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An Application of Conservative Scheme to Structure Problems (Elastic-Plastic Flows)

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We present an explicit high order accurate method to solve the dynamics of metal materials numerically. The governing equations for the dynamics consist of two parts. The first part is the conservation law of mass, momentum and energy. The second is the equation of state and Hook's law. For those equations we apply the method of retroactive characteristics [1] to establish high order accurate Godunov method. We finally verify our method through a few computational examples. The method gives rather good resolution for elastic and plastic waves.

1 Introduction

Godunov method [4] is a finite volume method mainly used in numerical simulation of conservation laws. In finite volume methods, we divide the space into small finite volumes (cells) and approximate the flux that passes the contacts between each pair of neighboring cells by some numerical flux. In Godunov method the numerical flux is estimated through the exact solution to the Riemann problem that is determined from the two states of neighboring cells that intersect at the contact. If an approximate solution to the Riemann solution is used instead of the exact solution, the algorithm is called Godunov type method.

The big advantage of Godunov method is a theoretical background derived from the exact Riemann solver, even though the convergence of method is still open in many cases. Especially when the nonlinearity is strong, like the compressible gas, Godunov method is rather reliable. But the order of accuracy is still of the first order.

We have already established high order accurate Godunov method for the compressible Euler equations using the retroactive characteristics method and the switching of accuracy based on parabolic spline criterion [1]. The retroactive characteristics method gives precise information on the region of independence at each contact of cells. As well known, the high order accuracy gives side effect of numerical oscilation where the spatial change of gradient of numerical data is large. We employ the swithing of accuracy based on parabolic spline criterion to suppress the inconvenience. The idea of this switching is rather natural and easy. It does not any harm with the accuracy in the region where the data is smooth. We also emphasize that in the practical coding our algorithm is almost like a 3-stencil shceme like Godunov method, while many high order accurate methods require us to treat 5 or more stencils in a complicated procedure. In brief, the methods employed are rather successful in the case of compressible Euler equations.

We here extend the methodology into the problems of elastic-plastic flow in solid continuum to develop a methodology to calculate the numerical solution for strong impact problems, where a piece of material collides with another at a very high speed or a fast and strong shockwave in fluid collides with some solid material etc. In the case, instead of the primitive variables, the Riemann invariants are interpolated by the method of retroactive characteristics. When we calculate the numerical flux, only the elastic part of Hook's law is taken into account. The plastic behavior of the material is included in the corrector step. Finally we show some numerical results to verify our methodology.

2 Equation Modeling Elasticity and Plasticity

The governing equations are wrriten in the following form with independent variables x_i $(i = 1, 2, 3)$ and t for space and time coordinates, respectively. While many different ways are proposed to model the plasticity, which is closely related with property of material, we employ the concept of so called ideal plasticity determined by von Mises criterion.

$$\frac{\partial \rho}{\partial t} + \sum_j \frac{\partial}{\partial x_j}(\rho u_j) = 0, \tag{1}$$

$$\frac{\partial(\rho u_i)}{\partial t} + \sum_j \frac{\partial}{\partial x_j}(\rho u_i u_j - \sigma_{ij}) = 0, \ i = 1, 2, 3 \tag{2}$$

$$\frac{\partial e}{\partial t} + \sum_j \frac{\partial}{\partial x_j}(eu_j - \sum_i u_i\sigma_{ij}) = 0 \tag{3}$$

$$\frac{D}{Dt}S_{ij} + \lambda S_{ij} = \mu e_{ij},\ i,j = 1,2,3 \tag{4}$$

$$\epsilon = \epsilon(p,\rho), \tag{5}$$

where

ρ:	density (mass per unit volume)
u_i:	the velocity component in the direction of x_i-axis
e:	total energy per unit volume. (specific energy and kinetic energy)
ϵ:	specific enerygy per unit volume
(σ_{ij}):	stress tensor
μ:	shear modulus
$\frac{D}{Dt}$:	Jaumann derivative.

We need some additional explanation. The stress tensor (σ_{ij}) is symmetric and devided into two parts, the part from pressure and that from deviatoric stress.

$$\sigma_{ij} = -p\delta_{ij} + S_{ij},\ p = -\frac{1}{3}\sum_i \sigma_{ii}, \tag{6}$$

where δ_{ij} is so called the Kronrcker's delta;

$$\delta_{ij} = \begin{cases} 1, & i = j \\ 0, & i \neq j. \end{cases} \tag{7}$$

The tensor (e_{ij}) is determined by

$$e_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{1}{3}\left(\sum_k \frac{\partial u_k}{\partial x_k}\right)\delta_{ij}. \tag{8}$$

The Jaumann detivative $\frac{D}{Dt}$ is determined by

$$\frac{D}{Dt}(S_{ij}) = \frac{\partial S_{ij}}{\partial t} + \sum_k \left\{u_k \frac{\partial}{\partial x_k} S_{ij} - S_{ik}\omega_{jk} - S_{jk}\omega_{ik}\right\}, \tag{9}$$

where $\omega_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i}\right)$. The Jaumann derivative is free from the rotation of stress tensor in Euler variables. For transition from elasticity to plasticity von Mises criterion is assumed; if $\sum_{i,j} S_{ij}S_{ij} \geq \frac{2}{3}{\sigma_s}^2$, the property changes to be plastic from elastic, where σ_s is the yield point of material that is subject to uniaxial dilatation-compresson. Then the components of the deviatoric stress are corrected by projecting themselves onto the yield surface, *i.e.* multiplying them by $\frac{1}{\sqrt{\lambda}}$.[1] The parameter characterizes the procedure associated with plastic deformation and is calculated by

$$\lambda = \frac{3}{2} \frac{\sum_{ij} S_{ij} S_{ij}}{{\sigma_s}^2}. \tag{10}$$

About the governing equations, especially the modeling of ideal plasticity. See [6].

3 Numerical Algorithm

As written in the beginning of previous section, there are many different modelings of plasticity, while the modeling of elastisity given in the governing equations is rather general. Therefore, we separate the discretized temporal evolution into two parts. The first part is the discretized temporal evolution governed by the equations (1)-(5) with $\lambda = 0$ in (4). It is the temporal evolution governed by the elasticity. The second is that governed by the equation

$$\frac{D}{Dt} S_{ij} + \lambda S_{ij} = 0, \tag{11}$$

where we take the evolution caused by plasticity into account. In other words, in the predictor step we only take the machinery of elasticity into account and the plasticity is included only in the corrector step.

In the cases of our interest the experience shows that the accuracy of calculation depends much more on the accuracy of the estimate of numerical flux in the first part than on the treatment of viscosity in the second part. The treatment of plasticity in the second part is free from the construction of numerical flux in the first part, and it means that many different modeling of plasticity can be used. Because of the reason above it is reasonable to divide the discretized temporal evolution into the two parts. Also in [6], they treat the discretized temporal evolution dividing them into the two parts.

3.1 Construction of Second Order Accurate Numerical Flux

Then we apply the idea to improve the accuracy of scheme by retroactive characteristics to the first part. We restrict ourselves into the two dimensional case with usual Descartes

[1] The (hyper) surface determined by $\sum_{ij} S_{ij} S_{ij} = \frac{2}{3} {\sigma_s}^2$ in the S_{ij}-space, which is 3 or 6 dimensional, is called von Mises surface. It is possible to understand that the plasticity works when the tensor (S_{ij}) grows to reach the surface. If $\lambda = 0$ in the equation (4), the governing equations (1)-(5) represent only the elastic motion.

coordinate (x, y). The equations (1)-(5) with $\lambda = 0$ in (4) is written in the form of conservation law

$$U_t + F_x + G_y = 0,\ U = \begin{bmatrix} p \\ \rho \\ u \\ v \\ S_{xx} \\ S_{yy} \\ S_{xy} \end{bmatrix} \tag{12}$$

and linearized into the following form.

$$U_t + AU_x + BU_y = 0 \tag{13}$$

The matrix A is given as follows.

$$A = \begin{bmatrix} u & 0 & \rho c^2 - fS_y y & -fS_{xy} & 0 & 0 & 0 \\ 0 & u & \rho & 0 & 0 & 0 & 0 \\ \frac{1}{\rho} & 0 & u & 0 & -\frac{1}{\rho} & 0 & 0 \\ 0 & 0 & 0 & u & 0 & 0 & -\frac{1}{\rho} \\ 0 & 0 & -\frac{4}{3}\mu & S_{xy} & u & 0 & 0 \\ 0 & 0 & \frac{2}{3}\mu & -S_{xy} & 0 & u & 0 \\ 0 & 0 & 0 & \frac{1}{2}(S_{yy} - S_{xx}) - \mu & 0 & 0 & u \end{bmatrix}, \tag{14}$$

where f is determined by $f = \left\{\rho\left(\frac{\partial\epsilon}{\partial p}\right)_\rho\right\}^{-1}$, but in the case of metal material it is enough to assume $f = 0$. The matrix B is given in a similar manner.

We come to the stage to discuss the construction of numerical flux. We assume structured mesh for the computation. Each cell (finite volume) is numbered (i, j) by a pair of integers i and j. Each contact is naturally numbered like $(i + \frac{1}{2}, j)$ or $(i, j + \frac{1}{2})$. The contact $(i + \frac{1}{2}, j)$ is the boundary of neighboring cells (i, j) and $(i + 1, j)$, $(i, j + \frac{1}{2})$ is that of (i, j) and $(i, j + 1)$. To estimate the numerical flux at the contact $(i + \frac{1}{2}, j)$, we may assume that the contact is perpendicular to x-axis without the loss of generality.

Let $U^n_{i,j}$ and $U^n_{i+1,j}$ be numerical data of U over a pair of finite volumes (i, j) and $(i + 1, j)$ at the time step n. The size of finite volumes in x-direction is Δx^n_i and Δx^n_{i+1}, respectively. To construct the numerical flux $\bar{F}^n_{i+\frac{1}{2},j}$ at the contact $(i + \frac{1}{2}, j)$ we consider the initial value problem

$$U_t + AU_x = 0, \tag{15}$$

$$U(x, 0) = U^n_i + \frac{U^n_{i+1} - U^n_i}{\left(\frac{\Delta x_i + \Delta x_{i+1}}{2}\right)}\left(x + \frac{1}{2}\Delta x_i\right). \tag{16}$$

Then we determine $U^{n+\frac{1}{2}}_{i+\frac{1}{2},j}$ by $U^{n+\frac{1}{2}}_{i+\frac{1}{2},j} = U(\frac{w}{2}\Delta t^n, \frac{1}{2}\Delta t^n)$, using the exact solution to the initial value problem above, where w is the moving speed in x-direction of the contact[2] and Δt^n is the time increment between the time steps n and $n+1$. Finally $\bar{F}^n_{i+\frac{1}{2},j}$ is given by

$$\bar{F}^n_{i+\frac{1}{2},j} = F(\bar{U}^{n+\frac{1}{2}}_{i+\frac{1}{2},j}). \tag{17}$$

Because the problem (15), (16) is linear, we obtain $U^{n+\frac{1}{2}}_{i+\frac{1}{2},j}$ by the following procedure.

The characteristic speeds of the linearized system (15) are equal to the eigenvalues of matrix A; $c_1 = u - a$, $c_2 = u - b$, $c_3 = u$, $c_4 = u$, $c_5 = u$, $c_6 = u + b$, $c_7 = u + a$, where u, a, b are the x-component of velocity of material itself, the longitudinal sound wave, the shear sound wave, respectively. A is diagonalizable. Then we decompose (15) into the form;

$$(\alpha_i)_t + c_i(\alpha_i)_x = 0, \;\; i = 1,2,3,4,5,6,7, \tag{18}$$

where each α_i is a function of (x,t); $\alpha_i = \alpha_i(x,t)$, so that U is a linear combination of some set of linearly independent seven vectors r_i, $i = 1,2,3,4,5,6,7$;

$$U = \sum_i \alpha_i r_i. \tag{19}$$

Then we obtain $U^{n+\frac{1}{2}}_{i+\frac{1}{2},j}$ by

$$U^{n+\frac{1}{2}}_{i+\frac{1}{2},j} = \sum_i \alpha_i(0, \tfrac{1}{2}(w - \lambda_i)\Delta t) \cdot r_i, \tag{20}$$

where the "initial value" $\alpha_i(0,*)$ is naturally given by the initial value of U given by (16).

We easily observe that the conservative difference scheme with the numerical flux determined above is of the second order accuracy.

3.2 Switching between Second and First Order Accuracy

If we apply the second order accurate numerical flux given by (15)-(20) everywehere, the numerical oscilation occurs where the spatial change of gradient of numerical data is large. To avoid the inconvenience, we have to go down to the first order accuracy at such exceptional points. Various algorithms to switch the accuracy are proposed. We here apply the method based on the monotonicity of parabolic spline, which is already discussed in [1]. (See also [2].)

[2]We assume that the change of normal of the contact is small enough even if the contact moves.

The discussion is given in the case of numerical flux in x (or i)-direction. The case of that in y (or j)-direction is similar.

Let numerical data of $S_{xx}-p$ be $(S_{xx}-p)^n_{i-1,j}$, $(S_{xx}-p)^n_{i,j}$, $(S_{xx}-p)^n_{i+1,j}$, $(S_{xx}-p)^n_{i+2,j}$ for each finite volumes $(i-1,j)$, (i,j), $(i+1,j)$, $(i+2,j)$, respectively. Also assume the size of finite vlumes are Δx^n_{i-1}, Δx^n_i, Δx^n_{i+1}, Δx^n_{i+2}, respectively. Then we take two parabolic splines

$$p_\pm(x) = a_\pm x^2 + b_\pm x + c_\pm$$

satisfying

$$\begin{cases} p_-\left(-\frac{1}{2}(\Delta x^n_{i-1}+\Delta x^n_i)\right) = (S_{xx}-p)^n_{i-1,j} \\ p_-(0) = (S_{xx}-p)^n_{i,j} \\ p_-\left(\frac{1}{2}(\Delta x^n_i+\Delta x^n_{i+1})\right) = (S_{xx}-p)^n_{i+1,j}, \end{cases}$$
$$\begin{cases} p_+\left(-\frac{1}{2}(\Delta x^n_i+\Delta x^n_{i+1})\right) = (S_{xx}-p)^n_{i,j} \\ p_+(0) = (S_{xx}-p)^n_{i+1,j} \\ p_+\left(\frac{1}{2}(\Delta x^n_{i+1}+\Delta x^n_{i+2})\right) = (S_{xx}-p)^n_{i+2,j}. \end{cases}$$

If the both parabolic splines $p_-(x)$, $-\frac{1}{2}(\Delta x^n_{i-1}+\Delta x^n_i) < x < \frac{1}{2}(\Delta x^n_i+\Delta x^n_{i+1})$ and $p_+(x)$, $-\frac{1}{2}(\Delta x^n_i+\Delta x^n_{i+1}) < x < \frac{1}{2}(\Delta x^n_{i+1}+\Delta x^n_{i+2})$ are monotone, we take the second order accurate numerical flux. Otherwise, we go down to the first order accuracy. The first order accurate numerical flux is given by the same procedure as the second order accurate one. But the initial condition (16) is replaced by the following.

$$U(x,0) = \begin{cases} U^n_{i,j}, & x < 0 \\ U^n_{i+1,j}, & x > 0. \end{cases} \tag{21}$$

The advantage of method is that the decision which accuracy should be taken is very simple. Just observing the data distribution over the four finite volumes around the contact concerned, we decide the formula to obtain the numerical flux. It means that we do not have to include the data from outer stencils $i-1, i+2$ in the main part to calculate the numerical flux applying the initial value problem (15), (16) or (15), (21). The complexity of the program coding is almost the same as that in the case of usual first order accurate Godunov method.

Finally we mention that from theoretical viewpoint we whould have to take the procedure to examine the monotonicity of parabolic splines for the seven variables p, ρ, u, v, S_{xx}, S_{yy}, S_{xy}. But, from the experience of practical computation, it seems enough to examine it only for the numerical data of $S_{xx}-p$.

4 Examples of Computation.

"Wilkins's flying plate problem" [6] is simulated by our method. In the problem, a 5mm thick alminium plate (A) that is assumed infinitely wide impacts from the left to another piece of alminium (B) that is assumed to occupy a half space to the right.

Both the elasticity and plasticity work in the phenomenon. As soon as the collision occurs, the shockwave is made and propagates from the contact to the left and right. The left boundary of (A) reflects shockwave changing it into rarefaction wave. The material of alminium is modeled as follows. The pressure $p = p(\rho) = 73.0 * \left(1 - \frac{\rho_0}{\rho}\right)$ is a function of the density ρ, where p is measured in GPa and $\rho_0 = 2700\text{kg/m}^3$. The sheer modulus $\mu =$ 24.8GPa. The constant for von Mises criterion is $\sigma_s = 0.2976$GPa. 500(in x-direction) $\times$ 10(in y-direction) cells of the size 0.1mm$\times$0.1mm are used in the computation. In x-direction 50 cells are in the 5mm thick plate (A) and 450 cells in the half space (B). The left boundary is treated with the free boundary condition with 0.1MPa. The right boundary treatment is done in the outflow manner, but it has no importance until the shockwave arrives there. The upper and bottom boudaries are just virtual. At the both we assume the reflecting boundary condition.

In Fig.1, we show the density in the case of initial collision speed 2km/sec. In the figure, we compare the first and second order methods. The second order method is what is introduced in the article. The first order method is usual Godunov scheme, which is given by numerical flux (17) with (15) and (21). We observe that the second order method gives separation of two sound waves, the longitudinal and shear, rather well.

5 Concluding Remarks

While the retroactive characteristics are used to construct a modified Riemann problem whose exact solution gives the numerical flux in the case of compressible Euler flow, they are rather directly used to determine the numerical flux via $U^{n+\frac{1}{2}}_{i+\frac{1}{2},j}$ in the case of elastic-plastic flow. But the methodology still works well because the nonlinearity is not so complicated as in the case of compressible Euler equations. It implies that the combination of retroactive characteristics may be widely applied together with the accuracy switching based on parabolic spline criterion.

Beside what is already mentioned in section 3, we mention that numerical boundary treatment is rather easy in this method, because we are still based on the idea of Godunov method that are rather physical *i.e.* that are based on the exact solution to Riemann solver.

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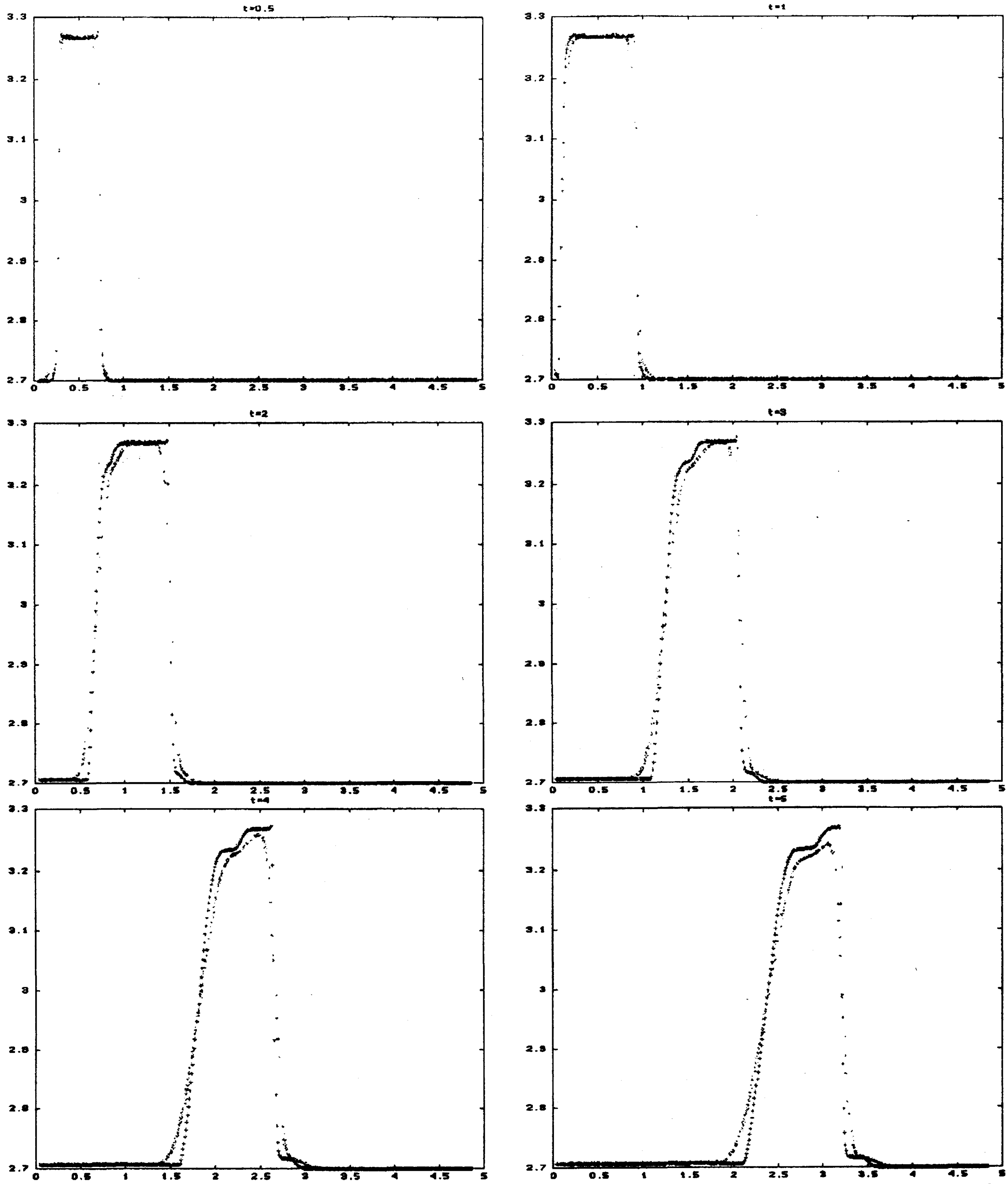

FIG. 1. Density for Wilkins's problem with impact velocity 2 km/s, comparison of first and second order accuracy schemes.