Second Order Spatial Accuracy in Spray Calculations

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When properly constructed, Lagrangian particle tracking should provide grid-independent results. Unfortunately, the numerical methods used in spray simulations are still somewhat ad-hoc. The current work attempts to (1) verify the order of accuracy of existing methods and (2) establish the simplest possible techniques for achieving second-order accuracy.

1. Introduction

Grid dependency, one of the problems faced by spray modelers, seriously undermines the ability to predict sprays accurately. It is unpredictable in nature and confounds the modeling of the physics of spray. Grid dependent computational models of sprays might lead to incorrect conclusions, eventually leading to expensive engineering mistakes.

Among all numerical methods used for spray simulations, the Eulerian-Lagrangian method has been the most popular. Eulerian-Lagrangian methods typically use the idea of statistical representation of the spray [1]. Lagrangian particle tracking is simple to implement and fast. Also, Monte Carlo Lagrangian particle tracking efficiently samples the multi-dimensional spray. Lagrangian particle tracking, though widely used, can demonstrate strong grid dependence [2, 3, 4, 5 and 6].

KIVA [7], which has been extensively used to simulate sprays (mainly sprays in internal combustion engines), implements Lagrangian particle tracking. Subramanian and O'Rourke [3] attempted to demonstrate that the KIVA code was convergent, but did not observe any such convergence in their tests. One of the main conclusions of their work was a recommendation of better coupling of the two phases.

Aneja and Abraham [6] concluded that the grid dependence is mainly because of the various sub models involved and inadequate spatial resolution hindering the coupling between the gas and liquid phase. Beard et al [4] developed a new Lagrangian-Eulerian Coupling method (CLE). The approach introduces gaseous particles and a sphere of momentum influence retaining vapor and momentum along the parcel trajectories. This improves liquid vapor transport and the momentum coupling between liquid-gas interactions. The model also addressed the issue of over-prediction of the drag because of the incorrect relative velocity between the two phases. However, some details of this model were necessarily ad hoc. Hieber [5] studied grid dependency in KIVA. She implemented a Void Fraction Compensation to correct for under resolution. In her conclusions Hieber identified coupling between the gas and liquid phase as the reason for mesh dependence. One of the few successes in testing for accuracy and achieving grid independent solutions was Sirignano [10]. Sirignano was able to demonstrate second order convergence. However many of the details of his test were never reported. Also, his simulations did not include any stochastic components, such as staggered injection and drop size sampling. Sirignano does not present a theoretical basis for why his approach should be second order.

In view of the above requirement for convergent, consistent and accurate spray simulations, the present work attempts to establish minimal standards by which second-order spatial accuracy can be achieved. This work will show that the Monte-Carlo sampling of sprays method can produce second order accurate results. Secondly, we question some of the observations of Sirignano. Toward this end, the liquid-phase simulation is divided into four parts: particle tracking, gas-to-liquid interpolation, liquid-to-gas distribution, and physical models. Each of these parts is tested independently for second-order accuracy.

2. Methodology

2.1. Gas Phase Solver

A new code, MOSES, is used, which is based on the Eulerian-Lagrangian framework. MOSES is a new code being developed at Convergent Thinking LLC in collaboration with University of Massachusetts. Currently it employs a regular block-structured mesh in a regular domain. All convective terms are third-order upwinded and the diffusive terms are second-order central differenced. With minor variations, the PISO method of Issa [8] is used for solving the gas phase conservation equations for both incompressible and compressible solvers.

2.2. Liquid Phase

As mentioned earlier, the liquid-phase simulation can be divided into four parts: particle tracking, gas-to-liquid interpolation, liquid-to-gas distribution, and physical models. Each of these is addressed below.

2.2.1. Particle tracking

Several methods were investigated and, surprisingly, the semi-implicit method employed by O'Rourke, turned out to be ideal. The semi-implicit method for updating the droplet velocity was employed by O'Rourke because it is unconditionally stable and also one of the simplest possible methods. This is the method implemented in KIVA. This method is the exact solution for a constant coefficient of drag, C_d, and constant gas velocity, u_g. O'Rourke was concerned only with stability, but this high accuracy is a fortuitous benefit of his choice [13].

2.2.2. Gas to Liquid Coupling

Gas-to-liquid interpolation involves interpolating the gas-phase velocity (flow quantities) to the parcel location to calculate the relative velocity. Relative velocity is an important parameter in the other spray sub models (breakup, vaporization) and hence gas-to-liquid interpolation is critical aspect in pursuing accurate spray calculations.

2.2.3. Liquid to Gas Coupling

Liquid to gas coupling is mainly the distribution of various source terms (mass, momentum and energy) to the gas phase nodes. In addition, since the mass and heat exchanges between the two phases are analogous to the momentum coupling, conclusions reached for momentum coupling are likely to be applicable to the others. In Eulerian-Langrangian, techniques since the spray is represented by particles, the momentum lost by the spray is now treated as point sources in the gas field. The distribution of these source terms is important to get the right gas field and spray solution. There are several different ways of doing this. The simplest approach

is to give all the momentum lost by droplets to the nearest gas phase node. This is called the "nearest node" approximation and is implemented in KIVA. Sirignano [9] advocated a distribution method based on distance from the surrounding gas phase nodes. The two approaches differ in the kernels they use to distribute the source terms in a cell to the nearby nodes.

2.2.4. Physical Models

No physical models were used in any of the tests below. Future numerical tests will include the Enhanced Taylor Analogy Breakup model, which is used to model jet and droplet breakup [11]. The NTC collision algorithm developed by Schmidt and Rutland [2] will be used to calculate collision incidence. This algorithm has a computational cost linearly proportional to the total number of parcels in the cell. The NTC algorithm is first order accurate in time and second order accurate in space.

3. Analysis and Results

3.1. Particle and Trajectory

The basic equations governing the parcel velocity and trajectory can be expressed as the following ODE's [3]:

$$\left.\begin{aligned} \frac{d\vec{x}_p}{dt} &= \vec{u}_p \\ \frac{d\vec{u}_p}{dt} &= -C_d (u_p - u_g)^2 \end{aligned}\right\} \qquad [3]$$

The variable $\vec{V}_{rel}$ represents the relative velocity of the gas and parcel. Hence if u_g^n, the gas velocity at the nth timestep, is taken to be a constant then the drag equation [4] is a linear ODE. Even though this ODE appears to be a three-dimensional, it is really one-dimensional because the relative velocity is in the direction of the force acting on the parcel.

$$\frac{d\vec{V}_{rel}}{dt} = -C_d \vec{V}_{rel}^{\,2} \qquad [4]$$

The analytical solution is easy to calculate by direct integration. Integration of equation [4] gives equation [5] which is nothing but the semi implicit method implemented in KIVA by O'Rourke.

$$\vec{V}_{rel}^{\,n+1} - \vec{V}_{rel}^{\,n} = -C_d * \Delta t * \vec{V}_{rel}^{\,n+1} \vec{V}_{rel}^{\,n} \qquad [5]$$

$$\text{i.e. } \vec{V}_{rel}^{\,n+1} = \frac{\vec{V}_{rel}^{\,n}}{1 + C_d * \Delta t * \vec{V}_{rel}^{\,n}}$$

$$u_p^{n+1} - u_p^n = \left(u_p^{n+1} - u_g^n\right) - \left(u_p^n - u_g^n\right) = \vec{V}_{rel}^{\,n+1} - \vec{V}_{rel}^{\,n} = -C_d * \Delta t * \vec{V}_{rel}^{\,n+1} \vec{V}_{rel}^{\,n}. \qquad [6]$$

To include changes in C_d and u_g^n, we use a predictor-corrector implementation of this method. Accuracy tests performed showed that this implementation was second order accurate.

3.2. Coupling of the gas phase and spray: Tests of linear interpolation

For coupling between gas phase and spray tri-linear interpolation was used, and accuracy tests showed that the interpolation scheme was second order accurate with respect to spatial variations. The tests were performed by injecting a single parcel into a fixed quiescent gas field with no collision or breakup. The gas field was generated using a Gaussian function. This profile is a rigorous test because it cannot be represented exactly by any polynomial. The Gaussian is a function of radial and axial distance from the injector.

3.3. Liquid-to-gas coupling

Sirignano, in his tests, had observed that nearest node momentum coupling is not sufficient for second-order accuracy. He compared fine mesh calculations to coarser-mesh calculations and noted the rate of convergence. In this present work, theoretical analysis and different numerical tests were performed using the nearest node method and Sirignano's method of distribution of the source term. Our results suggest that nearest node is indeed second order accurate. Sirignano's method is also found to be second-order accurate. Thus, the more sophisticated smoothing kernel demonstrates no higher formal accuracy than the simple nearest-node kernel. Numerical noise may have prohibited Sirignano from observing this in his numerical tests since he used relatively few parcels. Consequently, the spray exerts a non-smooth influence on the gas. In the current tests, the number of parcels per cell is kept high enough to suppress random error.

3.3.1. Theoretical Analysis

The following analysis is easy to visualize in the 1-D and can easily be extended to 2-D or 3-D. If x_p represents the parcel position and x_i represents the node position of the gas phase node, then the weight of the parcel on the node is given by $W(x_i - x_p)$, where W is the kernel of the weighting method. If $f(x)$ is the source function and N is the number of parcels, the value of the function at the node can be calculated to be

$$f(x_i) = \sum_{p=1}^{N} W(x_i - x_p) * f(x_p) \qquad [7]$$

The kernel for nearest node is given by:

$$W(x_i - x_p) = \begin{cases} 1.0 & |x_i - x_p| \le dx/2 \\ 0 & \text{otherwise} \end{cases} \qquad [8]$$

The kernel for Sirignano's method is given by:

$$W(x_i - x_p) = \begin{cases} (dx - |x_i - x_p|)/dx & |x_i - x_p| \le dx \\ 0 & \text{otherwise} \end{cases} \qquad [9]$$

Now if we assume perfect (continuous) approximation of the source function using an infinite number of parcels, the value of the function at the node is given by

$$f(x_i) = \int W(x_i - x_p) * f(x_p) dx_p \Big/ \int W(x_i - x_p) dx_p \qquad [10]$$

If the nearest node approximation is used the function value will be

$$f(x_i) = \frac{1}{dx} \int_{x_i - dx/2}^{x_i + dx/2} 1 * f(x_p) dx_p \qquad [11]$$

Thus, the nearest node method collects the average value of the source function in its vicinity. It can be shown that the nearest node method gives an exact answer when the source is constant or linear. A constant source function would just be a constant *A*. Evaluation of the above integral, assuming perfect sampling, and $f(x_p)=A$ gives the exact answer. Similarly, if a linear function is used, where $f(x_p)=Bx$, then the integral also gives the exact answer. Since any function can locally be approximated as a linear function with error $O(dx^2)$, then the leading truncation error term must be, at a minimum, second order. Similar analysis using Sirignano's methods showed that it was also second accurate.

3.3.2. Analytical Test based on the drag approximation

In this 1-D test case the parcels were stochastically distributed using an exponentially varying number density (equation [12]) along a 1-D domain of length L. The velocity field and the parcel velocities were fixed using an exponential function (equation [13]). Hence we have the exact (analytical) value of the drag at each node. The drag is also evaluated using both the nearest node method and Sirignano's method.

$$N(x) = 10^6 * \exp^{-\left(\frac{x}{L}\right)}. \qquad [12]$$

$$V(x) = 10 * \exp^{-\left(\frac{x}{L}\right)}. \qquad [13]$$

The total drag over the whole domain is calculated analytically and is also approximated using the different drag terms at each node and the trapezoidal rule. The approximations of the total drag are then compared to the analytical value. The relative errors observed in each case are plotted (Figure 3*)* as function of varying mesh size (*dx*). As shown, all the three curves have the same slopes, and hence we can claim that the nearest node method is second order accurate.

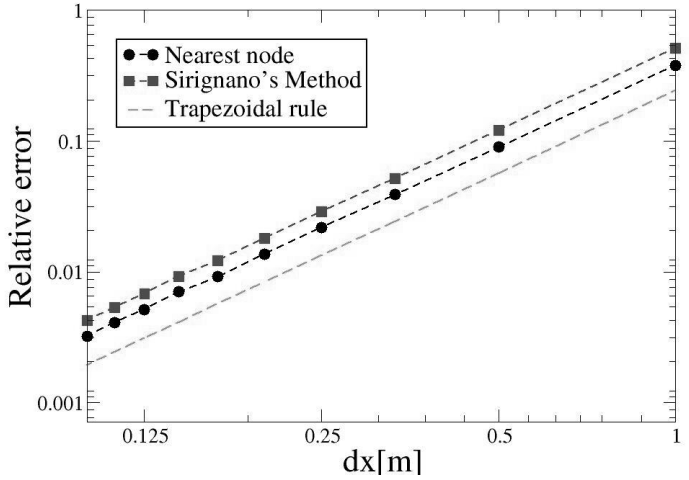

Figure 3. Comparison of error in the total drag approximation of Sirignano's method and nearest node to the error obtained when using trapezoidal method for varying dx.

4. Convergence Tests

All the parts of the spray model are tested together to demonstrate the collective behavior. Now that each method has individually been shown to be second order accurate, this should translate into second order accuracy when tested together. Since it is difficult to have an analytical solution for a real spray problem, only convergence can be tested for the collective code. This is done by testing the order of convergence to a numerical solution created with a

very fine mesh. Two different tests were performed using two different types of spray driven flows.

4.1. Swirling Spray Test

In this first test case an actual gas flow field with particles in a two dimensional domain of size *0.1m×0.1m* was simulated. All the particles were initialized to have an angular velocity and injected into the domain at the beginning. This test is relevant to swirling sprays, a respectable challenge for a Cartesian mesh. The source term was calculated again using nearest node approximation and Sirignano's methods. Five different mesh sizes were used: *dx=0.01m, dx=0.005m, dx=0.002m, dx=0.001m* and *dx=0.0005m.* One hundred thousand parcels were used in all of these simulations. The goal is here is to show that this variation in the angular momentum predictions for varying mesh sizes is proportional to dx^2.

For this test, Sirignano's method was clearly demonstrated to be second order accurate. The nearest-node method was found to be second order accurate for well-resolved cases, but performed badly with a coarse mesh. The smoother kernel of Sirignano's method is closer to being isotropic than the nearest-node method, which likely explains its superior performance in swirling flow.

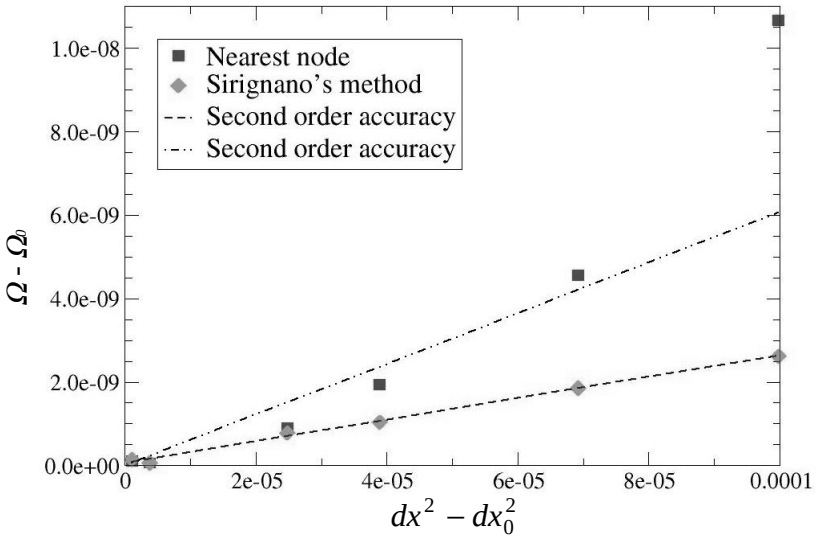

Figure 4. Plot showing that Sirignano's method and nearest node are second order accurate.

4.2. Plain Orifice Test

In the second test, particles are injected into gas flow field in a two dimensional domain of size *0.02m×0.04m.* This test was run with a planar, two-dimensional spray source that resembles a plain-orifice atomizer with a width of *4mm*. The source term was calculated again using nearest node approximation and Sirignano's method. Five different mesh sizes were used: *dx=0.005m, dx=0.0025m, dx=0.002m, dx=0.001m, dx=0.0005m, dx=0.00025m, dx=0.0002m, dx=0.0001m* and *dx=0.00005m.* Four hundred thousand parcels were used in all of these simulations. Figure 5 shows the plots of the gas phase kinetic energy summed over all nodes in the domain as a function of different mesh sizes. The plot also shows that the predictions of both methods are second order accurate.

Interestingly, Figures 6 and 7 show an order of convergence that is different than that of the gas phase. The order one-half convergence of spray tip penetration is common for Monte Carlo methods. However in the present work, it was observed even when the number of parcels was held constant. The first order convergence of the spray center of mass is also intriguing.

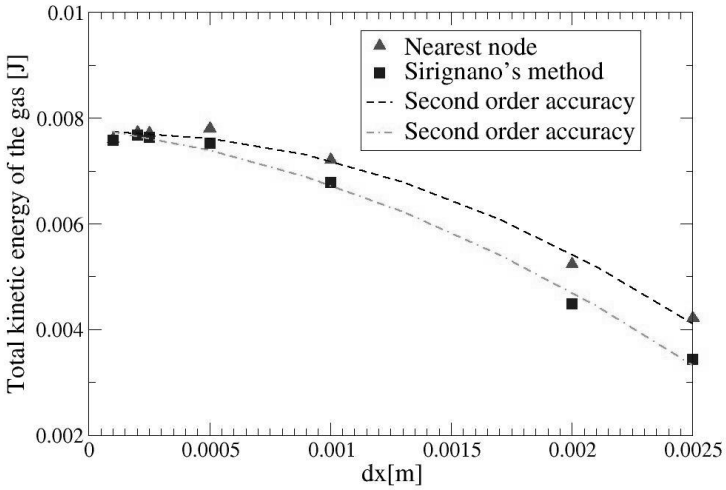

Figure 5. Log plot showing that predictions of nearest node and Sirignano's method are second order accurate.

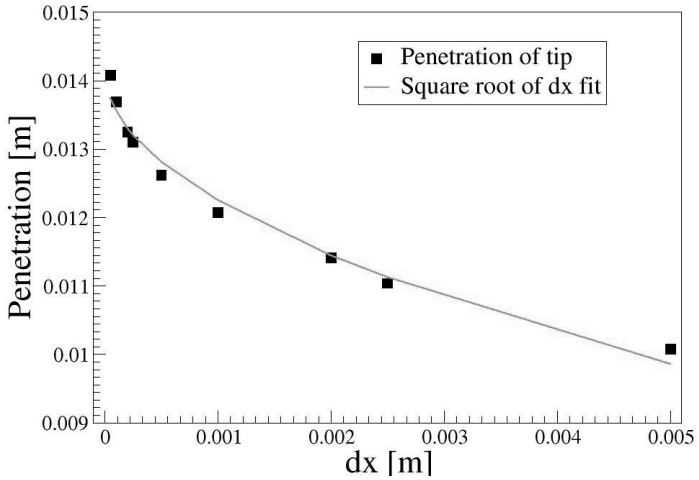

Figure 6. Plot showing variation of penetration of the tip with varying mesh size.

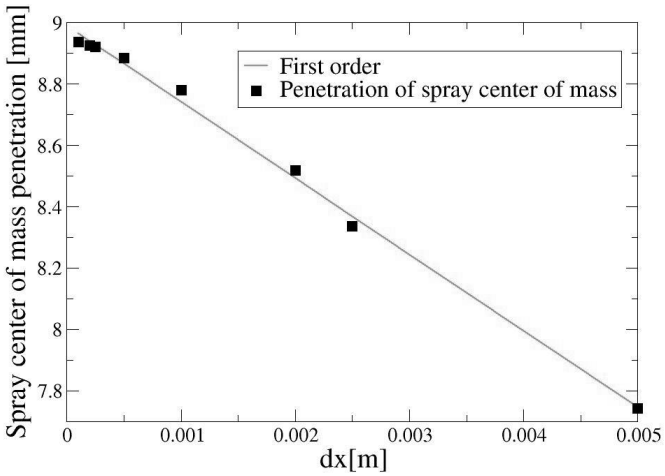

Figure 7. Plot showing variation of penetration of spray center of mass with varying mesh size.

5. Conclusions

In this work we explore the grid dependency of sprays simulations. One of the main conclusions is that nearest node method is second order accurate, contrary to the popular

belief that it is first order. But even though the nearest node method is second accurate, it is slightly inferior to Sirignano's method in swirling sprays due to the fact that Sirignano's method is smooth and less anisotropic.

As shown in the convergence tests, this work has partially established second order accuracy and convergence of spray simulations. This work also highlights techniques required to achieve second accuracy. The results are not conclusive in addressing the order of accuracy, as there seemed to be a dependence of the convergence on the metric that is chosen. These convergence rates appear related to the Monte Carlo nature of the spray simulation. The dependence of convergence rate on the metric chosen is clear from the different rates of convergence of penetration of the tip of the spray and penetration of the center of mass of the spray, which converge at rates proportional to $dx^{1/2}$ and dx (linear) respectively. The improved order of accuracy of penetration of the center of mass of the spray is likely due to the averaging process that is used for calculating the center of mass location.

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