

A FINITE POINT METHOD IN COMPUTATIONAL MECHANICS. APPLICATIONS TO CONVECTIVE TRANSPORT AND FLUID FLOW

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SUMMARY

The paper presents a fully meshless procedure for solving partial differential equations. The approach termed generically the 'finite point method' is based on a weighted least square interpolation of point data and point collocation for evaluating the approximation integrals. Some examples showing the accuracy of the method for solution of adjoint and non-self adjoint equations typical of convective-diffusive transport and also to the analysis of a compressible fluid mechanics problem are presented.

KEY WORDS: least squares; finite point method; mesh free techniques

1. INTRODUCTION

The Finite Element Method (FEM)¹ and its subclass the Finite Volume Method (FVM)^{2–4} are well-established numerical techniques in computational mechanics (though the latter is not used widely in solid mechanics) whose main advantage is their ability to deal with complicated domains in a simple manner while keeping a local character in the approximation. Both methods divide the total domain volume into a finite number of subdomains on which a volume integration is performed. The subdomains are constrained by some geometrical regularity conditions such as having a positive volume or a limit aspect ratio between the element dimensions and angles, etc. Although this poses no serious difficulties for 2D situations, the lack of robust and efficient 3D mesh generators makes the solution of 3D problems a more difficult task.

It is widely acknowledged that 3D mesh generation remains one of the big challenges in both FE and FV computations. Thus, given enough computer power even the most complex problems in computational mechanics, such as the 3D solution of Navier–Stokes equations in fluid flow can be tackled accurately providing an acceptable mesh is available. The generation of 3D meshes, however, is despite major recent advances in this field, certainly the bottle neck in most industrial FE and FV computations and, in many cases, it can absorb far more time and cost than the numerical solution itself.

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Considerable effort has been devoted during recent years to the development of the so-called mesh-free methods. The first attempts were reported by some Finite Difference (FD) practitioners deriving FD schemes in arbitrary irregular grids.^{5–12} Here typically the concept of ‘star’ of nodes was introduced to derive FD approximations for each central node by means of local Taylor series expansions using the information provided by the number and position of nodes contained in each star.¹² Similar procedure was developed for thin plate problems solved by a variational approach by Nay and Utku¹³ using a least-squares fit to nodal values and contributing domain concepts for deriving the approximation integrals.

An alternative class of methods named Smooth Particle Hydrodynamics (SPH), sometimes called the Free Lagrange methods, depend only on a set of disordered point or particles and has enjoyed considerable popularity in computational physics and astrophysics to model the motion and collision of stars.^{14–17} These methods work well in the absence of boundaries, although they are not as accurate as the regular finite element methods.¹⁸

Different authors have recently investigated the possibility of deriving numerical methods where meshes are unnecessary. Nayroles *et al.*¹⁹ proposed a technique which they call the Diffuse Element (DE) method, where only a collection of nodes and a boundary description is needed to formulate the Galerkin equations. The interpolating functions are polynomials fitted to the nodal values by a weighted least-squares approximation. Although no finite element mesh is explicitly required in this method, still some kind of ‘auxiliary grid’ was used in Reference 19 in order to compute numerically the integral expressions derived from the Galerkin approach, thus eliminating many of the advantages of the original mesh-free philosophy.

Belytschko *et al.*^{20,21} have proposed an extension of the DE approach which they call the Element-Free Galerkin (EFG) method. This provides additional terms in the derivatives of the interpolant considered unnecessary by Nayroles *et al.*¹⁹ In addition, a regular cell structure is chosen as the ‘auxiliary grid’ to compute the integrals by means of high-order quadratures. Duarte and Oden²² and Babuska and Melenk²³ have recently formalized this type of approximation as a subclass of the so-called ‘Partition of Unity’ (PU) methods and they propose meshless and enhanced FE procedures using hierarchical PU interpolations.

Liu *et al.*^{18,24–26} have developed a different class of ‘gridless’ multiple-scale methods based on reproducing kernel and wavelet analysis. This technique termed Reproducing Kernel Particle (RKP) method allows one to develop a new type of shape functions using an integral window transform. The window function can be *translated* and *dilated* around the domain thus replacing the need to define elements and providing refinement. Comparative study of RKP, SPH, DE and EFG methods can be found in Reference 27.

The objective of this paper is two fold. First, a brief overview of some point data interpolation-based procedures termed here generically ‘finite point methods’²⁸ is presented. Then, a particularly simple finite point method based on

- (a) weighted least-squares interpolation using a ‘fixed’ Gaussian weighting function, and
- (b) point collocation for evaluating the approximation integrals

is proposed. Some examples showing the accuracy of the method for solution of adjoint and non-self adjoint equations typical of convective–diffusive transport and also to the analysis of a compressible fluid mechanics problem are then presented.

2. BASIC CONCEPTS OF MESH FREE TECHNIQUES

Let us assume a scalar problem governed by a differential equation

$$A(u) = b \quad \text{in } \Omega \tag{1}$$

with boundary conditions

$$B(u) = t \quad \text{in } \Gamma_t \tag{2}$$

$$u - u_p = 0 \quad \text{in } \Gamma_u$$

to be satisfied in a domain Ω with boundary $\Gamma = \Gamma_t \cup \Gamma_u$. In the above A and B are appropriate differential operators, u is the problem unknown and b and t represent external forces or sources acting over the domain Ω and along the boundary Γ_t , respectively. Finally, u_p is the prescribed value of u over the boundary Γ_u .

The most general procedure of solving numerically the above system of differential equations is the weighted residual method in which the unknown function u is approximated by some trial approximation \hat{u} and equations (1) and (2) are replaced by¹

$$\int_{\Omega} W_i[A\hat{u} - b] d\Omega + \int_{\Gamma_t} \bar{W}_i[B\hat{u} - t] d\Gamma + \int_{\Gamma_u} \bar{\bar{W}}_i[\hat{u} - u_p] d\Gamma = 0 \tag{3}$$

with the weighting functions W_i , \bar{W}_i and $\bar{\bar{W}}_i$ defined in different ways FE, FV and FD methods can be considered as particular cases of (3) and indeed so can all the meshes approximation procedures.

In order to keep a local character of the problem (leading to a banded matrix), function u must be approximated by a combination of locally defined functions as

$$u(x) \cong \hat{u}(x) = \sum_{i=1}^{n_p} N_i(x)u_i^h = \mathbf{N}^T(u) \mathbf{u}^h \tag{4}$$

with n_p being the total number of points in the domain and the interpolation function $N_i(x)$ satisfy

$$\begin{aligned} N_i(x) &\neq 0 && \text{if } x \in \Omega_i \\ N_i(x) &= 0 && \text{if } x \notin \Omega_i \end{aligned} \tag{5}$$

Here Ω_i is a subdomain of Ω containing n points, $n \ll n_p$. In (4) u_i^h is the approximate value of u at point i such that $u(x_i) \simeq u_i^h$.

In FE and FV methods the Ω_i subdomains are divided into elements and the N_i function may have some discontinuities (in the function itself or in its derivatives) on the element interfaces. In the FE method the weighting functions W_i are defined in 'weighting domains' which usually coincide precisely with the interpolating domains Ω_i . In cell vertex FV the interpolation and integration domains also coincide, however in the cell centered case they are different²⁻⁴ (see Figure 1).

A common feature of FE and FV methods is that they both require a mesh for interpolation purposes and also to compute the integrals in equation (3).

In meshless (or element free) methods the subdomains Ω_i are frequently termed interpolation domains or 'clouds'.²²

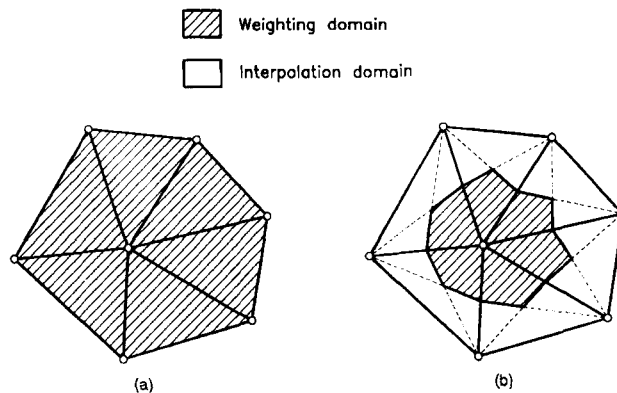


Figure 1. Interpolation and weighting domains in finite element (FE) and finite volume (FV) methods: (a) FEM and FVM (cell vertex); (b) FVM (cell centered)

On the basis of the above remarks, a mesh-free numerical procedure should satisfy the following conditions:

- I. (a) The discretization of the unknown function and its derivatives must be defined *only* by the position of points located within the analysis domain and parameters specified at these.
(b) The weighting function and its derivatives must be defined *only* by the position of points located within the analysis domain.
- II. (a) No volume or surface integration is needed, or
(b) Any volume or surface integration should be independent of the interpolation procedure chosen.

Condition II(a) is satisfied by finite difference and point collocation procedures. Other methods like subdomain collocation, or meshless methods which are based on the use of auxiliary background grids for integration purposes (i.e. DEM,¹⁹ EFG,²⁰ RPK¹⁸) satisfy condition II(b).

Condition I(a) is satisfied by classical use of Rayleigh–Ritz method in which the N_i functions are defined over the whole domain Ω , thus precluding the local character of the approximation. FE methods define the shape functions N_i over non-overlapping regions (elements) the assembly of which constitutes the domain Ω_i .^{2–4} Different interpolations are therefore possible for a given number of points simply by changing the orientation or the form of these regions, thus violating the necessary requirement of condition I(a). Although FV techniques do not explicitly define an interpolation of the form (4), it is well-known that they are equivalent to using linear shape functions over domains Ω_i defined in the same manner as in the FE method.^{2–4}

In next section some of the more popular approximations used to build interpolations based on a finite number of points (hereafter termed generically ‘finite point methods’) are briefly reviewed.

3. LEAST-SQUARES, DIFFUSE LEAST-SQUARES, MOVING LEAST-SQUARES AND REPRODUCING PARTICLE KERNEL APPROXIMATIONS

Let Ω_k be the interpolation domain (cloud) of a function $u(x)$ and let s_j with $j = 1, 2, \dots, n$ be a collection of n points with coordinates $x_j \in \Omega_k$. The unknown function u may be approximated within Ω_k by

$$u(x) \cong \hat{u}(x) = \sum_{i=1}^m p_i(x) \alpha_i = \mathbf{p}(x)^T \boldsymbol{\alpha} \quad (6)$$

where $\alpha = [\alpha_1, \alpha_2, \dots, \alpha_m]^T$ and vector $\mathbf{p}(x)$ contains typically monomials, hereafter termed 'base interpolating functions', in the space co-ordinates ensuring that the basis is complete. For a 2D problem we can specify

$$\mathbf{p} = [1, x, y]^T \quad \text{for } m = 3 \tag{7a}$$

and

$$\mathbf{p} = [1, x, y, x^2, xy, y^2]^T \quad \text{for } m = 6, \text{ etc.} \tag{7b}$$

Function $u(x)$ can now be sampled at the n points belonging to Ω_k giving

$$\mathbf{u}^h = \begin{Bmatrix} u_1^h \\ u_2^h \\ \vdots \\ u_n^h \end{Bmatrix} \cong \begin{Bmatrix} \hat{u}_1 \\ \hat{u}_2 \\ \vdots \\ \hat{u}_n \end{Bmatrix} = \begin{Bmatrix} \mathbf{p}_1^T \\ \mathbf{p}_2^T \\ \vdots \\ \mathbf{p}_n^T \end{Bmatrix} \alpha = \mathbf{C} \alpha \tag{8}$$

where $u_j^h = u(x_j)$ are the unknown but sought for values of function u at point j , $\hat{u}_j = \hat{u}(x_j)$ are the approximate values, and $\mathbf{p}_j = \mathbf{p}(x_j)$.

In the FE approximation the number of points is chosen so that $m = n$. In this case, \mathbf{C} is a square matrix and we can obtain *after equaling \mathbf{u}^h with $\mathbf{C} \alpha$* in (8)

$$\alpha = \mathbf{C}^{-1} \mathbf{u}^h \tag{9}$$

and

$$u \cong \hat{u} = \mathbf{p}^T \mathbf{C}^{-1} \mathbf{u}^h = \mathbf{N}^T \mathbf{u}^h = \sum_{j=1}^n N_j u_j^h \tag{10}$$

with

$$\mathbf{N}^T = [N_1, \dots, N_n] = \mathbf{p}^T \mathbf{C}^{-1} \text{ and } N_j = \sum_{i=1}^m p_i(x) C_{ij}^{-1} \tag{11}$$

The shape functions $N_j(x)$ satisfy the standard condition¹

$$\begin{aligned} N_j(x) &= 1 \quad j = i \\ &= 0 \quad j \neq i, \quad i, j = 1, \dots, n \end{aligned} \tag{12}$$

The development of the N_j can often be performed directly using interpolation methods and/or isoparametric concepts.¹

3.1. Least Squares (LSQ) approximation

If $n > m$, \mathbf{C} is no longer a square matrix and the approximation cannot fit all the u_j^h values. This problem can simply be overcome by determining the \hat{u} values by minimizing the sum of the square distances of the error at each point

$$J = \sum_{j=1}^n (u_j^h - \hat{u}(x_j))^2 = \sum_{j=1}^n (u_j^h - \mathbf{p}_j^T \alpha)^2 \tag{13}$$

with respect to the α_i parameters (least-squares fit).

Standard minimization gives

$$\alpha = \bar{\mathbf{C}}^{-1} \mathbf{u}^h \quad \text{with } \bar{\mathbf{C}}^{-1} = \mathbf{A}^{-1} \mathbf{B} \tag{14}$$

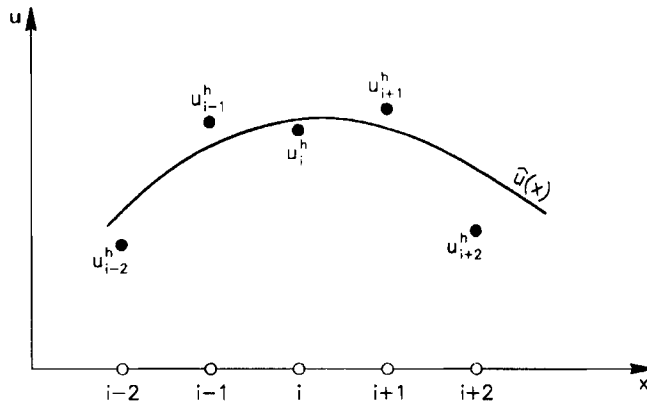


Figure 2. Unknown function $\hat{u}(x)$ and unknown parameters u_i^h

where

$$\mathbf{A} = \sum_{j=1}^n \mathbf{p}(x_j) \mathbf{p}^T(x_j) \tag{15a}$$

$$\mathbf{B} = [\mathbf{p}(x_1), \mathbf{p}(x_2), \dots, \mathbf{p}(x_n)] \tag{15b}$$

The final approximation is still given by equation (10) now however substituting matrix \mathbf{C} by $\bar{\mathbf{C}}$ of equation (14). The new shape functions are, therefore,

$$N_j^k = \sum_{i=1}^m p_i(x) \bar{C}_{ij}^{-1} \tag{16}$$

where superindex k emphasizes that the shape function N_j^k can now be defined differently for each cloud Ω_k .

It must be noted that accordingly to the least-squares character of the approximation

$$u_j = u^h(x_j) \neq \hat{u}(x_j) \tag{17}$$

i.e. the local values of the approximating function do not fit the nodal unknown values (Figure 2). Indeed \hat{u} is the true approximation for which we shall seek the satisfaction of the differential equation and boundary conditions and u_j^h are simply the unknown parameters sought!

However, if $n = m$ the FEM-type approximation is recovered. Then $\hat{u}(x_j) = u^h(x_j)$ and once again conditions (12) are satisfied.

Note again that according to (6), the approximate function $\hat{u}(x)$ is defined in each interpolation domain Ω_k . In fact, different interpolation domains can yield different shape functions N_j^k . As a consequence a point belonging to two or more overlapping interpolation domains has different values of the shape functions. The interpolation is now multivalued within Ω_k and, therefore, for any useful approximation a decision must be taken limiting the choice to a single value.

Indeed, the approximate function $\hat{u}(x)$ will be typically used to provide the value of the unknown function $u(x)$ and its derivatives in only specific regions within each interpolation domain. For instance by using point collocation we may limit the validity of the interpolation to a single point i .

LSQ approximation has enjoyed some popularity in deriving point data interpolations for numerical computation in solid and fluid mechanics. Nay and Utku¹³ used quadratic LSQ interpolations to fit the deflection field giving constant curvature for thin plate bending analysis.

More recently, Batina²⁹ has used LSQ fits based on linear polynomial to approximate the fluxes in the solution of high-speed compressible flows.

The main drawback of the LSQ approach is that the approximation rapidly deteriorates if the number of points used, n , largely exceeds that of the m polynomial terms in \mathbf{p} . Some examples of this kind are given in a later section. This deficiency can be overcome by using a weighted least-squares interpolation as described next.

3.2. Weighted least-squares (WLS) approximation

The LSQ approximation can be enhanced in a region in vicinity of point i where, for instance, the derivatives of the unknown are to be evaluated, by weighting the squared distances with a function φ_i so that, we minimize

$$J_i = \sum_{j=1}^n \varphi_i(x_j - x_i)(u_j^h - \hat{u}(x_j))^2 = \sum_{j=1}^n \varphi_i(x_j - x_i)(u_j^h - \mathbf{p}_j^T \boldsymbol{\alpha})^2 \tag{18}$$

Function $\varphi_i(x - x_i)$ is usually built in such a way that it takes a unit value in the vicinity of the point i (typically called ‘star node’¹²) where the function (or its derivatives) are to be computed and vanishes outside a region Ω_i surrounding the point (Figure 3). The region Ω_i can be used to define the number of sampling points n in the interpolation region (i.e. $\Omega_i = \Omega_k$ in this case). A typical choice for $\varphi_i(x - x_i)$ is the normalized Gaussian function. Of course, $n \geq m$ is always required in the sampling region and if equality occurs no effect of weighting is present and the interpolation is the same as in the LSQ scheme.

Standard minimization of equation (18) with respect to $\boldsymbol{\alpha}_i$ gives the same form of the shape functions as defined in equations (14)–(16) but with matrices \mathbf{A} and \mathbf{B} given now by

$$\mathbf{A} = \sum_{j=1}^n \varphi_i(x_j - x_i) \mathbf{p}(x_j) \mathbf{p}^T(x_j) \tag{19a}$$

$$\mathbf{B} = [\varphi_i(x_1 - x_i) \mathbf{p}(x_1), \varphi_i(x_2 - x_i) \mathbf{p}(x_2), \dots, \varphi_i(x_n - x_i) \mathbf{p}(x_n)] \tag{19b}$$

Note that also again a multivalued interpolation is obtained in this case and some definition of Ω_k is required as in the LSQ approach.

3.3. Moving Least-Squares (MLS) approximation

In the Moving Least-Squares (MLS) approach the weighting function φ is defined in shape and size and is translated over the domain so that it takes the maximum value over the point k identified by the co-ordinate x_k where the unknown function \hat{u} is to be evaluated.

As shown in Figure 3 we now minimize for every point k the following functional:

$$J = \sum_{j=1}^n \varphi_k(x_j - x_k)(u_j^h - \mathbf{p}_j^T \boldsymbol{\alpha}) \tag{20}$$

where φ_k can in general change its shape and span depending on the position of point k . Note that x_k is now an arbitrary coordinate position and it can be simply replaced by the global co-ordinate x . We will however retain the form $\varphi_k(x_j - x_k)$ to emphasise the possibility of changing function φ at each position within the approximation domain. In the simplest case of constant grid spacing it is possible to take

$$\varphi_k(x_j - x_k) = \varphi(x_j - x) \tag{21}$$

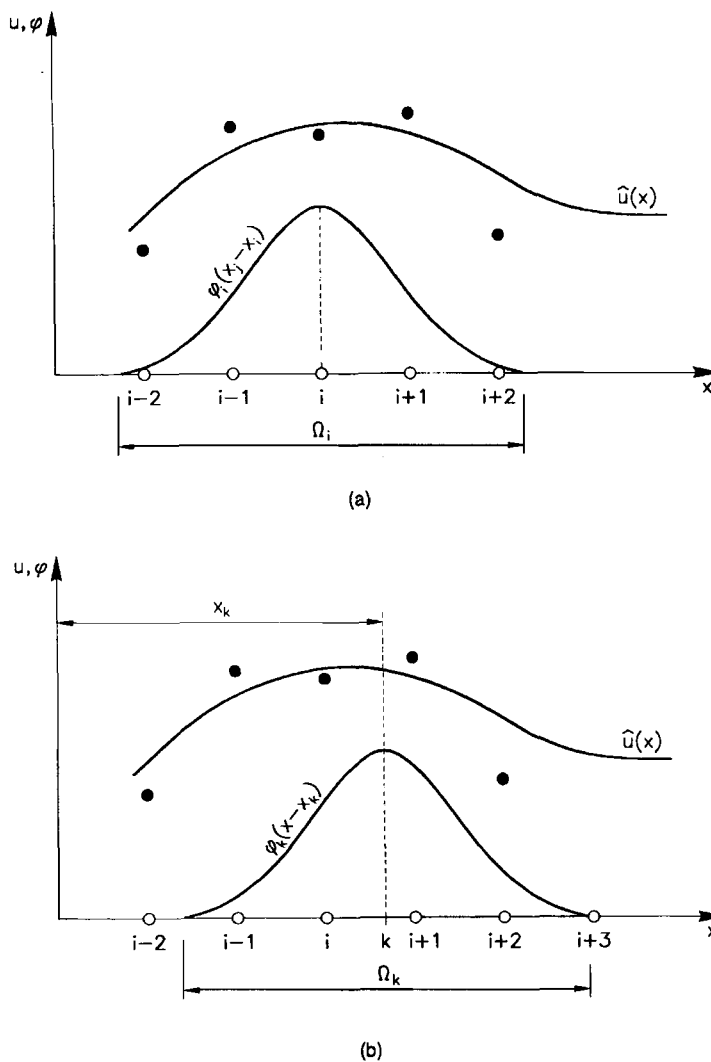


Figure 3. Fixed and moving weighting functions: (a) fixed φ corresponding to point x_i ; (b) moving φ

and assume the shape of the weighting function *invariant*. It is precisely for this case that the name MLS is derived.

In general, with an arbitrary position of points the problem of specifying φ_k at every position x is very difficult and presents an infinite number of possibilities. It is convenient instead to specify only the weighting function at the finite number of points chosen and derive similar to the WLS, weightings of the type $\varphi_i(x_j - x_i)$. With this definition, a possible and computationally useful procedure is to define

$$\varphi_k(x_j - x_k) = \varphi_j(x_k - x_j) \quad (22)$$

Note again that k denotes an arbitrary location (i.e. $x_k = x$) whereas j is a fixed point in the domain. With this assumption the function to be minimized in place of that of equation (20) is

now the following:

$$J(x) = \sum_{j=1}^n \varphi_j(x - x_j) [u_j^h - \mathbf{p}_j^T \boldsymbol{\alpha}(x)] \tag{23}$$

This gives immediately

$$\mathbf{A} = \sum_{j=1}^n \varphi_j(x - x_j) \mathbf{p}(x_j) \mathbf{p}^T(x_j) \tag{24a}$$

$$\mathbf{B} = [\varphi_1(x - x_1) \mathbf{p}(x_1), \varphi_2(x - x_2) \mathbf{p}(x_2), \dots, \varphi_n(x - x_n) \mathbf{p}(x_n)] \tag{24b}$$

Observe that in this case the parameters α_i are no longer constants but vary continuously with position x and that inversion of matrices is required at every point where \hat{u} is to be evaluated. Furthermore, a unique global definition of the shape functions can be now obtained provided:

- (a) the weighting function φ_i is continuous and differentiable in Ω_i ,
- (b) the weighting function φ_i vanishes on the boundary of Ω_i and outside,
- (c) the number of points n within Ω_i is equal or greater than the parameters m at all points in Ω_i .

This method has been successfully used by Nayroles *et al.*¹⁹ with the name of Diffuse Finite Element (DFE) method and later by Belytschko *et al.*²⁰ in the context of the so-called Element Free Galerkin (EFG) method. In the DFE method reported in Reference 19, the derivatives of φ_i were omitted when computing the derivatives of the unknown function, whereas the full expression was used in the EFG method. In order to avoid the need of inverting matrix \mathbf{A} for each quadrature point where the discrete equations are assembled, Lu *et al.*²¹ proposed to use a weighted orthogonal basis functions using a Schmidt orthogonalization technique though the computational advantage seems to be small. A generalization of the MLS approach using the concept of partition of unity functions can be found in Reference 22. Indeed that paper introduces a very simple possibility of increasing the polynomial order of the shape functions hierarchically as illustrated in Reference 37.

3.4. Reproducing Kernel Particle (RPK) methods

An alternative procedure to derive point data interpolation of the form (6) is to use multiple-scale methods based on reproducing kernel and wavelet analysis. This approach has been successfully exploited by Liu *et al.*^{18,24-26} under the name of RKP methods for the solution of some solid and fluid flow problems.

A reproducing kernel is a class of operators that reproduces the function itself by integrating through the domain. The Fourier transform is a typical example of a reproducing kernel. In general form, we can write

$$f(x) = \int_{\Omega} \phi(x - y) f(y) dy \tag{25}$$

where $\phi(x)$ is an appropriate window function defined with a compact support and which can be translated around the domain. A dilation parameter is also used to provide refinement. The parameters α_i in (6) can be obtained by applying the integral window transform to equation (6) and after discretization an approximation identical to equation (4) can be obtained.^{18,28} A comparison of RPK, SPH, MLS and WLS methods can be found in References 18 and 27.

3.5. Comparison of FE, LSQ, WLS and MLS approximations

Independently of the method chosen to solve the global problem (equation (3)), the accuracy of the solution will very much depend on the shape functions used in each approximation. One of the main differences between FE and LSQ, WLS and MLS methods is that in the FE approach the local value of the approximating function is coincident with the unknown parameters, i.e.

$$\hat{u}(x_i) = u_i^h \quad (26)$$

whereas in finite point-based methods (FPM) such as LSQ, WLS and MLS methods

$$\hat{u}(x_i) \neq u_i^h \quad (27)$$

Summarizing the 'freedom' for choosing the approximation in the different methods considered we can list

- (a) In FE methods
 - (1) the mesh,
 - (2) the polynomial order (m in equation (6))
- (b) In Finite Point Methods (FPM)
 - (1) the point position (in LSQ, WLS and MLS methods),
 - (2) the polynomial order (in LSQ, WLS and MLS methods),
 - (3) the shape of the weighted least square function $\varphi_i(x)$ (in WLS and MLS methods),
 - (4) the span of $\varphi_i(x)$ (in WLS and MLS methods), and
 - (5) the choice of fixed or moving least-squares weighting functions $\varphi_i(x)$ (in WLS and MLS methods).

To understand better these differences we will plot some of the shape functions resulting from these methods in one dimension.

We choose for simplicity a collection of equally spaced points at a distance h from each other. Figure 4 shows the weighting least-squares function $\varphi_i(x)$ used for WLS and MLS methods given by the Gaussian expression

$$\varphi_i(x) = \frac{e^{-(x/c)^2} - e^{-(xm/c)^2}}{1 - e^{-(xm/c)^2}} \quad (28)$$

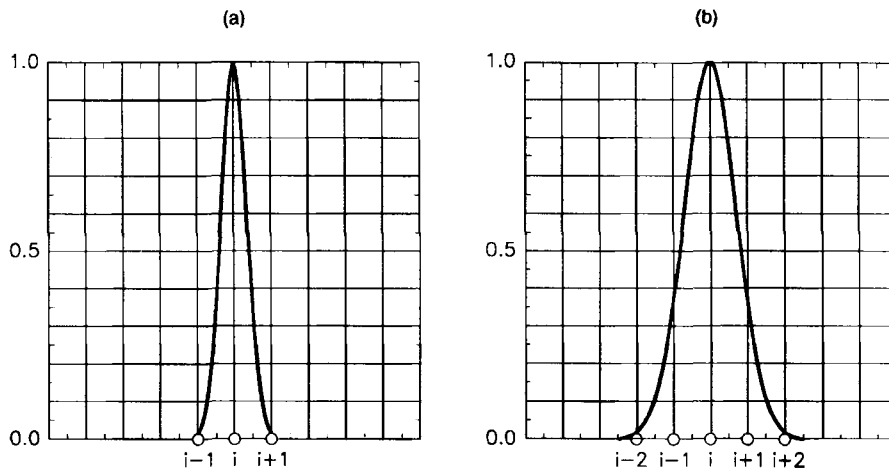


Figure 4. Gaussian weighting functions for three and five points clouds: (a) $n = 3$; (b) $n = 5$

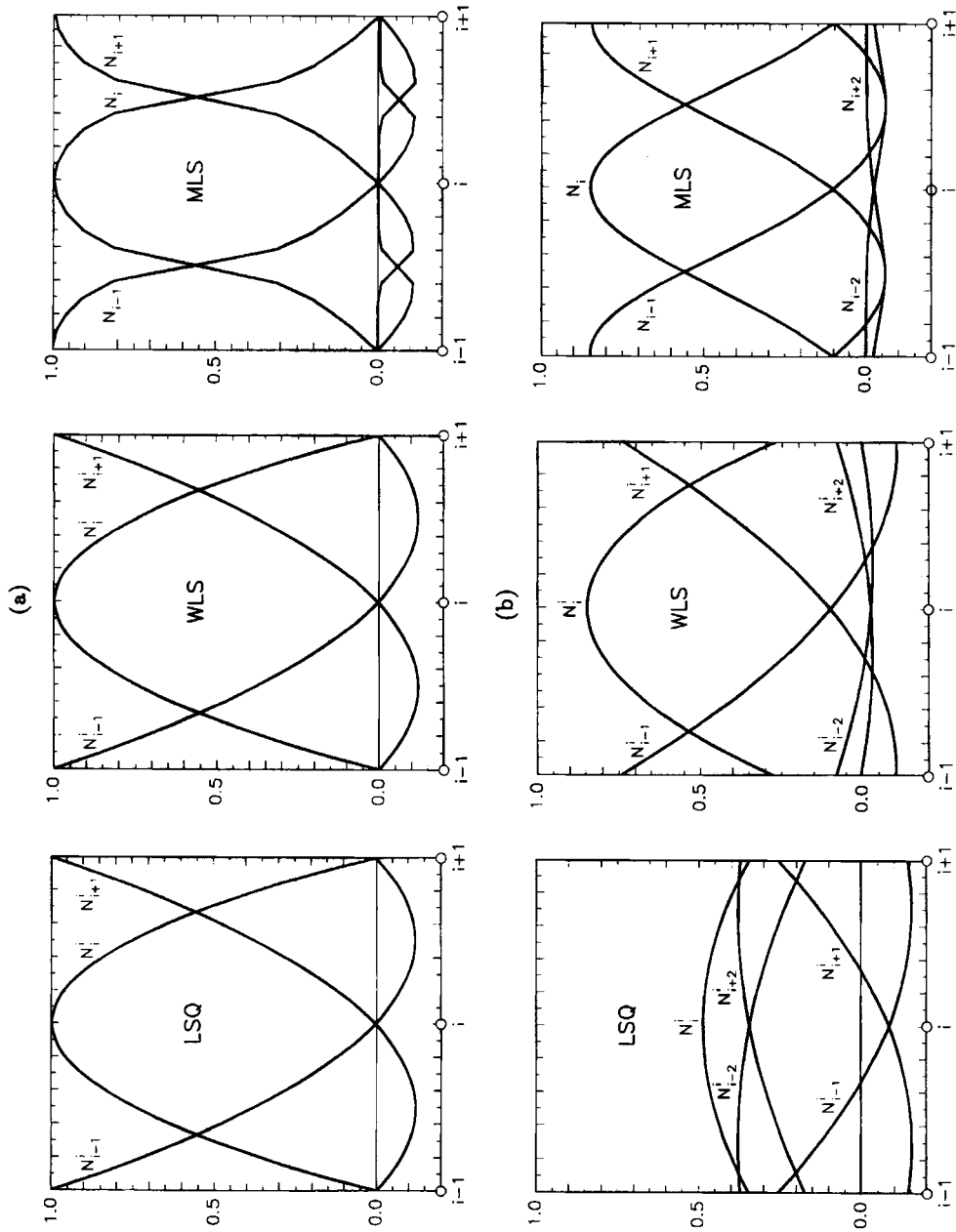


Figure 5. Shape functions $N_i(x)$ for $\mathbf{p} = [1, x, x^2]$: (a) three-points clouds ($m = 3$) ($n = 3$); (b) five-points clouds ($m = 3$) ($n = 5$). $\Omega_k = \Omega_i$ is the domain from $i - 1$ to $i + 1$ in (a) and $i - 2$ to $i + 2$ in (b)

where x_m is the half size of the support and c is a parameter determining the shape. We will choose $c = x_m/2$.

The following weightings will be considered:

- (a) $x_m = 1.6h$. This defines three-point clouds ($n = 3$) for both LSQ and WLS methods. It also defines a *minimum* number of three-point clouds for the MLS method, although four points occur for some particular positions. For consistency the name *three-point cloud* will be given to this option in all cases.
- (b) $x_m = 2.5h$. This generally defines a five point cloud ($n = 5$). Note that now four points may occur for one position in the MLS method.

Figure 5 shows the shape functions for a quadratic base function polynomial ($m = 3$) and clouds of three and five points, respectively. Note that with three-points clouds LSQ and WLS methods yield interpolating functions similar to the standard FE quadratic shape functions as expected. The MLS method gives global interpolating functions of higher order than quadratic. When $n = 5$ (five-points cloud) none of the methods gives $N_i(x) = 1$ at $x = x_i$ nor is $N_i(x) = 0$ at $x = x_j, j \neq i$. In particular, the LSQ method yields very inaccurate interpolating functions in this case with the value $N_i(x_i)$ equal to less than 0.5 everywhere.

Note that, as previously mentioned, the global interpolation is multivalued in the LSQ and WLS approaches. This is illustrated in Figure 6(a) where the global expressions of the shape functions are plotted for the case $m = 3, n = 3$. A mid-point rule has been chosen in Figure 6(b) to preserve a single value of the shape function in the vicinity of each point. Note also that the first derivative is undetermined at $x = (x_i + x_{i-1})/2$ which limits the validity of LSQ and WLS methods to point or subdomain collocation procedures.^{33,34}

Similar results can be obtained with linear base functions ($m = 2$) as shown in Figure 7. Here again, the shape functions provided by the LSQ method attenuate when the number of points within the cloud n is changed from 3 to 5. This attenuation is also noted in WLS and MLS methods where the $N_i(x_i)$ value decreases from 0.97 to 0.57.

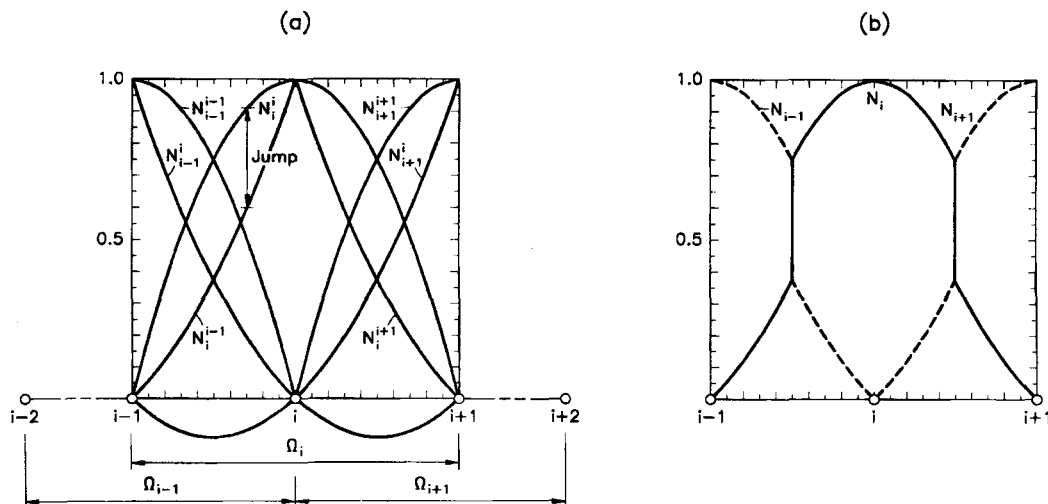


Figure 6. (a) Multivalued definition of the shape function in LSQ and WLS methods for $m = 3, n = 3$, and (b) global definition of the interpolation using a mid-point rule

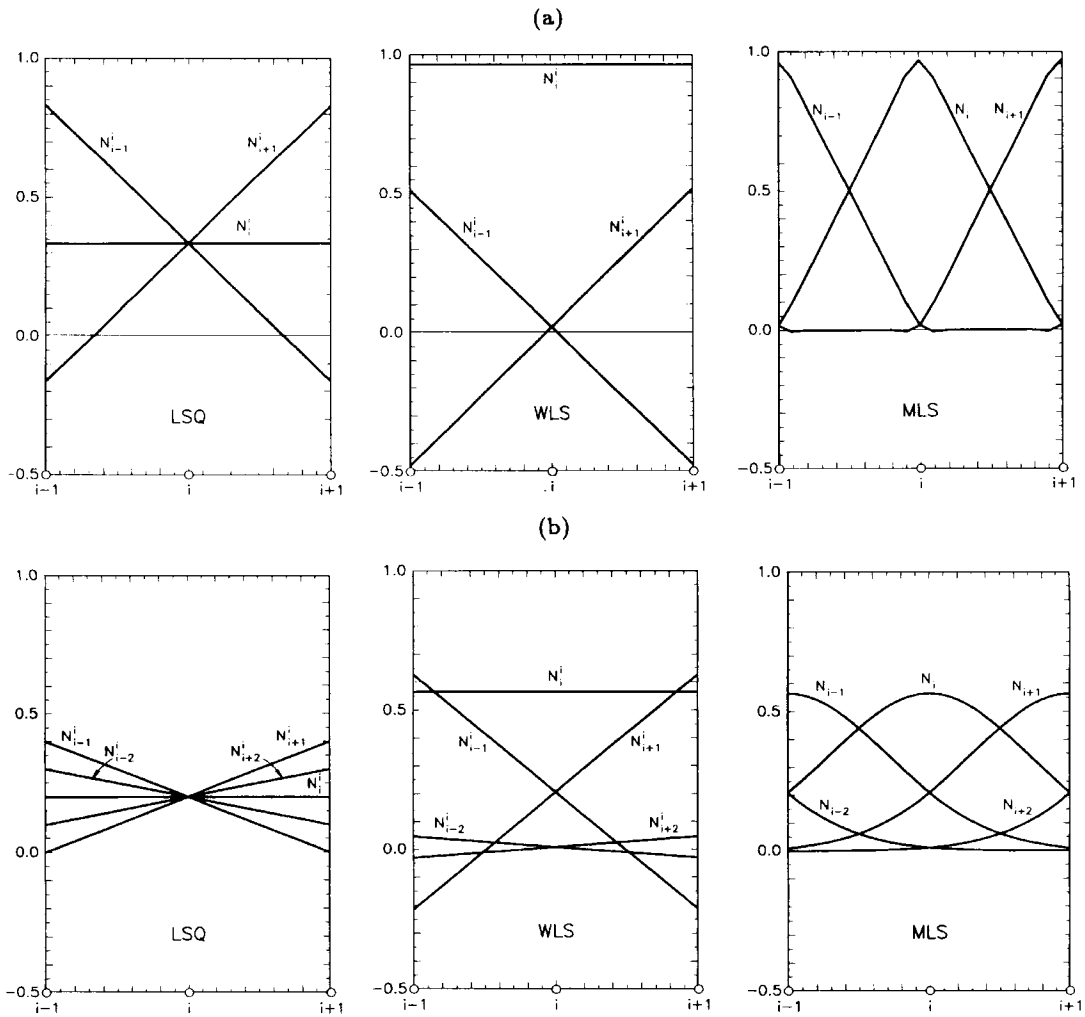


Figure 7. Shape functions $N_i(x)$ for $\mathbf{p} = [1, x]$; (a) three-points clouds ($m = 2$) ($n = 3$); (b) five-points clouds ($m = 2$) ($n = 5$). $\Omega_k = \Omega_i$ is the domain from $i - 1$ to $i + 1$ in (a) and $i - 2$ to $i + 2$ in (b)

It can be concluded that the selection of the more adequate approximation for point data interpolation should be based on its *insensitivity* to the number of points chosen within the approximating region (cloud). In order to preserve the freedom of adding, moving or removing points for a given order of interpolation, the approximating functions should be as insensitive as possible to the number of points within the cloud. We have found that the LSQ method is very sensitive to the number of cloud points chosen and the approximation rapidly deteriorates as the number of points increases. The MLS and WLS approximations with linear base polynomials seem to also be quite sensitive to the number of cloud points. Conversely, the MLS and WLS methods with quadratic base functions seem to be best suited for point data interpolation using blendings of approximations based on three and five points for each cloud (see Table I).

Table I. Sensitivity of the quality of the approximation when the number of cloud points n is changed from 3 to 5

Method	Order of the base interpolating polynomial (m)	Sensitivity of the approximation
LSQ	Linear ($m = 2$)	Very large
LSQ	Quadratic ($m = 3$)	Very large
WLS	Linear ($m = 2$)	Large
WLS	Quadratic ($m = 3$)	Low
MLS	Linear ($m = 2$)	Large
MLS	Quadratic ($m = 3$)	Low

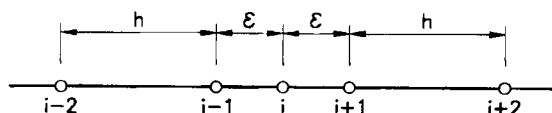


Figure 8. Point distribution with variable distance

Another important property of a good Finite Point Method (FPM) is the possibility to introduce (or to translate) new points independently of the distance between existing points. In the FE method, two nodes that are very close together, generate a gradient in the shape function which can introduce numerical error. This adds severe limitations in the mesh generator and adaptivity criteria. In a good FPM, a close distance between two points should not affect the numerical results.

Figure 8 shows a set of points with two points placed at a variable distance ε from a central point i . Figure 9 shows the shape functions when this distance ε tends to zero for two different cases: (a) WLS interpolation with quadratic base functions ($m = 3$) and (b) MLS interpolations function with a linear base function ($m = 2$). Again a truncated Gaussian weighting (equation (28)) was chosen in both cases. For $h/\varepsilon = 2$ the shape functions in the WLS approach are coincident with the quadratic FE shape functions. Alternatively, when the three points $i - 1$, i and i tend to coincide, the three corresponding shape functions tend to take the same expression in both WLS and MLS cases, thus avoiding the sharp gradients typical in FE approximation.

4. DERIVATION OF THE DISCRETIZED EQUATIONS

The selection of different weighting functions in the general weighted residual form of equation (3) yields different sets of discretized equations. In order to preserve the mesh-free character of the method, the weighting function must satisfy Condition II(b) of Section 2 and the weighting domain must be defined independently of any mesh. All approximation methods of integral type (i.e. Galerkin, area collocation, etc.) are costly and necessitate the introduction of complex procedures for integration (i.e. background grid, etc.¹⁸⁻²¹). Some of these procedures are reviewed in Reference 28. In this paper we shall therefore limit the choice to *point collocation* methods where we feel the advantages of Finite Point Methods are best realized.

Such point collocation has recently been used with success by Batina,²⁹ who however limited his work to the use of LSQ and linear approximation. We shall show that considerable improvement can be gained using WLS or MLS procedures.

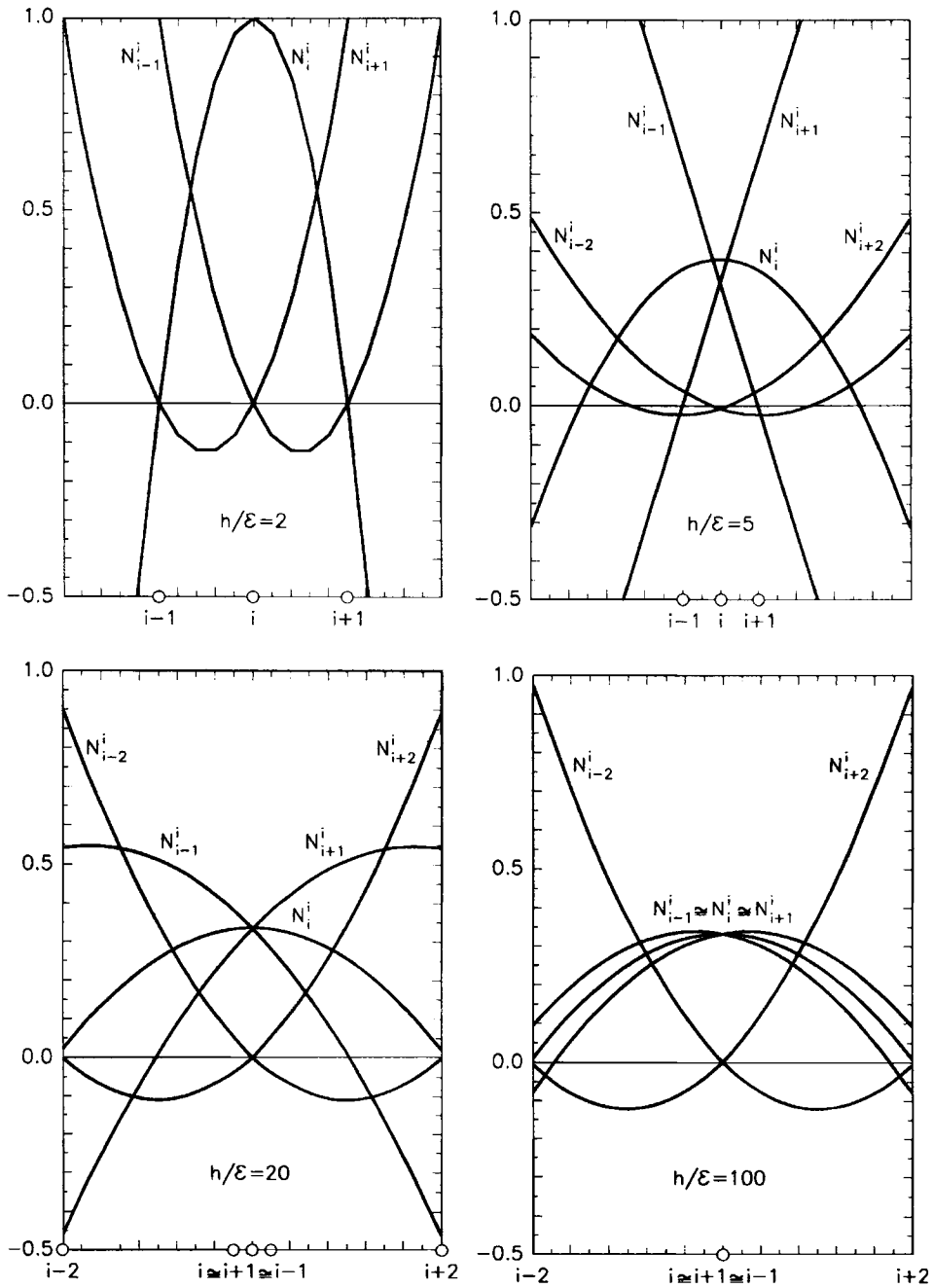


Figure 9a. Shape functions for 3 very close points, WLS method ($m = 3$)

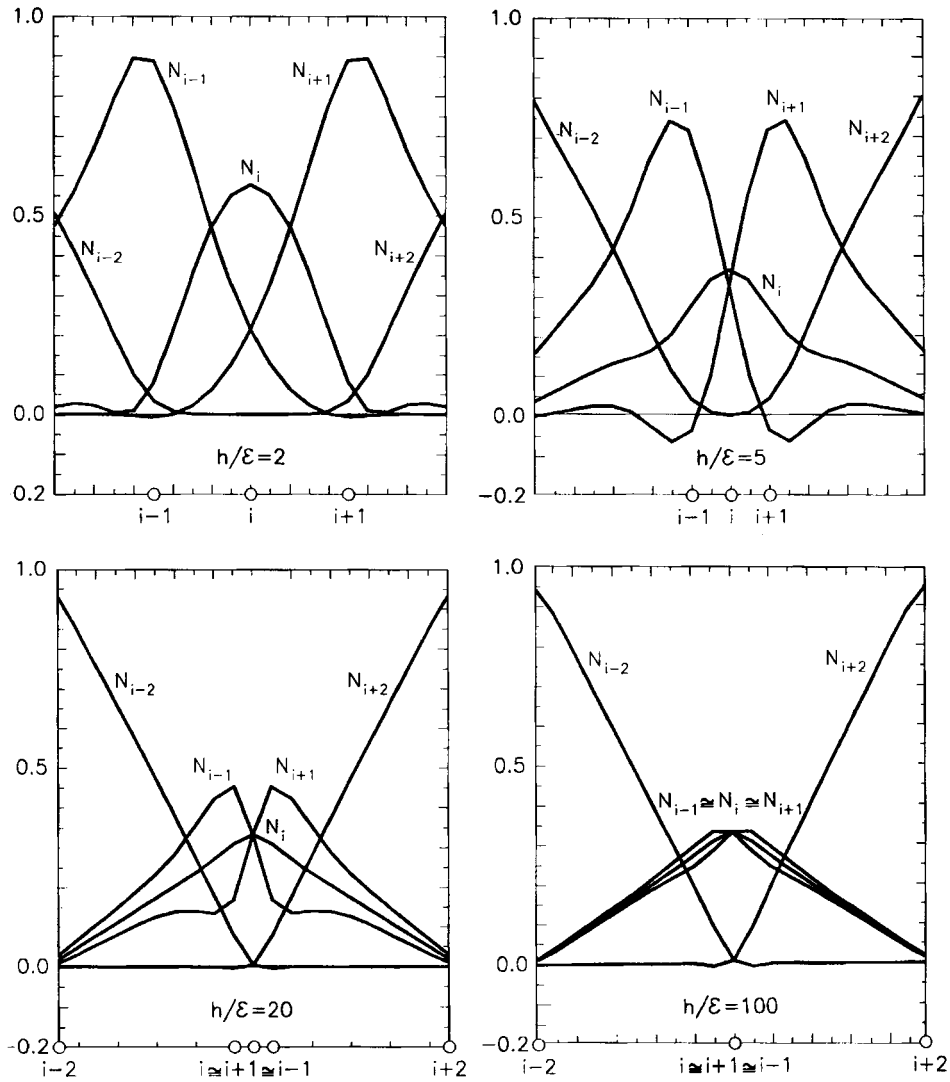


Figure 9b. Shape functions for 3 very close points, MLS method ($m = 2$)

4.1. Point collocation

The simplest choice that satisfies the mesh-free condition is making $W_i = \bar{W}_i = \bar{\bar{W}}_i = \delta_i$ where δ_i is the Dirac delta. This gives the set of equations

$$[A(\hat{u})]_i - b_i = 0 \quad \text{in } \Omega \tag{29}$$

$$[B(\hat{u})]_i - t_i = 0 \quad \text{in } \Gamma_t \tag{30}$$

$$\hat{u}_i - u_p = 0 \quad \text{in } \Gamma_u \tag{31}$$

Any of the previous shape functions may be used to approximate \hat{u} leading in all cases to the system of equations

$$\mathbf{K} \mathbf{u}^h = \mathbf{f} \tag{32}$$

with $K_{ij} = [A(N_j)]_i + B(N_j)_i$ and where the symmetry of the ‘coefficient’ matrix \mathbf{K} is not generally achieved. Vector \mathbf{u}^h contains the problem unknowns, u_i^h , and \mathbf{f} is a vector containing the contributions from the force terms b and t and the prescribed values u_p .

Taking a particular set of nodes and shape functions, this method is coincident with the generalized Finite Difference Methods of the type described in References 7–12. However, the approach proposed here offers more possibilities. Indeed any of the interpolation techniques described in Section 3 can be used.

5. BOUNDARY CONDITIONS

The boundary conditions given by (2) are imposed by the second and third integral of (3). If a *unique* solution to (3) is to be achieved using approximations of the type given by (4), the total number of *independent* W_i , \bar{W}_i and $\bar{\bar{W}}_i$ functions must be exactly n_p (the number of parameters defining $\hat{u}(x)$). In point collocation methods each W is a Dirac delta function and the above can be achieved by ensuring that the number of point used to approximate the differential equations is $n_p - n_b$, where n_b is the total number of points at which the boundary conditions Γ_t and Γ_u are constructed.

The satisfaction of the essential boundary conditions

$$u - u_p = 0 \quad \text{in } \Gamma_u$$

can be approximated for points x_i placed on Γ_u as

$$\hat{u}(x_i) = u_p(x_i) \quad x_i \quad \text{on } \Gamma_u \tag{33}$$

Similarly, the other boundary conditions on Γ_t may be approximated as

$$B(\hat{u}(x_i)) = t(x_i) \quad x_i \quad \text{on } \Gamma_t \tag{34}$$

If n_u is the number of points where (29) is given and n_t the number of points where (34) is given, then

$$n_b = n_u + n_t \tag{35}$$

and the differential equation is approximated (collocated) at only $n_p - n_b$ points.

The approximation of $\hat{u}(x_i)$ on Γ_u can be performed using different least-squares approximations than that used for the differential equation. For example, approximating the essential boundary conditions

$$u(x_i) = u_p(x_i) \quad \text{on } \Gamma_u \tag{36}$$

by

$$u(x) \simeq \hat{u}(x) = 1 \cdot \alpha_1 \tag{37}$$

and using a cloud which includes only x_i (i.e. one point) gives

$$u(x_i) \simeq \hat{u}(x_i) = u_i^h. \tag{38}$$

Thus, an approximation using

$$u_i^h = u_p(x_i) \quad x_i \quad \text{on } \Gamma_u \tag{39}$$

may be used. In this case, however, the approximation chosen for the domain will *not* be identical to the interpolation given above at the boundary points.

Further details on the treatment of the essential boundary conditions can be found in Reference 28.

6. THE FINITE POINT METHOD IN CONVECTION-DIFFUSION PROBLEMS

For non-self-adjoint problems such as those which occur in fluid mechanics special treatment is needed to stabilize the numerical approximation. As a typical example, we shall outline the special feature on the convection-diffusion equation given by

$$\begin{aligned} c\phi, t + \mathbf{u} \cdot \nabla \phi - \nabla \cdot (k \nabla \phi) - Q &= 0 \quad \text{in } \Omega \\ \mathbf{n} \cdot k \nabla \phi + \bar{q}_n &= 0 \quad \text{in } \Gamma_r \\ \phi - \bar{\phi}_p &= 0 \quad \text{in } \Gamma_u \end{aligned} \quad (40)$$

with the initial condition

$$\phi = \phi_0(\mathbf{x}) \quad \text{for } t = t_0$$

where ∇ is the gradient operator, c , u and k are known physical parameters, ϕ the unknown field and Q a source term. \bar{q}_n and $\bar{\phi}_p$ are known values of the flux and the unknown function at the boundaries Γ_r and Γ_u , respectively.

It is well-known that the numerical solution of non-self-adjoint equations must be stabilized in order to avoid oscillations.¹ Upwind finite difference derivatives, anisotropic balancing diffusion, Petrov-Galerkin weighting functions or characteristic time integration are some of the standard techniques used to stabilize FD, FE and FV methods.^{1,30-35} We will test some of these approaches in the context of a FPM using a WLS approximation and point collocation.

Let us consider for simplicity the case of the stationary 1D equation

$$\begin{aligned} u \frac{\partial \phi}{\partial x} - k \frac{\partial^2 \phi}{\partial x^2} &= 0 \\ \phi &= 0 \quad \text{in } x = 0 \\ \phi &= 1 \quad \text{in } x = L \end{aligned} \quad (41)$$

The FD and FV method stabilize the numerical solution of this equation by evaluating the first derivative upwind each point as

$$\left(\frac{\partial \phi}{\partial x} \right)_i = \frac{\phi_i - \phi_{i-1}}{h} \quad (42)$$

in which h is the distance between two points.

The FE method with linear approximation uses Petrov-Galerkin weighting functions defined as¹

$$W = N + \frac{h}{2} \alpha \frac{\partial N}{\partial x} \quad (43)$$

where N are the linear shape function. Exact nodal solution are obtained if

$$\alpha = \coth |Pe| - \frac{1}{|Pe|} \quad (44)$$

with the Peclet number defined as

$$Pe = \frac{uh}{2k} \tag{45}$$

Both upwind derivative and Petrov–Galerkin weighting procedures can be interpreted as the addition of a balancing diffusion term to the original differential equation.¹

Quadratic finite elements typically require the definition of *two upwind* parameters. In Reference 31, a single parameter is proposed for quadratic elements with an expression identical to equation (44) and *h* given now by half the element length. Exact nodal values are not obtained in this case, but the superconvergence is preserved and the method is very simple to use.

Let us try to generalize these concepts for the FPM using point collocation.

6.1. *Upwind computation of first derivative*

A simple stabilization procedure in the FPM can be derived by evaluating the first derivative upwind of each approximating point. This is in fact similar to some standard FD stabilization procedures.³² Taking advantage of the continuity of the field around each point the upwind distance ξ from point x_k can be evaluated in order to obtain exact nodal values (Figure 9).

For *quadratic* base interpolating functions ($m = 3$)

$$p^T = [1, x, x^2]$$

and choosing three point clouds ($n = 3$), we have found that *exact* nodal values are obtained if

$$\xi = \frac{h}{2} \alpha \tag{46}$$

$$\left(\frac{\partial\phi}{\partial x}\right)_i = \left(\frac{\partial\phi}{\partial x}\right)_{x_i - \xi}$$

where *h* is defined as

$$h = (x_{i+1} - x_{i-1})/2 \tag{47}$$

Using again quadratic base interpolating functions and five point clouds ($n = 5$), acceptable results are obtained as in quadratic finite elements (also linking five nodes) using

$$\xi = \frac{h}{4} \alpha \tag{48}$$

and evaluating now α by equation (44) with the distance *h* defined as

$$h = (x_{i+2} - x_{i-2})/2 \tag{49}$$

An identical approach can be followed in two and three-dimensional problems. In two-dimensional problems the critical distance *h* is defined now as shown in Figure 10.

6.2. *Characteristic approximation*

Other possibility to solve equation (40) is eliminating the convective term using a Lagrangian description. In this way, the operator becomes self-adjoint, and a central difference scheme may be used. This method is also known as characteristic approach.^{1,35}

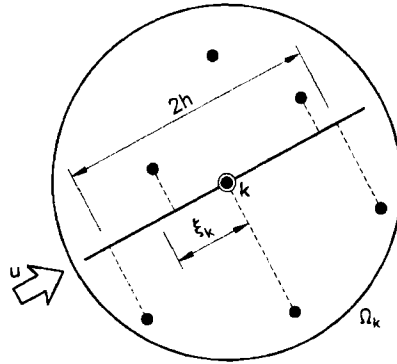


Figure 10. Definition of the critical distance h

Let

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \frac{d\phi}{dt} \tag{50}$$

where the right-hand side represents the temporal variation along the particle path (or characteristic).

Along this path equation (40) now becomes

$$\frac{d\phi}{dt} - \nabla \cdot (k \nabla \phi) - Q = 0 \tag{51}$$

Considering $\phi^n(\mathbf{x})$, the unknown function in a co-ordinate (\mathbf{x}) at time t_n and $\phi^n(\mathbf{x} - \delta)$ the same function at the co-ordinate $\mathbf{x} - \delta$, where $\delta = \mathbf{u}\Delta t$ is a distance along the characteristic. Then

$$\phi^{n+1}(\mathbf{x}) - \phi^n(\mathbf{x} - \delta) = \Delta t [\nabla \cdot k \nabla \phi + Q]^{n+1/2} \tag{52}$$

The following Taylor expansion can now be written in component form^{1,35}

$$\phi^n(x_i - u_i \Delta t) = \phi^n(x_i) - \Delta t u_j \frac{\partial \phi^n}{\partial x_j} + \frac{\Delta t^2}{2} u_i \frac{\partial}{\partial x_i} \left(u_j \frac{\partial \phi}{\partial x_j} \right)^n \tag{53}$$

$$Q^{n+1/2} = Q \left(x - \frac{\delta}{2} \right) = Q^n - u_i \frac{\Delta t}{2} \frac{\partial Q^n}{\partial x_i} \tag{54}$$

Substituting (53) and (54) into (52) finally gives³⁵

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} + \mathbf{u} \cdot \nabla \phi^n - \nabla \cdot (k \nabla \phi)^n - Q^n - \frac{\Delta t}{2} \mathbf{u}^T \nabla [\mathbf{u} \cdot \nabla \phi + Q]^n = 0 \tag{55}$$

Note that the last term may be interpreted as an artificial diffusion in which the term $\Delta t \mathbf{u}$ is a characteristic distance. An interesting particular case arises for $\Delta t \mathbf{u} = \mathbf{h}$ with \mathbf{h} defined (in component form) as shown in Figure 10. The stabilization algorithm is now similar to the upwinding approach described in previous section and identical results are obtained for the examples shown next if Δt is taken to be equal to the critical time step.^{1,35} A generalization of this procedure can be found in Reference 38.

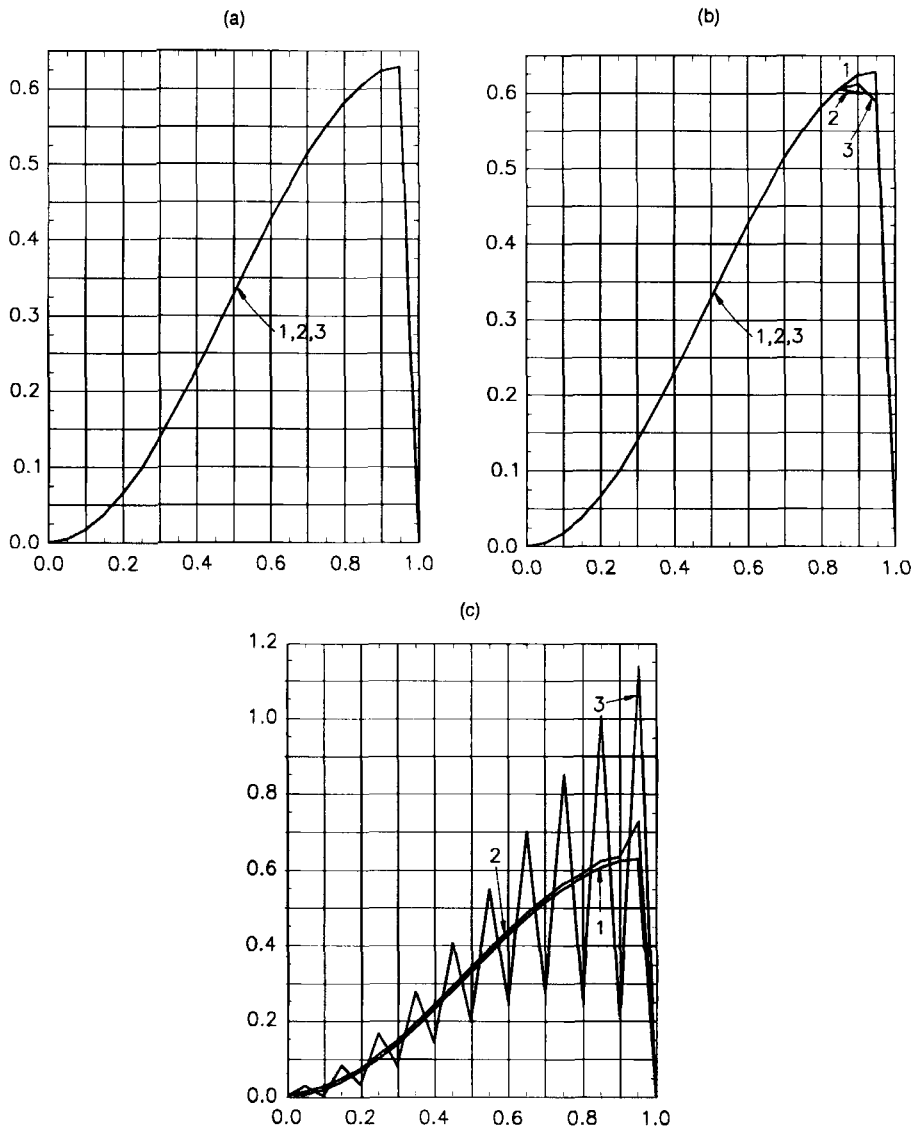


Figure 11. One-dimensional convection–diffusion problem with sinusoidal source term analysed with different clouds: (a) WLS, $n = 3$; (b) WLS, $n = 5$; (c) WLS, $n = 7$. Quadratic base interpolation ($m = 3$) is used in all cases. Curve 1: Analytical curve. Curve 2: Unknown function values $\hat{\phi}(x_i)$. Curve 3: Unknown parameters curve ϕ_i^h

6.3. Numerical examples

Numerical solutions presented here onwards have been obtained with a FPM based on a WLS interpolation using a fixed Gaussian weighting and point collocation. The essential boundary condition have been imposed by using equation (39)²⁸. Numerical results obtained with the standard LSQ approach (and point collocation) are shown in some cases for comparison purposes.

Figure 11 shows steady-state results for equation (40) with a source term

$$Q = \sin \pi x \tag{56}$$

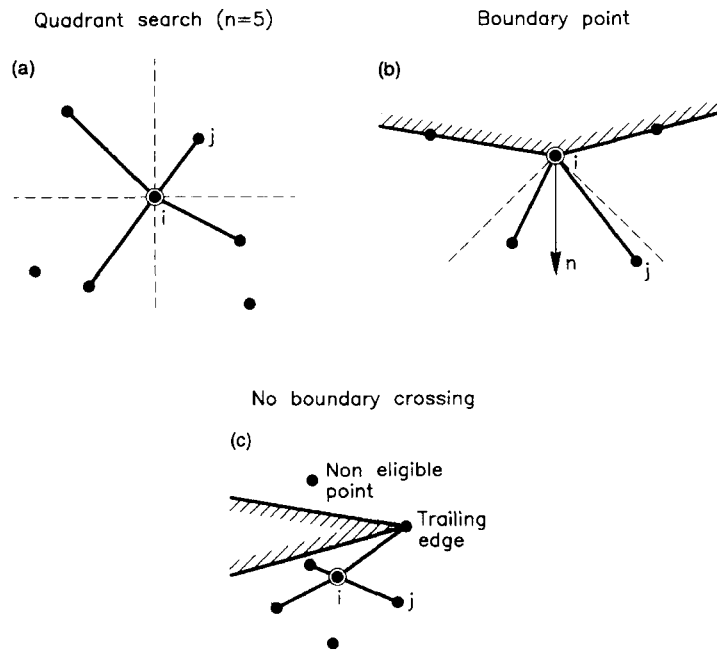


Figure 12. Quadrant technique for selection of points within a cloud: (a) quadrant search ($n = 5$); (b) boundary point; (c) no boundary crossing

and boundary conditions

$$\phi_{(x=0)} = \phi_{(x=1)} = 0 \tag{57}$$

Twenty-one equally spaced points have been used in this case giving

$$Pe = \frac{uh}{2k} = 2.5 \tag{58}$$

Figures 11(a)–11(c) show the numerical results using quadratic interpolation ($m = 3$) and clouds with $n = 3, 5$ and 7 points, respectively. In each figure, the exact results, the approximate function $\hat{\phi}(x_i)$ and the parameters ϕ_i^h are shown. For $n = 3$ both solutions are coincident with the analytical one. A small overdiffusion appears for $n = 5$. Finally, for $n = 7$, the unknown parameters ϕ_i^h are inaccurate but the values obtained for the unknown function $\hat{\phi}$ are acceptable.

The next example is the analysis of a pure two-dimensional thermal diffusion problem in a square domain under a uniform heat source $Q = 10$ using a regular square grid of 7×7 points. A prescribed zero value of the temperature at the boundary has been taken. A quadratic base interpolation ($m = 6$) and clouds containing 10 points ($n = 10$) have been chosen. This test shows the importance of using a WLS approach with ϕ_i functions as described in equation (28) rather than the standard LSQ method ($\phi_i = 1$). In order to select the points involved in each cloud a technique of quadrants has been used consisting in defining a system of orthogonal axes in each point and taking the closest point to the origin of each quadrant. The first set of n points are selected with this criteria (the ‘star’ node and one in each quadrant for $n = 5$). New points must be added to the cloud if the \mathbf{A} matrix defined in (19a) is singular or near singular. The new points were added using the same quadrant criteria for the next nearest points (Figure 12). Figures 13(a)

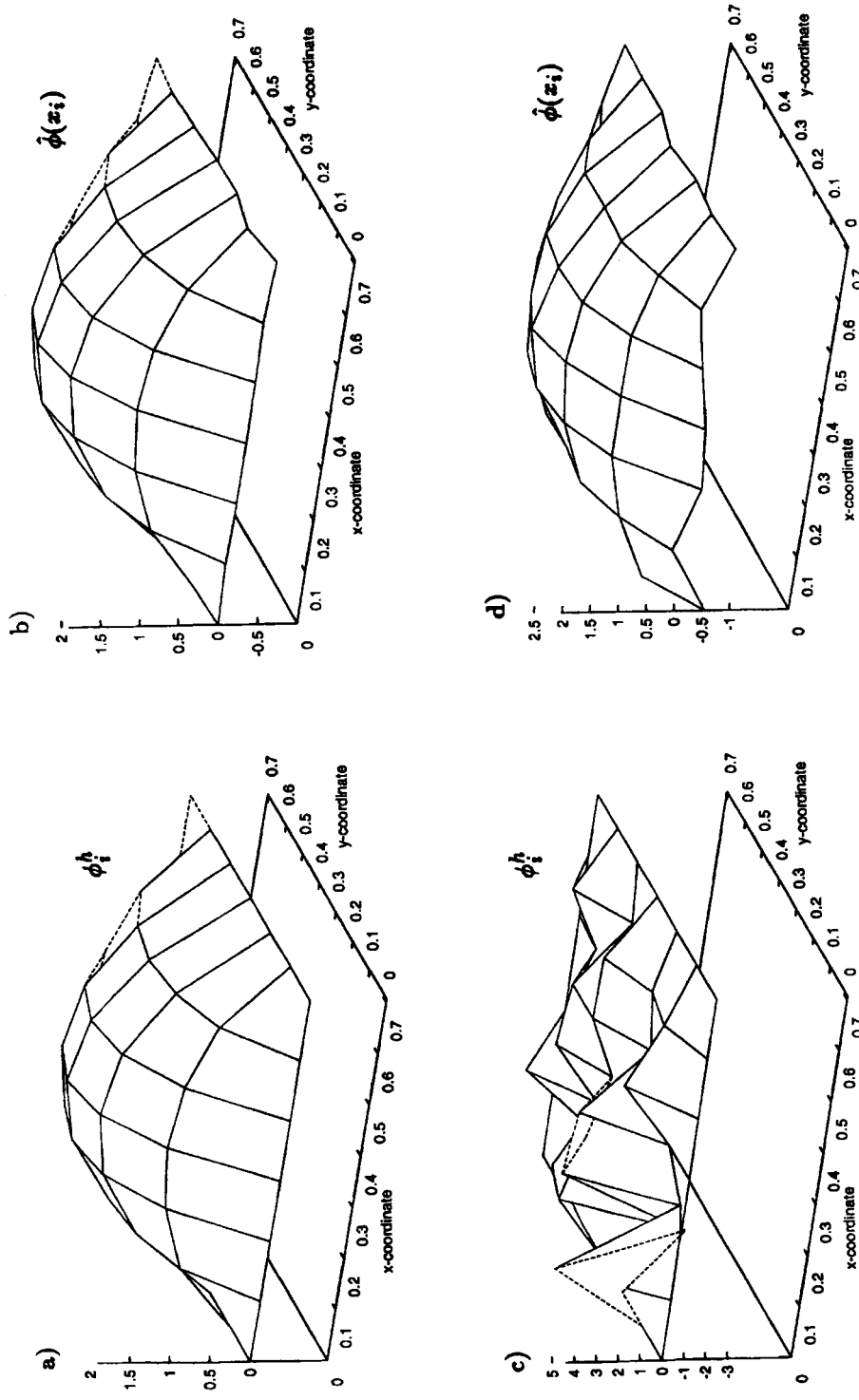


Figure 13. Pure thermal diffusion under constant heat source. 7×7 points grid. Quadratic base interpolation ($m = 6$). Ten points clouds ($n = 10$). Results for ϕ_i^h and $\hat{\phi}(x_i)$ with WLS and LSQ methods: (a) WLS method; (b) WLS method; (c) LLS method; (d) LQ method

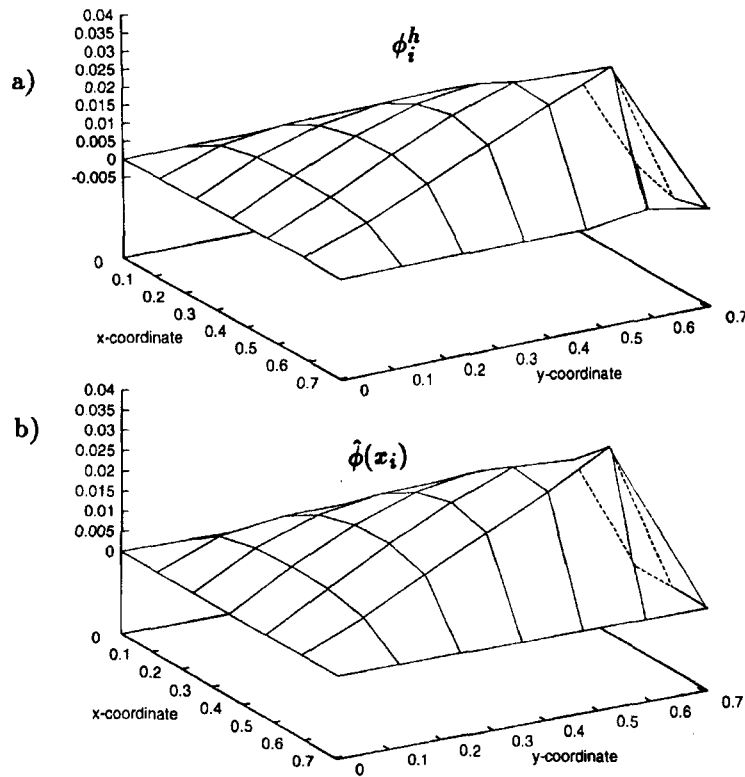


Figure 14. Convection–diffusion problem with diagonal velocity field. 7×7 points grid. Quadratic base interpolation ($m = 6$). Nine points clouds ($n = 9$). Results for ϕ_i^h and $\hat{\phi}(x_i)$ obtained with WLS interpolations and point collocation

and 13(b) show results for the unknown function $\hat{\phi}(x)$ and the unknown parameters ϕ_i^h when φ_i is taken equal to a fixed Gaussian function (equation (28)). Figures 13(c) and 13(d) display the same results for $\varphi_i = 1$ (LSQ method). Note the deterioration of the solution giving non-physical results for the unknown parameters ϕ_i^h for the second case ($\varphi_i = 1$).

Figure 14 shows results for the same example taking into account convection effects. A diagonally oriented field has been chosen giving $Pe = 10$. Quadratic base interpolating polynomials are again used ($m = 6$) and each cloud contains now nine points ($n = 9$). Figure 14(a) shows the unknown function and Figure 14(b) the unknown parameters. The numerical solution is free of oscillations and coincides with the expected result.³⁴

Further evidence of the importance of using a weighted least-squares approximation for solving convection–diffusion problems with this FP method can be found in References 33, 34 and 38.

7. COMPRESSIBLE FLUID FLOW

The proposed FPM will be used now to solve fluid mechanics problems governed by the generalized Navier–Stokes equation

$$\frac{\partial \mathbf{U}}{\partial t} + \mathbf{F}_i \frac{\partial \mathbf{U}}{\partial x_i} + \mathbf{K}_{ij} \frac{\partial^2 \mathbf{U}}{\partial x_i \partial x_j} + \mathbf{Q} = 0 \quad (59)$$

with $\mathbf{U} = [\rho, \rho \mathbf{u}^T]^T$, where ρ and \mathbf{u} are density and the velocity vector, respectively and \mathbf{F}_i and \mathbf{K}_{ij} denote the standard convective and diffusive matrix operators.^{1,35}

The well-known Lax-Wendroff scheme³² has been used giving now after some algebra,¹

$$\frac{\mathbf{U}^{n+1} - \mathbf{U}^n}{\Delta t} + \mathbf{F}_i^n \frac{\partial \mathbf{U}^n}{\partial x_i} + \mathbf{K}_{ij}^n \frac{\partial^2 \mathbf{U}^n}{\partial x_i \partial x_j} + \mathbf{Q}^n + \underline{(\Delta t/2)(\partial/\partial x_i)[\mathbf{F}_i(\partial/\partial x_j)(\mathbf{F}_j \mathbf{U})]^n} + \underline{(\Delta t/2) \mathbf{F}_i^n (\partial/\partial x_i) \mathbf{Q}^n} = 0 \tag{60}$$

where the underline identifies the stabilization terms which have some similarity with those emerging from the characteristic approach (see equation (55)).^{1,35}

This approach has been followed to solve the steady-state Euler equation [$\mathbf{K}_{ij} = \mathbf{0}$] around a NACA 0012 profile with a Mach number at infinity of 0.3 and an angle of attack = 10°.

The problem has again been solved with the FPM and point collocation using both LSQ and WLS (fixed Gaussian weighting) interpolation procedures. The initial distribution of 6694 points was generated with a standard unstructured advancing front triangular mesh generator.³⁶ The essential boundary conditions around the profile and in the incoming flow were imposed by equation (39). A linear base interpolating polynomial ($m = 3$) and clouds of a minimum of five points ($n = 5$) have been chosen.

Second derivatives corresponding to the stabilization diffusion terms in equation (60) were computed by constructing first a linear interpolation of the obtained solution gradients using the same FP procedure as

$$\frac{\partial \hat{\mathbf{U}}}{\partial x_k} = \sum_{i=1}^n N_i \left(\frac{\partial \hat{\mathbf{U}}}{\partial x_k} \right)_i \tag{61}$$

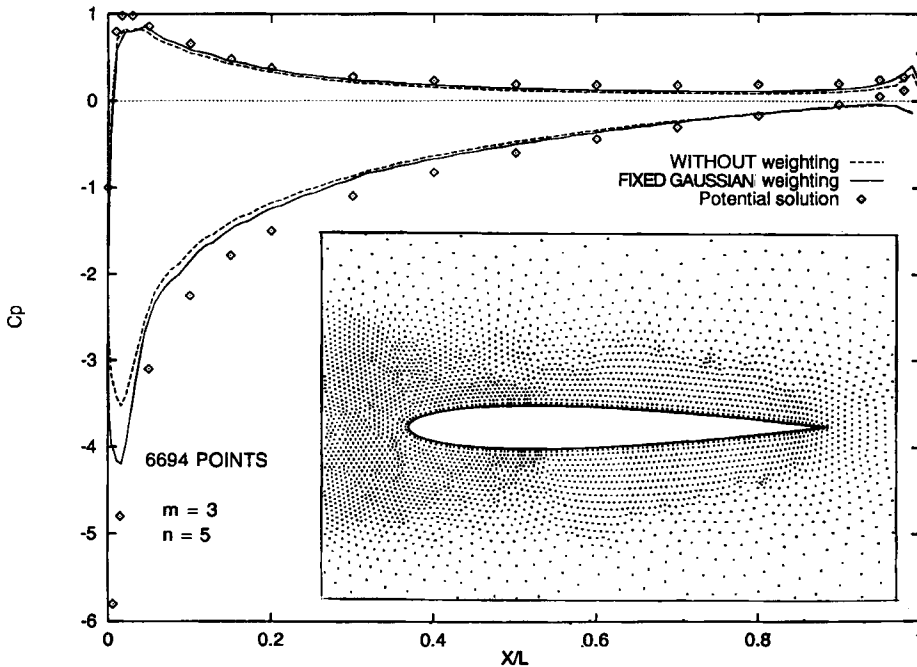


Figure 15. NACA 0012 profile, Mach = 0.3, $\alpha = 10^\circ$. C_p distribution: (- - -) Constant weighting (LSQ), (—) fixed Gaussian weighting (WLS), (\diamond) potential solution

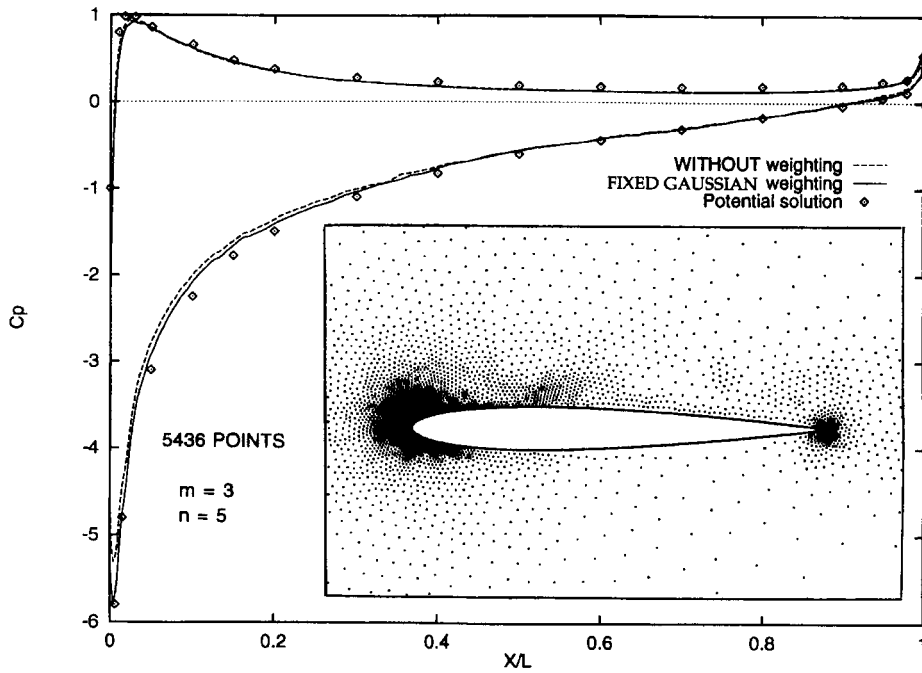


Figure 16. NACA 0012 profile, Mach = 0, 3, $\alpha = 10^\circ$. C_p distribution for an adaptive distribution of points (---) Constant weighting (LSQ), (—) fixed Gaussian weighting (WLS), (\diamond) potential solution

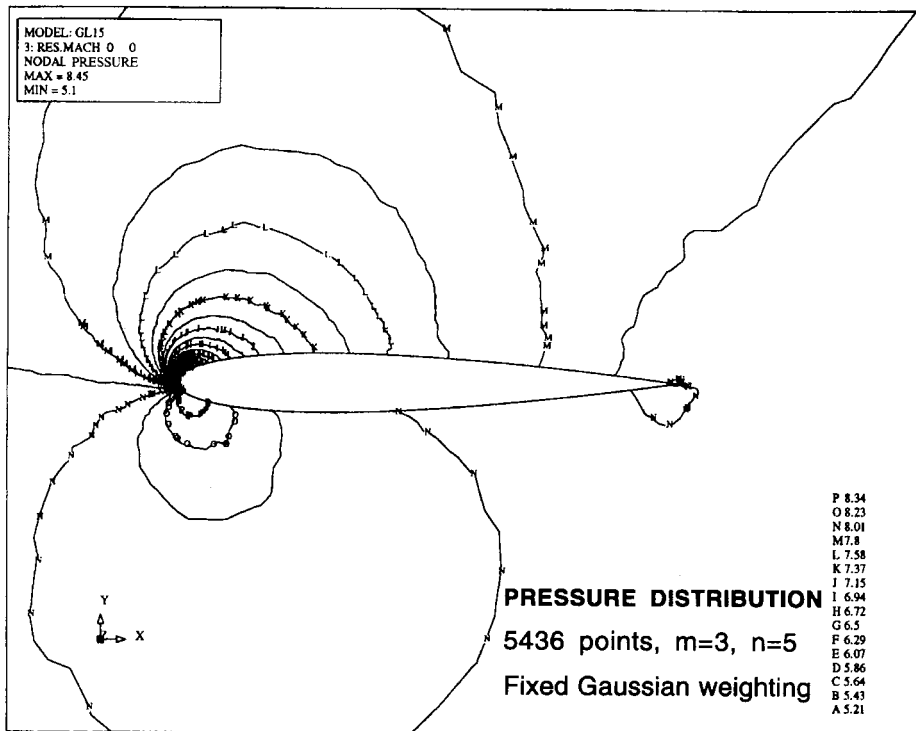


Figure 17. NACA 0012 profile, Mach = 0.3. Pressure distribution

which finally gives

$$\frac{\partial}{\partial x_j} \left(\frac{\partial \hat{U}}{\partial x_k} \right) = \sum_{i=1}^n \frac{\partial N_i}{\partial x_j} \left(\frac{\partial \hat{U}}{\partial x_k} \right)_i^h \quad (62)$$

Figure 15 shows the distribution of the pressure coefficient C_p around the profile obtained with the FPM with Gaussian weighting (WLS) and constant weighting (LSQ). The potential solution is also plotted in the figure for comparison purposes. Note the higher accuracy of the WLS method as expected. This difference becomes greater if the number of points is increased. It was found that for $n \geq 10$ the results become unstable for the LSQ approximation.

Figure 16 shows a more accurate solution using a cloud of 5436 points obtained after an adaptivity criteria based on the curvature of the solution as suggested in Reference 1. Figure 17 shows the pressure distribution which also agrees with the expected result.³²

Further examples of the solution of fluid flow problems using the FPM can be found in References 33, 34 and 38.

8. CONCLUDING REMARKS

The weighted least-squares interpolation combined with a simple point collocation technique is a promising Finite Point Method for the numerical solution of computational mechanics problems. The advantage of the method compared with standard FEM is to avoid the necessity of mesh generation and compared with classical FDM is the facility to handle the boundary conditions and the non-structured distribution of points.

The method proposed seems to be as accurate as other numerical methods for convective transport and fluid flow problems and the computing time to solve the differential equation is of the same order as for methods using non-structured grids.

Another interesting conclusion is the comparison with other FPM presented in the literature. Firstly, the use of a Gaussian weighting function improves considerably the results with respect to the standard LSQ approach.^{29,33} Secondly, the sensitivity of a FPM to a variable number of points in each cloud must be low enough to preserve the freedom of adding, moving or removing points. This sensitivity is very high in FPM using the LSQ approximation, it is large in WLS and MLS methods with linear base interpolations and it quite low in WLS and MLS methods using quadratic base interpolations.

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