

## 16. The MPM mapping

For the MPM method, the basis used for the approximation function is selected independently from the particle locations. The problem is:

*Given a set of particle locations  $\{\mathbf{x}_1, \dots, \mathbf{x}_N\}$  at which data  $\{f_1, \dots, f_N\}$  are known, construct a function  $F(\mathbf{x})$  that approximates a function  $f(\mathbf{x})$  for which  $f(\mathbf{x}_p) = f_p$ . Since the equations of physics are most general in integral form (and since, in practice, nothing is ever measured at a point), it is not necessary for  $F(\mathbf{x}_p) = f_p$ , but it is desirable to minimize error over a finite domain containing the particle.*

At each time step MPM makes use of an overlay grid that is selected for convenience. The key feature of MPM is that the approximating function  $F(\mathbf{x})$  is constructed at each time step in terms of basis functions defined with respect to the nodes of the *overlay grid*.

Suppose that the particle data correspond to discrete values of some desired function  $f(\mathbf{x})$ . We seek to construct a function  $F(\mathbf{x})$  that approximates the exact function  $f(\mathbf{x})$ . In particular, using the overlay grid, we seek to construct an approximating function  $F$  of the form

$$F(\mathbf{x}) = \sum_{j=1}^n F_j N_j(\mathbf{x}) \quad (16.1)$$

where  $N_j(\mathbf{x})$  are nodal basis functions on the grid.

The approximation error can be quantified by a mass-weighted\* least-squares residual functional as

$$E = \int_{\Omega} [F(\mathbf{x}) - f(\mathbf{x})]^2 \rho dV \quad (16.2)$$

Thus, the error depends on the nodal values assigned for the approximation function:

$$E(F_1, \dots, F_n) = \int_{\Omega} \left[ \left( \sum_{i=1}^n F_i N_i(\mathbf{x}) \right) - f(\mathbf{x}) \right]^2 \rho dV \quad (16.3)$$

To minimize the error, we set

$$\frac{\partial E}{\partial F_j} = 0 \quad (16.4)$$

or

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\* This analysis can be easily revised to use volume weighting.

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$$2 \int_{\Omega} \left[ \left( \sum_{i=1}^n F_i N_i(\mathbf{x}) \right) - f(\mathbf{x}) \right] N_j(\mathbf{x}) \rho dV = 0 \quad (16.5)$$

Rearranging a bit gives

$$\sum_{i=1}^n F_i m_{ij} = b_j, \quad (16.6)$$

where  $m_{ij}$  is the consistent mass matrix defined by

$$m_{ij} \equiv \int_{\Omega} N_i(\mathbf{x}) N_j(\mathbf{x}) \rho dV \quad (16.7)$$

and

$$b_j \equiv \int_{\Omega} f(\mathbf{x}) N_j(\mathbf{x}) \rho dV \quad (16.8)$$

To simplify these integrals, the overlay grid's nodal basis functions are typically selected to have compact support. In conventional practice, the above integrals over the entire domain are split without loss of generality into integrals over element sub-domains  $\Omega_e$ :

$$\begin{aligned} m_{ij} &= \sum_e m_{ije}, \text{ where } m_{ije} \equiv \int_{\Omega_e} N_i(\mathbf{x}) N_j(\mathbf{x}) \rho dV \\ \text{and } b_j &= \sum_e b_{je}, \text{ where } b_{je} \equiv \int_{\Omega_e} f(\mathbf{x}) N_j(\mathbf{x}) \rho dV \end{aligned} \quad (16.9)$$

The summation over  $e$  ranges from 1 to the number of elements. Consider, for example, one dimensional problems. Let the nodes be ordered sequentially from 1 to  $n$ . Let the  $i^{\text{th}}$  element be defined as the region between  $x_i$  and  $x_{i+1}$ . Then within that element, only two nodal shape functions are nonzero:

$$\begin{aligned} N_i(x) &= 1 - \left( \frac{x - x_i}{h_i} \right) \quad \text{over the } i^{\text{th}} \text{ element} \\ N_{i+1}(x) &= \frac{x - x_i}{h_i} \quad \text{over the } i^{\text{th}} \text{ element} \\ \text{all other } N_i &= 0 \quad \text{over the } i^{\text{th}} \text{ element} \end{aligned} \quad (16.10)$$

where  $h_i \equiv x_{i+1} - x_i$ . Consequently, for constant mass density  $\rho = \rho_e$  within the element (which is used here only for illustration),

$$m_{ije} = \begin{cases} \frac{\rho_e h_e}{3} & \text{if } i=j \\ \frac{\rho_e h_e}{6} & \text{if } i \neq j \end{cases} \quad \text{for } i \text{ and } j \text{ taking values } e \text{ and } e+1 \quad (16.11)$$

and  $m_{ije} = 0$  for any other values of  $i$  and  $j$ .

and, for a constant  $f(x) = f_e$  within the element (again, assumed here only for illustration),

$$b_{je} = f_e \rho_e \int_{\Omega_e} N_j(x) dx \quad (16.12)$$

If the density field and the exact field  $f(\mathbf{x})$  were known for all points  $\mathbf{x}$ , then the integral of Eq. (16.8) could be computed exactly and Eq. (16.6) could then be solved for the approximation coefficients  $\{F_i\}_{i=1}^n$ . The resulting coefficients would then minimize the error of the approximating function. If, for example, the grid basis functions are simple linear tent functions, then the resulting approximation gives an the optimal piecewise linear fit to the data.

For the discrete problem, neither the function  $f(\mathbf{x})$  nor the density field is known for all positions  $\mathbf{x}$ . Instead, the values of these fields are known only at the discrete particle positions  $\{\mathbf{x}_p\}_{p=1}^N$ . Each particle  $\mathbf{x}_p$  is presumed to lie at the center of a compact subregion of space  $\Omega_p$  that does not overlap (or form gaps) with the similar subregions of other particles. Because these subregions tessellate the total domain  $\Omega^*$ , there is no loss in generality in writing Eq. (16.8) as

$$b_j \equiv \sum_{p=1}^N \int_{\Omega_p} f(\mathbf{x}) N_j(\mathbf{x}) \rho(\mathbf{x}) dV \quad (16.13)$$

Now we only need a good approximation for the integral over a single particle's domain. The lowest fidelity approach is to use a single Gauss point at the single location where the function is known. Namely

$$\int_{\Omega_p} f(\mathbf{x}) N_j(\mathbf{x}) \rho(\mathbf{x}) dV \approx f(\mathbf{x}_p) N_j(\mathbf{x}_p) M_p \quad (16.14)$$

Without examining the values of the  $f$  and  $\rho$  fields at neighboring points, we have no information about how these fields vary over the particle domain  $\Omega_p$ . However, relative to the peak values of these fields over the entire domain  $\Omega$ , it is reasonable to assume that their variation over any particle domain  $\Omega_p$  is a miniscule percentage of their peak value in the total domain  $\Omega$ . Variation of the element shape functions, on the other hand, is not

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\* These subregions might be, say, Voronoi cells about the particles, and these subregions should not be confused with the influence domains for particles, which do overlap [see Fig. 16.4].

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reasonably assumed negligible (if, for example, the particle domain is half as large as the element domain,  $N_j(\mathbf{x})$  can vary over a particle domain by as much as 50% of its peak value of 1. Therefore, assuming that only the physical fields ( $f$  and  $\rho$ ) are approximately constant over the particle, but the shape function are not constant,

$$\int_{\Omega_p} f(\mathbf{x}) N_j(\mathbf{x}) \rho dV \approx f(\mathbf{x}_p) M_p v_{jp}, \quad (16.15)$$

where  $v_{jp}$  is the average of the  $j^{\text{th}}$  shape function over the physical (e.g. Voronoi) domain associated with particle  $p$ .

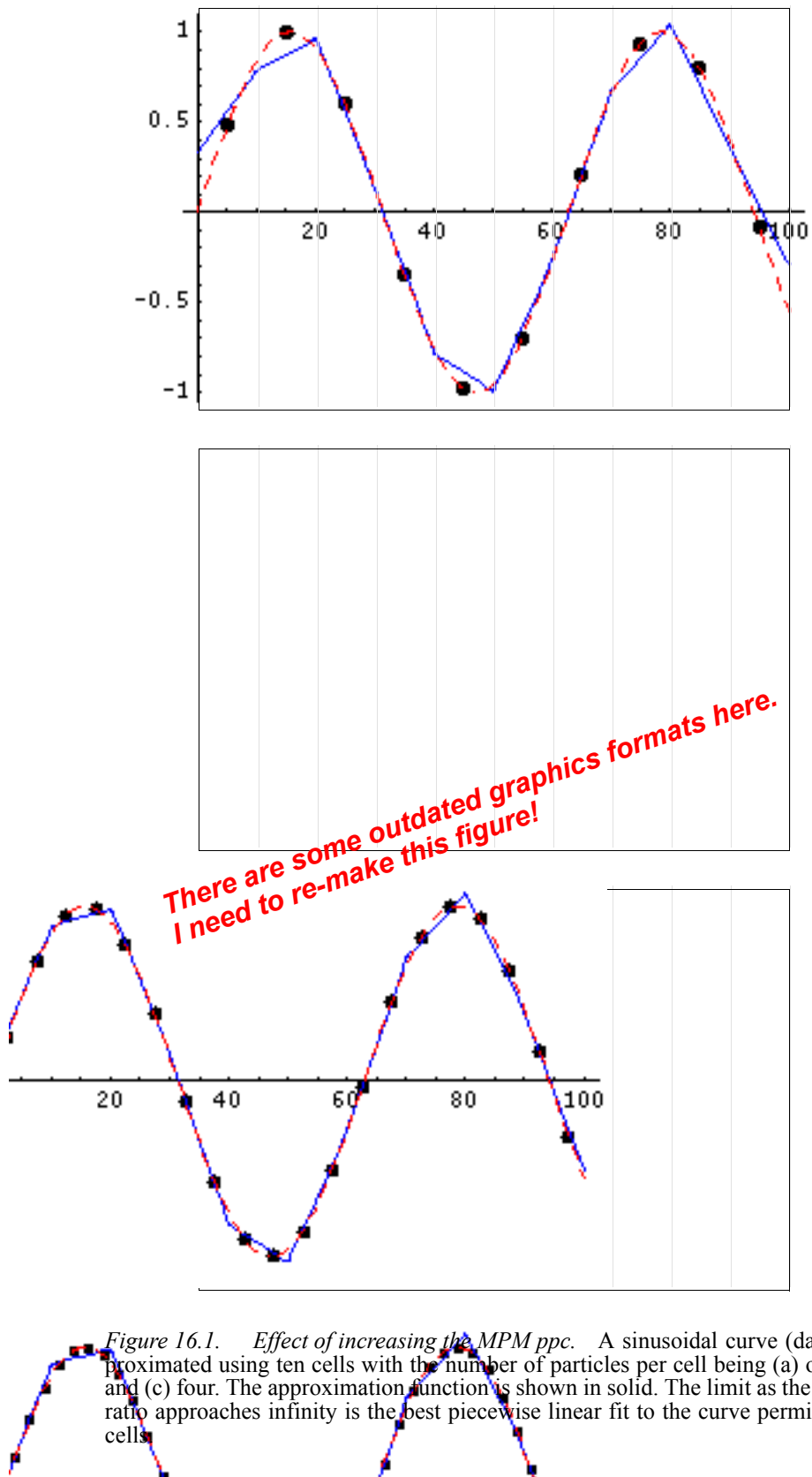
$$v_{jp} \equiv \frac{1}{V^p} \int_{\Omega_p} N_j(\mathbf{x}) dV \quad (16.16)$$

The final expression for the approximation coefficients follows from substituting (16.15) into (16.13), which is then substituted back into (16.6) to give

$$\sum_{i=1}^n F_i m_{ij} = \sum_{p=1}^N f_p M_p v_{jp} \quad (16.17)$$

This equation must be solved for the approximation coefficients  $\{F_i\}_{i=1}^n$ .

**The approximation function  $F(\mathbf{x})$  does not equal the data at  $F(\mathbf{x}_p)$ , nor was it intended to. Error in the approximation should not be considered pointwise. Instead, a better quantifier of the local error at a point is an integral norm of  $F(\mathbf{x}) - f(\mathbf{x})$  over the particle's implied influence domain (which, as discussed in the next section, is larger than the particle's physical domain -- see Fig. 16.4).**



## Effect of using lumped integrals

*Effect of lumped mass.* Recall the definition

$$m_{ij} \equiv \int_{\Omega} N_i(\mathbf{x}) N_j(\mathbf{x}) \rho dV \quad (16.18)$$

Without loss in generality, we may break this integral into a sum over particle sub-domains to give

$$m_{ij} \equiv \sum_{p=1}^N M_p \mu_{ijp}, \quad (16.19)$$

where  $\mu_{ijp}$  is the mass average of the nodal basis product over the particle domain:

$$\mu_{ijp} \equiv \frac{1}{M_p} \int_{\Omega_p} N_i(\mathbf{x}) N_j(\mathbf{x}) \rho dV \quad (16.20)$$

The lumped mass matrix is the diagonal matrix obtained by a row sum of the consistent mass matrix:

$$m_i \equiv \sum_{j=1}^n m_{ij} = \int_{\Omega} N_i(\mathbf{x}) \left( \sum_{j=1}^n N_j(\mathbf{x}) \right) \rho dV \quad (16.21)$$

Assuming the nodal basis functions have the partition of unity property, the summation inside the integral is given by simply

$$m_i = \int_{\Omega} N_i(\mathbf{x}) \rho dV \approx \sum_{p=1}^N M_p v_{ip}, \quad \text{where } v_{ip} \equiv \frac{1}{V} \int_{\Omega_p} N_i(\mathbf{x}) \rho dV \quad (16.22)$$

With a lumped mass, the approximation coefficients are easily computed by

$$F_i = \frac{1}{m_i} \left( \sum_{p=1}^N f_p M_p v_{ip} \right) = \frac{\sum_{p=1}^N f_p M_p v_{ip}}{\sum_{p=1}^N M_p v_{ip}} = \sum_{p=1}^N f_p \psi_{ip} \quad (16.23)$$

where

$$\psi_{ip} \equiv \frac{M_p v_{ip}}{\sum_{q=1}^N M_q v_{iq}} \quad (16.24)$$

**Implied particle basis function.** It will be shown in this section that MPM falls into the general category of particle methods that approximate fields by a sum of coefficients times compact *particle* basis functions. The beauty of MPM is that, even though particle basis functions exist, they are never constructed explicitly, which gives MPM an “efficiency edge” over other particle methods.

As illustrated in Figs. 16.2 and 16.4, particles in MPM have *non-overlapping* physical domains (e.g. Voronoi cells), which likewise are not usually computed explicitly\* — they merely exist. In addition to the non-overlapping physical domains, particles in MPM have *overlapping* domains of influence with compact support (i.e., domains over which the implied particle basis function is nonzero). When a Dirac formulation is used [i.e., when  $v_{jp}$  in Eq. 16.16 is approximated by  $N_j(\mathbf{x}_p)$ ], the influence domain of an MPM particle is the union of the support domains of any overlay grid node that is nonzero at the particle. Suppose, for example, that a particle lies between nodes  $k$  and  $k+1$  in a 1D simulation. Then the influence domain for the particle basis function lies between nodes  $k-1$  and  $k+2$  because the grid’s nodal shape functions  $N_k(x)$  and  $N_{k+1}(x)$  are nonzero between those nodes. If a particle resides exactly at node  $k$ , then its influence domain is identical to the support domain (from node  $k-1$  to  $k+1$ ) of node  $k$ .

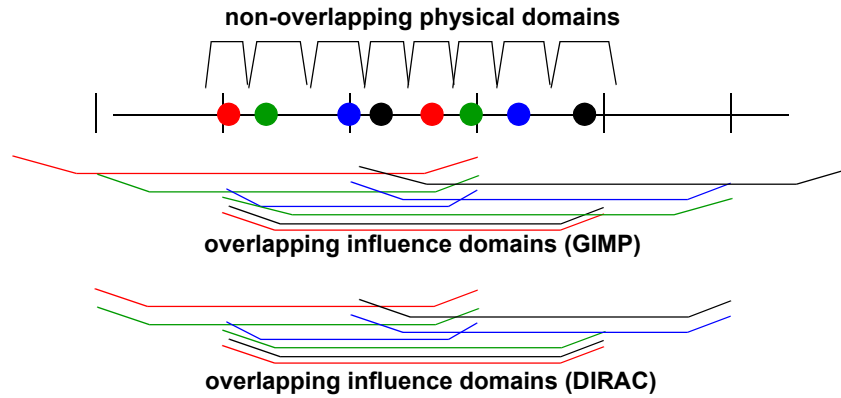


Figure 16.2. Distinction between physical domains and influence domains. In this figure, the influence domains for all particles overlap in the center. Hence, all of those particles influence the approximation function at the center. The relative weight of each contribution increases with proximity to the evaluation point.

When a GIMP-like scheme is used for  $v_{jp}$  in Eq. 16.16, then the particle’s influence domain is the union of nodal support domains associated with each nodal shape function that is nonzero *anywhere* on the particle’s physical domain  $\Omega_p$ .

\* The compact domain over which an interpolation function is unity in a GIMP method can be viewed as an approximation to the particle’s non-overlapping physical domain, which is why it is advisable to evolve these domains with the deformation so that they remain non-overlapping.

## The MPM mapping

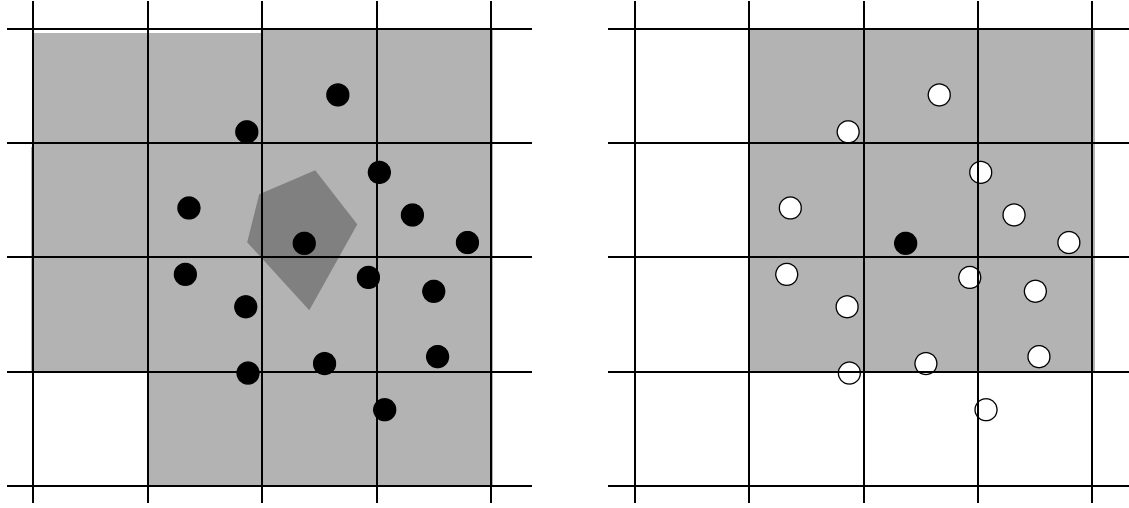


Figure 16.3. LEFT: Physical domain (dark gray) and influence domain (light gray) for piecewise constant GIMP-style weighting over the Voronoi-based physical domain. The influence domain is the union of support domains for all nodal basis functions that are nonzero over any part of the physical domain. RIGHT: influence domain when using a Dirac delta formulation (which, in essence, shrinks the physical domain to a Dirac delta point at the particle location)

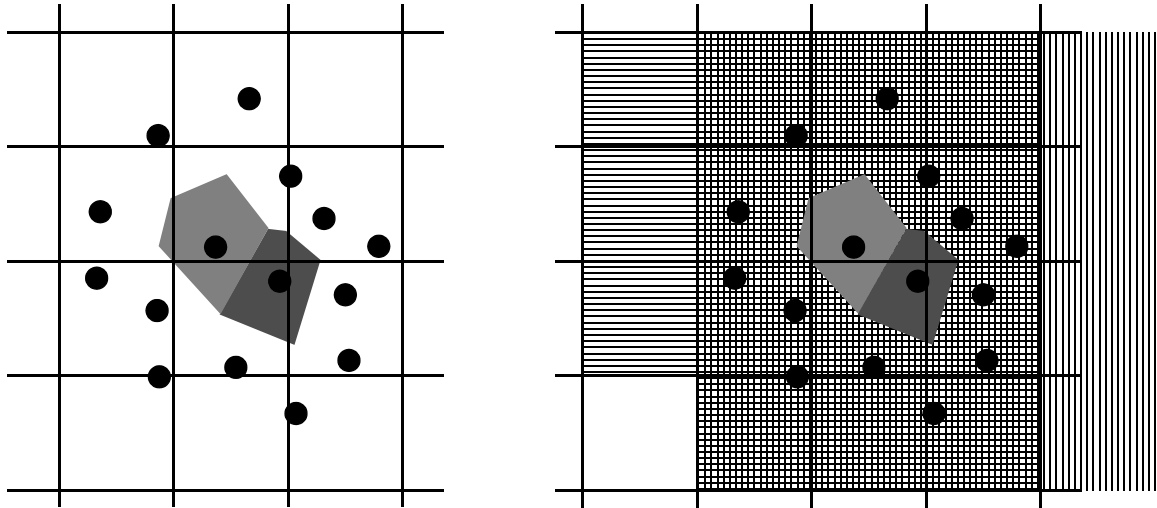


Figure 16.4. LEFT: Non-overlapping physical domains. RIGHT: overlap of influence domains (cross-hatched)

Recall that the approximation field is carried on the grid so that

$$F(\mathbf{x}) = \sum_{i=1}^n F_i N_i(\mathbf{x}) \quad (16.25)$$

where  $N_i(\mathbf{x})$  is the  $i^{\text{th}}$  nodal basis function on the grid and  $F_i$  is the nodal value of the field on the grid. Substituting (16.17) into (16.25),



$$F(\mathbf{x}) = \sum_{i=1}^n \sum_{j=1}^n m_{ij}^{-1} \left( \sum_{p=1}^N f_p M_p v_{jp} \right) N_i(\mathbf{x}) \quad (16.26)$$

Here,  $f_p$  is the field value at the  $p^{\text{th}}$  particle,  $M_p$  is the particle mass,  $m_{ij}^{-1}$  is the  $ij$  component of the inverse of the consistent mass matrix, and

$$v_{jp} \equiv \frac{1}{V_p} \int_{\Omega_p} N_j(\mathbf{x}) dV, \quad (16.27)$$

where  $\Omega_p$  is the particle's physical domain and  $V_p$  is its volume. The summation order in Eq. (16.26) can be rearranged without loss to write

$$F(\mathbf{x}) = \sum_{p=1}^N f_p \sum_{i=1}^n m_{ij}^{-1} M_p v_{jp} N_i(\mathbf{x}) \quad (16.28)$$

The *particle* basis function  $\Phi_p(\mathbf{x})$  is defined such that

$$F(\mathbf{x}) = \sum_{p=1}^N f_p \Phi_p(\mathbf{x}) \quad (16.29)$$

Comparing the coefficients of  $f_p$  in the above two equations gives

**Implied particle basis function**

$$\Phi_p(\mathbf{x}) = \sum_{i=1}^n N_i(\mathbf{x}) \psi_{ip}, \quad \text{where } \psi_{ip} = \sum_{j=1}^n m_{ij}^{-1} M_p v_{jp}. \quad (16.30)$$

If a lumped mass is used, then

$$\psi_{ip} \equiv \frac{M_p v_{ip}}{m_i} = \frac{M_p v_{ip}}{\sum_{q=1}^n M_q v_{iq}} \quad (16.31)$$

The particle influence domain is the set of points in space over which  $\Phi_p(\mathbf{x})$  is nonzero. Hence, the particle influence domain is the union of nodal support domains associated with the smallest set of grid elements that fully enclose  $\Omega_p$ .

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The implied MPM particle basis functions have the following properties (at least for a lumped mass): *(I need to double check these claims because it has been years since I first wrote this set of notes!)*

- (i)  $\Phi_p(\mathbf{x}_q) \neq \delta_{pq}$  (UNLIKE nodal basis functions, the MPM mapping is not an interpolation, but that's a *good* thing -- the MPM mapping better preserves *integrals* by also minimizing overall error for most non-pathological functions)
- (ii) Partition of unity:  $\sum_{p=1}^N \Phi_p(\mathbf{x}) = 1$  (inherited from nodal basis functions)
- (iii) Linear completeness:  $\sum_{p=1}^N \mathbf{x}_p \Phi_p(\mathbf{x}) = \mathbf{x}$  (inherited)
- (iv) Piecewise differentiable. (inherited)
- (v) The basis  $\Phi_p(\mathbf{x})$  is not symmetric about the particle, not even for uniform particle spacings. (UNLIKE nodal basis functions)
- (vi) Two particles with identically shaped physical domains will not generally have identically shaped particle basis functions unless their positions relative to the overlay grid are identical.
- (vii) Two particles will have identical influence domains if their physical domains are contained (entirely) within a shared grid element.
- (viii) Positivity:  $0 \leq \Phi_p(\mathbf{x}) \leq 1$  for all  $\mathbf{x}$ .
- (ix) Monotonicity (inherited): within the particle's influence domain, there exists a point  $\mathbf{x}_\Pi$ , not generally coincident with  $\mathbf{x}_p$ , for which  $\Phi_p(\mathbf{x}_\Pi)$  is maximum and, for any unit vector  $\mathbf{u}$ ,  $\Phi_p(\mathbf{x}_\Pi + \alpha \mathbf{u})$  decreases monotonically to a minimum value of 0 over all  $\alpha > 0$ . *I'm not absolutely sure about this one in 2D and 3D since, for a non-rectangular grid, the influence domain is not necessarily convex.*
- (x) Galilean invariant if both the grid and particles translate rigidly *together* (i.e.,  $\Phi_p(\mathbf{x})$  becomes  $\Phi_p(\mathbf{x} - \mathbf{u})$  in response to a rigid displacement  $\mathbf{u}$ ). (inherited)
- (xi) Not Galilean invariant if the particles translate rigidly relative to the grid or vice versa. If all particles are translating with velocity  $\dot{\mathbf{x}}_p$  relative to a fixed grid, the quantity  $v_{ip}$  varies with time according to  $\dot{v}_{ip} = \bar{\mathbf{G}}_i \bullet \dot{\mathbf{x}}_p$ , where  $\bar{\mathbf{G}}_i$  is the average of the  $i^{\text{th}}$  shape function gradient over the particle's physical domain.
- (xii) Globally Galilean:  $\frac{d}{dt} \int_{\Omega^*} \Phi_p(\mathbf{x}; t) dV = 0$  over any compact domain  $\Omega^*$  that encloses the particle's influence domain.  
(i.e., even though the function  $\Phi_p(\mathbf{x}; t)$  varies pointwise with time and even though the particle's physical influence and physical domains change over time) this volume integral remains constant, which is what

is really important physically in conservation principles — the concept of function values at a point is unnecessary and nonphysical. All that matters is moving averages over small domains).

- (xiii) Lagrangian invariant (i.e.,  $\frac{D\Phi_p}{Dt} = 0$ ) under homogeneous deformation if the grid also moves with the material. Otherwise, not Lagrangian invariant.
- (xiv) The particle basis function  $\Phi_p(\mathbf{x})$  equals the approximation function  $F(\mathbf{x})$  corresponding to  $f_p = 1$  and zero at all other particles.

The solid lines in Fig. 16.5 show the 1-dimensional MPM particle basis functions corresponding to simple linear grid basis functions and three particles per cell with a Dirac evaluation of  $v_{ip}$ . This figure illustrates how simple translation of the particles relative to the grid causes the particle basis functions to change even though the particle data do not change. Importantly, however, the *integral* over the particle basis does *not* vary with particle motion.

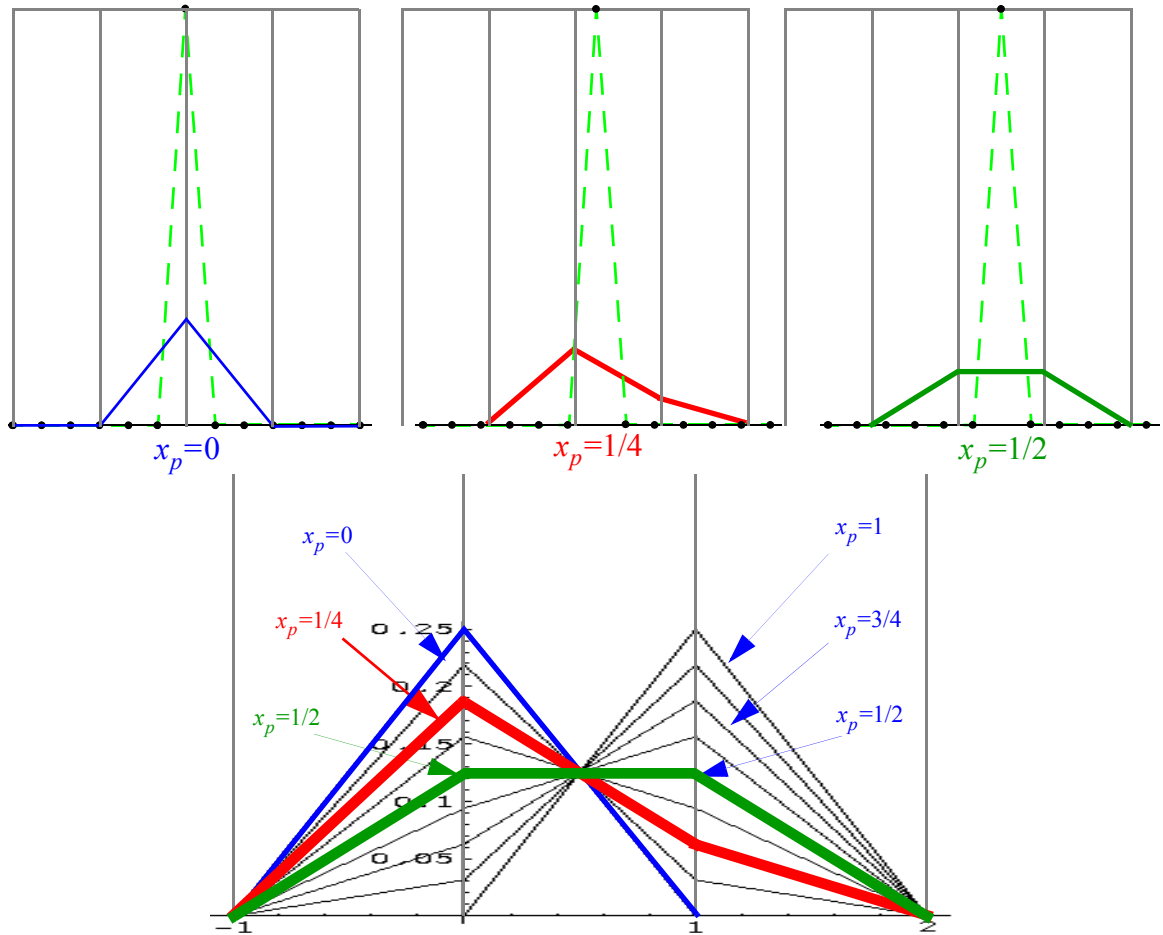


Figure 16.5. Effect of particle translation on particle basis. This figure shows how the particle basis function  $\Phi_p(x)$  changes as  $x_p$  and all other particles translate rigidly relative to a fixed grid. The dashed line shows an ordinary point-to-point interpolation and the solid line shows the MPM approximation to the data.