Volumetric radial basis function methods applied to gas dynamics

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Abstract: *A set of rotational and translation transformations are applied to the Euler gas dynamic equations. In such a transformed coordinate frame, the partial differential equations (PDEs) appear as a set of steady ordinary differential equations (ODEs) in the rotating, translating frame. By using appropriate linear combinations of the ODEs, we obtain a transformed set of ODEs that resemble the compatibility equations from the method of characteristics plus additional terms for the angular momentum or streamline bending. The new dependent variables are cast into radial basis functions that are volumetrically integrated over each piecewise continuous subregion. At discontinuities such as shocks or contact surfaces, these discontinuities are propagated by the Rankine-Hugoniot jump conditions. For the case of weak shocks that are not important to track, they are captured and dampened away by the use of artificial viscosity. Knots over each continuous subregion may be added, deleted, or redistributed while constraining the appropriate volumetric dependent variables to be strictly conservative. Because volumetric integration is a smoothing operation, the numerical solutions converge faster compared with simple collocation.*

Introduction

Radial basic functions (RBFs) have been successfully applied to many areas of engineering and science over the last decade. Two of the most notable advantages are that RBFs are mesh-free and can be extended to any dimension of space; they are generally higher order than the typical finite difference, linear finite element, or finite volume methods. However, there is one major of applications that RBF methods have not been demonstrated yet, namely hyperbolic aerodynamics. It shall be argued that when carefully applied, RBF methods will also exhibit superior performance.

The topics that will be covered in this presentation are:

1. Why are aerodynamics different from typical PDE applications?
2. Why do we want interior points to move and what are the advantages?
3. What are the computational bottlenecks and how can they be overcome?
4. What do we want a volumetric formulation of the governing PDEs?
5. *What are some preliminary results?*

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1. Why are aerodynamics different from typical PDE applications?

Idealized aerodynamics are described by nonlinear wave equations that can develop shock and contact surface discontinuities, and rarefaction waves whose endpoints have discontinuous derivatives. Let F_k and U_k represent the kth normal flux vector and the kth dependent, respectively. Furthermore, let the superscripts "+" and "−" represent the above quantities to the right and left of the discontinuity. Then the propagation speed is given by the Rankine-Hugoniot jump condition:

$$V_D = (F_k^+ - F_k^-)/(U_k^+ - U_k^-)$$

An error in the endpoint conditions creates errors in the speed of propagation of the discontinuity.

Landau and Lipshitz (1959) show that the shock thickness due to molecular viscosity and thermal conduction (increasing the system entropy) is approximately a mean free path length of the air molecules, $O(10^{-7}$ cm). An ideal shock of zero thickness yields an increase of entropy. Ideally, one desires to have a sufficiently fine mesh so as to capture the shock as it propagates in a passive mode. Given the dimensions of a supersonic aircraft can range from 6-120 m, we will still need to wait many years to adequately resolve shock waves by shock capturing. Rarefaction wave fans are different in that they represent regions of constant entropy and are continuous within the limits of the fans. Rarefaction waves become progressively steeper as the geometry goes from planar, cylindrical, or spherical.

Standard shock capturing methods smear out the step functions over one or two meshes in the propagating direction by introducing an artificial viscosity that is typically several orders of magnitude greater than that of air at sea level. In order words, to perform the calculations using the standard mesh based schemes; the physics is modified to accommodate the numerical scheme chosen. Physics is also modified by the introduction of upwind differencing to prevent destabilizing truncation errors contaminating the solution. Other problems are the wave dispersion problems whenever the mesh spacing is nonuniform, and the flow skewness problem when the mesh axes are not aligned with the flow. For this reason, multi-level adaptive mesh refinement with its complex bookkeeping has been used to zone those regions with step gradients to minimize the various numerical artifacts. With sufficient experience and intuition, uniformly fine meshing is avoided by gradually allowing the mesh to become coarser in region of little physical interest such as the far field boundaries.

Since the 1940's, and with millions of dollars of research support, shock-capturing methods have been rather successful in describing the steady state locations of shocks and interacting shocks, and Mach stems. Boundaries, especially those representing fixed far-field boundaries, pose a problem since out-going waves can reflect off the boundaries and contaminate the interior solution. The price for this success is much effort in the very high front-end overhead of generating a problem free mesh that is several times longer than actually longer than the calculation itself. In theory, the standard mesh based schemes will represent the actual partial differential equations in the limit as the mesh cells in each dimension goes uniformly to zero; in practice, there is no computer existing that can or will be conceivably compute infinitely fast with infinite memory.

Lagrangian methods are more useful in problems with multiple materials in which the interfaces must be tracked by permitting interior points to move at the fluid velocity. The benefit of this approach is that no upwind differencing is used for the advective flux transport better representing the physics. The disadvantage is that meshes eventually become so distorted that the order of convergence of a scheme that is initially second order accurate drops to first order or even zeroth order accurate. Those mesh cells that undergo a severe amount of distortion must be interpolated onto regular mesh typically by first order interpolation known to be diffusive.

2. Why do we want interior points to move and what are the advantages?

The governing equations of inviscid gas dynamics are:

$$\frac{\partial U}{\partial t} + \nabla \bullet \mathbf{F}(U) = 0$$

where $U = [\ \rho,\ E,\ m_1,\ m_2,\ m_3]^T$ where ρ is the mass density, E is the total energy density, and m_1, m_2, m_3 are the components of the momentum densities along the 1, 2, and 3 coordinate axes, and $\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{e}_3$ are the corresponding unit vectors along the 1, 2, and 3 coordinate axes, The flux vector, $\mathbf{F}(U)$, is a three dimensional nonlinear vector represent the advective transport of mass, total energy, and the components of the momentum vector.

At an arbitrary point, x_i , one can find two consecutive rotations having angles, θ and ψ, of the principal momentum vector and local coordinate system that transforms the three-dimensional conservation equations into (1) one-dimensional time dependent PDEs for the conservation of mass, total energy, and principal momentum densities, and (2) two different two dimensional PDEs for the angular momentum component conservation equations. This is a local reduction of the dimensionality of the problem. Scalar quantities are invariant under rotation, but vectors are not. Note that the flux vector $\mathbf{F}(U)$ is transformed under rotation into a new vector $\mathbf{F}'(U)$.

Rather than keeping the positions of the discretization points always fixed, a simple alternative would be to permit points to move to regions that have steepening gradients moving at a velocity, $\boldsymbol{\lambda}$, that will be determined. In a local moving frame, the rotated conservation equations become

$$\frac{\partial U}{\partial t} + \boldsymbol{\lambda} \bullet \nabla'' U + \{\ \nabla'' \bullet \mathbf{F}'(U) - \boldsymbol{\lambda} \bullet \nabla'' U\ \} = 0$$

Choose $\boldsymbol{\lambda}$ so that

$$\nabla'' \bullet \mathbf{F}'(U) - \boldsymbol{\lambda} \bullet \nabla'' U = 0$$

then

$$dU/dt = 0$$

along $d\mathbf{x}''/dt = \boldsymbol{\lambda},$

and where $dU/dt = \dfrac{\partial U}{\partial t} + \boldsymbol{\lambda} \bullet \nabla'' U.$

By taking linear combinations of the dependent variables, we obtain the compatibility equations along the familiar characteristic velocities, $u''+a$, u'', $u''-a$. Additional two angular momentum components that account for streamline bending.

$d\theta/dt = 0$,
along $dx'_1/dt = u'$ and $dx'_2/dt = p_{x'2}/m'\theta_{x'1}$, and

$d\psi/dt = 0$,
along $dx''_1/dt = u''$ and $dx''_3/dt = p_{x3''}/m''\psi_{x''3}$.

Details of these transformations can be found in Kansa(2002) and Kansa,
Power, Fasshauer and Ling (2003).

Since the conservation equations are nonlinear and hyperbolic, it is possible that wave steepening may occur, eventually steeping so much, that the wave breaks and forms a shock. The conservation PDEs also apply at the boundaries, and the usual Dirichlet or Neumann boundary conditions are algebraic constraints that are solved in addition to the PDEs at the boundaries. Thus, with simple local and translational transformations upon the system of PDEs, we have reduced the entire problem to a set of ordinary differential equations (ODEs). Note that at each $\mathbf{x}_i$, these local transformations are applied without an imposed ordering of a mesh. This can be readily achieve by a meshless method to solve the system of PDEs or transformed ODEs using radial basis functions (RBFs).

3. What are the computational bottlenecks and how can they be overcome?

One misperception is that low order schemes yielding sparse systems are always more computationally efficient than arbitrarily higher order RBF schemes having very broad banded or even full systems of equations. However, we argue that the true test is whether the total number of operations is measured and compared. Consider the case in which we have an exact analytic solution, U_{exact}, and we wish to calculate the approximate solution U_{approx}, so that $|U_{exact} - U_{approx}| < \varepsilon$. To achieve this precision, the low order scheme requires O_L operations per point, and N_L points, whereas the higher order RBF scheme requires O_{RBF} operations per point and N_{RBF} points. It was common to assume $O_{RBF} \propto (NRBF)^3$, so the RBF method is more efficient if $N_{RBF} < [N_L O_L]^{1/4}$. Even with Gaussian elimination of full matrices, there are documented cases that RBFs are more efficient.

Although RBFs are meshless and converge faster than standard methods, some bad publicity has been associated with them. Namely, the complaint is that they give rise to systems of very large equations that are horribly ill conditioned and too expensive to be seriously used. However, this perception is out-dated.
▪   Domain decomposition, using small ranked matrices per subdomain, not only lowers condition numbers and flop rates, but also is essential for parallelization.
▪   Preconditioners developed by Beatson and coworkers and Ling and Kansa transform matrices with very large condition numbers to ones have condition numbers of $O(10)$. Solution of expansion coefficients is achieved by GMRES iteration. (Note preconditioning and domain decomposition can be combined). The number of operations is $O(N^2)$
▪   Fast multipole expansions reduce vector-matrix multiplies considerably reduce the number of operations to $O(N\log N)$.

▪   Appending appropriate asymptotic terms to RBF expansion can introduce a tunable degree of sparsity, even lower the estimates further.

Research is required to establish bounds to the question of which method is more efficient and under what circumstances.

4. What do we want a volumetric formulation of the governing PDEs?

There are two basic reasons to prefer a volumetric formulation in solving PDEs. First, density is a mathematical construct whereas volume extensive quantities such as mass, momentum, and total energy are measurable physical quantities. These total quantities must be conserved as a basic tenant of physics. No matter how points are moved, added, or deleted numerically, the total quantities must be invariant. The local velocities associated with the characteristic velocities are not calculated by gradients, but integrated quantities. In fact, integration is defined a discontinuity whereas differentiation is not.

Second, volume integration is a smoothing anti-differentiation method that increases, rather than decreases the rate of convergence. The objective is to obtain very highly accurate numerical solutions with the least amount of effort. So higher convergence rates are welcome. The drawback is that the search for nearest neighbors about a test point, x_i, is required; however, this search is parallelizable.

5. What are some preliminary results?

The problem that was examined is planar 1D geometry problem in which there are a right traveling rarefaction fan followed by a contact surface and a strong shock at the initial time, t_0. At the far right boundary is a rigid wall. The purposes of the calculations were to determine the convergence rates of the RBF collocation method with the volumetric RBF collocation methods and compute the errors in the conservation of mass, momentum, and total energy. Discretization nodes were allowed to move in time. An ideal gas was assumed having $\gamma=7/5$.

The rarefaction wave remains at constant entropy even though it may reflect off the rigid wall. The discretization was performed over piece-wise continuous regions. The mass, momentum, and total energy densities of the shock and contact surface are essentially constant functions within the continuous regions, and only a minimum of two RBF basis functions are required in these continuous regions. On the other hand, the mass, momentum, and total energy densities are continuous within the endpoints of the rarefaction fan. They vary as a fifth, sixth, and seventh degree polynomial for the mass, momentum, and total energy densities, respectively. So a minimum number of 14 points were used to discretize the rarefaction fan containing 14 RBFs within the fan.

We know that within a rarefaction fan, the entropy is constant. Although the fluid velocity, u, and sound speed, a, vary at each discretization point, the sum $u - \dfrac{2}{\gamma-1}a$ is constant. Each discretization point moves at a characteristic velocity, $dx_i/dt = u_i+a_i$. Before the rightmost point in the rarefaction wave hits the rigid wall, the solution is a trivial self-similar.

However, the situation becomes much more interesting when the rightmost part of the rarefaction waves collides with the rigid wall, reflects, and interacts with the parts of the rarefaction wave on the left. The reflected characteristic that had be previously a right traveling characteristic now becomes a left traveling characteristic. However, entropy does remain constant but a new Riemann invariant $u_r + \dfrac{2}{\gamma-1} a_r = u_{in} + \dfrac{2}{\gamma-1} a_{in}$ where the subscript r refers to the reflect portion of the rarefaction fan, and "in" refers to the right incoming portion of the fan. The compatibility equations for ith reflected wave and the jth incoming wave must be solved simultaneously to determine the result of the interacting waves.

The interactions were solved by RBF and volumetric RBF collocation. It was found that the results from volumetric RBF collocation were superior in preserving conservation and were more accurate. The small inaccuracies observed with the volumetric RBF scheme are on the order of machine round-off errors.

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