# Grid Alignment Effects and Rotated Methods for Computing Complex Flows in Astrophysics 

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Seminar für Angewandte Mathematik
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#### Abstract

We discuss some advantages and difficulties of Cartesian grid calculations on high Mach number flows. We show and explain strong grid alignment effects even in smooth flow regions and in steady state solutions. We present first order rotated schemes for the Euler equations which are able to overcome some of the difficulties, but still display strong dependence of shock positions and speeds on the underlying scheme.


Keywords: gas dynamics, grid alignment effects, transonic rarefaction, rotated schemes, flows in astrophysics

Subject Classification: 65M06, 76J20, 76M10

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## Introduction

This work is inspired by astrophysical calculations showing severe grid alignment problems with high Mach number flows. In particular, we have studied colliding stellar winds in a double star system and also point blasts into different surrounding density distributions. These are important astrophysical problems since over 50 percent of all stars exist in double star systems and are typically losing mass due to stellar winds. Supernovae- and novae explosions are the most important examples of astrophysical point blasts.

Below we will present calculations from symbiotic double star systems in the latest stage of stellar evolution, where stellar winds are an important determining factor in the interaction and the evolution of the double star system. Figure 2 illustrates the situation. The density contours in a logarithmic scale shows the two bow shocks and the slip line in between, where the two flows come together. The star on the right side of the figure is a Red Giant that produces a strong stellar wind, losing about $10^{-5}-10^{-7}$ solar masses per year. This mass flow is slightly supersonic (around Mach 2 or 3) and is the source of a dense nebula which surrounds both stars. Suddenly, by processes which are still not well understood, the other (left) star also begins to lose mass. This new flow drives a shock into the surrounding nebula. The characteristics of this wind are very different from those of the other: it is much less dense (by a factor of perhaps 100), but highly supersonic with Mach numbers in the region of 100 . The momenta of the two winds may be of similar magnitude. Heat transfer via radiation is an important factor in these flows, but one which has not yet been included in our model.

The numerical calculations involve a number of difficulties. One wind is highly supersonic, producing very strong shocks and strong convection. The gradients of density in the winds are very steep: the density of one wind is about two orders of magnitude higher than the other and densities over the entire computational domain differ by 6 or 7 orders of magnitude. There are several different time and length scales involved. Moreover, we would like to do simulations advancing to times at which the interesting shock structure is far from the stars.

We have chosen to use a Cartesian grid refinement method based on a code developed by Berger and LeVeque[1]. Grid refinement is necessary for this problem in order to efficiently capture the interesting features. Although the flow in the region of each star is radially symmetric, the interesting shock features are not aligned with either of these directions. The Cartesian grid approach has the advantage that automatic grid refinement is easily implemented and that very efficient vectorized integrators can be used on each grid. The Cartesian grid is cut by two circles representing boundaries of each star along which the flow is assumed to be known. This results in some rectangular cells being replaced by irregular polygons that may be arbitrarily small relative to the regular cells. We need to specify boundary conditions in these cells that are accurate and stable with a time step chosen relative to the regular cells.

For solid wall boundaries (e.g. an airfoil embedded in a Cartesian grid), Berger and LeVeque[2] have developed such boundary conditions. In this work we have successfully modified these boundary conditions to simulate the stellar wind from
the stars. The fluxes at the solid wall segments of Cartesian cells used in [2] have been replaced by the given supersonic outflow fluxes.

This approach has been tested and works well with moderate Mach numbers. Unfortunately, difficulties appear with the very high Mach number flows that are physically relevant for this problem, as seen in Figures 2 for example. Results show a large grid alignment effect due to the use of a Cartesian grid in a region where the flow is radially symmetric with very steep density gradients. The method used in the original code is a typical high resolution method, based on work of Colella [3]. This is a very good method for moderate problems, but breaks down for the problems considered here.

To avoid this difficulty, we have implemented a rotated method following ideas of [5], [8] and [10]. In this method, Riemann problems are solved in directions relevant to the flow direction, rather than in the coordinate directions. The work reported here is for first order accurate methods. We are currently working on extending these ideas to high resolution second order accurate methods. In the next section, we will give a brief review of the Godunov scheme and describe the basic ideas of rotated difference schemes.

In Section 3 we will show that a first order rotated difference scheme can give a significant improvement over the standard Godunov method. However, the use of rotated schemes gives rise to some interesting new difficulties. In particular, we see that the computed solution (on underresolved grids) can be highly dependent on the particular rotation method used. For example, in stationary solutions the locations of the shock and contact discontinuities can depend on the particular method used and the choice of rotation angle.

In Section 4 we describe and explain one grid alignment effect seen in the figures, the appearance of "bumps" along the coordinate axes that result from strong supersonic outflow that is interpreted as transonic expansions in the one dimensional problems solved to compute the numerical fluxes.

## First order Godunov and rotated schemes

We consider the Euler equations in two space dimensions,

$$
\begin{equation*}
\vec{u}_{t}+f(\vec{u})_{x}+g(\vec{u})_{y}=0, \tag{1}
\end{equation*}
$$

where $\vec{u}=(\rho, \rho u, \rho v, E)$ is the vector of conserved quantities and $f$ and $g$ are the flux functions. As a simplified model we consider an ideal gamma-law gas.

We consider finite volume methods on Cartesian grids, taking the form

$$
\begin{equation*}
U_{i j}^{n+1}=U_{i j}^{n}-\frac{\Delta t}{A}\left[F_{i+1 / 2, j}-F_{i-1 / 2, j}+G_{i, j+1 / 2}-G_{i, j-1 / 2}\right] . \tag{2}
\end{equation*}
$$

Here $U_{i j}^{n}$ represents the cell average over the $(i, j)$ cell $\left[x_{i-1 / 2}, x_{i+1 / 2}\right] \times\left[y_{j-1 / 2}, y_{j+1 / 2}\right]$ on a uniform grid with spacing $\Delta x=\Delta y=h$. The numerical flux $F_{i+1 / 2, j}$ is an approximation to

$$
\begin{equation*}
\frac{1}{\Delta t} \int_{t_{n}}^{t_{n+1}} \int_{y_{j-1 / 2}}^{y_{j+1 / 2}} f\left(u\left(x_{i+1 / 2}, y, t\right)\right) d y d t \approx h f\left(u\left(x_{i+1 / 2}, y_{j}, t_{n+1 / 2}\right)\right) \tag{3}
\end{equation*}
$$

at the right side of the $(i, j)$ cell. Similarly, $G_{i, j+1 / 2}$ is an approximation to the flux at the upper boundary.

Godunov's method is a standard first order numerical method in which $F_{i+1 / 2, j}$ is computed by solving the one-dimensional Riemann problem $u_{t}+f(u)_{x}=0$ with data $u_{l}=U_{i j}^{n}$ and $u_{r}=U_{i+1, j}^{n}$. See, e.g., [6] for a description of such methods.

In the one-dimensional analog of Godunov's method, the wave structure in the solution of the Riemann problem is very revealing and gives a method that is strongly based on physics and behaves quite well, although solutions are strongly smeared due to the inherent dissipation of the method.

In two space dimensions, however, the structure of the solution to a one-dimensional Riemann problem obtained by taking data from adjacent cells in the $x$ - or $y$-direction can be misleading in terms of understanding the two-dimensional structure of the flow. This leads to the grid alignment effects seen in Figure 2 in a way that will be explained.

In two dimensional flow there is often a single direction which is the "dominant" direction in some sense. Examples include the radial direction away from a star or the direction normal to a shock. An attractive idea is to use a method that makes use of this dominant direction.

Rotated schemes take advantage of the fact that the form of the Euler equations remains invariant under rotation by an arbitrary angle. We can define a new coordinate system with axes in some $\xi$-direction (at angle $\Theta$ to the $x$-axis) and an orthogonal $\eta$-direction. The equation (1) then becomes

$$
u_{t}+f^{\xi}(u)_{\xi}+g^{\eta}(u)_{\eta}=0
$$

where

$$
\begin{aligned}
f^{\xi}(u) & =f(u) \cos \Theta+g(u) \sin \Theta \\
g^{\eta}(u) & =-f(u) \sin \Theta+g(u) \cos \Theta .
\end{aligned}
$$

If we can compute numerical fluxes $F^{\xi}$ and $G^{\eta}$ in the $\xi$ - and $\eta$-directions, then we can recover fluxes $F$ and $G$ (see Figure 1a for an example) in the $x$ - and $y$-directions using

$$
\begin{align*}
& F=F^{\xi} \cos \Theta-G^{\eta} \sin \Theta  \tag{4}\\
& G=F^{\xi} \sin \Theta+G^{\eta} \cos \Theta \tag{5}
\end{align*}
$$

In a first order rotated generalization of Godunov's method, we continue to use (2), but now determine $F$ or $G$ by performing the following steps at each interface:

1. Choose appropriate directions $\xi$ and $\eta$, based on the flow.
2. Compute data $u_{l}^{\xi}, u_{r}^{\xi}$ in the $\xi$-direction and solve the Riemann problem $u_{t}+f^{\xi}(u)_{\xi}=0$ with this data to find $F^{\xi}$. Repeat in the $\eta$-direction to find $G^{\eta}$.
3. Use (4) or (5) to compute the flux normal to the interface.

Figure 1: a) Transformation of fluxes, b) and c) Interpolation methods A, B

Clearly there are several choices to be made. The physical properties of a complex flow may suggest several different rotation angles and it is not clear which should be used. As we will see, the choice of angle can make a dramatic difference in the computed solution.

In Step 2 of the algorithm, we must interpolate the data from the underlying Cartesian grid to obtain appropriate data in the $\xi$ - and $\eta$-directions. There are several ways that we might do this. Here we mention two possibilities. Method A is illustrated in Figure 1b. We construct a box extending distance h in the $\xi$-direction and use the areas of overlap with each cell to determine interpolation weights. This gives

$$
\begin{equation*}
u_{r}^{\xi}=\left(A_{2} \times U_{i+1, j}+A_{1} \times U_{i+1, j+1}\right) /\left(A_{1}+A_{2}\right)=(1-\sin \Theta) U_{i+1, j}+\sin \Theta U_{i+1, j+1} . \tag{6}
\end{equation*}
$$

In the same way one gets $u_{l}^{\xi}$, and $u_{l}^{\eta}, u_{r}^{\eta}$ in the $\eta$-direction.
Method B is illustrated in Figure 1c. A box of size $h^{2}$ is centered distance $h / 2$ from the interface in the $\xi$-direction, and the overlap with each of four cells are used to define weights,

$$
\begin{equation*}
u_{r}^{\xi}=\left(A_{1} \times U_{i, j+1}+A_{2} \times U_{i+1, j+1}+A_{3} \times U_{i+1, j}+A_{4} \times U_{i, j}\right) / h^{2} . \tag{7}
\end{equation*}
$$

This is equivalent to bilinear interpolation between the four neighboring cell centers to the point lying distance $h / 2$ from the center of the interface in the $\xi$-direction.

In smooth regions the results with Method B are much better. On problems with strong shocks, however, we see oscillations near the shocks. This is presumably due to the fact that (7) takes data from both sides of the shock and does not fully preserve the upwind nature of Godunov's method.

## Numerical results

Figure 2 shows the steady state solutions for a double star calculation with different methods on a $200 \times 200$ grid. On the boundary of the two stars we set the densities $\rho_{\text {left }}=0.0067$ and $\rho_{\text {right }}=1$, with velocities $v_{\text {left }}=39.1$ and $v_{\text {right }}=2.17$ and pressures $p_{\text {left }}=0.04$ and $p_{\text {right }}=0.6$. The polytropic index $\gamma$ is 1.6. The flow from the left star has a Mach number of 12.65 , from the right one of 2.14 . The separation

Figure 2: a) Solution of colliding winds using standard Godunov method compared with b) solution using a rotated scheme with rotation in radial direction with respect to the left star and c) solution using a rotated scheme, with rotation in velocity direction.
of the stars is 0.2 and each star has a radius of 0.038 in a domain which is the unit square.

With Godunov's method 2a we see strong bumps aligned with the $\mathrm{x}-\mathrm{and} \mathrm{y}$-axis, which are the directions in which the Riemann problems are solved.

We also see grid alignment effects in the plots of the solution, calculated with the rotated scheme (method A), but they look different. Instead of bumps we have depressions. Figure 2 b using the rotated scheme with $\Theta$ chosen based on the radial direction relative to the star on the left. In Figure 2c we have instead chosen the rotation angle at each interface based on the average flow direction from the cells on either side.

The difference between these solutions is quite striking. In particular, notice that the shock location is different in each case. Also significant is the different resolution of the slip line where the two flows come together. This phenomenon has not yet been studied in sufficient depth. One interesting question is whether the choice of rotation angle based on the characteristics of the flow might cause some form of feedback that in turn affects the flow.

The use of an appropriate rotated scheme seems to alleviate some of the difficulties seen with bumps in the above calculations. To see that it can also improve the location of shocks, we show another set of calculations.

In Figure 3 we present solutions of a point blast calculated with different methods. The initial data of the point blast are : density $\rho=0.1$, velocity $v \equiv 0$ in the whole domain and pressure $p_{i n}=600$ inside of a circle with radius $r_{0}=0.05$ and $p_{\text {out }}=0.06$ outside of this circle. The polytropic index $\gamma$ is equal to 1.6 . The figure shows plots from calculations with different methods on a $100 \times 100$ grid, all taken at the same computational time. The first plot shows calculatons with Godunov's method, the second one with a rotated scheme, where the rotation angle was chosen to be 45 degrees everywhere. The third plot shows results obtained with the rotated scheme in which the $\xi$-direction at each interface is chosen in the direction of velocity. One can see clearly the dependence of the shock position of the rotation angle. The shock should be circular. With Godunov's method it tends to become

Figure 3: Point blast calculated with Godunov method, scheme with 45 degree rotation and scheme with rotation in flow direction.
diamond shaped, indicating that propagation is faster along the coordinate axes than at $45^{\circ}$. With rotation at $45^{\circ}$ the propagation is now fastest in this direction, and so the shock becomes square. Rotating in the velocity direction gives relatively nice results, with a roughly circular shock.

## Description of the grid alignment effects

One of the obvious grid alignment effects seen in the above experiments is the appearance of "bumps" along the coordinate axes. This can be explained by the fact that one-dimensional cross-sections of the flow can exhibit quite different physical flow characteristics than the full two dimensional flow. In particular, a flow that is everywhere highly supersonic in two dimensions can yield transonic behavior in computing the one-dimensional fluxes. This type of difficulty is well-known in other contexts, [4], [9], [11].

This effect can be nicely illustrated with a simple model problem, a single time step on a flow with energy and pressure that are initially uniform and should remain roughly so over short times, but for which steep gradients in density and velocity give rise to the bump phenomenon in a striking way. Here we can explicitly calculate the energy flux and see that bumps arise from one-dimensional transonic rarefaction waves.

To isolate the grid alignment effects from other possible sources of difficulty, such as boundary effects from the star boundaries, we use a radially symmetric outflow problem with the star center off the grid, at $\left(x_{0}, y_{0}\right)=(0.5,-0.2)$, while the computational grid is the unit square. We use the following initial conditions:

$$
\begin{array}{cl}
\rho(\vec{x}, 0)=\rho_{0} / r^{2} & u(\vec{x}, 0)=\tilde{x} q_{0} \\
p(\vec{x}, 0)=p_{0} & v(\vec{x}, 0)=\tilde{y} q_{0}
\end{array}
$$

with $r^{2}=\left(x-x_{0}\right)^{2}+\left(y-y_{0}\right)^{2}$ and $\tilde{x}=x-x_{0}, \tilde{y}=y-y_{0}$. We use $\rho_{0}=1.4$, $p_{0}=1$, and various values for $q_{0}$. For a gamma-law gas with $\gamma=1.4$, the Mach number is then $q_{0}$ everywhere. Energy is inintially also constant in $x$ and $y$ with the value

$$
\begin{equation*}
E(\vec{x}, 0)=E_{0}=\frac{p_{0}}{\gamma-1}+\frac{1}{2} \rho_{0} q_{0}^{2} . \tag{8}
\end{equation*}
$$

With these initial conditions, we can easily compute that at time $t=0$,

$$
\begin{array}{ll}
\rho_{t}=0 & (\rho u)_{t}=-\rho_{0} q_{0}^{2} \tilde{x} / r^{2} \\
p_{t}=(\gamma-1)\left(-2 K+\rho_{0} q_{0}^{3}\right) & (\rho v)_{t}=-\rho_{0} q_{0}^{2} \tilde{y} / r^{2}  \tag{9}\\
E_{t}=-2 K &
\end{array}
$$

where $K=q_{0}\left(E_{0}+p_{0}\right)$. In particular, the derivatives of pressure and energy are spatially uniform, so that these quantities should remain nearly spatially uniform over small times. With an explicit numerical method we might expect these quantities to remain uniform at the end of one time step, particularly the energy which is itself one of the conserved variables. However, the energy flux depends on the velocity, which has steep gradients. We can at least hope for smooth solutions after one time step.

Figures 4 a and 4 b show results with the standard Godunov method for $q_{0}=4$ and $q_{0}=10$, respectively. We see that $E$ remains constant only outside of the wedge

$$
\begin{equation*}
\left|x-x_{0}\right|<\frac{\left|y-y_{0}\right|}{\sqrt{q_{0}^{2}-1}} \tag{10}
\end{equation*}
$$

A discontinuity arises along the boundary of this wedge. The pressure remains only approximately constant outside the wedge and again displays discontinuties at the wedge boundary. For large values of the Mach number $q_{0}$, this wedge shrinks to a thin strip along the coordinate axis $x=x_{0}$, giving bumps of the form seen in the earlier results.

The appearance of these discontinuities is easy to predict if we compute the numerical fluxes being used. The true energy flux in the $x$ - and $y$-directions is given by

$$
\begin{align*}
u(E+p) & =\left(x-x_{0}\right) K \\
v(E+p) & =\left(y-y_{0}\right) K \tag{11}
\end{align*}
$$

With Godunov's method, we solve 1D Riemann problems in the $x$ - and $y$-directions separately. For $q_{0}$ large enough, the flow is everythere supersonic in the $y$-direction. So the computed flux at the top of each cell is simply the flux function evaluated at the cell value. In particular, the energy flux is

$$
\begin{equation*}
G_{i, j+1 / 2}=\left.h v(E+p)\right|_{\left(x_{i}, y_{j}\right)}=h K\left(y_{j}-y_{0}\right) . \tag{12}
\end{equation*}
$$

In solving the $x$-Riemann problems, the flow is only supersonic for $|\tilde{x}|$ large enough, since $u=0$ at $\tilde{x}=0$. For supersonic flow we require ( $c$ is the adiabatic sound speed)

$$
\begin{equation*}
u=\tilde{x} q_{0}>c=\sqrt{\frac{\gamma p}{\rho}}=\sqrt{\frac{\gamma p_{0}}{\rho_{0}}\left(\tilde{x}^{2}+\tilde{y}^{2}\right)}=\sqrt{\left(\tilde{x}^{2}+\tilde{y}^{2}\right)} \tag{13}
\end{equation*}
$$

From this, we see that the region where the flow appears to be subsonic in the $x$-direction is precisely the wedge (10).

Figure 4: Results for the model problem. Energy contour plots and a slice at $y=0.2$ are shown after one time step with various methods. a) Godunov method for Mach number $q_{0}=4$. b) Godunov method for $q_{0}=10$. c) Rotated method with $\Theta=45^{\circ}$ everywhere $\left(q_{0}=10\right)$. d) Rotated method with rotation in the radial direction ( $q_{0}=10$ ).

Outside of this wedge, where the flux is supersonic in both $x$ and $y$, solving the Riemann problem in $x$ will return the flux at the upwind cell center as the interface flux $F_{i+1 / 2, j}$. For example, for $\tilde{x}>|\tilde{y}| / \sqrt{q_{0}^{2}-1}$ we will obtain

$$
\begin{equation*}
F_{i+1 / 2, j}=\left.h u(E+p)\right|_{\left(x_{i}, y_{j}\right)}=h K\left(x_{i}-x_{0}\right) . \tag{14}
\end{equation*}
$$

Combining this with (12) and computing the updated cell value via (2), we obtain

$$
E_{i j}^{1}=E_{i j}^{0}-\frac{\Delta t}{h^{2}}\left(2 h^{2} K\right)=E_{0}-2 \Delta t K
$$

This is constant in $x$ and $y$ and is consistent with the value of $E_{t}$ from (9).
Inside the wedge, where the flow is subsonic in $x$, the flux is not simply the flux function evaluated at the upwind cell center. Instead, solving the Riemann problem at the interface will give an intermediate value somewhere between the values at the neighboring cell centers.

As an extreme example, consider the case where $q_{0}$ is very large, large enough that the only subsonic cell interfaces are along the coordinate line $\tilde{x}=0$. Let $I$ be the index for which $\tilde{x}_{I-1 / 2}=0$. Then we have

$$
\begin{aligned}
& F_{i+1 / 2, j}=h(i+1 / 2) K \text { for } i \geq I, \\
& F_{i+1 / 2, j}=h(i+3 / 2) K \text { for } i \leq I-2
\end{aligned}
$$

from (14), while

$$
F_{I-1 / 2, j}=0 .
$$

As a result, flux differencing gives

$$
F_{i+1 / 2, j}-F_{i-1 / 2, j}=h^{2} K \quad \text { for } \quad i \neq I-1, I
$$

as desired away from the central cells, but

$$
F_{i+1 / 2, j}-F_{i-1 / 2, j}=\frac{1}{2} h^{2} K \quad \text { for } \quad i=I-1 \text { and } I .
$$

The flux difference in these cells is only half what it should be, leading to

$$
E_{i j}^{1}=E_{0}-\frac{3}{2} \Delta t K
$$

for $i=I-1$ and $I$. This leads to the bump along the coordinate line $x=x_{0}$.
The fact that Godunov's method gives nonsmooth fluxes in transonic rarefaction waves is also responsible for the appearance of so-called "entropy glitches" or "doglegs" in certain calculations. See [7] for a description of this problem and some analysis similar to what is presented here.

Figure 4c shows results computed with the rotated scheme presented above, where we have first chosen a rotation angle $\Theta=45^{\circ}$ everywhere. We now see bumps appearing along the edges of wedges $|\tilde{x}-\tilde{y}|<|\tilde{y}| / \sqrt{q_{0}^{2}-1}$ at $45^{\circ}$ to the grid. In the rotated Riemann problems, the flow is supersonic in both the $\xi$ and $\eta$ directions outside these wedges, while inside the wedges the flow in the $\eta$ direction appears as a transonic rarefaction. Rotating at other fixed angles gives bumps
in the corresponding direction. This is also true for the steady state double star calculations.

For the model problem, the most natural choice of rotation direction would be the radial direction. In this case the Riemann problem in the $\eta$-direction gives a transonic rarefaction everywhere. This gives results that are no longer exactly constant anywhere, but are nearly constant everywhere, as seen in Figure 4d. This is a substantial improvement over the other calculations.

Clearly much work remains to be done in developing high resolution methods to solve these difficult problems. It seems that rotated difference methods have some advantages, but there are still many intriguing difficulties to be understood and overcome.

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