Solving Godunov-Romenski-Type Continuum Models by Eigendecomposition of the Cauchy Tensor

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Abstract

A formulation of the Godunov-Peshkov-Romenski model of continuum mechanics based upon the Cauchy deformation tensor, rather than the distortion tensor, is used to model simple laminar flow. Rather than evolving the Cauchy deformation tensor itself, evolution equations are presented and solved for its eigendecomposition. This form of the model obviates the repeated calculations that are required in the canonical model to find the eigenvalues of the full system. Thus, a significant speedup is obtained, as demonstrated numerically in this study.

Keywords: Godunov-Peshkov-Romenski, GPR, Continuum Mechanics, Distortion Tensor, Cauchy Deformation Tensor, Eigendecomposition

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1. Background

1.1. Motivation

Motivation goes here.

1.2. The GPR Model

The GPR model, first introduced in Peshkov and Romenski [5], has its roots in Godunov and Romenski's 1970s model of elastoplastic deformation (see Godunov and Romenski [3]). It was expanded upon in Dumbser et al. [1] to include thermal conduction. This expanded model takes the following form:

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho v_k)}{\partial x_k} = 0 \tag{1a}$$

$$\frac{\partial (\rho v_i)}{\partial t} + \frac{\partial (\rho v_i v_k + p\delta_{ik} - \sigma_{ik})}{\partial x_k} = 0 \tag{1b}$$

$$\frac{\partial A_{ij}}{\partial t} + \frac{\partial (A_{ik} v_k)}{\partial x_j} + v_k \left(\frac{\partial A_{ij}}{\partial x_k} - \frac{\partial A_{ik}}{\partial x_j} \right) = -\frac{\psi_{ij}}{\theta_1(\tau_1)} \tag{1c}$$

$$\frac{\partial (\rho J_i)}{\partial t} + \frac{\partial (\rho J_i v_k + T\delta_{ik})}{\partial x_k} = -\frac{\rho H_i}{\theta_2(\tau_2)} \tag{1d}$$

$$\frac{\partial (\rho E)}{\partial t} + \frac{\partial (\rho E v_k + (p\delta_{ik} - \sigma_{ik}) v_i + q_k)}{\partial x_k} = 0 \tag{1e}$$

ρ,$\mathbf{v}$,p,δ,σ,T,E,$\boldsymbol{q}$ retain their usual meanings. θ_1 and θ_2 are positive scalar functions, chosen according to the properties of the material being modeled. A is the distortion tensor (containing information about the deformation and rotation of material elements), $\mathbf{J}$ is the thermal impulse vector (a thermal analogue of momentum), τ_1 is the strain dissipation time, and τ_2 is the thermal impulse relaxation time. $\psi = \frac{\partial E}{\partial A}$ and $\boldsymbol{H} = \frac{\partial E}{\partial \boldsymbol{J}}$.

The following definitions are given:

$$p = \rho^2 \frac{\partial E}{\partial \rho} \tag{2a}$$

$$\sigma = -\rho A^T \frac{\partial E}{\partial A} \tag{2b}$$

$$T = \frac{\partial E}{\partial s} \tag{2c}$$

$$\boldsymbol{q} = \frac{\partial E}{\partial s} \frac{\partial E}{\partial \boldsymbol{J}} \tag{2d}$$

To close the system, the equation of state must be specified, from which the above quantities and the sources can be derived. E is the sum of the contributions of the energies at the molecular scale (microscale), the material element[1] scale (mesoscale), and the flow scale (macroscale):

[1]The concept of a *material element* corresponds to that of a fluid parcel from fluid dynamics, applied to both fluids and solids.

$$E = E_1(\rho, p) + E_2(A, \boldsymbol{J}) + E_3(\boldsymbol{v}) \tag{3}$$

For an ideal or stiffened gas, E_1 is given by:

$$E_1 = \frac{p + \gamma p_\infty}{(\gamma - 1)\rho} \tag{4}$$

where $p_\infty = 0$ for an ideal gas.

E_2 is chosen to have the following quadratic form:

$$E_2 = \frac{c_s^2}{4}\left\|\operatorname{dev}(G)\right\|_F^2 + \frac{\alpha^2}{2}\left\|\boldsymbol{J}\right\|^2 \tag{5}$$

c_s is the characteristic velocity of propagation of transverse perturbations. α is a constant related to the characteristic velocity of propagation of heat waves:

$$c_h = \frac{\alpha}{\rho}\sqrt{\frac{T}{c_v}} \tag{6}$$

$G = A^T A$ is the Gramian matrix of the distortion tensor, and $\operatorname{dev}(G)$ is the deviator (trace-free part) of G:

$$\operatorname{dev}(G) = G - \frac{1}{3}\operatorname{tr}(G)\, I \tag{7}$$

E_3 is the usual specific kinetic energy per unit mass:

$$E_3 = \frac{1}{2}\left\|\boldsymbol{v}\right\|^2 \tag{8}$$

The following forms are chosen:

$$\theta_1(\tau_1) = \frac{\tau_1 c_s^2}{3|A|^{\frac{5}{3}}} \tag{9a}$$

$$\theta_2(\tau_2) = \tau_2 \alpha^2 \frac{\rho T_0}{\rho_0 T} \tag{9b}$$

$$\tau_1 = \frac{6\mu}{\rho_0 c_s^2} \tag{10a}$$

$$\tau_2 = \frac{\rho_0 \kappa}{T_0 \alpha^2} \tag{10b}$$

The justification of these choices is that classical Navier–Stokes–Fourier theory is recovered in the stiff limit $\tau_1, \tau_2 \rightarrow 0$ (see Dumbser et al. [1]). This results in the following relations:

$$\sigma = -\rho c_s^2 G \operatorname{dev}(G) \tag{11a}$$

$$\boldsymbol{q} = \alpha^2 T \boldsymbol{J} \tag{11b}$$

$$-\frac{\psi}{\theta_1(\tau_1)} = -\frac{3}{\tau_1}|A|^{\frac{5}{3}} A \operatorname{dev}(G) \tag{11c}$$

$$-\frac{\rho \boldsymbol{H}}{\theta_2(\tau_2)} = -\frac{T\rho_0}{T_0 \tau_2}\boldsymbol{J} \tag{11d}$$

The following constraint also holds (see Peshkov and Romenski [5]):

$$\det(A) = \frac{\rho}{\rho_0} \tag{12}$$

The GPR model and Godunov and Romenski's 1970s model of elastoplastic deformation are very similar in structure. The differences lie in the physical interpretation of A, the appearance of algebraic source terms in the evolution equations for A, and the inclusion of thermal conduction by the evolution of $\boldsymbol{J}$. Whereas the earlier model described only solids, the new model seeks to describe fluids as well. In the former, A was viewed as describing the global deformation of the medium; it is now regarded as describing the local distortion of the material elements comprising the medium, containing information about their rotation and deformation. Unlike in previous continuum models, material elements have not only finite size, but also internal structure.

The strain dissipation time τ_1 of the GPR model is a continuous analogue of Frenkel's "particle settled life time" Frenkel [2]; the characteristic time taken for a particle to move by a distance of the same order of magnitude as the particle's size. Thus, τ_1 characterizes the time taken for a material element to rearrange with its neighbors. $\tau_1 = \infty$ for solids and $\tau_1 = 0$ for inviscid fluids. It is in this way that the GPR model seeks to describe all three major phases of matter, as long as a continuum description is appropriate for the material at hand.

The evolution equation for $\boldsymbol{J}$ and its contribution to the energy of the system are derived from Romenski's model of hyperbolic heat transfer, originally proposed in Malyshev and Romenskii [4], Romenski [8], and implemented in Romenski et al. [7, 6]. In this model, $\boldsymbol{J}$ is effectively defined as the variable conjugate to the entropy flux, in the sense that the latter is the derivative of the specific internal energy with respect to $\boldsymbol{J}$. Romenski remarks that it is more convenient to evolve $\boldsymbol{J}$ and E than the heat flux or the entropy flux, and thus the equations take the form given here. τ_2 characterizes the speed of relaxation of the thermal impulse due to heat exchange between material elements.

1.3. The Cauchy Deformation Tensor

It is noted by Peshkov and Romenski [5]:

> As long as a fluid under consideration is simple and a flow is laminar, the information about rotations of fluid particles stored in the distortion A can be ignored and, for example, the [Cauchy] deformation tensor $G = A^T A$ can be used as the state variable instead of A. The situation becomes quite different if we consider complex fluids, e.g., liquid crystals, where the orientation of particles plays an important role, and therefore, particle rotations cannot be ignored. One may expect that the same is true for turbulent flows of simple Newtonian fluid.

Thus, for simple laminar flows, (1c) can be replaced with the following evolution equation for G, which is easily derived from (1c):

$$\frac{\partial G_{ij}}{\partial t} + v_k \frac{\partial G_{ij}}{\partial x_k} + G_{ik}\frac{\partial v_k}{\partial x_j} + G_{jk}\frac{\partial v_k}{\partial x_i} = \frac{2\sigma_{ij}}{\rho\theta_1(\tau_1)} \tag{13}$$

Ortega et al. [REF] advise against using this formulation in the context of elastic-plastic solid mechanics, owing to the fact that this formulation is not fully conservative, leading to the incorrect weak solution across discontinuities. However... [talk about DLM].

2. Evolution Equations for the Eigendecomposition

2.1. Decoupling the Eigenvalues and Eigenvectors

As G is symmetric positive definite, it has the following eigendecomposition:

$$G = U\Lambda U^T \tag{14}$$

where Λ is the diagonal matrix of eigenvalues and U is orthonormal. Note that:

$$G \operatorname{dev}(G) = U\Lambda U^T \left(U\Lambda U^T - \frac{\operatorname{tr}\left(U\Lambda U^T\right)}{3} I \right) = U\Lambda \operatorname{dev}(\Lambda)\, U^T \tag{15}$$

Thus, (13) becomes:

$$\dot{U}\Lambda U^T + U\dot{\Lambda}U^T + U\Lambda\dot{U}^T + U\Lambda U^T\nabla\boldsymbol{v} + \nabla\boldsymbol{v}^T U\Lambda U^T = \frac{-2c_s^2}{\theta_1(\tau_1)} U\Lambda \operatorname{dev}(\Lambda)\, U^T \tag{16}$$

where $\dot{X}$ is the material derivative of quantity X. Therefore:

$$U^T\dot{U}\Lambda + \dot{\Lambda} + \Lambda\dot{U}^T U + \Lambda U^T\nabla\boldsymbol{v}U + U^T\nabla\boldsymbol{v}^T U\Lambda = \frac{-2c_s^2}{\theta_1(\tau_1)} \Lambda \operatorname{dev}(\Lambda) \tag{17}$$

Thus, (17) is equivalent to the set of six equations:

$$\dot{\Lambda}_{ii} + \left(\Lambda U^T\nabla\boldsymbol{v}U + U^T\nabla\boldsymbol{v}^T U\Lambda\right)_{ii} = \frac{-2c_s^2}{\theta_1(\tau_1)} \left(\Lambda \operatorname{dev}(\Lambda)\right)_{ii} \tag{18a}$$

$$\left(U^T\dot{U}\Lambda + \Lambda\dot{U}^T U\right)_{jk} + \left(\Lambda U^T\nabla\boldsymbol{v}U + U^T\nabla\boldsymbol{v}^T U\Lambda\right)_{jk} = 0 \tag{18b}$$

where $i = 1,2,3$ and $(j,k) = (1,2),(1,3),(2,3)$. Note that these equations can be written in the more succint form:

$$\dot{\lambda}_i + \lambda_i \|\boldsymbol{u_i}\|^2_{\operatorname{sym}(\nabla\boldsymbol{v})} = \frac{-2c_s^2}{\theta_1(\tau_1)} \lambda_i \left(\lambda_i - \bar{\lambda}\right) \tag{19a}$$

$$\operatorname{sym}\left(U^T\dot{U}\Lambda\right)_{jk} + \operatorname{sym}\left(\Lambda U^T\nabla\boldsymbol{v}U\right)_{jk} = 0 \tag{19b}$$

where:

$$\bar{x} = \frac{x_1 + x_2 + x_3}{3} \tag{20a}$$

$$\operatorname{sym}(X) = X + X^T \tag{20b}$$

$$\|\boldsymbol{u}\|^2_X = \boldsymbol{u}^T X \boldsymbol{u} \tag{20c}$$

Note that as we have $U_i^T U_j = \delta_{ij}$, we have $\dot{U}_i^T U_j + U_i^T \dot{U}_j = 0$ for $i,j = 1,2,3$. Combining these 6 independent relations with the 3 relations found in (19b) we have:

$$\begin{pmatrix} u_{12} & u_{22} & u_{32} & u_{11} & u_{21} & u_{31} & 0 & 0 & 0 \\ u_{13} & u_{23} & u_{33} & 0 & 0 & 0 & u_{11} & u_{21} & u_{31} \\ 0 & 0 & 0 & u_{13} & u_{23} & u_{33} & u_{12} & u_{22} & u_{32} \\ u_{11} & u_{21} & u_{31} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & u_{12} & u_{22} & u_{32} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & u_{13} & u_{23} & u_{33} \\ u_{12}\lambda_1 & u_{22}\lambda_1 & u_{32}\lambda_1 & u_{11}\lambda_2 & u_{21}\lambda_2 & u_{31}\lambda_2 & 0 & 0 & 0 \\ u_{13}\lambda_1 & u_{23}\lambda_1 & u_{33}\lambda_1 & 0 & 0 & 0 & u_{11}\lambda_3 & u_{21}\lambda_3 & u_{31}\lambda_3 \\ 0 & 0 & 0 & u_{13}\lambda_2 & u_{23}\lambda_2 & u_{33}\lambda_2 & u_{12}\lambda_3 & u_{22}\lambda_3 & u_{32}\lambda_3 \end{pmatrix} \frac{d}{dt} \begin{pmatrix} u_{11} \\ u_{21} \\ u_{31} \\ u_{12} \\ u_{22} \\ u_{32} \\ u_{13} \\ u_{23} \\ u_{33} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ u_1^T \left(\lambda_1 \nabla \boldsymbol{v} + \lambda_2 \nabla \boldsymbol{v}^T\right) u_2 \\ u_3^T \left(\lambda_3 \nabla \boldsymbol{v} + \lambda_1 \nabla \boldsymbol{v}^T\right) u_1 \\ u_2^T \left(\lambda_2 \nabla \boldsymbol{v} + \lambda_3 \nabla \boldsymbol{v}^T\right) u_3 \end{pmatrix} \tag{21}$$

It is straightforward to verify that the inverse of this system matrix is:

$$\begin{pmatrix} -\frac{u_{12}\lambda_2}{\lambda_1-\lambda_2} & -\frac{u_{13}\lambda_3}{\lambda_1-\lambda_3} & 0 & u_{11} & 0 & 0 & \frac{u_{12}}{\lambda_1-\lambda_2} & \frac{u_{13}}{\lambda_1-\lambda_3} & 0 \\ -\frac{u_{22}\lambda_2}{\lambda_1-\lambda_2} & -\frac{u_{23}\lambda_3}{\lambda_1-\lambda_3} & 0 & u_{21} & 0 & 0 & \frac{u_{22}}{\lambda_1-\lambda_2} & \frac{u_{23}}{\lambda_1-\lambda_3} & 0 \\ -\frac{u_{32}\lambda_2}{\lambda_1-\lambda_2} & -\frac{u_{33}\lambda_3}{\lambda_1-\lambda_3} & 0 & u_{31} & 0 & 0 & \frac{u_{32}}{\lambda_1-\lambda_2} & \frac{u_{33}}{\lambda_1-\lambda_3} & 0 \\ \frac{u_{11}\lambda_1}{\lambda_1-\lambda_2} & 0 & -\frac{u_{13}\lambda_3}{\lambda_2-\lambda_3} & 0 & u_{12} & 0 & -\frac{u_{11}}{\lambda_1-\lambda_2} & 0 & \frac{u_{13}}{\lambda_2-\lambda_3} \\ \frac{u_{21}\lambda_1}{\lambda_1-\lambda_2} & 0 & -\frac{u_{23}\lambda_3}{\lambda_2-\lambda_3} & 0 & u_{22} & 0 & -\frac{u_{21}}{\lambda_1-\lambda_2} & 0 & \frac{u_{23}}{\lambda_2-\lambda_3} \\ \frac{u_{31}\lambda_1}{\lambda_1-\lambda_2} & 0 & -\frac{u_{33}\lambda_3}{\lambda_2-\lambda_3} & 0 & u_{32} & 0 & -\frac{u_{31}}{\lambda_1-\lambda_2} & 0 & \frac{u_{33}}{\lambda_2-\lambda_3} \\ 0 & \frac{u_{11}\lambda_1}{\lambda_1-\lambda_3} & \frac{u_{12}\lambda_2}{\lambda_2-\lambda_3} & 0 & 0 & u_{13} & 0 & -\frac{u_{11}}{\lambda_1-\lambda_3} & -\frac{u_{12}}{\lambda_2-\lambda_3} \\ 0 & \frac{u_{21}\lambda_1}{\lambda_1-\lambda_3} & \frac{u_{22}\lambda_2}{\lambda_2-\lambda_3} & 0 & 0 & u_{23} & 0 & -\frac{u_{21}}{\lambda_1-\lambda_3} & -\frac{u_{22}}{\lambda_2-\lambda_3} \\ 0 & \frac{u_{31}\lambda_1}{\lambda_1-\lambda_3} & \frac{u_{32}\lambda_2}{\lambda_2-\lambda_3} & 0 & 0 & u_{33} & 0 & -\frac{u_{31}}{\lambda_1-\lambda_3} & -\frac{u_{32}}{\lambda_2-\lambda_3} \end{pmatrix} \tag{22}$$

Define:

$$b_1 = u_2^T \left(\lambda_2 \nabla \boldsymbol{v} + \lambda_3 \nabla \boldsymbol{v}^T\right) u_3 \tag{23a}$$

$$b_2 = u_3^T \left(\lambda_3 \nabla \boldsymbol{v} + \lambda_1 \nabla \boldsymbol{v}^T\right) u_1 \tag{23b}$$

$$b_3 = u_1^T \left(\lambda_1 \nabla \boldsymbol{v} + \lambda_2 \nabla \boldsymbol{v}^T\right) u_2 \tag{23c}$$

Thus,we have:

$$\frac{d}{dt} \begin{pmatrix} u_{11} \\ u_{21} \\ u_{31} \\ u_{12} \\ u_{22} \\ u_{32} \\ u_{13} \\ u_{23} \\ u_{33} \end{pmatrix} = \begin{pmatrix} \frac{b_3 u_{12}}{\lambda_1-\lambda_2} + \frac{b_2 u_{13}}{\lambda_1-\lambda_3} \\ \frac{b_3 u_{22}}{\lambda_1-\lambda_2} + \frac{b_2 u_{23}}{\lambda_1-\lambda_3} \\ \frac{b_3 u_{32}}{\lambda_1-\lambda_2} + \frac{b_2 u_{33}}{\lambda_1-\lambda_3} \\ \frac{b_1 u_{13}}{\lambda_2-\lambda_3} - \frac{b_3 u_{11}}{\lambda_1-\lambda_2} \\ \frac{b_1 u_{23}}{\lambda_2-\lambda_3} - \frac{b_3 u_{21}}{\lambda_1-\lambda_2} \\ \frac{b_1 u_{33}}{\lambda_2-\lambda_3} - \frac{b_3 u_{31}}{\lambda_1-\lambda_2} \\ -\frac{b_2 u_{11}}{\lambda_1-\lambda_3} - \frac{b_1 u_{12}}{\lambda_2-\lambda_3} \\ -\frac{b_2 u_{21}}{\lambda_1-\lambda_3} - \frac{b_1 u_{22}}{\lambda_2-\lambda_3} \\ -\frac{b_2 u_{31}}{\lambda_1-\lambda_3} - \frac{b_1 u_{32}}{\lambda_2-\lambda_3} \end{pmatrix} \tag{24}$$

This can be expressed succinctly as:

$$\frac{du_i}{dt} = u_i \times B \tag{25}$$

$$B_i = \frac{u_j^T \left(\lambda_j \nabla \boldsymbol{v} + \lambda_k \nabla \boldsymbol{v}^T\right) u_k}{\lambda_j - \lambda_k} \tag{26}$$

where i, j, k should be taken to be cyclic permutations of $1, 2, 3$.

Whilst it is possible to use this equation to calculate the components of U, it is unnecessarily computationally expensive. As an orthogonal matrix, U represents a rotation of $\mathbb{R}^3$, and thus only has 3 degrees of freedom. Calculating U in matrix forms requires the computation of 9 components. Whilst it is tempting to devise instead evolution equations for the Euler angles that specify U, one runs into the Gimbal lock [REF], making certain calculations impossible. Thus, these evolution equations will now be formulated in terms of quaternions.

2.2. *The Quaternion Representation*

Let $\boldsymbol{q} = s + x\boldsymbol{i} + y\boldsymbol{j} + z\boldsymbol{k}$ be the unit quaternion (so that $s^2 + x^2 + y^2 + z^2 = 1$) corresponding to the rotation matrix U. Then we have:

$$U = \begin{pmatrix} 1 - 2y^2 - 2z^2 & 2xy - 2sz & 2zx + 2sy \\ 2xy + 2sz & 1 - 2z^2 - 2x^2 & 2yz - 2sx \\ 2zx - 2sy & 2yz + 2sx & 1 - 2x^2 - 2y^2 \end{pmatrix} \tag{27}$$

Noting that $s\dot{s} + x\dot{x} + y\dot{y} + z\dot{z} = 0$, it is straightforward to confirm that we have:

$$U^T \dot{U} \Lambda + \Lambda \dot{U}^T U = 2 \begin{pmatrix} 0 & (s\dot{z} - z\dot{s} + y\dot{x} - x\dot{y})(\lambda_1 - \lambda_2) & (s\dot{y} - y\dot{s} + x\dot{z} - z\dot{x})(\lambda_3 - \lambda_1) \\ (s\dot{z} - z\dot{s} + y\dot{x} - x\dot{y})(\lambda_1 - \lambda_2) & 0 & (s\dot{x} - x\dot{s} + z\dot{y} - y\dot{z})(\lambda_2 - \lambda_3) \\ (s\dot{y} - y\dot{s} + x\dot{z} - z\dot{x})(\lambda_3 - \lambda_1) & (s\dot{x} - x\dot{s} + z\dot{y} - y\dot{z})(\lambda_2 - \lambda_3) & 0 \end{pmatrix} \tag{28}$$

Elements $(2,3), (1,3), (1,2)$ of $\operatorname{sym}\left(U^T \dot{U} \Lambda\right)$ can be written in the following form:

$$2 \begin{pmatrix} (s\dot{x} - x\dot{s} + z\dot{y} - y\dot{z})(\lambda_2 - \lambda_3) \\ (s\dot{y} - y\dot{s} + x\dot{z} - z\dot{x})(\lambda_3 - \lambda_1) \\ (s\dot{z} - z\dot{s} + y\dot{x} - x\dot{y})(\lambda_1 - \lambda_2) \end{pmatrix} = 2 \begin{pmatrix} \left(s\dot{x} + x\frac{x\dot{x}+y\dot{y}+z\dot{z}}{s} + z\dot{y} - y\dot{z}\right)(\lambda_2 - \lambda_3) \\ \left(s\dot{y} + y\frac{x\dot{x}+y\dot{y}+z\dot{z}}{s} + x\dot{z} - z\dot{x}\right)(\lambda_3 - \lambda_1) \\ \left(s\dot{z} + z\frac{x\dot{x}+y\dot{y}+z\dot{z}}{s} + y\dot{x} - x\dot{y}\right)(\lambda_1 - \lambda_2) \end{pmatrix} \tag{29}$$

Denoting elements $(2,3), (1,3), (1,2)$ of $\operatorname{sym}\left(\Lambda U^T \nabla \boldsymbol{v} U\right)$ by $\boldsymbol{b}$, from (18b) we have:

$$2 \begin{pmatrix} \lambda_2 - \lambda_3 & 0 & 0 \\ 0 & \lambda_3 - \lambda_1 & 0 \\ 0 & 0 & \lambda_1 - \lambda_2 \end{pmatrix} \begin{pmatrix} \frac{x^2}{s} + s & \frac{xy}{s} + z & \frac{xz}{s} - y \\ \frac{yx}{s} - z & \frac{y^2}{s} + s & \frac{yz}{s} + x \\ \frac{zx}{s} + y & \frac{zy}{s} - x & \frac{z^2}{s} + s \end{pmatrix} \begin{pmatrix} \dot{x} \\ \dot{y} \\ \dot{z} \end{pmatrix} = -\boldsymbol{b} \tag{30}$$

Thus, using the fact that $s^2 + x^2 + y^2 + z^2 = 1$:

$$\begin{aligned} \begin{pmatrix} \dot{x} \\ \dot{y} \\ \dot{z} \end{pmatrix} &= -\frac{1}{2} \begin{pmatrix} s & -z & y \\ z & s & -x \\ -y & x & s \end{pmatrix} \begin{pmatrix} \frac{1}{\lambda_2 - \lambda_3} & 0 & 0 \\ 0 & \frac{1}{\lambda_3 - \lambda_1} & 0 \\ 0 & 0 & \frac{1}{\lambda_1 - \lambda_2} \end{pmatrix} \boldsymbol{b} \\ &= -\frac{1}{2} \begin{pmatrix} s & -z & y \\ z & s & -x \\ -y & x & s \end{pmatrix} \begin{pmatrix} \frac{U_2^T\left(\lambda_2 \nabla \boldsymbol{v} + \lambda_3 \nabla \boldsymbol{v}^T\right) U_3}{\lambda_2 - \lambda_3} \\ \frac{U_3^T\left(\lambda_3 \nabla \boldsymbol{v} + \lambda_1 \nabla \boldsymbol{v}^T\right) U_1}{\lambda_3 - \lambda_1} \\ \frac{U_1^T\left(\lambda_1 \nabla \boldsymbol{v} + \lambda_2 \nabla \boldsymbol{v}^T\right) U_2}{\lambda_1 - \lambda_2} \end{pmatrix} \end{aligned} \tag{31}$$

In non-conservative block-matrix form, this is:

$$\begin{pmatrix} \dot{x} \\ \dot{y} \\ \dot{z} \end{pmatrix} = -\frac{1}{2} \begin{pmatrix} s & -z & y \\ z & s & -x \\ -y & x & s \end{pmatrix} \begin{pmatrix} \frac{1}{\lambda_2-\lambda_3} & 0 & 0 \\ 0 & \frac{1}{\lambda_3-\lambda_1} & 0 \\ 0 & 0 & \frac{1}{\lambda_1-\lambda_2} \end{pmatrix} \begin{pmatrix} \lambda_2 U_{i2} U_{k3} + \lambda_3 U_{i3} U_{k2} \\ \lambda_3 U_{i3} U_{k1} + \lambda_1 U_{i1} U_{k3} \\ \lambda_1 U_{i1} U_{k2} + \lambda_2 U_{i2} U_{k1} \end{pmatrix} \partial_k \boldsymbol{v}_i \tag{32}$$

The six equations contained in (19a), (31) will in this study be used to replace the nine equations contained in (1c). The advantage of this is that the eigendecomposition of G is readily calculated as part of the evolution of the system, rather than having to be calculated separately at each time step.

It should be noted that the right hand side of (31) is undefined when $\lambda_i = \lambda_j$ for some $i \neq j$. This is because the eigenvectors of G are not uniquely defined when one or more eigenvalues take the same value (as the corresponding eigenspaces have dimension $d > 1$). This issue is treated numerically by taking:

$$\frac{1}{\lambda_i - \lambda_j} \approx \operatorname{sign}\left(\frac{1}{\lambda_i - \lambda_j}\right) \times \min\left(\left|\frac{1}{\lambda_i - \lambda_j}\right|, \Theta\right) \tag{33}$$

where Θ is a large number, less than or equal to the largest representable number available on the computational platform being used.

2.3. Perturbative Approximate Solution

3. Numerical Results

3.1. Validation of the Eigendecomposition ODEs

This test case is undertaken to determine the results of using the split evolution equations for the eigenvalues and eigenvectors of G (as given in Section 2), under a flow with a constant strain rate tensor. The value of the strain rate tensor was taken from Peshkov and Romenski [5]:

$$\frac{\partial v_i}{\partial x_j} = \begin{pmatrix} 0.62 & 0.40 & 1.14 \\ -0.28 & -1.41 & 0.59 \\ -0.19 & -0.72 & -1.28 \end{pmatrix} \tag{34}$$

These values were determined randomly in the cited paper, and they are used here only for comparability. The particle settled life time was $\tau = 1.45 \times 10^{-9} s$. The results of this test are presented in Figure 1 on page 9. As can be seen, the obtained values for the eigenvalues exactly match those obtained with the original ODEs. Under the original formulation, as soon as the flow starts, the eigenvectors “snap” to their constant values after the first time step. Under the new formulation, the eigenvectors relax to their true values in a continuous manner. The larger the parameter Θ in (33), the faster this relaxation occurs, but the stiffer the ODEs that need to be solved become.

3.2. Stokes’ First Problem

3.3. Viscous Shock Problem

4. Conclusions

Conclusions go here.

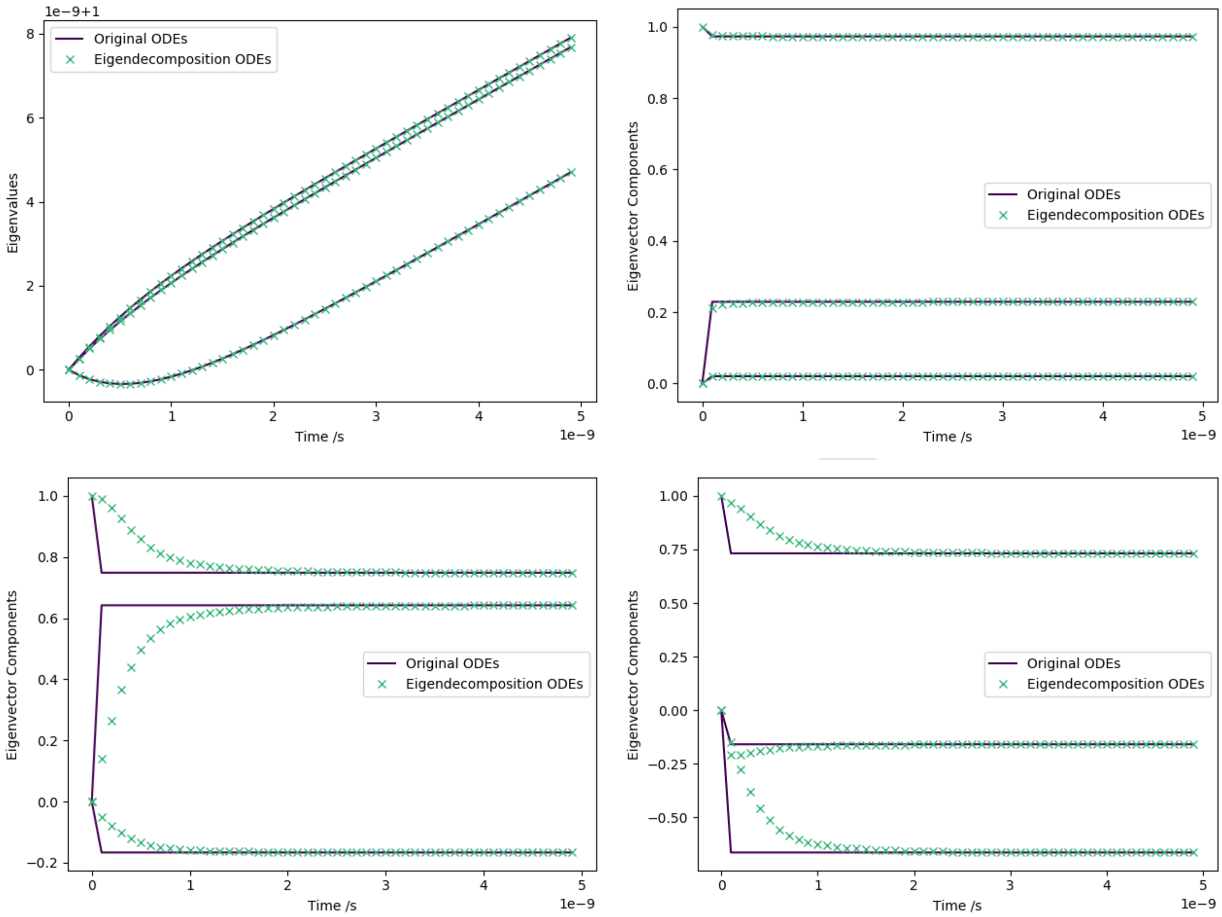

Figure 1: The evolution of the eigenvalues and eigenvectors of the Cauchy Deformation Tensor using the canonical ODEs and the new ODEs

5. References

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