Time Marching Kernel Approximated PDE Solutions for Meshfree Computational Fluid Dynamics

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Abstract

This paper will address the problem of time marching function approximated solutions inherent in emerging meshfree Computational Fluid Dynamics (CFD) solution techniques. The numerical solutions of partial differential equations (PDEs) of CFD has been dominated by either finite difference methods (FDM), finite element methods (FEM), and finite volume methods (FVM). These methods can be derived from the assumptions of the Taylor expansion based local interpolation schemes and they require a mesh to support the local approximation. The problem is that in complex shaped domains, the construction of the mesh is a non-trivial problem. Typically with these methods, only the function is continuous across meshes, but not its partial derivatives. The difficulties of mesh construction and discontinuous derivatives has led to the development of mesh independent methods or meshfree (MF). These new meshfree methods represent the next generation of CFD solvers as they mature. In these methods the local function approximation method is independent of the mesh (or design points) of the geometric domain in which a solution is sought. In this paper we investigate the approximation of the local function by the kernel based statistical method of Nadaraya and Watson (NW). We show how the approximated solution in an arbitrary mesh can be matched in time to obtain the steady state and/or time dependent solution of the PDE.
KeyWords: Meshfree, CFD, Kernel Smoothers, Complex Variables, Time Marching, Derivatives

Introduction

Most practical engineering problems can be modeled by PDEs with the appropriate boundary and initial conditions. Approximating solutions to these relies heavily on numerical methods because of the non-linear nature of the problem, the complexity of the boundary and initial conditions, and/or the irregular geometry.

Types of schemes utilized with these numerical solution techniques are categorized as either implicit or explicit. If the scheme is implicit, the length of the time-step cannot be chosen at random. It is limited by the Courant-Friedrichs-Lewy (CFL) stability criteria. On the other hand if the scheme is explicit, then there is no bound on the length of the time-step. However, this scheme is limited because it requires solving simultaneously for all the unknown values of the variables at a particular time-step.

The numerical solutions of PDEs of CFD has been dominated by either FDM, FEM, and FVM. The FDM approximates the derivatives in the differential equations by truncating a Taylor series expansion in terms of the values at a number of discrete mesh points. The result is a set of algebraic equations to which the boundary and initial conditions are then applied to approximate the solution of the differential equations. The FEM approximates the unknown functions over each element, or sub domain, in terms of polynomial interpolation functions. This method also results in a set of algebraic equations to which the boundary and initial conditions are applied when discretized.

A numerical technique which has been receiving increasing attention among scientists and engineers is the boundary element method (BEM), also called the boundary integral equation method. It has become a viable alternative to FDM and FEM for solving engineering problems. The BEM theory dates to 1903 with Fredholm, who established the existence of solutions on the basis of his limiting discretization procedure. The emergence of computers in the 1950s stimulated the development of numerical methods including the BEM. Tosaka and Onishi [1,2] are given credit for first introducing an approach of implementing time differencing before deriving an integral equation. Su [3] developed a similar technique to obtain time marching integral equations for the solution of two and three dimensional unsteady transonic flows around wings. The main procedures are as follows: 1) time discretize the differential equations by replacing the time derivatives with finite difference, 2) transform the time discretized differential equation into an equivalent integral equation by applying the Green's function method, 3) discretize the integral equation in space and solve it using numerical integration techniques in each time step.

A method of simplifying complex PDEs is by first discretizing the spatial operators ($\partial x, \partial xx$, etc) on a chosen grid. This converts the PDE into a system of ordinary differential equations (ODE) to which an appropriate time integration method is applied to obtain a numerical solution. It is important to note that a single ODE system is not being considered but rather a family of systems which are parameterized by the grid parameter, step-size. In this paper, instead of approximating derivatives within the computational domain, the function itself is approximated by the statistical approach of kernel smoothing [9]. The function is then differentiated to obtain the required derivatives. To differentiate the function, the novel approach of complex variables method (CVM) will be used. Once the derivatives have been obtained, then an appropriate time marching approach can be chosen and implemented to solve the resulting system of ODEs. In this paper, the standard modified Runga Kutta approach will be used to march the solution in time.

Runge Kutta Method

Consider an ODE of the form:

$$\frac{dy}{dx} = f(x, y)$$

The Runge-Kutta method (RKM) computes the value of f(x,y) at strategic points in the rectangle bounded by the points [x, x+h, y(x), y(x+h)] and then combines them in such a way so to increase the order of accuracy. The formula involves a weighted average of values of f(x,y) inside this domain. In order to determine a point in this rectangle, it is necessary to compute the unknown y(x+αh) where α is a coefficient between 0 and 1. The RK scheme involves several stages or applications. As each stage is added, the order of accuracy increases by 1. Selection of the coefficient is cumbersome. These may be obtained by straightforward Taylor series expansion. More information can be obtained from numerical analysis textbooks.
An m-stage RK scheme (which is slightly different from standard formulation) used in this paper is of the form [5]:

$$\begin{aligned}
&y_1 = y(x) + \alpha_1 hf(y) \\
&y_2 = y(x) + \alpha_2 hf(y_1) \\
&\ldots \\
&\ldots \\
&y_{m-1} = y(x) + \alpha_{m-1} hf(y_{m-2}) \\
&y(x+h) = y_m = y(x) + \alpha_m hf(y_{m-1})
\end{aligned}$$

This RK method uses the classical approach and adds steps between y(x) and y(x+h). It achieves increased accuracy due to weighting more recent calculations. In general, the RKM is preferred to a Taylor series formula of same order accuracy because the RKM does not require that the higher partial derivatives be computed. Furthermore, the RKM is a very accurate formula, halving the time-step reduces the local formula error by the factor 1/32.

Kernel Methods

Non-parametric regression (NPR) belongs to the data analytic methodology known as local modeling [12]. NPR techniques consist of fitting a curve to a data set where there is little or no knowledge about its shape. The basic idea behind local regression consists of obtaining the prediction for a data point x by fitting a function. According to Cleveland and Loader [19], local regression dates back to the nineteenth century. The modern work on local modeling starts in the 1950's with the kernel methods introduced within the probability density estimation setting (Rosenballat, [14]; Parzen,[13]), and within the regression setting (Nadaraya, [10]; Watson, [11]).

Two of the most commonly used approaches to non-parametric regression are smoothing splines and kernel regression. Smoothing splines minimize the sum of the squared residuals plus a term, which penalizes the roughness of the fit. Kernel regression involves making smooth composites by applying a weighted filter to the data. The Kernel Smoother describes the trend in the dependent variable Y, as a function of one or more regressors. It helps to reduce the amount of horizontal scatter in the data. And, thus allows trends in the data to be easily seen.

Complex Variables Method for Obtaining Derivatives

The complex variables method, is somewhat similar to the automatic differentiation technique using the popular software tool ADIFOR, to obtain sensitivities (derivatives) from source codes. Application of automatic differentiation to an existing source code, (that evaluates output functions) automatically generates another source code that can be used to evaluate both output functions and derivatives of those functions with respect to specified code input or internal parameters. The pre-compiler software tool, ADIFOR is usually used to obtain derivatives from CFD and grid generation codes. On the other hand, the complex variables approach is simpler and easier to implement [15]. The application of complex variables to obtain derivatives has been described recently by Squire and Trapp, [16]. In addition, the method has been applied to obtain aerodynamic sensitivities for the Navier Stokes equations for use in aerodynamic shape optimization, [8]. This approach will be implemented to obtain derivatives in our meshfree solution approach.

Results and Discussions

The following problem is posed to illustrate the approximation of a function using kernel smoothers. Given is a data set of the form {(X_i,Y_i), i=1,2,…n, i∈N} which is assumed to occur in predictor-response pairs. The Gaussian kernel used to approximate the function $f(x,y) = y\cos x + 3x^2 e^y$ where x∈[0,7] and y∈[0,7] is

$$f_{estimate}(x,y) = \frac{\sum_{i=1}^{n} h_i Y_i}{\sum_{i=1}^{n} h_i} \quad \text{where} \quad h_i = e^{\frac{D_{i(x)}^2 + D_{i(y)}^2}{2\sigma^2}}, \qquad D_{i(x)}^2 = (x - X_i)^T (x - X_i),$$

$D_{i(y)}^2 = (y - Y_i)^T (y - Y_i)$, and σ=0.100.

Function approximations are generated using a Fortran code. The results follows:

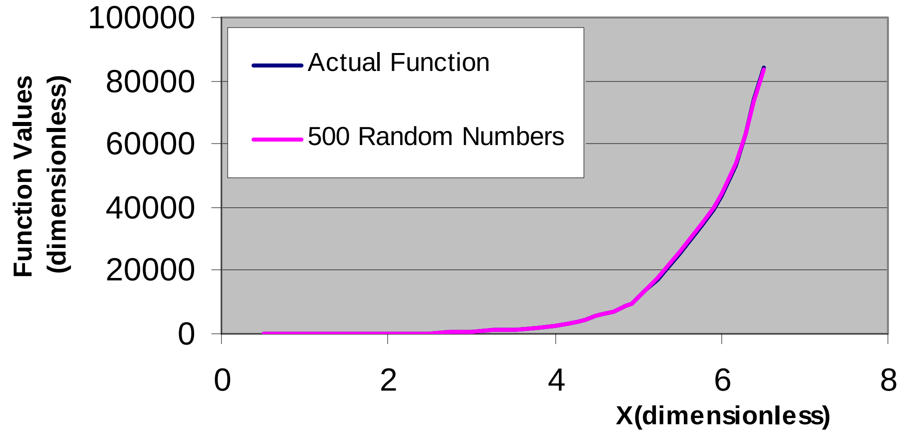

Figure 1. Actual Function Values versus Estimated Values using 500 Random Numbers in Computation

Figure 1 shows the function values versus the estimated function value using 500 randomly generated points (RGP) in the computation. The chart indicates that the approximation is close to the actual functional values. Figure 2 shows the relative errors when approximating the function using 20, 250, 400, and 500 RGPs. For 500 RGPs, the relative error ranges from -0.0280 to +0.0209 with an average of -.0007. For 20 RGPs the average relative error ranges from -0.5492 to +0.2784 with an average of -.0021. For 250 RGPs the average relative error ranges from -0.0550 to +0.0412 with an average of +0.0113. And, for 400 RGPs the average relative error ranges from -0.0596 to +0.0217 with an average of -0.0113. Clearly, the 500 RGPs resulted in the closest function approximation having the smallest relative error. In addition, this approximation had the smallest relative error range of 0.0489 versus 0.8276 for 20 RGPs, 0.0962 for 250 RGPs, and 0.0813 for 400 RGPs.

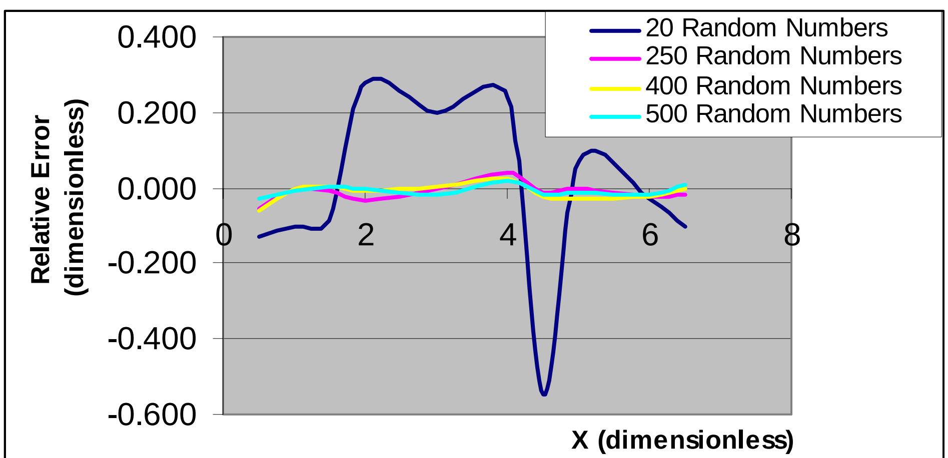

Figure 2. Relative Error for Estimated Function Values using Random Numbers Equal 20, 250, 400, 500 in Computation

Conclusions

Preliminary results for our new meshfree method for solving PDEs has been presented. We have shown the accuracy of the kernel approximator using a two dimensional mathematical function to simulate 2-D CFD. Complete results will be presented in a followup paper

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