = \underline{p}^T \underline{A}^{-1}$$

Applying transpose and differentiating w.r.t. x

$$\underline{A} \underline{\gamma} = \underline{p}$$

$$\underline{A} \underline{\gamma}_{,x} = \underline{p}_{,x} - \underline{A}_{,x} \underline{\gamma}$$

$$\underline{\gamma}_{,x} = \underline{A}^{-1} (\underline{p}_{,x} - \underline{A}_{,x} \underline{\gamma})$$

Handwritten notes:

$$\underline{\gamma}^T = \underline{p}^T \underline{A}^{-1}$$

$$\underline{\gamma} = \underline{A}^{-1} \underline{p}$$

$$\underline{A} \underline{\gamma} = \underline{p}$$

$$\underline{A} \underline{\gamma}_{,x} = \underline{p}_{,x} - \underline{A}_{,x} \underline{\gamma}$$

$$(\underline{A} \underline{\gamma})_{,x}$$

$$\Rightarrow \underline{A} \underline{\gamma}_{,x} + \underline{A}_{,x} \underline{\gamma} = \underline{p}_{,x}$$

$$\underline{\gamma}_{,x} = \underline{A}^{-1} (\underline{p}_{,x} - \underline{A}_{,x} \underline{\gamma})$$

Now similarly we can write the same thing. So if we have A gamma comma x equals to P comma x, A comma x into gamma. Now in this case we can again differentiate that means if we have A gamma twice, differentiate the same thing. So this is A comma x into gamma plus A gamma comma x. And this whole thing is again comma x. This comma is our first derivative.

So this is $A \gamma_{,xx}$, this is $\gamma_{,xx} + A \gamma_{,xx}$ plus, from the second term we get $A \gamma_{,xx}$ plus $A \gamma_{,xx}$ equals to $P_{,xx}$. So from this one we can simplify $A \gamma_{,xx}$ plus $2 A \gamma_{,xx}$ plus $A \gamma_{,xx}$ equals to $P_{,xx}$. So from this one we can directly calculate the second order derivative of $\gamma_{,xx}$, like this.

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Derivative Computation

$$A\gamma_{,xx} = p_{,xx} - A_{,xx}\gamma$$

Similarly,

$$A\gamma_{,xxx} + 2A_{,xx}\gamma_{,xx} + A_{,xxx}\gamma = p_{,xxx}$$

$$\gamma_{,xxx} = A^{-1}(p_{,xxx} - 2A_{,xx}\gamma_{,xx} - A_{,xxx}\gamma)$$

$$(A\gamma)_{,xx} = p_{,xx}$$

$$\text{or } (A_{,xx}\gamma + A\gamma_{,xx})_{,x} = p_{,xx}$$

$$\text{or } A_{,xxx}\gamma + A_{,xx}\gamma_{,xx} + A_{,xx}\gamma_{,xx} + A\gamma_{,xxx} = p_{,xx}$$

$$\text{or } A_{,xxx}\gamma + 2A_{,xx}\gamma_{,xx} + A\gamma_{,xxx} = p_{,xx}$$

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So this is all about calculation by indirect method. We are not directly differentiating the W with individual terms. We have transformed it with a new variable γ . And we are calculating the derivative of that function. So first and second order derivatives can be calculated like this. So now the full thing is $\gamma_{,xx}$. This is our first derivative and this is second derivative.

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Discretization

Derivative Computation

Similarly,

$$\mathbf{A}\gamma_{,xxx} + 2\mathbf{A}_{,x}\gamma_{,xx} + \mathbf{A}_{,xx}\gamma = \mathbf{p}_{,xxx}$$

$$\gamma_{,xx} = \mathbf{A}^{-1}(\mathbf{p}_{,xxx} - 2\mathbf{A}_{,x}\gamma_{,xx} - \mathbf{A}_{,xx}\gamma)$$

The first and second order derivatives can be calculated as,

$$\mathbf{W}_{,x}^T = \underline{\underline{\gamma_{,x}^T \mathbf{B} + \gamma^T \mathbf{B}_{,x}}}$$

$$\mathbf{W}_{,xxx}^T = \underline{\underline{\gamma_{,xxx}^T \mathbf{B} + 2\gamma_{,xx}^T \mathbf{B}_{,x} + \gamma^T \mathbf{B}_{,xxx}}}$$

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We already know the value of gamma comma x and gamma comma xx. We can utilize that value for calculation of first and second order derivative of our weight functions.

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Discretization

Derivative Computation

Similarly,

$$\mathbf{A}\gamma_{,xxx} + 2\mathbf{A}_{,x}\gamma_{,xx} + \mathbf{A}_{,xx}\gamma = \mathbf{p}_{,xxx}$$

$$\gamma_{,xx} = \mathbf{A}^{-1}(\mathbf{p}_{,xxx} - 2\mathbf{A}_{,x}\gamma_{,xx} - \mathbf{A}_{,xx}\gamma)$$

The first and second order derivatives can be calculated as,

$$\left\{ \begin{array}{l} \mathbf{W}_{,x}^T = \underline{\underline{\gamma_{,x}^T \mathbf{B} + \gamma^T \mathbf{B}_{,x}}} \\ \mathbf{W}_{,xxx}^T = \underline{\underline{\gamma_{,xxx}^T \mathbf{B} + 2\gamma_{,xx}^T \mathbf{B}_{,x} + \gamma^T \mathbf{B}_{,xxx}}} \end{array} \right. \quad \text{✓}$$

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Now in this case again let us consider our original problem. Original problem is one dimensional groundwater flow equation. Mathematical conceptualization is in terms of second order derivative. And a support domain we can have 2-3 or number of points in this case. Using mesh free shape function, we can represent it like this.

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Numerical Discretization

Using mesh-free shape function, h can be approximated as,

$$h^h(x_i) = \mathbf{W}_i^T \mathbf{h}_S$$

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Now in this case derivative can be approximated like this. Now derivative calculation we have already performed using that by introducing new variable gamma. If we have N_s number of nodes present in the local support domain, obviously we should include all points.

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Numerical Discretization

Using mesh-free shape function, h can be approximated as,

$$h^h(x_i) = \mathbf{W}_i^T \mathbf{h}_S$$

Similarly, derivatives can be approximated as,

$$\left. \frac{dh}{dx} \right|_i = \frac{d\mathbf{W}_i^T}{dx} \mathbf{h}_S$$

$$\left. \frac{d^2h}{dx^2} \right|_i = \frac{d^2\mathbf{W}_i^T}{dx^2} \mathbf{h}_S$$

where \mathbf{W}_i is the vector of shape functions, and \mathbf{h}_S is the vector that collects nodal values of the unknown function. If N_s number of nodes are present in the local support domain, then

$$\mathbf{W}_i^T = \{\dots w_{i-1} \ w_i \ w_{i+1} \ \dots\}_{1 \times N_s}$$

$$\mathbf{h}_S^T = \{\dots h_{i-1} \ h_i \ h_{i+1} \ \dots\}_{1 \times N_s}$$

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Now in this case our calculation is not straight forward like our finite difference of mesh free method of polynomial interpolation. If you have N_s number of nodes present in the local support domain, for interior nodes equation is not simplified form. Only thing is that problematic term is this one. Because it involves the calculation of our shape functions.

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Numerical Discretization

Governing Equation

If N_s number of nodes are present in the local support domain, then
For interior nodes at x_i , the discretized governing equation can be obtained by simple collocation at x_i .

$$\frac{d^2 \mathbf{W}_i^l}{dx^2} \mathbf{h}_{S_i} - \frac{C_{\text{conf}}}{T} h_i = -\frac{C_{\text{conf}}}{T} h_{wt} \Big|_i$$

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So in this case polynomial basis of order 2 can be used. So if we use polynomial basis of order 2 that means we are using in this case 1, x, x square. So let us say that L is the index for support domain or points in the support domain. So L equals to 1 to N_s . That means all points in the support domain. We can directly write this or if you multiply this two terms, we can directly write this thing. Problem is with the structure of this $\omega(x - x_L)$.

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$$P(x) = \begin{Bmatrix} 1 \\ x \\ x^2 \end{Bmatrix}$$

The polynomial basis of order 2 can be used.

$$\mathbf{A}(x) = \sum_{l=1}^{N_s} \omega(x - x_l) \begin{bmatrix} 1 \\ x_l \\ x_l^2 \end{bmatrix} \begin{bmatrix} 1 & x_l & x_l^2 \end{bmatrix} = \sum_{l=1}^{N_s} \omega(x - x_l) \begin{bmatrix} 1 & x_l & x_l^2 \\ x_l & x_l^2 & x_l^3 \\ x_l^2 & x_l^3 & x_l^4 \end{bmatrix}$$

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Now we need to define the structure of this one. Because this is a given function u_h for our problem. Only A was a variable. So BL again, structure of BL for any arbitrary L. There is $x - x_L$, 1, x_L , x_L square.

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The polynomial basis of order 2 can be used.

$$\mathbf{A}(\mathbf{x}) = \sum_{l=1}^{N_n} \omega(\mathbf{x} - \mathbf{x}_l) \begin{bmatrix} 1 \\ x_l \\ x_l^2 \end{bmatrix} \begin{bmatrix} 1 & x_l & x_l^2 \end{bmatrix} = \sum_{l=1}^{N_n} \omega(\mathbf{x} - \mathbf{x}_l) \begin{bmatrix} 1 & x_l & x_l^2 \\ x_l & x_l^2 & x_l^3 \\ x_l^2 & x_l^3 & x_l^4 \end{bmatrix}$$

$$\mathbf{B}_l = \omega(\mathbf{x} - \mathbf{x}_l) \mathbf{p}(\mathbf{x}_l) = \omega(x - x_l) \begin{bmatrix} 1 \\ x_l \\ x_l^2 \end{bmatrix}$$

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Now characteristic of this weight function, $\omega(x - x_i)$ should be greater than zero within support domain. Should be zero outside support domain and is sufficiently smooth. That means smooth function is required for this weight calculation. And this $\omega(x - x_i)$, this one is monotonically decreasing from point of interest towards boundary. So if we have $x - x_i$ by r_w , this is our radius.

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Characteristics of Weight Function

- $\omega(|\mathbf{x} - \mathbf{x}_i|) > 0$ within support domain.
- $\omega(|\mathbf{x} - \mathbf{x}_i|) = 0$ outside support domain.
- $\omega(|\mathbf{x} - \mathbf{x}_i|)$ is sufficiently smooth.
- $\omega(|\mathbf{x} - \mathbf{x}_i|)$ is monotonically decreasing from point of interest towards boundary.

$$\bar{r}_i = \frac{\mathbf{x} - \mathbf{x}_i}{r_w}$$

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So we can use different weight functions. So in this case our first representation is in terms of cubic spline. So if r greater than 1, r greater than 1 means outside support domain. So outside support domain it is zero. That is r_i barequals $(x - x_i) / r_w$, this is normalized

one. Radius starting from zero to 1. From 0.5 to 1 we have one variation and below this 0.5 we have another kind of variation.

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The screenshot shows a presentation slide with the following content:

- Top navigation: Moving Least Squares Method, Problem Definition, Discretization, References.
- Institution: I.I.T. Kharagpur.
- Slide Title: Choice of Weight Function.
- Section: Cubic Spline.
- Equation for weight function $\omega(x - x_i)$:

$$\omega(x - x_i) = \begin{cases} \frac{2}{3} - 4\bar{r}_i^2 + 4\bar{r}_i^3, & \bar{r}_i \leq 0.5 \\ \frac{4}{3} - 4\bar{r}_i + 4\bar{r}_i^2 + 4\bar{r}_i^3, & 0.5 < \bar{r}_i \leq 1 \\ 0, & \bar{r}_i > 1 \end{cases}$$
- Handwritten notes: $\bar{r}_i = \frac{x - x_i}{\Delta x}$ and a checkmark next to the third case.
- Bottom navigation: Dr. Anirban Dhar, NPTEL, Computational Hydraulics.

So this is continuous function. Again we can use this weight functions for calculation of our problems. We can have exponential function where alpha is some defined value. R_i again greater than 1, this is zero. And within this domain or r_i less than equals to 1, we have this exponentially decaying function. That means at point of interest this is equal to 1. A to the power zero is 1.

And then exponentially decaying value. If we have quartic spline. In this case again we have, within support domain it is defined in terms of some function which is varying with r_i . And outside support domain again this is zero. So these three are typical example for choice of weight function or for the MLS approximation.

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Choice of Weight Function

Cubic Spline

$$\omega(\mathbf{x} - \mathbf{x}_i) = \begin{cases} \frac{2}{3} - 4\bar{r}_i^2 + 4\bar{r}_i^3, & \bar{r}_i \leq 0.5 \\ \frac{4}{3} - 4\bar{r}_i + 4\bar{r}_i^2 + 4\bar{r}_i^3, & 0.5 < \bar{r}_i \leq 1 \\ 0, & \bar{r}_i > 1 \end{cases}$$

Exponential Function

$$\omega(\mathbf{x} - \mathbf{x}_i) = \begin{cases} e^{-\left(\frac{\bar{r}_i}{\alpha}\right)}, & \bar{r}_i \leq 1 \\ 0, & \bar{r}_i > 1 \end{cases} \quad \text{MLS}$$

Quartic Spline

$$\omega(\mathbf{x} - \mathbf{x}_i) = \begin{cases} 1 - 6\bar{r}_i^2 + 8\bar{r}_i^3 - 3\bar{r}_i^4, & \bar{r}_i \leq 1 \\ 0, & \bar{r}_i > 1 \end{cases}$$

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So we can see that in our MLS approximation, we are not getting any explicit form like P polynomial interpolation. In case of polynomial interpolation we got our two things that is for interior points and for boundary points two equations or expressions which are similar to finite difference method. But in case of MLS we are not getting any explicit form of the equation. Indirectly we need to solve the equation and then only we can get the solution out of this method. Thank you.