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An Angular Weighting Approach for Calculating Gradients and Divergences

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Abstract: There are several desirable properties for a free Lagrange algorithm: 1) a Lagrangian nature, 2) reciprocity, 3) minimization of numerical noise, 4) numerical efficiency, and 5) the ability to extend the algorithms to 3-D. In addition, some integral hydro formulations allow the mass points to drift among the other points because the divergences and gradients do not depend explicitly on the position of a mass point between two other mass points. Therefore, another desirable property is 6) a restoring force that keeps the mesh regular. An algorithm based on the angles subtended by the Voronoi polygon sides satisfies all the above criteria, except the fourth; this is because of the necessity of using trigonometric functions. Nevertheless, this loss of efficiency may be compensated by the avoidance of reconnection noise.

1 Introduction

Some current implementations of the free Lagrange method use the Voronoi mesh for nearest neighbor definition, but use a median mesh for computation of the hydrodynamic quantities. As long as the nearest neighbors don't change, the computational mesh is purely Lagrangian, but when the flow is such that neighbors change, then there is an abrupt change in the computational mesh, and fluxing must be done to preserve the integrity of the calculation and to minimize the resultant noise of reconnection. Since the apexes of the Voronoi polyhedra (the centers of spheres defined by the apexes of the associated tetrahedral mesh) are not Lagrangian, the use of a median mesh with fluxing when reconnection occurs is an improvement over the use of the Voronoi mesh as a computational mesh. However, in cases of extreme shear flow, the fluxing can lead to considerable diffusion as the calculation takes on a more Eulerian nature. Thus, current free Lagrange implementations are pure Lagrangian only in the limit of no shear flow, hence only in the regime more efficiently handled by logical mesh Lagrangian codes. It may be more correct to classify current implementations of free Lagrange as adaptive mesh algorithms.

Is it possible to avoid fluxing when neighbors change in the presence of shear flow? Clearly, the Voronoi polyhedra or their associated tetrahedra cannot be used as control volumes if a Lagrangian nature is to be retained.

2 A Different Perspective

It seems profitable to consider a close cousin of free Lagrange, the smooth particle hydrodynamics (SPH) method. The SPH method uses the particles as data points of an interpolation scheme based on weighting functions (or smoothing kernels) centered on each particle. The particles correspond to the mass points in free Lagrange. The weighting functions ideally have scale lengths on the order of the local mean distance between particles, and thus use only the particle and its closest neighbors for the local interpolation necessary to obtain the divergences and gradients needed for the hydro. Early implementations of SPH used a gaussian weighting function, and as the distance between particles increased the weight decreased and quickly became negligible beyond the closest neighbors, but in current implementations a weighting function is often used that is zero beyond twice the local mean spacing. Because in most implementations of SPH the weighting functions are spherically symmetric, an inordinately large number of particles may be needed to represent an object with a large aspect ratio. A highly anisotropic distribution of mass points necessary to economically represent a large aspect ratio object presents no difficulty for free Lagrange.

Is there a scheme which utilizes the strong points of SPH and free Lagrange without inheriting the less desirable features? We will explore this possibility.

3 Weighted Sums

While the conservation equations for hydrodynamics are differential, and the implementation in computer codes are often referred to as difference equations, many implementations are actually integral (that is, numerically expressed as sums). With the integral formulation it is easier to insure reciprocity and conservation. Mathematically there is an equivalence between the integral and the differential formulations. The divergence theorem relates the divergence to an areal integral, and through a generalization of the divergence theorem [1] one can relate the gradient to an integral over an area:

$$\nabla P = \lim_{V \rightarrow 0} \frac{1}{V} \int P d\hat{A} \quad (1)$$

$$\nabla \cdot \hat{v} = \lim_{V \rightarrow 0} \frac{1}{V} \int \hat{v} \cdot d\hat{A} \quad (2)$$

The procedure for obtaining the divergence is analogous to that for the gradient, so henceforth only the gradient will be illustrated. Also, only the 2-D analysis

will be presented here. In the early implementations of free Lagrange [2] the force acting on a mass point was computed by summing the product of the pressure and the areas represented by the Voronoi polygon sides:

$$\hat{F} = \sum P_n \hat{A}_n = \sum P_n L_n \hat{1}_H \quad (3)$$

Division by the control volume $\frac{1}{2} \sum_n L_n H_n$ provides an approximation to the gradient:

$$\nabla P = \frac{1}{V} \sum_n P_n \hat{A}_n = \frac{1}{\frac{1}{2} \sum_n L_n H_n} \sum P_n L_n \hat{1}_H \quad (4)$$

where P is the pressure mid-way between two neighbors, H is half the distance between them, and L is the length of a Voronoi polygon side. Because the apex is not Lagrangian, this implementation is not Lagrangian and is not used in current implementations of the free-Lagrange method. A variation on this involves inscribing a circle around a mass point, bi-linearly interpolating the pressure along the circle, and taking the limit:

$$\lim_{V \rightarrow 0} \int_S P d\hat{A} = \frac{1}{\pi R^2} \int_{2\pi} P_c \hat{1}_R R d\theta, \quad (5)$$

where the pressures and other quantities are defined in figure 1:

Fig. 1. Triangular element of a Voronoi polygon

It is not necessary to take the limit numerically, since $P_c = P_o + \frac{P_p - P_o}{D} R$ and analytically the R dependence drops out:

$$\nabla P = \frac{1}{\pi} \sum \int \left[\frac{P_m - P_o}{H} \cos \theta + \frac{P_p - P_m}{L} \sin \theta \right] \hat{1}_R d\theta. \quad (6)$$

This relation may be thought of as a weighted sum of simple gradients derived from the data at the mass points. Upon performing the indicated integration one obtains for the x-component of the gradient:

$$\nabla_x P = \frac{1}{2\pi} \sum [(Q_a - Q_d)\theta_A + (Q_a + Q_d)\sin\theta_A \cos\theta_A + (Q_c - Q_b)\sin^2\theta_A], \quad (7)$$

$$\text{where } Q_a = \frac{P_m - P_o}{H} \cos\theta_n,$$

$$Q_b = \frac{P_m - P_o}{H} \sin\theta_n,$$

$$Q_c = \frac{P_A - P_m}{L} \cos\theta_n,$$

$$Q_d = \frac{P_A - P_m}{L} \sin\theta_n,$$

θ_n is the angle between the x axis and the line between the two mass points bisected by the polygon side, and θ_A is the angle between the connecting line and the polygon apex. In order to insure a Lagrangian nature, P_A must be interpolated properly from the pressures of the mass points that surround it. In order to avoid reconnection noise the interpolation must give zero weight to any newly acquired or just lost mass point in the collection of mass points used for the interpolation. An appropriate interpolation scheme might be a weighting function based on the distance of each mass point from the apex. If the scale length were the distance from the apex to any of the three mass points that define it, then in the limit of infinitesimal time steps, the scale length doesn't change when reconnection occurs, and since the new neighbor was included in the previous interpolation no noise comes from the change in the mass points used for the interpolation. A Gaussian or similar function could be used for the interpolation, but the B-spline used in some SPH codes would seem to be a logical choice. For an isotropic distribution of mass points, only the neighbors of the mass points defining the apex should be needed for the interpolation. Reciprocity is guaranteed because the same value of P_A is used in the evaluation of the gradient for all three mass points that define the apex.

What are the relative contributions of the terms in equation (7)? Can some be neglected?

4 Term Contributions

Equation (7) can be rewritten as

$$\begin{aligned} \nabla_x P = \frac{1}{2\pi} \sum \frac{1}{\Delta x_n^2 + \Delta y_n^2} \{ & (P_m - P_o)(\theta_{A2} - \theta_{A1})\Delta x_n \\ & - \left(\frac{P_{A2} - P_m}{\tan\theta_{A2}} \theta_{A2} - \frac{P_{A1} - P_m}{\tan\theta_{A1}} \theta_{A1} \right) \Delta y_n \\ & + (P_m - P_o)(\sin\theta_{A2} \cos\theta_{A2} - \sin\theta_{A1} \cos\theta_{A1})\Delta x_n \\ & + (P_m - P_o)(\cos^2\theta_{A2} - \cos^2\theta_{A1})\Delta y_n \\ & + ((P_{A2} - P_m) \sin\theta_{A2} \cos\theta_{A2} - (P_{A1} - P_m) \sin\theta_{A1} \cos\theta_{A1})\Delta x_n \\ & + ((P_{A2} - P_m) \cos^2\theta_{A2} - (P_{A1} - P_m) \cos^2\theta_{A1})\Delta y_n \} \end{aligned} \quad (8)$$

If one defines the values of the apex and midpoint pressures P_A and P_m to conform to a specified linear gradient, the contributions of the various terms to the gradient can be compared. Also, the calculated gradient can be compared with the specified linear gradient. For the case of the Voronoi polygon being a regular triangle, square, or hexagon (centered on the mass point for which the gradient is desired), only the first two terms make a net contribution to the gradient. Both of the first two terms are necessary to obtain the correct value of the gradient. If only one of the first two is used, then the resulting gradient is just half the specified value, which might lead one to speculate that the computational burden could be eased by keeping only the first term and doubling the result. The last four terms sum to zero.

For an irregular Voronoi polygon the last four terms still sum to zero, even when the pressures at the apexes and mid-points don't conform to a linear gradient, suggesting that these four terms may be neglected with impunity. The gradient resulting from using only the first term no longer yields just one half of the specified gradient; both of the first two terms are necessary. Keeping only the first two terms, equation (8) can be rewritten as:

$$\nabla_x P = \frac{1}{2\pi} \sum \left[\frac{P_m - P_o}{H} \Delta\theta_A \cos \theta_n - \left(\frac{P_{A2} - P_m}{L_2} \theta_{A2} - \frac{P_{A1} - P_m}{L_1} \theta_{A1} \right) \sin \theta_n \right], \quad (9)$$

an expression surprisingly similar in appearance to equation (6), but an expression involving angular weights of simple gradients between mass points and along the Voronoi polygon sides.

5 The Properties Of Angular Weighting

Since a) the angles associated with the polygon sides smoothly approach zero for two mass points that are disconnecting and grow smoothly from zero for the two that become newly connected, and b) the value of P_m does not change due to reconnection, in the limit of infinitesimal time steps, there is no reconnection noise associated with the first term of equation (9). Figure 2 illustrates the smoothness of the reconnection.

The second term of equation (9) involves apex pressures, so despite the geometrical smoothness of reconnection, reconnection noise could occur if the value of P_A changes due to reconnection. As mentioned above the proper specification of the apex pressure P_A is crucial to the success of equation (7), hence to the success of angular weighting as represented by equation (9). The value used must be Lagrangian, which also means that it cannot change due to reconnection. This means that when the set of points used to interpolate for P_A changes, the weights of those points lost and gained must be negligible (preferably zero). A test should be made for this condition each time reconnection occurs. If this condition is violated it can be corrected in one of two ways: a) by increasing the number in the set of mass points used for the interpolation (perhaps by reaching beyond

Fig. 2. The reconnection process

the neighbors of the three points that define the apex) or b) by reducing the scale length of the interpolation. The zero weight loss and gain condition should be guaranteed throughout the calculation, so it may be necessary to restart a calculation. In principle the interpolation function could have a sharply decreasing spatial dependence outside the apex radius, but it is impractical to have a scale length which allows a mass point that did not previously contribute importantly to the value of P_A to suddenly contribute to that value, when due to a finite time step it substantially changes its position. For too sharp a spatial dependence of the interpolation function this could happen even when no reconnection occurs.

For the 1-D case of one mass point mid-way between two others the gradient will be zero if the pressures of the outside mass points is the same. If the middle mass point has a pressure that differs from that of the two outside points and it is moved one direction or the other with no change in its pressure, then equation (4) gives no change in the gradient – it is still zero. This means that there is no restoring force on the middle mass point and it can freely drift between the outside two. Equation (9) does generate a gradient, hence a restoring force. This is illustrated in figure 3.

Thus the distribution of mass points should tend to remain more uniform with angular weighting.

Extension to 3-D depends on the ability to calculate solid angles for the Voronoi polyhedra. The equation that relates the angles between the planes that define the solid angle and the value of the solid angle is [3]:

$$\Omega = \sum_n \theta_n - (n - 2)\pi. \quad (10)$$

For each polyhedron there is an associated gradient which may be derived by angular weighting of the simple gradients associated with each polygon face of the polyhedron. In addition there is a simple gradient between the central mass point and the ("mid") point defined by the connecting line and its polyhedron

Fig. 3. Generation of a restoring force

face plane. These two gradients (eg., the associated face gradient and the simple central gradient) must be weighted by the solid angle of the polyhedron face. The analysis has not been done for 3-D, so there may be some surprises.

6 Conclusion

Analysis shows that angular weighting has a firm basis. The sine and cosine terms that arise from the angular integration around the mass point for which the gradient is desired cancel exactly, leaving only the angularly weighted contributions. Only the x-component of the gradient has been analyzed completely, but the modification for the y-component is obvious. Also, it is clear that the divergence is very analogous. A crucial aspect is the interpolation scheme for the apex pressures. Although several schemes may be candidates, the one used must be rigorously Lagrangian. Angular weighting offers a desirable property that is missing from simpler free-Lagrange implementations – a restoring force that will tend to regularize the distribution of mass points.

The next important step is to implement angular weighting in a code in order to test the algorithm. It is important to test alternative interpolation schemes for obtaining the apex pressures and velocity components. In addition, one must ask whether interpolation for the apex quantities is equivalent to fluxing on a median mesh. Does this necessary aspect of angular weighting introduce diffusion into the calculation? Clearly, additional work is needed to understand this angular weighting approach for calculating gradients and divergences.

References

1. Harry Lass (1950) *Vector and Tensor Analysis*, (McGraw-Hill Book Company, Inc., New York)
2. M.J. Fritts, W.P. Crowley, and H. Trease (1987) Lecture Notes in Physics 238, *The Free-Lagrange Method*, (Springer-Verlag, New York)
3. C.D. Hodgman (1957) *CRC Standard Mathematical Tables* (Chemical Rubber Publishing Co., Cleveland, Ohio)

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