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Conservation of Momentum and Tensile Instability in Particle Methods

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ABSTRACT

This paper considers conservation of momentum and tensile instability in transient dynamic particle methods. Local particle methods are defined as representing a continuous body with particles which discretize the body. The particles carry the field variables and are used for interpolation purposes. They also are discrete chunks of matter which must have mass and volume which in sum represent the total mass and volume of the body. In particle methods, a function is approximated by summing data-weighted shape functions over the particles. Conservation of momentum is considered from the standpoint of Newton's third law, and the conditions which the shape functions must satisfy in order to conserve momentum are derived. The tensile instability is considered from the standpoint of the strength of interaction between particles, and the concept of area vectors which define the surfaces on which the stresses act is introduced. The local nature of the approximation is shown to produce area vectors and forces which decrease as the distance between particles increases. This situation is shown to be similar to other particle systems, such as gravitational systems of particles or molecular dynamics. The instability is shown to be the expected behavior of the physical system represented by the discretization scheme. Finally, these concepts are applied to a specific example, that of moving least squares.

1. Introduction

This paper considers conservation of momentum and tensile instability in transient dynamic particle methods. Local particle methods are defined as representing a continuous body with particles which discretize the body. The particles carry the field variables and are used for interpolation purposes. They also are discrete chunks of matter which must have mass and volume which in sum represent the total mass and volume of the body. If a background mesh is used for integration, the particles are really only generalized integration points, and the background mesh discretizes the body. Such a technique does not constitute a particle method as defined here. In particle methods, a function is approximated by summing data-weighted shape functions over the particles. If the shape functions are non-zero only over a finite range, the method is called local. Conservation of momentum is considered from the standpoint of Newton's third law, and the conditions which the shape functions must satisfy in order to conserve momentum are derived. The tensile instability is considered from the standpoint of the strength of interaction between particles, and the concept of area vectors which define the surfaces on which the stresses act is introduced. The local nature of the approximation is shown to produce area vectors and forces which decrease as the distance between particles increases. This situation is shown to be similar to other particle systems, such as gravitational systems of particles or molecular dynamics. The instability is shown to be the expected behavior of the physical system represented by the discretization scheme. Finally, these concepts are applied to a specific example, that of moving least squares.

2. Definition of Local Particle Method

The definition of a local particle method starts from Smoothed Particle Hydrodynamics, or SPH [Swegle et al. 1994], a gridless Lagrangian transient dynamics numerical technique suitable for large deformation situations in which mesh distortion would render a grid-based method useless. Mesh distortion is circumvented by replacing grid-based approximations for spatial derivatives with a kernel-based approximation applicable to an arbitrary distribution of data points. Thus, the grid is replaced with a set of particles which carry all the field variables of interest, such as position, velocity, stress, mass, density, etc. From one perspective, the particles are interpolation points to which the kernel-based approximation is applied to produce spatial gradients. However, since the particles discretize the body, they are also discrete chunks of matter which must have mass and volume which in sum represent the total mass and volume of the body. The particles must be distributed so that the number density of particles represents the density of the body, and the mass and volume of each particle reflect the correct density at that location. For equal mass particles, fewer particles means lower density, and where there are no particles, there is no body (a void). If the particles are unevenly distributed, the masses and volumes must be adjusted to reflect the actual material density at each spatial location. The particles have a volume which extends for some distance (radius) from the center of the particle, which defines the particle coordinates. At a boundary, the edge (outer radius) of the particle must coincide with the boundary, not the center of the particle.

Thus, there are no particles whose coordinates lie on the boundary. If there were, a somewhat larger body would actually be represented.

Thus, even though the method is gridless, there is still a form of meshing which must be done to ensure that the spatial extent of the body and variations in density are correctly represented by the particles. In other words, the particles must be initially distributed so that they discretize the bodies involved in much the same way that a grid does. This may be less difficult than filling the volume of the body with polygons due to fewer constraints on the connectivity of the particles, but it is still a type of meshing.

The motion of the particles is governed by the divergence of the stress tensor. In other words, the particles move in response to the stress gradient, which is found by performing a local fit to the stresses carried by the particles in the neighborhood of the particle being accelerated. Since SPH is intended for large deformations, each particle's neighbor set must be allowed to vary as deformation and flow occur. Thus, a search for the neighbors of a given particle must be performed at each time step, and the stress gradient determined by the neighbor set is used to move the particle.

The kernel-based spatial gradient approximation used in SPH is basically a curve fit to the data values at the interpolation points in the neighborhood of the location at which the gradient is being approximated. The fit is performed by first multiplying the data value at each neighboring point by an SPH kernel function (usually a cubic b-spline), so that the kernel function at each particle is in effect weighted by the data value at that particle. The kernel function has compact support (is zero beyond some radius), so that only local neighbors enter into the sums. A continuous function is obtained from the discrete data by summing the weighted kernels, so that

$$f(x) = \sum_{J=1}^N Vol^J f^J W(|x - x^J|, h), \quad (EQ 1)$$

where bold-face symbols indicate a vector quantity, the volume is given by

$$Vol^J = \frac{m^J}{\rho}, \quad (EQ 2)$$

the f^J are the discrete data values, W is the kernel function, $|x - x^J|$ is the distance from x to x^J , and h is the smoothing length, related to the radius beyond which the kernel function is zero. This process is illustrated graphically in Figure 1. This continuous function is then differentiated to find spatial derivatives. Only the kernel function itself depends on the spatial coordinate with respect to which the derivative is taken, so derivatives can be found from the data values and the gradient of the kernel function, as in

Figure 1. Continuous function from summing weighted kernels

$$\nabla \cdot f(x) = \sum_{J=1}^N Vol^J f^J \cdot \nabla W(|x - x^J|, h), \quad (\text{EQ } 3)$$

where the gradient is taken with respect to x . The above definition of SPH involves a specific interpolation scheme based on a kernel function approximation. However, the gridless concept can be generalized by allowing interpolation schemes other than the specific SPH form. A generalized interpolation scheme can be written in the form

$$f(x) = \sum_{J=1}^N Vol^J f^J \phi^J, \quad (\text{EQ } 4)$$

where the f^J are the discrete nodal values and the ϕ^J are shape functions. The volume appears explicitly to maintain connection with the SPH form, since it can without loss of generality be factored into the shape function. This general form can describe many interpolation schemes, including SPH, moving least squares, reproducing kernel methods, and partition of unity methods. See (Belytschko et al. 1996) for a description of these methods and the specific shape functions associated with each.

Transient dynamic numerical methods using a generalized interpolation scheme may be referred to in general as particle methods. If the shape functions have compact support, such schemes may be called local particle methods. However, there is one more restriction to be applied, which is that the method is truly gridless. Many 'meshless' techniques actually use a background mesh to evaluate interpolated quantities. We consider here only truly gridless methods in which the particles themselves constitute the

only discretization of the bodies. Therefore, the equation of motion (conservation of momentum) in the form

$$\rho a = \nabla \cdot \sigma \quad (\text{EQ 5})$$

must be evaluated directly on the particles, using an interpolation scheme of the above form. Thus, the acceleration of particle I will be given by

$$\rho^I a^I = \sum_{J=1}^N \text{Vol}^J \sigma^J \cdot \nabla_I \phi^J. \quad (\text{EQ 6})$$

This completes the definition of a local particle method.

3. Conservation of Momentum

This section will consider the momentum conserving properties of particle methods. The generalized interpolation scheme defined above allows for a variety of curve fitting algorithms depending on the choice of the shape functions. However, there are some limitations that must be placed on the schemes if the numerical method is to be consistent with the physical laws that are being solved, namely conservation of mass, momentum, and energy. The acceleration of a given particle involves sums over neighbors. Multiplying by the mass gives the total force on particle I,

$$F^I = m^I a^I = \frac{m^I}{\rho^I} \sum_{J=1}^N \text{Vol}^J \sigma^J \cdot \nabla_I \phi^J, \quad (\text{EQ 7})$$

or

$$F^I = \sum_{J=1}^N \text{Vol}^I \text{Vol}^J \sigma^J \cdot \nabla_I \phi^J. \quad (\text{EQ 8})$$

Isolating just the term in the sum due to particle J, the force on particle I due to particle J is given by

$$F^{IJ} = \text{Vol}^I \text{Vol}^J \sigma^J \cdot \nabla_I \phi^J \quad (\text{EQ 9})$$

In the case of SPH, this becomes

$$F^{IJ} = \text{Vol}^I \text{Vol}^J \sigma^J \cdot \nabla_I W(|x^I - x^J|, h) \quad (\text{EQ 10})$$

Since it has long been recognized that a symmetrized form is required to conserve momentum exactly (Monaghan 1988), the stress is symmetrized. This is usually done by adding a constant σ^I into the stress term so that the force on I due to J is

$$F^{IJ} = Vol^I Vol^J (\sigma^I + \sigma^J) \bullet \nabla_I W(|x^I - x^J|, h) \quad (EQ 11)$$

This is equivalent to adding a constant σ^I to the stress field so that the stress gradient is unchanged. As can be seen, this form is anti symmetric in I and J due to the fact that the same kernel function is used at each particle, and the gradient of $W(|x^I - x^J|, h)$ with respect to x^I is the negative of the gradient with respect to x^J , so that

$$F^{IJ} = -F^{JI} \quad (EQ 12)$$

Newton's third law is satisfied, and momentum is exactly conserved.

Now consider the more general interpolation schemes above. If the stress is symmetrized, the force on I due to J becomes

$$F^{IJ} = Vol^I Vol^J (\sigma^I + \sigma^J) \bullet \nabla_I \phi^J. \quad (EQ 13)$$

Note that in general, this is not anti-symmetric in I and J, since in the general case, the shape functions are not necessarily the same at each particle. Thus, such a scheme cannot conserve momentum in general. In fact, in order for Newton's third law to be always satisfied, and thus the demonstration of global momentum conservation to be a trivial matter, Eq. 12 must always be satisfied. From Eq. 13 this means

$$\nabla_I \phi^J = -\nabla_J \phi^I, \quad (EQ 14)$$

where the subscript indicates which coordinate the gradient is with respect to, so the shape functions at every particle must be the same to within a constant. However, since the shape functions must go to zero outside the region of support, the constants must be zero. Thus, for Newton's third law to be always satisfied, the shape functions must be the same at every particle.

The above argument means that no scheme which attempts to improve some aspect of SPH by 'correcting' or normalizing the kernel function, or which for whatever reason does not have the same shape function at each particle, can conserve momentum in general. This does not mean that such schemes can never conserve momentum. If particles are uniformly distributed and all shape functions are the same, then momentum will be conserved. However, when distortion occurs and the shape functions change, momentum will no longer be conserved. This is somewhat ironic, since it is the distorted particle distributions which are usually used as examples of the shortcomings of SPH, and to demonstrate the need for 'corrections'. Yet it is in these situations that the 'corrected' schemes will not conserve momentum.

There is an obvious way in which schemes with the possibility of different shape functions at each particle can be modified to always conserve momentum. The shape functions themselves can be symmetrized, so that Eq. 13 becomes

$$\mathbf{F}^{IJ} = Vol^I Vol^J (\boldsymbol{\sigma}^I + \boldsymbol{\sigma}^J) \bullet \nabla \phi^{IJ}, \quad (\text{EQ 15})$$

where

$$\phi^{IJ} = \phi^{JI} = \frac{1}{2}(\phi^I + \phi^J) \quad (\text{EQ 16})$$

This form will always conserve momentum, but it must then be determined whether or not the shape functions ϕ^{IJ} have the same properties as the original ϕ^I and ϕ^J which were chosen for some 'corrective' purpose, or indeed whether or not the solution obtained with the ϕ^{IJ} makes any sense at all.

The bottom line is that when the conservation laws of continuum mechanics are discretized for purposes of numerical solution, the first step which should be done is a sanity check to ensure that the discretized equations still have the same properties as the original conservation laws. A discretization that results in a local particle method with potentially different shape functions at every particle does not satisfy this condition, since the discretization no longer satisfies Newton's third law.

4. Tensile Instability

A major difficulty with SPH is the behavior of the method in tension. In (Swegle, et al. 1995) it was shown that the method can be unstable in tension, and a rigorous stability analysis showed that the condition for instability is

$$W''\sigma > 0 \quad (\text{EQ 17})$$

where W'' is the second derivative of the kernel function and the stress, σ , is taken negative in compression. It was also shown that the instability is due to an effective stress-strain relation in which the stress decreases with increasing strain. Here additional insight into the source of the instability is provided by considering the stability of particle methods in general and by comparison with other particle-particle interaction phenomena such as molecular dynamics and gravitational systems of particles.

Discussion of the source of the instability can be enhanced by introduction of the concept of area vectors. The fundamental definition of the stress tensor shows that the force exerted on a surface due to a stress σ is given by

$$\mathbf{F} = \boldsymbol{\sigma} \bullet \mathbf{A} \quad (\text{EQ 18})$$

where the area vector $\mathbf{A}$ has a direction normal to the surface and a magnitude equal to the area of the surface. In the context of particle methods this means that the force between two particles is determined from the stress tensor at the particles and the

interaction area between the particles, as shown in Fig. 2. Comparing Eqs. 10 and 18, it

Figure 2. Area vector for particle interactions

can be seen that in SPH, the interaction area vector is given by

$$\mathbf{A}^{IJ} = Vol^I Vol^J \nabla_I W(|\mathbf{x}^I - \mathbf{x}^J|, h) \quad (\text{EQ 19})$$

Thus, the gradient of the kernel function can be thought of as defining the area on which the stress acts to produce a force between the particles. Put another way, the kernel gradient defines the interaction strength between particles. One of the fundamental tenets of SPH and local particle methods as defined here is that the kernel function has compact support so that the kernel and its derivatives are zero beyond some distance, usually referred to as the smoothing length. This guarantees that only local neighbors will contribute to the sums in the interpolations, since a single fit to all particles simultaneously would be undesirable. This also is critical to the ability to do large deformation problems in that it allows neighbor sets to change so that particles which were originally interacting neighbors do not have to remain neighbors forever, and particles which originally did not interact can interact at later times as distortion and flow occurs which brings the particles into proximity. An additional requirement is that the kernel function and its derivatives go continuously to zero at the smoothing length. This guarantees that the interaction between particles changes in a continuous manner, and interactions do not jump discontinuously from zero to some large value, or vice versa, as a limiting distance between the particles is reached.

The fact that the kernel derivative must go smoothly to zero at the smoothing length means that its magnitude must be decreasing in that region. If the kernel gradient had its maximum at zero separation, and went continuously to zero at the smoothing length, then its magnitude would be decreasing at all separations, as would the magnitude of the area vectors and the interaction strength between particles. However, the maximum of the kernel derivative need not be at zero separation, nor need there be only one maximum. In any case, since the kernel derivative is not identically zero, there must be some region

where its magnitude is decreasing in order for it to go continuously to zero at the smoothing length. In the specific case of the SPH cubic b-spline kernel, the single maximum of the kernel function is at a particle separation smaller than the normal initial particle spacing, so the area vector is decreasing for all particle separations greater than or equal to the normal initial spacing.

The area vector concept can be applied to the generalized interpolation schemes as well, and the area vector can be related to the shape functions. In order to have a local particle method and the ability to handle arbitrary distortions, the same local support and smoothness of the shape functions defining the interaction area is required. Thus, whether SPH specifically or a more general interpolation method is considered, the kernel or shape function defines the area vector and thus the interaction strength. The area vectors must go smoothly to zero at the smoothing length in order to have compact support and a local method, and thus they must be decreasing in some region.

The fact that there are regions in which the area vectors and thus the interaction strength must be decreasing is the fundamental source of the tension instability. Consider the case in which the particles represent a fluid under compression. The forces between the particles are repulsive, since the stress gradient acts to drive material from high pressure regions to low pressure. Thus, as particles get nearer, the density and stress increases and the force between particles is in a direction to drive them apart. Thus, where the area vectors are decreasing, there is in effect a repulsive force law with the repulsive force increasing as the particles approach, and decreasing as they separate. The repulsive force must go continuously to zero at the smoothing length.

Now suppose that the fluid is in tension, rather than under compression. The interaction between the particles is similar to the compression case, except that the force between the particles is attractive instead of repulsive. Thus, where the area vector is decreasing, there is an attractive force between the particles which increases as they approach, and decreases as they separate. The situation is stable if the force is repulsive, but is unstable if the force is attractive. That is, the closer two particles get, the more they are attracted, and vice versa. If three particles form a line with equal spacing, the attraction of the center particle to the left and right particles is equal. However, if the center particle moves very slightly off-center, say to the right, it will be more attracted to the right particle and less attracted to the left particle. It will thus move to the right, and the more it moves, the greater the force to the right, until it joins the particle on the right. So, if a small perturbation is applied to a uniform distribution of particles in tension, particles will tend to clump together. This is in contrast to the case in which the force is repulsive, where the center particle will be more strongly repelled by the particle it is nearer to, so the repulsive forces will drive the center particle to be equidistant from the other particles so that the forces are equal.

The nature of the instability can be better appreciated by comparison with other types of particle systems. Consider a system of particles in which the only interaction between the particles is due to gravitational forces. The force is always attractive, and is inversely proportional to the square of the distance between the particles, so it is everywhere

decreasing with increasing separation. The above description of the three-particle problem also applies here, but it is more easily understood that three particles under the force of gravity do not have a three-in-line equilibrium configuration which will be maintained if the particle positions are perturbed. Clearly, the particles will tend to group together under the attractive forces, although the kinematics of the situation may result in stable orbital motion, rather than all particles coming together at rest.

A similar situation holds for molecular dynamics, which has been shown to have an isomorphism with SPH (Hoover, 1998). In molecular dynamics the force between particles is determined from an interaction potential, typically something similar to the Lennard-Jones potential. There is an equilibrium particle separation at which the force between particles is zero. For smaller interparticle distances, there is a repulsive force which increases as the particle separation decreases. For interparticle distances larger than the equilibrium separation, there is an attractive force between the particles. At particle separations just larger than the equilibrium, the attractive force increases as the separation increases. However, the force between particles eventually goes to zero as the particle separation goes to infinity, so the attractive force must at some point begin to decrease as particle separation increases. In fact, for the Lennard-Jones potential, this occurs at a particle separation about 10 percent greater than the equilibrium separation. At larger separations than this, the situation is analogous to SPH in tension. The attractive force increases as the particles approach, and decreases as they separate. Thus, if in a molecular dynamics simulation the particles have a spacing greater than 10 percent of the equilibrium spacing, the above three-particle description applies, and the system of particles is unstable to clumping. For instance, if an elastic filament is represented with molecular dynamics with the particles distributed on a cubic lattice it can only stretch 10 percent of its length before coming apart. Presumably, to represent a rubber band with molecular dynamics and get the real stretching behavior, it would be necessary to represent the polymer chains actually present in the rubber.

The above examples demonstrate that the SPH instability in tension is not due to the numerics of the solution scheme, but is in fact a necessary consequence of the local nature of the method. It is the result of an attractive force which increases as particles approach, and decreases as they separate. There are analogs of the instability in both molecular dynamics and gravitational systems. The fact that the force must decrease with increasing separation follows from the fact that a local method is required so that a particle does not interact with every other particle in the problem, but only with its local neighbors. Thus particles not initially interacting will begin to interact as they get closer, and particles initially interacting will stop interacting when they get far enough apart. This is what gives gridless particle methods an advantage over gridded methods for large deformations.

In fact, it can be seen that local particle methods do not represent the same physical model as gridded methods. In a gridded method, zones or elements only interact with nearest neighbors, and must always interact with those neighbors, absent remeshing. Thus, if a rubber band is represented with a gridded method, it can be stretched any amount, and neighbor elements will continue to interact and support the increasing tension. In this case neighbor elements are expected to continue to interact and support

tension until the constitutive relation says otherwise. Local particle methods do not support this physical model. It is inherent in the method that interactions decrease and eventually go to zero as particles separate, regardless of the constitutive relation. This is inconsistent with the physical model implicit in the assumption that neighbors can keep supporting increasing tension as they are pulled apart, as with a gridded method.

In fact, it has been previously pointed out (Duvall, 1971) that when discretizing the conservation laws of continuum mechanics using a grid the resulting finite difference or finite element equations actually represent a spring-mass system. The springs connect only nearest neighbors, and always connect the same neighbors regardless of deformation. This allows, for example, the treatment of a stretching rubber band, as mentioned above. The discretization in local particle methods does not represent a spring mass system, but rather a physical system of particles interacting by means of an action-at-a-distance force law, with the interaction force a decreasing function of interaction distance. Thus, it is more representative of a gravitational system of particles than a spring-mass system. When the behavior of the physical systems the discretizations represent is considered, it is clear that a gridded method is applicable to solids in tension, but a local particle method is not. Thus, the instability of SPH in tension cannot be fixed by an improved integration scheme involving different shape functions, because the instability is the true behavior of the physical system represented by the discretization scheme.

5. Example: Moving Least Squares

In this section the above concepts are applied to a specific example, that of moving least squares. In this method, the discrete data are represented by a continuous approximation function found by minimizing the least squares form

$$G = \sum_{J=1}^N W^J (f(x^J) - f^J)^2, \quad (\text{EQ 20})$$

where $f(x)$ is the continuous approximation, usually consisting of polynomial basis functions with unknown coefficients, f^J are the discrete data values, and W are weight functions with compact support, which can be chosen to be the SPH kernel functions. This is similar to a standard least squares method, except for the weight functions. Without the weights, all data values in the body would be fit by a single function. The weights allow for a different approximation at each point, with only neighboring data values contributing to the fit. If the basis functions are linear, the approximation function is of the form

$$f(x) = a_0 + a_1 x, \quad (\text{EQ 21})$$

where the coefficients a_0 and a_1 will in general be different at each spatial location, since the weights will change with position. Basically, this corresponds to fitting the local tangent line to the data at each point, rather than fitting all the data with a single linear function.

After solving the least squares problem, the coefficients in the approximation function $f(x)$ are determined, and with some manipulation, it can be expressed in the form of Eq. 4. The resulting shape functions involve the basis and weight functions evaluated at the particle positions, but not the data values (Belytschko 1996). However, although the approximation can be expressed in this form, there is a fundamental difference between the SPH fitting procedure and the moving least squares procedure. In SPH, the approximation function is built by summing data weighted kernel functions as shown in Fig.1, with the same kernel function used at each particle. In moving least squares, the approximation function is found by solving the least squares problem, and writing the approximation function in the form of Eq. 4 essentially amounts to building shape functions at each particle which will add up to the approximation function. Thus, as discussed in the previous section, SPH uses the same kernel function at each particle, so that Eqs. 11 and 12 apply, and momentum is always conserved. In moving least squares, the shape functions are in general different at each particle, and will change if a particle's position changes, so that momentum conservation is not guaranteed in general.

The lack of momentum conservation with moving least squares applied to particle methods makes it a non-viable option for transient dynamics. Again, this does not mean that the method can never conserve momentum or that the answers obtained with the method are always wrong. In regions where particles are evenly distributed, as would often be the case in the initial configuration, the shape functions will be the same, the forces between particle pairs will be equal and opposite, and momentum will be conserved. Test calculations can give the right answer in such situations, and the method can appear to be working correctly. However, when a simple analysis such as the above can demonstrate the potential for lack of momentum conservation and incorrect answers, the method should clearly not be used for important large deformation problems when the correct answer is not known and the code must be relied on.

Moving least squares thus illustrates the issues involved with momentum conservation in particle methods, but it also is informative to consider it from the standpoint of the tensile instability. It turns out that moving least squares does not exactly correspond to the previous definition of a local method. Although the fit can be expressed in terms of shape functions with compact support, the interaction forces between particles do not depend on the distance between the particles as in SPH. As a simple example of this, consider the case in which the data values can be exactly represented by the basis functions. That is, if the basis functions are linear, then data which lie on a plane will be fit exactly, regardless of the particle positions. Put another way, if all the squared error terms in Eq. 20 are zero, then the weights are irrelevant, so long as they are not all zero. This is shown graphically in Fig. 3, which compares SPH and moving least square fits to data points which all have the same stress value, but whose spacing is non-uniform. In regions where the particle spacing is uniform, the data-weighted kernels are the same at each point, and they sum

Figure 3. Comparison of SPH and MLS for irregular particle spacing

up to a constant value. However, if the spacing is non-uniform, or the particles move apart, a straight line fit is no longer obtained everywhere. This is not the case with a moving least squares fit, since the same straight line fit is produced everywhere, regardless of particle spacing, so long as there are enough neighbors with non-zero weights to determine the fit. The proviso that not all weights are zero is the key to the previous statement that moving least squares does not exactly fit the definition of a local method. The weights are irrelevant and the fit is independent of particle spacing so long as all the weights are non-zero. If all weights are zero, the problem is indeterminate, since Eq. 20 is zero regardless of the basis functions or the data values, so there can be no interaction defined between particles.

As an example, consider equally-spaced particles which all have the same data value. Take the range of the weight functions to be h , which means that they are zero for distances larger than h . So long as the distance between particles is less than h , the same straight-line fit is obtained and there is no distance dependence to particle interactions. When the distance between particles becomes equal to h , a linear fit becomes undefined, since there can be no more than a single particle within a distance h of any location, and a unique straight line cannot be fit through a single point. Thus, at a spacing of h , the particles cease to interact. The method is local in that particle interactions go to zero at h , but since the interaction is independent of distance for separations less than h , they do not go to zero continuously. So, moving least squares does not fully meet the previously stated requirements for a local method.

Thus, while there is a distance dependence to interactions between particles in SPH, this example shows a case in which there is a regime where there is no distance dependence with a least squares fit. The SPH fit is unstable in tension because of the distance dependence of the particle interactions, just as in gravitational systems or large distention molecular dynamics. With no distance dependence to particle interactions in moving least squares, the method is stable in tension, even though it is not conservative. Unfortunately, conservation cannot be abandoned, even to gain stability. If an attempt is made to regain conservation of momentum by symmetrizing the shape functions as in Eq. 16, the

modified shape functions will no longer necessarily add up to the approximation function. The least squares fit is no longer obtained, so there is a distance dependence to the particle interactions, and the method is again unstable.

It might seem that the fact that the lack of distance dependence to interactions with moving least squares is desirable, since it removes the tensile instability. This is due to the fact that the basis functions are always reproduced, regardless of particle spacing. However, this reproducing condition involves an invalid assumption. Forcing the basis functions to be reproduced, regardless of particle spacing, implicitly assumes that the region covered by the interpolation points represents a continuous material body with no included voids or gaps. If so, the fit should extend across the domain of the body, regardless of the position of the interpolation points. However, the assumption of a continuous body does not hold for the type of large deformation problems for which SPH is intended. An essential feature of SPH is that the number density of particles is related to the material density of the body being represented, that is

$$\rho(x) = \sum_{J=1}^N m^J W(|x - x^J|, h), \quad (22)$$

where m^J is the mass of particle J.

For equal mass particles, a region of fewer particles represents a region of lower density material, and a region of no particles means no material, or a void. Outside the boundaries of the body, all field variables should go to zero. Unfortunately, the reproducing condition not only does not recognize low particle number density regions as internal voids, it does not even recognize the absence of particles exterior to the body as a boundary, as shown in Figure 3. The SPH fit falls off in the interior where there are no particles, while the MLS fit does not. However, the MLS fit does not even fall off at the exterior boundary, represented by the vertical lines. The SPH fit has a non-zero stress gradient at the boundary, while the MLS fit does not. Since stress gradients are evaluated at the particles themselves, particles on the boundary must have a stress gradient appropriate to a boundary. Consider the case of a body initially at some non-zero pressure, such as the gas in a balloon. At time zero, the balloon is removed, and the gas begins to expand. In SPH, the lack of particles outside the boundary causes the stress to go to zero, producing a stress gradient on the boundary particles, causing outward motion. In MLS, the linear fit to the constant stress field at time zero extends beyond boundary particles, with the result that there are no stress gradients at the boundaries, and nothing moves. In order to implement MLS, an algorithm must be added to place zero stress particles at all boundaries and in internal voids so that the stress will go to zero in these regions and the proper boundary stress gradients will be obtained. For example, in Figure 3 zero stress particles would have to be placed at the locations marked with a cross in the MLS fit in order for boundaries and internal voids to be treated correctly. No algorithm to do this in the general case of large deformation with boundary motion, creation, and removal has been discovered which is both correct and efficient, especially in three dimensions.

6. Conclusion

This paper considers transient dynamic particle methods from the point of view of conservation of momentum and tensile instability. Particle methods represent a continuous body with particles which discretize the body. The particles carry the field variables and are used for interpolation purposes. They also are discrete chunks of matter which must have mass and volume which in sum represent the total mass and volume of the body. If a background mesh is used for integration, the particles are really only generalized integration points, and the background mesh discretizes the body. Such a technique does not constitute a particle method as defined here.

Consideration of particle methods starts from SPH, a gridless Lagrangian transient dynamics numerical technique suitable for large deformation situations. Mesh distortion is circumvented by replacing grid-based approximations for spatial derivatives with a kernel-based approximation, which is basically a curve fit obtained by multiplying the data value at each point by an SPH kernel function and summing the weighted kernels. This concept can be generalized by allowing the SPH kernel to be replaced by shape functions, resulting in a general form which can describe many interpolation schemes, including SPH, moving least squares, reproducing kernel methods, and partition of unity methods. Transient dynamic numerical methods using a generalized interpolation scheme may be referred to in general as particle methods. If the shape functions have compact support, such schemes may be called local particle methods.

When the discretized equation of motion is applied to the particles, there result conditions that must be placed on the scheme if the numerical method is to be consistent with the physical laws that are being solved, namely conservation of mass, momentum, and energy. In particular, Newton's third law must be satisfied so that the force on particle I due to J is equal and opposite to that on J due to I , and global momentum is exactly conserved. It is shown that in order for Newton's third law to be always satisfied, the shape functions must be the same at every particle. Thus, no scheme which attempts to improve some aspect of SPH by correcting or normalizing the kernel function, or which for whatever reason does not have the same shape function at each particle, can conserve momentum in general. The lack of momentum conservation in a particle method makes it a non-viable option for transient dynamics. It should go without saying that a scheme which purports to solve the conservation laws of continuum mechanics but does not conserve momentum is incorrect and should not be used. The bottom line is that when evaluating a numerical method, the first step which should be done is a sanity check to ensure that the discretized equations still have the same properties as the original conservation laws. A discretization that results in a local particle method with potentially different shape functions at every particle does not satisfy this sanity check, since the discretization no longer satisfies Newton's third law.

Tensile instability in particle methods is discussed from the point of view of area vectors which define the area on which the stress acts to produce a force between the particles. The area vector is related to the gradient of the kernel function, so the kernel gradient defines the interaction strength between particles. One of the fundamental tenets of SPH

and local particle methods as defined here is that the kernel or shape function has compact support so that the kernel and its derivatives are zero beyond some distance, and go continuously to zero at that distance. Thus, the area vectors and the interaction strength must go smoothly to zero there. This is the fundamental source of the tension instability, which is thus a necessary consequence of the local nature of the method. It is the result of an attractive force which increases as particles approach, and decreases as they separate. There are analogs of the instability in both molecular dynamics and gravitational systems. The fact that the force must decrease with increasing separation follows from the fact that a local method is required so that a particle does not interact with every other particle in the problem, but only with its local neighbors. Thus particles not initially interacting will begin to interact as they get closer, and particles initially interacting will stop interacting when they get far enough apart. This is what gives gridless particle methods an advantage over gridded methods for large deformations.

In fact, it can be seen that local particle methods do not represent the same physical model as gridded methods. In a gridded method, zones or elements only interact with nearest neighbors, and must always interact with those neighbors, absent remeshing. Local particle methods do not support this physical model. It is inherent in the method that interactions decrease and eventually go to zero as particles separate, regardless of the constitutive relation. This is inconsistent with the physical model implicit in the assumption that neighbors can keep supporting increasing tension as they are pulled apart, as with a gridded method. The discretization in local particle methods represents a physical system of particles interacting by means of an action-at-a-distance force law, with the interaction force a decreasing function of interaction distance. When the behavior of the physical systems the discretizations represents is considered, it is clear that a gridded method is applicable to solids in tension, but a local particle method is not.

Moving least square methods are an example of attempts to improve particle methods and remove the tension instability. However, the moving least squares fit will not conserve momentum, and is in fact not really a local particle method as defined herein. The distance dependence of the interaction between particles is removed, so there is no recognition of voids or boundaries. Since moving least squares fits remove the property of decreasing particle interaction with distance, the method is stable in tension. Unfortunately, conservation cannot be abandoned, even to gain stability.

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