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Interfacial transfer in Tryggvason's method

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SUMMARY

Tryggvason's method computes two phase flows by smoothing the regions near the boundaries between the two fluids. This requires averaging of the fluid properties, which may differ by orders of magnitude and can lead to large errors. Traditional linear averaging produces a first order error that can be extremely large. In this paper, we show that for a number of simple test cases, averaging of the inverses of the properties can lead to a significant improvement in the quality of the results. Copyright © 2003 John Wiley & Sons, Ltd.

1. INTRODUCTION

Numerical methods for simulating two-phase flows have received increased attention in recent years. Methods that have been proposed can be broken into two major categories. In the first group are methods that advance the Navier–Stokes equations as if the two phases comprise a single fluid. In the second type of method, the two phases are treated separately and the phase boundary is explicitly taken into account. These may be called front capturing and front tracking methods, respectively.

Among the front tracking methods are the Chimera method developed by Dwyer and others (for example, Reference [1]) and the moving finite element method proposed by Helenbrook among others (for example, Reference [2]). Chimera methods use a body fitted grid overlaid on a coarser outer grid and the solution is obtained by iterating between the two grids and passing information between them. The major problem in this approach is that it is difficult (but not impossible) to take deformation of the phase boundary into account. The finite element method has the potential to handle a wider range of problems but is likely to be more expensive computationally.

The principal types of front capturing methods are the volume of fluid methods that have been worked on by many people (Reference [3] and others). In these methods, each cell

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carries a parameter that represents the fraction of a cell filled with one of the fluids. The major disadvantage in this approach is that the interface needs to be reconstructed after each time step and this is difficult to do accurately.

Tryggvason's method [4, 5] also treats the entire system as a single fluid, advancing the solution at all grid points simultaneously, but avoids use of an auxiliary variable. Numerical oscillations are suppressed by smoothing all of the fluid properties over several computational cells in the direction normal to the interface. To prevent it from being smoothed excessively by diffusion, the interface is explicitly tracked. Use of a level set method has been suggested as an alternative to tracking. As is true of many methods that deal with sharp interfaces, this method is only first order accurate in the region of the interface. Decreased accuracy near the interface is deemed acceptable (if not necessary) when compressible flows containing shocks are simulated. However, in two-phase flows, the rate of exchange of important physical properties such as momentum, energy, and species between the phases is often one of the significant quantities to be computed and it is predicted to only first order accuracy by Tryggvason's method.

In this note we will first give a demonstration that the method is first order accurate in the exchanged properties. For steady one-dimensional heat conduction (or its mathematical equivalent, two-layer Couette flow) it is possible to modify the method so that the computed heat (momentum) flux is exact even though the temperature (velocity) field is not. We shall show that the accuracy is also improved when the new procedure is applied to the unsteady heat equation and stratified unsteady Couette flow.

2. STEADY ONE-DIMENSIONAL HEAT CONDUCTION

2.1. Dependence of the heat flux on the averaging procedure

To begin, let us consider a simple problem, steady heat conduction in a two-layer medium. It is not much more difficult (and is more useful) to consider the heat equation with arbitrarily variable thermal conductivity:

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(k(x)\frac{\mathrm{d}T}{\mathrm{d}x}\right)=0 \tag{1}$$

This equation is to be solved together with the boundary conditions:

$$T(0)=T_0; \quad T(L)=T_1 \tag{2}$$

In the two layer case:

$$k=\begin{cases} k_1 & x<L/2 \\ k_2 & x>L/2 \end{cases} \tag{3}$$

The reason for using a heat transfer setting rather than the apparently more relevant fluid mechanical one will become obvious below.

The problem posed by Equations (1) and (2) is easily solved in closed form for any distribution of k. In fact, the non-dimensional temperature distribution is:

$$\frac{T - T_0}{T_1 - T_0} = \frac{\int_0^x \mathrm{d}x/k(x)}{\int_0^L \mathrm{d}x/k(x)} \tag{4}$$

while the heat flux (which is independent of x) is:

$$q = \frac{T_1 - T_0}{\int_0^L \mathrm{d}x/k(x)} \tag{5}$$

These results are easily specialized to the case of a two-layer medium.

The largest error in Tryggvason's method for this problem is not due to the method used to discretize the equations. The essential element of the method, whose effect needs to be investigated, is the replacement of the exact thermal conductivity k by a smoothed one. The smoothing can be represented by a filtering operation:

$$\bar{k}(x) = \int G(|x - x'|)k(x')\,\mathrm{d}x' \tag{6}$$

Typically, one might use a simple volume average which corresponds to $G(x) = 1$ for $|x| < L$ and $G(x) = 0$ for $|x| > L$.

This smoothing is the principal source of error. The effect of smoothing the conductivity on the temperature field was analysed by Tryggvason himself. The analysis is relatively straightforward. One assumes that the difference between k and $\bar{k}$ and the resulting change in the temperature profile are both small i.e.

$$\bar{k} = k + \delta k; \quad \bar{T} = T + \delta T \tag{7}$$

and ignores second order terms. When Equation (7) is substituted into the heat equation (1), the result is easily solved for the perturbation to the temperature. This is not difficult to do but we are more interested in the change in the heat flux; it is not difficult to show that:

$$\delta q = \frac{\int_0^L \frac{\delta k(x)}{k(x)}\,\mathrm{d}T/\mathrm{d}x\,\mathrm{d}x}{\int_0^L \mathrm{d}x/k(x)} \tag{8}$$

The denominator of this expression is constant and, for the two layer case, the functions $\mathrm{d}T/\mathrm{d}x$ and k in the numerator are both piecewise constant. If $k_1 < k_2$, then δk is positive for $x < 0$ and $\delta k(x) = -\delta k(-x)$. Using this observation, it is not difficult to show that δq is proportional to the size of the region over which k is smoothed. Since, in Tryggvason's method, this is a fixed number of grid sizes, we see that the error is proportional to the grid size i.e. the heat flux is computed with first order accuracy.

To perform calculations with the method, we used a conservative second order central finite volume method in which the temperature is given at the grid points and the thermal conductivity is given midway between the grid points [6]; a temperature node is located at the interface but we shall discuss the issue further below. The smoothing is accomplished by averaging the thermal conductivity over five points with a weighting of 1/8, 1/4, 1/4, 1/4, and 1/8. These calculations (and all subsequent ones) were run on an SGI workstation using

Table I. Steady one-dimensional heat flux.

Grid size	Heat flux	Error/$q_{ex}h$
0.1	2.0486	−1.2693
0.05	1.9265	−1.1918
0.025	1.8708	−1.1573
0.01	1.8389	−1.1375
0.005	1.8285	−1.1311
0.0025	1.8233	−1.1279
0.001	1.8202	−1.1260

Matlab. For the case shown in the table, we took $k_1 = 1$, $k_2 = 10$, and $L = 2$. For this case, the exact heat flux is 1.8182. Table I presents both the heat flux and the relative error divided by the grid size. As expected, the results show that the method is first order accurate and that the errors are quite large for moderate grid sizes.

A way to improve the accuracy to which the heat flux is computed can be based on a method presented in many elementary heat transfer textbooks. Indeed, the method has been known for a sufficiently long time that it is not clear to whom it should be attributed. This approach can also be found by inspection of Equation (5). The idea is that the heat flux will be exact if $1/k$ is averaged rather than k. In other words, the resistance, not the conductance, must be averaged; this leads to the well-known analogy between conductive heat transfer and resistive electrical circuits and is the reason why the problem was cast in heat transfer terms. In fact, if we repeat the calculation done above and average $1/k$ rather than k, the heat flux is computed exactly with any grid size. The temperature profile is, of course, not computed exactly. Indeed, the error in the temperature distribution remains first order in the grid size but the actual error, at least for this problem, is reduced by about an order of magnitude. The temperature profiles are shown in Figure 1.

The figure also shows that the error created by averaging k is largely a shift of the solution curve into the region of lower thermal conductivity. This can be attributed to the fact that this method of averaging produces a larger k in the part of this region close to the boundary.

We should also mention that Tryggvason [7] himself recognized that averaging $1/k$ rather than k should produced improved results but did not use the procedure recommended here in place of his method.

2.2. *Another view of the problem*

We can repeat the analysis of the preceding section in a way that will be useful later. In problems whose solutions have discontinuities, for example problems with shocks or reaction fronts, it is necessary to smooth or filter the solution in order to render it resolvable on the numerical grid. This may be accomplished by adding a diffusive (dissipative) term to the differential equation or by using a dissipative numerical method. A related technique is used in turbulent flows. Because it is impossible to capture the smallest scales, they are filtered out and a model (which often takes the form of an increased or eddy viscosity) is added to the equations. In the present case, it is only the derivative of the solution that has a discontinuity so the issue is somewhat simpler.

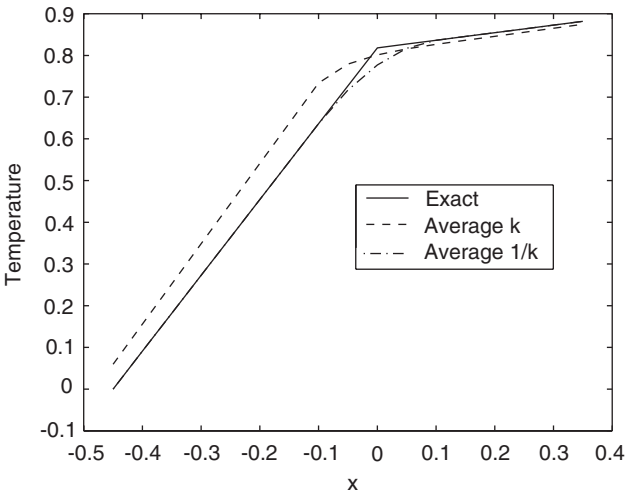

Figure 1. The temperature profile produced by Tryggvason's method with averaging of k and $1/k$ compared with the exact solution. The solid line is the exact solution, the dashed line was obtained by averaging k, and the dash-dot line is the solution obtained by averaging $1/k$. The method described in the text was used in each case with grid size, $h = 0.05$.

Let us filter Equation (1). Since a filter of the form (6) commutes with differentiation, the result is

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(\overline{k\,\frac{\mathrm{d}T}{\mathrm{d}x}}\right) = 0 \tag{9}$$

Our objective is to select $\bar{k}$ so that

$$\bar{k}\,\frac{\mathrm{d}\bar{T}}{\mathrm{d}x} = \overline{k,\frac{\mathrm{d}T}{\mathrm{d}x}} \tag{10}$$

In the present case, this is easily accomplished. Because $k\,\mathrm{d}T/\mathrm{d}x = -q$, the heat flux which is constant, we can write:

$$\bar{k} = -\frac{q}{\mathrm{d}\bar{T}/\mathrm{d}x} = \frac{q}{\overline{q1/k}} = \frac{1}{\overline{1/k}} \tag{11}$$

This is, of course, the result we found earlier.

The interpretation of this result is that, if the thermal conductivity (11) is used, the solution (in the absence of numerical errors) should be the filtered temperature field

$$\bar{T} = \int G(|x - x'|)T(x')\,\mathrm{d}x' \tag{12}$$

Since the width of the filter need not be related to the grid size, this is the temperature profile to which an accurate numerical solution will converge. This view shows that there are two sources of difference between the exact solution of the differential equation and the numerical solution: filtering and numerical error. The filtered temperature distribution is

computed exactly (to machine accuracy) by the method described above, as it should be because $\bar{k}\mathrm{d}\bar{T}/\mathrm{d}x$ is constant.

In a more realistic problem, it would not be possible to place a grid point at the interface. If we use the method described above, this means that the interface cannot be localized to within less than a grid size and there is therefore an error of this order of magnitude in the resulting temperature profile. The heat flux remains exact, however.

In the calculations shown in the figure, the boundary between the two regions was placed on a grid point. When we repeated the calculations with the boundary half way between two grid points, nearly identical results were found.

3. UNSTEADY HEAT CONDUCTION

As the next example, let us consider the case of unsteady one-dimensional heat conduction with constant heat capacity and density:

$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(\alpha \frac{\partial T}{\partial x}\right) \tag{13}$$

where $\alpha = k/\rho c_p$ is the thermal diffusivity. This problem can also be interpreted as two-layer constant density Couette flow. For the initial temperature distribution, we take the step function:

$$T(x,0) = \begin{cases} -1 & x<0 \\ 1 & x>0 \end{cases} \tag{14}$$

This problem has an exact solution that is an error function on each side of the discontinuity. The solution is continuous everywhere, including at the property discontinuity, but its derivative is not. (The heat flux $q = -k\,\mathrm{d}T/\mathrm{d}x$ is continuous everywhere including at $x=0$ but is not constant in either space or time.)

In order to avoid the numerical problems associated with the discontinuity of α, we shall start the numerical solution with the exact solution at $t=0.2$ and run until $t=0.4$. We use $\alpha_1 = 1$ and $\alpha_2 = 0.1$. The exact heat flux at the final time is 0.5916.

It is again possible to use the perturbation method to show that the method based on averaging k is first order accurate in its prediction of the temperature.

If we filter Equation (13), the result can be written:

$$\frac{\partial \bar{T}}{\partial t} = \frac{\partial}{\partial x}\left(\bar{\alpha} \frac{\partial \bar{T}}{\partial x}\right) \tag{15}$$

where $\bar{\alpha}$ is defined in analogy with $\bar{k}$ of Equation (10). The important difference between this case and the preceding one is that, because the heat flux is not independent of either x and t, it is not possible to reduce this expression to the simple average in Equation (11).

Thus, to find $\bar{T}$ it would be necessary to re-evaluate $\bar{\alpha}$ at each time step using the instantaneous temperature profile, which would add a great deal of expense to the procedure. To avoid the necessity of doing this we shall use the averages that were applied in the preceding problem.

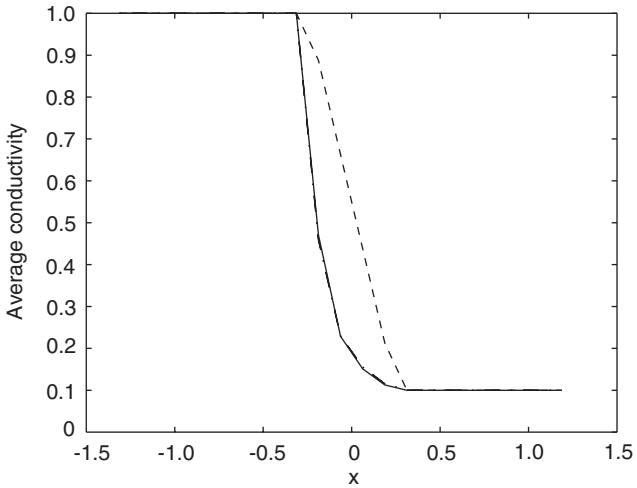

Figure 2. The average thermal diffusivity produced by simple averaging of $1/k$ (solid line) and k (dashed line) and by averaging with the exact temperature distributions at $t = 0.2$ and 0.4 (dash-dot lines).

We can get an idea of the effect of averaging by computing $\bar{\alpha}$ using the exact temperature distribution. Figure 2 shows the distribution of $\bar{\alpha}$ produced by simple averaging of $1/\alpha$ and α and by computing the average with the exact temperature profile for a grid size of 0.125. It is clear that averaging the inverse of α produces a better approximation to the actual average. We repeated this process at other times and with different grid sizes and found similar results in all cases.

For numerical solution of the problem, we used a slight extension of the method employed in the preceding section. The thermal conductivity (or its inverse) is smoothed in the way it was in the preceding case and the spatial derivative is discretized in the manner described earlier. The temperature profile is advanced in time using the Crank–Nicolson (trapezoid) method with a time step $\Delta t = 0.125h^2/\alpha_{\max}$ where h is the spatial grid size. This assures that the error due to the time advancement is smaller than that due to the spatial differencing.

In this case, there are three sets of results that may be compared. The first is the exact heat flux at the interface which is, of course, independent of the computational parameters. The second is the exact heat flux obtained with the filtered conductivity; it can also be obtained by filtering the exact heat flux. Finally, there is the numerical solution which, if discretization errors were removed, would agree with the second value.

The results obtained when the thermal diffusivity, α, is averaged are presented in Table II. We see that the error is quite large and is approximately proportional to the grid size i.e. the method appears to be first order accurate, as expected.

When we average $1/\alpha$ rather than α, we obtain the results shown in Table III. The errors are much smaller than those obtained by averaging α. However, there is a change in the sign of the error between the last two grid sizes so it is not possible to say that the method has a definite order. However, the error appears to decrease in magnitude at least as fast as the square of the grid size.

Table II. Unsteady one-dimensional heat flux with α averaged.

Grid size	Heat flux	Error/$q_{ex}h$
0.25	0.8186	−1.5353
0.125	0.7366	−1.9652
0.0625	0.6424	−1.3747

Table III. Unsteady one-dimensional heat flux with $1/\alpha$ averaged.

Grid size	Heat flux	Error/q_{ex}
0.25	0.4695	0.8257
0.125	0.5673	0.3247
0.0625	0.5945	−0.0796

4. UNSTEADY COUETTE FLOW

As the final example we consider a problem that is a slight mathematical variation on the preceding problem. This is stratified Couette flow, for which the differential equation is

$$\rho \frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(\mu \frac{\partial u}{\partial x}\right) \tag{16}$$

with both the viscosity μ and the density ρ having two-layer behaviour. The initial velocity distribution, is again a step function:

$$u(x,0) = \begin{cases} -1 & x<0 \\ 1 & x>0 \end{cases} \tag{17}$$

The solution is started with the exact solution at $t = 0.01$. We have chosen properties that approximate those of the water–water-vapour system:

$$\mu(x,0) = \begin{cases} 1 & x<0 \\ 100 & x>0 \end{cases} \qquad \rho(x,0) = \begin{cases} 1 & x<0 \\ 1000 & x>0 \end{cases} \tag{18}$$

For this case, the exact shear stress is $\tau = 2.4546$.

The only significant difference between this problem and the preceding one is the density variation. Since we are now certain that the inverse of the diffusive property (viscosity) should be averaged, the important question is whether to average the density itself or its inverse. We shall do this problem both ways.

Although we can be quite certain that averaging the properties themselves will not give good results, we tried that approach. The errors were very large; on the finest grid the shear stress at the boundary was 3.23 vs the exact value of approximately 2.45 given above. On coarser grids, the results were much worse. When one looks at the profiles, it is found that

Table IV. Unsteady one-dimensional shear stress with $1/\rho$ averaged.

Grid size	Shear stress	Error/$\tau_{ex}h$
0.25	2.5117	−0.0932
0.125	2.5118	−0.1903
0.0625	2.4693	−0.0959

Table V. Unsteady one-dimensional shear stress with ρ averaged.

Grid size	Heat flux	Error/$\tau_{ex}h$
0.25	5.5275	−5.08
0.125	6.4480	−13.03
0.0625	4.8402	−15.55

the reason for such large errors is that the profile is shifted to the left relative to the correct one just as was the case for the one-dimensional steady conduction problem.

The results obtained when both the inverses of the density and viscosity are averaged are shown in Table IV. We see that the quality of the results is approximately the same as those found in the preceding two cases. The error appears to decrease more rapidly than the grid size (at least for the finest grids used) but it is difficult to say anything about the order of the method.

When the density and the inverse of the viscosity are averaged, we obtain the results presented in Table V. They are obviously not of the quality obtained when the inverses of both properties are averaged. We conclude that the best procedure is to average the inverses of both the density and the viscosity. We believe that this result should apply to the Navier–Stokes equations as well.

An argument for favouring inverse averaging is that the acceleration is inversely proportional to the density and, to predict it correctly, it is necessary to use the correct average of the inverse density.

Another question is whether one should advance the velocity in time by treating the density as a coefficient or advance the momentum (ρu) in time. That question cannot be answered by using the test problem used in this paper because ρ is independent of time but experience with other problems suggests that one should update the conserved variable i.e. momentum.

5. SUMMARY AND DISCUSSION

We have shown that the use of averages of inverse properties rather than the properties themselves greatly reduces the error in the computed fluxes of important quantities at the interface between two phases. Use of these averages in Tryggvason's method is thus likely to bring a significant increase in the accuracy of these fluxes and in the overall quality of the results.

An issue that has not been considered in this paper is that of the effect of curvature of the interface. Interfaces in real two phase flows of the kind computed by Tryggvason and

his colleagues are, of course, strongly curved. We expect that, as long as the curvature of the surfaces is small relative to the inverse of the grid size, which is required for numerical accuracy, the effect of curvature should be limited.

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