

Lab Notes

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Chapter 1

To Do

1.1 Coding

- Test split-WENO in 2D
- Implement in CUDA
- Solid EOSs
- Implement Barton's damage model
- Test compressible Euler vs GPR - use narrowing domain from Toro's book
- Try conservative formulation [Peshkov, Grmela, Romenski]

1.2 Theoretical

- Investigate further methods of obtaining predictor with form $w_0 + w_1x + c_0t + c_0xt$
- MUSCL using some approximate Riemann solver (perhaps Dumbser's HLLEM) and operator splitting for source terms
- Try evolving in time by $\frac{\Delta t}{2}$ in split-WENO
- Convergence of conservation of mass in RGFM

1.3 Papers

- Application of ADER-WENO to equations in other areas of Physics, Biology, & Economics
- Split solver vs ADER-WENO
- Isobaric cookoff paper - make cookoff the focus
- HPR-RGFM paper (solve stationarity of interface solver under some conditions)

Chapter 2

Faster Solvers

2.1 Fast WENO Oscillation Indicator Calculation

The WENO oscillation indicator is defined as:

$$o = \Sigma_{mn} w_m w_n \quad (2.1)$$

where w_i are the WENO coefficients calculated for a particular stencil, and:

$$\Sigma_{mn} = \sum_{\alpha=1}^N \int_0^1 \psi_m^{(\alpha)} \psi_n^{(\alpha)} \quad (2.2)$$

By considering that:

$$o = \sum_{\alpha=1}^N \int_0^1 \left(\frac{d^\alpha w}{dx^\alpha} \right)^2 > 0 \quad (2.3)$$

we have that Σ is symmetric positive definite. Thus, it has a Cholesky decomposition $\Sigma = LL^T$. Thus:

$$o = \|w^T L\|^2 \quad (2.4)$$

L can be precalculated, and o calculated quickly as:

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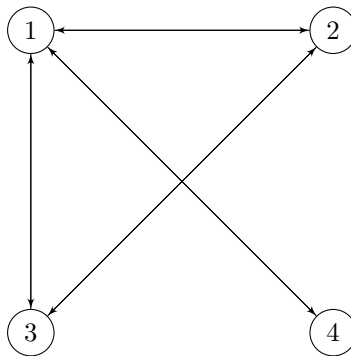
1: o = 0
2: for j = 1...n do
3:   tmp = 0
4:   for i = j...n do
5:     tmp = tmp + w(i) * L(i,j)
6:   end for
7:   o = o + tmp * tmp
8: end for

```

2.2 Perron-Frobenius Estimate for Rusanov Flux

The most expensive single part of the FV flux updates when using the Rusanov flux is the calculation of the maximum absolute eigenvalue of the system matrix. In my dissertation I showed that this is equal to $|v \pm \lambda_{max}|$ where λ_{max} is the maximum eigenvalue of the thermo-acoustic tensor X , and the sign depends on the sign of v . When $\alpha \neq 0$, by considering the fact that the graph of which X is the adjacency matrix is clearly strongly connected, it follows that X is irreducible. Additionally, it can be shown that its non-zero components are always positive.

$$\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix} \quad (2.5)$$



Thus, by the Perron-Frobenius Theorem, we have:

$$\min_i \sum_j X_{ij} \leq \lambda_{max} \leq \max_i \sum_j X_{ij} \quad (2.6)$$

These bounds are much more quickly calculated than explicitly finding the eigenvalues. I proposed using an average of the bounds as an estimate for λ_{max} . This results in $\sim 35\%$ speedup on the FV section of Stokes' First Problem.

NB this method can be used to obtain a conservative upper bound on λ_{max} when calculating the timestep.

2.3 Approximating Interface Terms in FV

Instead of calculating the following:

$$\int D(q^-(x_0, t), q^+(x_0, t)) dt \quad (2.7)$$

I propose calculating the following:

$$D\left(\frac{1}{\Delta t} \int q^-(x_0, t) dt, \frac{1}{\Delta t} \int q^+(x_0, t) dt\right) \quad (2.8)$$

This obtains a large speedup with no discernable difference in the results of Stokes' First Problem.

2.4 Analytical Results for Basis Vectors

For $N = 1$, the Gauss-Legendre nodes on $[0, 1]$ are $\left\{\frac{1}{2}\left(1 - \frac{1}{\sqrt{3}}\right), \frac{1}{2}\left(1 + \frac{1}{\sqrt{3}}\right)\right\}$. Thus:

$$\psi_1(x) = -\sqrt{3}x + \frac{1 + \sqrt{3}}{2} \quad (2.9a)$$

$$\psi_2(x) = \sqrt{3}x + \frac{1 - \sqrt{3}}{2} \quad (2.9b)$$

$$\psi_1(1) = \frac{1 - \sqrt{3}}{2} \quad (2.10a)$$

$$\psi_2(1) = \frac{1 + \sqrt{3}}{2} \quad (2.10b)$$

$$\psi_1(1)\psi_1(1) = 1 - \frac{\sqrt{3}}{2} \quad (2.11a)$$

$$\psi_1(1)\psi_2(1) = -\frac{1}{2} \quad (2.11b)$$

$$\psi_2(1)\psi_2(1) = 1 + \frac{\sqrt{3}}{2} \quad (2.11c)$$

$$\int_m^{m+1} \psi_1(x) dx = \frac{-\sqrt{3}}{2}(2m+1) + \frac{1 + \sqrt{3}}{2} = \frac{1}{2} - m\sqrt{3} \quad (2.12a)$$

$$\int_m^{m+1} \psi_2(x) dx = \frac{\sqrt{3}}{2}(2m+1) + \frac{1 - \sqrt{3}}{2} = \frac{1}{2} + m\sqrt{3} \quad (2.12b)$$

The WENO matrices are:

$$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} - \sqrt{3} & \frac{1}{2} + \sqrt{3} \end{pmatrix}, \begin{pmatrix} \frac{1}{2} + \sqrt{3} & \frac{1}{2} - \sqrt{3} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} \quad (2.13)$$

The inverses are:

$$\frac{1}{\sqrt{3}} \begin{pmatrix} \sqrt{3} + \frac{1}{2} & -\frac{1}{2} \\ \sqrt{3} - \frac{1}{2} & \frac{1}{2} \end{pmatrix}, \frac{1}{\sqrt{3}} \begin{pmatrix} \frac{1}{2} & \sqrt{3} - \frac{1}{2} \\ -\frac{1}{2} & \sqrt{3} + \frac{1}{2} \end{pmatrix} \quad (2.14)$$

The weights for both nodes are 0.5 so $\int_0^1 \psi_i \psi_j dx = \frac{\delta_{ij}}{2}$ and $\int_0^1 \psi_i \psi_j' dx = (-1)^j \frac{\sqrt{3}}{2}$.

$$\begin{aligned} I_{11} - I_2^T &= \frac{1}{2} \begin{pmatrix} 2 - \sqrt{3} & -1 \\ -1 & 2 + \sqrt{3} \end{pmatrix} - \frac{1}{2} \begin{pmatrix} -\sqrt{3} & -\sqrt{3} \\ \sqrt{3} & \sqrt{3} \end{pmatrix} \\ &= \frac{1}{2} \begin{pmatrix} 2 & -(1 - \sqrt{3}) \\ -(1 + \sqrt{3}) & 2 \end{pmatrix} \end{aligned} \quad (2.15)$$

$$(I_{11} - I_2^T)^{-1} = \frac{1}{3} \begin{pmatrix} 2 & 1 - \sqrt{3} \\ 1 + \sqrt{3} & 2 \end{pmatrix} \quad (2.16)$$

Using a precalculated, analytical form of U in the DG predictor for $N = 1$ obtains a ~30% speedup on Stokes' First Problem.

2.5 Operator Splitting

Noting that $\frac{d\rho}{dt} = 0$ over the ODE time step, we must solve the following system:

$$\frac{dA_{ij}}{dt} = \frac{-\psi_{ij}}{\theta_1(\tau_1)} = \frac{-3}{\tau_1} |A|^{\frac{5}{3}} A \operatorname{dev}(G) \quad (2.17a)$$

$$\frac{dJ_i}{dt} = \frac{-H_i}{\theta_2(\tau_2)} = -\frac{1}{\tau_2} \frac{T\rho_0}{T_0\rho} J_i \quad (2.17b)$$

Many different solvers can be used to solve the homogeneous part of the system. So far, this has been tested with SLIC, WENO, and DG. A split-WENO scheme seems to be the fastest and most accurate method available. The results using split-WENO to solve Stokes' First Problem with $N = 1$ are shown in 2.1. These results are comparable to the corresponding results using ADER-WENO, as seen in 2.2.

The results of using a 3rd-order split-WENO scheme to solve Stokes' First Problem are shown in 2.3. Note the close agreement with the Navier-Stokes solution, closely matching the result using ADER-WENO. The split-WENO scheme took 15 times less CPU time than the ADER-WENO scheme.

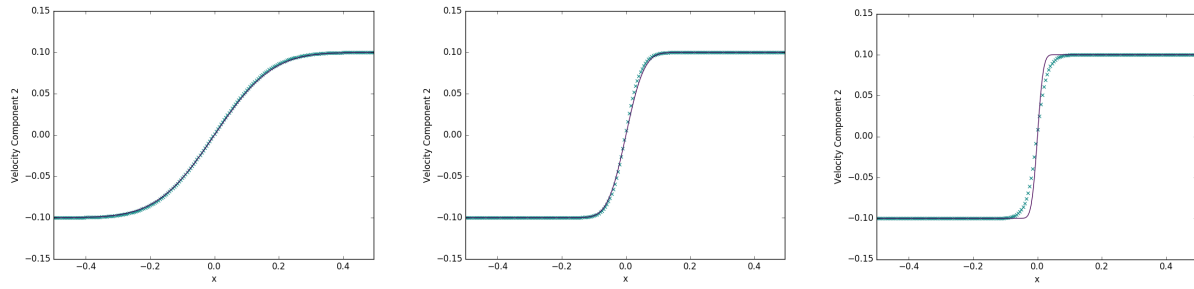


Figure 2.1: Results of solving Stokes' First Problem ($\mu = 10^{-2}, \mu = 10^{-3}, \mu = 10^{-4}$) with a split-WENO scheme ($N = 1$)

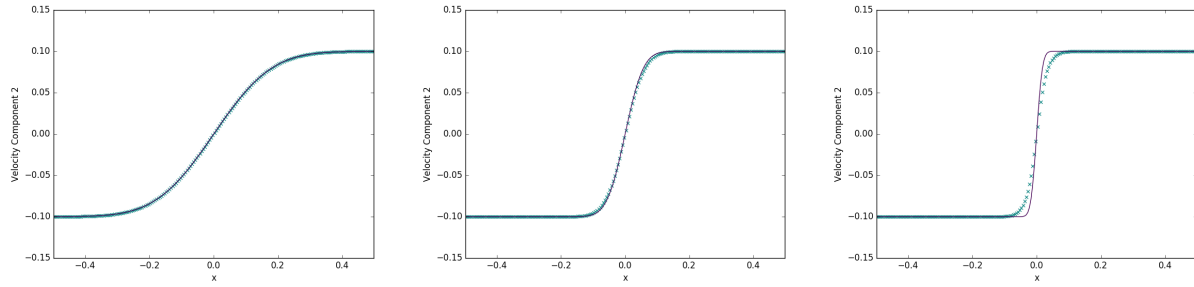


Figure 2.2: Results of solving Stokes' First Problem ($\mu = 10^{-2}, \mu = 10^{-3}, \mu = 10^{-4}$) with an ADER-WENO scheme ($N = 1$)

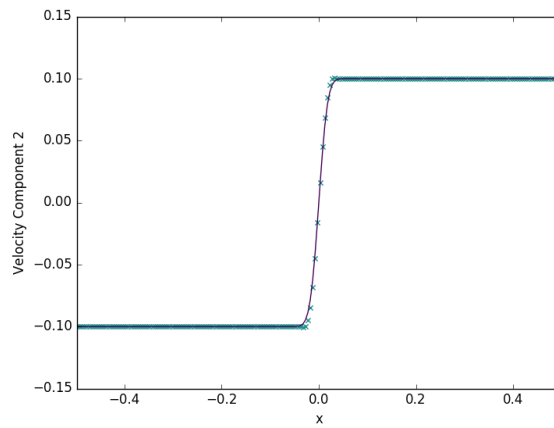


Figure 2.3: Results of solving Stokes' First Problem ($\mu = 10^{-4}$) with a split-WENO scheme ($N = 2$)

2.6 Distortion ODEs

2.6.1 Jacobian of Distortion ODEs

The Jacobian of the source function is used to speed up numerical integration of the ODE. It is derived thus:

$$\frac{\partial \operatorname{dev}(G)_{ij}}{\partial A_{mn}} = \delta_{in} A_{mj} + \delta_{jn} A_{mi} - \frac{2}{3} \delta_{ij} A_{mn} \quad (2.18)$$

Thus:

$$\begin{aligned} \frac{\partial (A \operatorname{dev}(G))_{ij}}{\partial A_{mn}} &= \frac{\partial A_{it}}{\partial A_{mn}} \operatorname{dev}(G)_{tj} + A_{it} \frac{\partial \operatorname{dev}(G)_{tj}}{\partial A_{mn}} \\ &= \delta_{im} \delta_{tn} \left(A_{kt} A_{kj} - \frac{1}{3} A_{kl} A_{kl} \delta_{tj} \right) \\ &\quad + A_{it} \left(\delta_{tn} A_{mj} + \delta_{jn} A_{mt} - \frac{2}{3} \delta_{tj} A_{mn} \right) \\ &= \left(\delta_{im} A_{kn} A_{kj} - \frac{1}{3} \delta_{im} \delta_{jn} A_{kl} A_{kl} \right) \\ &\quad + \left(A_{in} A_{mj} + \delta_{jn} A_{ik} A_{mk} - \frac{2}{3} A_{ij} A_{mn} \right) \end{aligned} \quad (2.19)$$

Thus:

$$\begin{aligned} J_A &\equiv \frac{-3}{\tau_1} \frac{\partial \left(\det(A)^{\frac{5}{3}} A \operatorname{dev}(G) \right)_{ij}}{\partial A_{mn}} \\ &= \frac{-3}{\tau_1} \det(A)^{\frac{5}{3}} \left(\frac{5}{3} (A \operatorname{dev}(G))_{ij} A_{mn}^{-T} + A_{in} A_{mj} + \delta_{jn} G'_{im} + \delta_{im} G'_{jn} - \frac{1}{3} \delta_{im} \delta_{jn} A_{kl} A_{kl} - \frac{2}{3} A_{ij} A_{mn} \right) \end{aligned} \quad (2.20)$$

$$(2.21)$$

where $G' = AA^T$.

2.6.2 Linearized Distortion ODEs Solver

Note that $A^* = \left(\frac{\rho}{\rho_0} \right)^{\frac{1}{3}} I$ is a stationary point of the ODE for A . Linearizing the ODE around A^* gives:

$$\begin{aligned}
\frac{dA}{dt} &\approx J_A(A^*)(A - A^*) \\
&= \frac{-3}{\tau_1} \left(\frac{\rho}{\rho_0} \right)^{\frac{5}{3}} \left(\left(\frac{\rho}{\rho_0} \right)^{\frac{2}{3}} \delta_{in} \delta_{mj} + \left(\frac{\rho}{\rho_0} \right)^{\frac{2}{3}} \delta_{jn} \delta_{im} + \left(\frac{\rho}{\rho_0} \right)^{\frac{2}{3}} \delta_{im} \delta_{jn} - \frac{1}{3} \left(\frac{\rho}{\rho_0} \right)^{\frac{2}{3}} \delta_{im} \delta_{jn} \delta_{kl} \delta_{kl} - \frac{2}{3} \left(\frac{\rho}{\rho_0} \right)^{\frac{2}{3}} \delta_{ij} \delta_{mn} \right) \\
&\quad \times \left(A_{mn} - \left(\frac{\rho}{\rho_0} \right)^{\frac{1}{3}} \delta_{mn} \right) \\
&= \frac{-3}{\tau_1} \left(\frac{\rho}{\rho_0} \right)^{\frac{7}{3}} \left(\delta_{in} \delta_{mj} + \delta_{im} \delta_{jn} - \frac{2}{3} \delta_{ij} \delta_{mn} \right) \left(A_{mn} - \left(\frac{\rho}{\rho_0} \right)^{\frac{1}{3}} \delta_{mn} \right) \\
&= \frac{-3}{\tau_1} \left(\frac{\rho}{\rho_0} \right)^{\frac{7}{3}} \left(A_{mn} \left(\delta_{in} \delta_{mj} + \delta_{im} \delta_{jn} - \frac{2}{3} \delta_{ij} \delta_{mn} \right) - \left(\frac{\rho}{\rho_0} \right)^{\frac{1}{3}} \delta_{mn} \left(\delta_{in} \delta_{mj} + \delta_{im} \delta_{jn} - \frac{2}{3} \delta_{ij} \delta_{mn} \right) \right) \\
&= \frac{-3}{\tau_1} \left(\frac{\rho}{\rho_0} \right)^{\frac{7}{3}} \left(\left(A_{ji} + A_{ij} - \frac{2}{3} \text{tr}(A) \delta_{ij} \right) - \left(\frac{\rho}{\rho_0} \right)^{\frac{1}{3}} (\delta_{ij} + \delta_{ij} - 2\delta_{ij}) \right) \\
&= \frac{-3}{\tau_1} \left(\frac{\rho}{\rho_0} \right)^{\frac{7}{3}} \left(A + A^T - \frac{2}{3} \text{tr}(A) I \right)
\end{aligned} \tag{2.22}$$

The matrix for this system, in row-major form, is:

$$\frac{-3}{\tau_1} \left(\frac{\rho}{\rho_0} \right)^{\frac{7}{3}} \begin{pmatrix} \frac{4}{3} & 0 & 0 & 0 & -\frac{2}{3} & 0 & 0 & 0 & -\frac{2}{3} \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ -\frac{2}{3} & 0 & 0 & 0 & \frac{4}{3} & 0 & 0 & 0 & -\frac{2}{3} \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ -\frac{2}{3} & 0 & 0 & 0 & -\frac{2}{3} & 0 & 0 & 0 & \frac{4}{3} \end{pmatrix} \tag{2.23}$$

The eigenvalues and eigenvectors are:

$$\{0, 0, 0, 0, -2k, -2k, -2k, -2k, -2k\} \tag{2.24}$$

$$\begin{pmatrix} 0 \\ 1 \\ 0 \\ -1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ -1 \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ -1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \begin{pmatrix} -1 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} -1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \tag{2.25}$$

where $k = \frac{3}{\tau_1} \left(\frac{\rho}{\rho_0} \right)^{\frac{7}{3}}$. Thus, the solution is:

$$\begin{aligned}
& \frac{A_{12} - A_{21}}{2} \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \frac{A_{13} - A_{31}}{2} \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix} + \frac{A_{23} - A_{32}}{2} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix} \\
& + \frac{A_{11} + A_{22} + A_{33}}{3} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \\
& + \frac{2A_{22} - A_{11} - A_{33}}{3} e^{-2kt} \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \frac{2A_{33} - A_{11} - A_{22}}{3} e^{-2kt} \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \\
& + \frac{A_{12} + A_{21}}{2} e^{-2kt} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \frac{A_{13} + A_{31}}{2} e^{-2kt} \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} + \frac{A_{23} + A_{32}}{2} e^{-2kt} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}
\end{aligned} \tag{2.26}$$

This is equal to:

$$\frac{1}{2} (A - A^T) + \frac{\text{tr}(A)}{3} I + e^{-2kt} \left(\frac{1}{2} (A + A^T) - \frac{\text{tr}(A)}{3} I \right) \tag{2.27}$$

Results with Stokes' First Problem look good with this linearisation. The ODE step takes a negligible amount of time, meaning that if accuracy is maintained to second order, the solver is now fast enough.

2.6.3 Reduced Distortion ODEs

By the Polar Decomposition Theorem, under an appropriate change of coordinates, $A = RS$ where R is a rotation matrix and S is a diagonal matrix with positive entries, representing the principle stretches. In this case, $G = A^T A = S^T R^T R S = S^2$. Then we have:

$$\frac{d(RS)}{dt} = -kRS \text{dev}(S^2) \tag{2.28}$$

where $k = \frac{3}{\tau_1} \left(\frac{\rho}{\rho_0} \right)^{\frac{5}{3}} > 0$. Note that $A(t) = R(0)S(t)$ is a solution if:

$$\frac{dS}{dt} = -kS \text{dev}(S^2) \tag{2.29}$$

Let the SVD of A be $U\Sigma V^T$. Then a change of coordinates under V gives $V^T A V = (V^T U) \Sigma = RS$. Thus, using a fast 3×3 SVD algorithm (such as in [1]), U, V, Σ can be obtained, after which the following procedure is applied to $\Sigma = S$, giving $A(t) = U\Sigma(t)V^T$.

Denote the singular values of A by a_1, a_2, a_3 . Then:

$$S \text{dev}(S^2) = \begin{pmatrix} a_1 \left(a_1^2 - \frac{a_1^2 + a_2^2 + a_3^2}{3} \right) & 0 & 0 \\ 0 & a_1 \left(a_1^2 - \frac{a_1^2 + a_2^2 + a_3^2}{3} \right) & 0 \\ 0 & 0 & a_1 \left(a_1^2 - \frac{a_1^2 + a_2^2 + a_3^2}{3} \right) \end{pmatrix} \tag{2.30}$$

Letting $x_i = a_i^2$ we have:

$$\frac{dx_i}{dt} = -3kx_i(x_i - \bar{x}) \quad (2.31)$$

where now $k = \frac{2}{\tau_1} \left(\frac{\rho}{\rho_0} \right)^{\frac{5}{3}} > 0$. Now, $\det(A) = a_1 a_2 a_3 = \sqrt{c}$ where $c = \left(\frac{\rho}{\rho_0} \right)^2$ is constant. The ODE system travels along the surface $x_1 x_2 x_3 = c$ to the point $x_1, x_2, x_3 = c^{\frac{1}{3}}$. Thus, we have:

$$\begin{cases} \frac{dx_1}{dt} = -kx_1(2x_1 - x_2 - x_3) = -kx_1 \left(2x_1 - x_2 - \frac{c}{x_1 x_2} \right) \\ \frac{dx_2}{dt} = -kx_2(2x_2 - x_3 - x_1) = -kx_2 \left(2x_2 - x_1 - \frac{c}{x_1 x_2} \right) \end{cases} \quad (2.32)$$

Thus, an ODE solver can be used on these two equations to effectively solve the ODEs for all 9 components of A . Alternatively, it can be noted that:

$$\frac{dx_2}{dx_1} = \frac{x_2}{x_1} \frac{2x_2 - x_1 - \frac{c}{x_1 x_2}}{2x_1 - x_2 - \frac{c}{x_1 x_2}} \quad (2.33)$$

This has solution:

$$x_2 = \frac{c_0 \pm \sqrt{c_0^2 + 4(c - c_0)x_1^3}}{2x_1^2} \quad (2.34)$$

where

$$c_0 = c - \frac{x_{1,0}^2 x_{2,0}^2 - c x_{2,0}}{x_{1,0} - x_{2,0}} \in [0, c] \quad (2.35)$$

Thus, the ODE system for A has been reduced to a single ODE, as $x_2(x_1)$ can be inserted into the RHS of the equation for $\frac{dx_1}{dt}$. It is probably less computationally expensive to evolve the system presented in (2.32).

2.6.4 Semi-Analytic Solution of Reduced Distortion ODEs

Letting $c = 1$, define the following variables:

$$m = x_1 + x_2 + x_3 \quad (2.36a)$$

$$e = (x_1 - x_2)^2 + (x_2 - x_3)^2 + (x_3 - x_1)^2 \quad (2.36b)$$

Then:

$$\frac{de}{dt} = m \left(m^2 - \frac{5}{2}e \right) - 27 \quad (2.37a)$$

$$\frac{dm}{dt} = -e \quad (2.37b)$$

This gives:

$$\frac{dm}{de} = \frac{e}{27 - m \left(m^2 - \frac{5}{2}e \right)} \quad (2.38a)$$

$$m(0) = 3 \quad (2.38b)$$

Note that $\frac{dm}{de}$ is undefined at $(m, e) = (3, 0)$ and in fact the solution to this ODE is the limit curve of the solutions as $m(0) \rightarrow 3$ from below. This solution can be calculated numerically. It is monotone increasing so the inverse $e(m)$ can also be calculated easily. $e(m)$ can now be used to obtain $m(t)$ from (2.37b), numerically. Note that m is monotone decreasing in time, and $\frac{dm}{dt}$ only depends on m . We now calculate $m^*(t)$ as the solution curve to this ODE with some large value for $m(0)$. This solution curve can be used to evaluate $m_{\Delta t} = m(\Delta t)$ for any $m(0) = m_0$, by finding t^* such that $m^*(t^*) = m_0$ and evaluating $m^*(t^* + \Delta t)$. Note that, as with $e(m)$, $m^*(t)$ is easily invertible, allowing t^* to be evaluated quickly.

Once $m_{\Delta t}$ has been found, we have:

$$x_1 + x_2 + x_3 = m_{\Delta t} \quad (2.39a)$$

$$x_1 x_2 x_3 = 1 \quad (2.39b)$$

$$x_2 = \frac{c_0 \pm \sqrt{c_0^2 + 4(c - c_0)x_1^3}}{2x_1^2} \quad (2.39c)$$

This yields:

$$x_1 + \frac{c_0 + \sqrt{c_0^2 + 4(1 - c_0)x_1^3}}{2x_1^2} + \frac{2x_1}{c_0 + \sqrt{c_0^2 + 4(1 - c_0)x_1^3}} = m_{\Delta t} \quad (2.40)$$

x_1 is in fact the root of the following polynomial in the region $x \in [1, x_{1,0}]$:

$$c_0^2 - c_0^2 m_{\Delta t} x^2 + (4(1 - c_0) + 2c_0^2) x^3 - m_{\Delta t}^2 (1 - c_0) x^4 + 2m_{\Delta t} (1 - c_0) x^5 - (1 - c_0) x^6 \quad (2.41)$$

x_2 and thus x_3 are found from x_1 with the available formulas. Thus, the calculation of the distortion factors has been reduced to 2 simple evaluations (to obtain t^* , $m_{\Delta t}$) and a polynomial root find (using e.g. Newton's Method). Note that if $|m_{\Delta t} - 3| < \epsilon_{machine}$ then the system can be considered to have converged, rendering the polynomial root-finding unnecessary, and saving more time.

Tighter bounds for the region in which x_1 lies are given by the roots of the following equations (corresponding to $c_0 = 1$ and $c_0 = 0$, respectively):

$$2x_1 + \frac{1}{x_1^2} = m_{\Delta t} \quad (2.42a)$$

$$x_1 + \frac{2}{\sqrt{x_1}} = m_{\Delta t} \quad (2.42b)$$

The following result may be useful in future:

$$\begin{aligned} \frac{d^2 m}{dt^2} &= -\frac{de}{dt} \\ &= 27c - m \left(m^2 - \frac{5}{2}e \right) \\ &= 27c - m^3 - \frac{5}{2}m \frac{dm}{dt} \end{aligned} \quad (2.43)$$

$$\therefore \frac{d^2 m}{dt^2} + \frac{5}{2}m \frac{dm}{dt} + (m^3 - 27c) = 0 \quad (2.44)$$

2.6.5 Bounds on Reduced Distortion ODEs

As previously noted, the ODE system is confined to the surface $\Psi = x_1 x_2 x_3 = c$ with $x_1, x_2, x_3 > 0$. This surface is symmetrical in the planes $x_1 = x_2$, $x_1 = x_3$, $x_2 = x_3$. As such, given that the system is autonomous, the paths of evolution of the x_i cannot cross the intersections of these planes with Ψ . Thus, any non-strict inequality of the form $x_i \geq x_j \geq x_k$ is maintained for the whole history of the system. By considering (2.31) it is clear that in this case x_i is monotone decreasing, x_k is monotone increasing, and the time derivative of x_j may switch sign. If any of these non-strict inequalities are in fact equalities, equality is maintained throughout the history of the system. This can be seen by noting that the time derivatives of the equal variables are in this case equal. If $x_j = x_k$ then $x_i = \frac{c}{x_j^2}$. Combining these results, the path of the system in (x_i, x_j) coordinates is in fact confined to the curved triangular region:

$$\left\{ (x_i, x_j) : x_i \leq x_i^0 \cap x_i \geq x_j \cap x_i \geq \frac{c}{x_j^2} \right\} \quad (2.45)$$

This is demonstrated in figure 2.4. By (2.32), the rate of change of x_i at a particular value $x_i = x_i^*$ is given by:

$$-kx_i \left(2x_i^* - x_j - \frac{c}{x_i^* x_j} \right) \quad (2.46)$$

Note that:

$$\begin{aligned} \frac{d}{dx_j} \left(2x_i^* - x_j - \frac{c}{x_i^* x_j} \right) &= -1 + \frac{c}{x_i^* x_j^2} = 0 \\ \Rightarrow x_j &= \sqrt{\frac{c}{x_i^*}} \end{aligned} \quad (2.47)$$

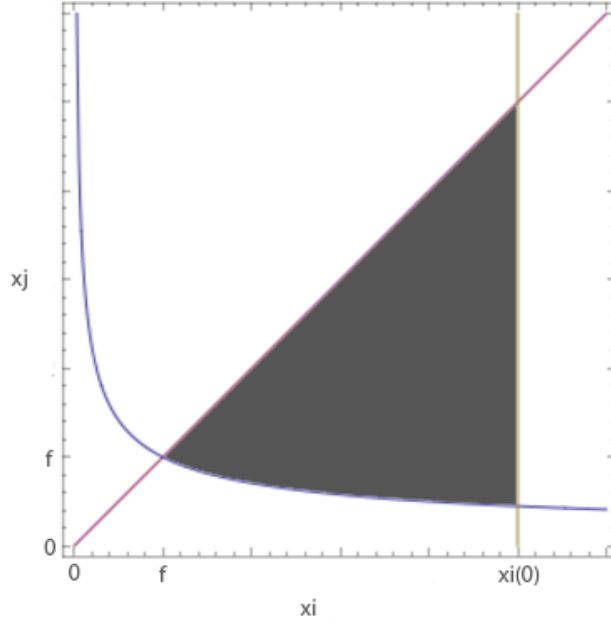


Figure 2.4: The (shaded) region to which x_i, x_j are confined in the evolution of the distortion ODEs. f represents the final value of x_i, x_j, x_k (i.e. $\sqrt[3]{c}$).

$$\frac{d^2}{dx_j^2} \left(2x_i^* - x_j - \frac{c}{x_i^* x_j} \right) = \frac{-2c}{x_i^* x_j^3} < 0 \quad (2.48)$$

Thus, x_i decreases fastest on the line $x_i = \frac{c}{x_j^2}$ (the bottom boundary of the region given in figure 2.4), and slowest on the line $x_i = x_j$. The rates of change of x_i along these two lines are given respectively by:

$$\frac{dx_i}{dt} = -2kx_i \left(x_i - \sqrt{\frac{c}{x_i}} \right) \quad (2.49a)$$

$$\frac{dx_i}{dt} = -kx_i \left(x_i - \frac{c}{x_i^2} \right) \quad (2.49b)$$

These have implicit solutions:

$$t = \frac{1}{6\sqrt[3]{ck}} \left(f \left(\sqrt{x_i}; \sqrt[3]{c} \right) + g \left(\sqrt{x_i}; \sqrt[3]{c} \right) - \left(f \left(\sqrt{x_i^0}; \sqrt[3]{c} \right) + g \left(\sqrt{x_i^0}; \sqrt[3]{c} \right) \right) \right) \equiv F_1(x_i; x_i^0, c) \quad (2.50a)$$

$$t = \frac{1}{6\sqrt[3]{ck}} \left(f(x_i; \sqrt[3]{c}) - g(x_i; \sqrt[3]{c}) - (f(x_i^0; \sqrt[3]{c}) - g(x_i^0; \sqrt[3]{c})) \right) \equiv F_2(x_i; x_i^0, c) \quad (2.50b)$$

where

$$f(x_i; l) = \log \left(\frac{x_i^2 + lx_i + l^2}{(x_i - l)^2} \right) \quad (2.51a)$$

$$g(x_i; l) = 2\sqrt{3} \tan^{-1} \left(\frac{2x_i + l}{\sqrt{3}l} \right) \quad (2.51b)$$

As (2.31) is an autonomous system of ODEs, it has the strange property that its limit $x_1 = x_2 = x_3 = \sqrt[3]{c}$ is never obtained in finite time, in precise arithmetic. In floating point arithmetic we may say that the system has converged when $x_i - \sqrt[3]{c} < \epsilon$ (machine epsilon) for each i . This happens when:

$$t > F_2(\sqrt[3]{c} + \epsilon; x_i^0, c) \quad (2.52)$$

This provides a quick method to check whether it is necessary to run the ODE solver in a particular cell. If $\Delta t > F_2(\sqrt[3]{c} + \epsilon; \max\{x_i^0\}, c)$ then we know the system in that cell converges to the ground state over the time interval in which the ODE system is calculated. If the fluid is very inviscid, resulting in a stiff ODE, the critical time is lower, and there is more chance that the ODE system in the cell reaches its limit in Δt . This check potentially saves a lot of computationally expensive stiff ODE solves. The same goes for if the flow is slow-moving, as the system will be closer to its ground state at the start of the time step and is more likely to converge over Δt .

Similarly, if $\Delta t < F_1(\sqrt[3]{c} + \epsilon; \max\{x_i^0\}, c)$ then we know for sure that an ODE solver is necessary, as the system certainly will not have converged over the system.

2.6.6 Linearized Reduced Distortion ODE Solver

Taking system (2.31), note that the Jacobian of the system is given by:

$$J = -k \begin{pmatrix} 4x_1 - x_2 - x_3 & -x_1 & -x_1 \\ -x_2 & 4x_2 - x_3 - x_1 & -x_3 \\ -x_3 & -x_3 & 4x_3 - x_1 - x_2 \end{pmatrix} \quad (2.53)$$

Evaluated at stationary point $x_i = \sqrt[3]{c}$ we have:

$$J(\mathbf{x}_0) = -k\sqrt[3]{c} \begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix} \quad (2.54)$$

Thus, the system is linearized to:

$$\begin{aligned} \frac{d\mathbf{x}}{dt} &\approx -k\sqrt[3]{c} \begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix} \left(\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} - \sqrt[3]{c} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \right) \\ &= k\sqrt[3]{c} \begin{pmatrix} -2 & 1 & 1 \\ 1 & -2 & 1 \\ 1 & 1 & -2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \end{aligned} \quad (2.55)$$

The eigenvalues of this system matrix are $\{-3k\sqrt[3]{c}, -3k\sqrt[3]{c}, 0\}$ and the eigenvectors are:

$$\begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix}, \begin{pmatrix} 0 \\ -1 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \quad (2.56)$$

Thus, the linearized solution is:

$$\mathbf{x}(t) = \frac{-2x_1 + x_2 + x_3}{3} e^{-3k\sqrt[3]{c}t} \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix} + \frac{x_1 - 2x_2 + x_3}{3} e^{-3k\sqrt[3]{c}t} \begin{pmatrix} 0 \\ -1 \\ 1 \end{pmatrix} + \frac{x_1 + x_2 + x_3}{3} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \quad (2.57)$$

This may represent a faster way to calculate the evolution of the stretch terms of A . Note that some kind of normalization will probably be necessary, as:

$$\frac{x_1 + x_2 + x_3}{3} \geq (x_1 x_2 x_3)^{\frac{1}{3}} \quad (2.58)$$

with equality if and only if $x_1 = x_2 = x_3$.

2.7 Thermal Impulse ODEs

Density does not change over the time period of the ODE. Assuming pressure (and therefore temperature) does not change also, we have the following:

$$\tilde{J}_i = \exp\left(-\frac{T\rho_0}{T_0\rho} \frac{\Delta t}{\tau_2}\right) J_i \quad (2.59)$$

Note that the constant pressure assumption may not always work well. Pressure (and temperature) increase over this time period, by conservation of energy (see the EOS), so the relaxation of \mathbf{J} is quicker than produced here. Ignoring the contribution from A , the EOS gives:

$$\begin{aligned} T &= \frac{E_1}{c_v} \\ &= \frac{E - E_{2A}(A) - E_3(\mathbf{v})}{c_v} - \frac{1}{c_v} E_{2J}(\mathbf{J}) \\ &= c_1 - c_2 \mathbf{J}^2 \end{aligned} \quad (2.60)$$

where:

$$c_1 = \frac{E - E_{2A}(A) - E_3(\mathbf{v})}{c_v} \quad (2.61a)$$

$$c_2 = \frac{\alpha^2}{2c_v} \quad (2.61b)$$

Over the time period of the ODE, $c_1, c_2 > 0$ are constant. We have:

$$\begin{aligned}\frac{dJ_1}{dt} &= -\frac{1}{\tau_2} \frac{\rho_0}{T_0 \rho} (c_1 J_1 - c_2 \mathbf{J}^2) \\ &= -c_3 J_1 + c_4 J_i (J_1^2 + J_2^2 + J_3^2)\end{aligned}\quad (2.62)$$

$$\therefore J_i \frac{dJ_i}{dt} = \frac{1}{2} \frac{d}{dt} (J_i^2) = -c_3 J_i^2 + c_4 J_i^2 (J_1^2 + J_2^2 + J_3^2) \quad (2.63)$$

$$\therefore \frac{d}{dt} (J_i^2) = J_i^2 (-a + b (J_1^2 + J_2^2 + J_3^2)) \quad (2.64)$$

Note that this is a generalized Lotka-Volterra system in $\{J_1^2, J_2^2, J_3^2\}$. It has solution:

$$J_i(t) = J_i(0) \sqrt{\frac{1}{e^{at} - \frac{b}{a}(e^{at} - 1) \mathbf{J}(\mathbf{0})^2}} \quad (2.65)$$

2.8 Primitive WENO and DG Reconstruction

As suggested in [2], the WENO and DG can be performed in primitive variables, which is less computationally expensive than evaluating fluxes using conserved variables. Achieves around 20% speedup in DG step, at double cost in WENO step. Minimal speedup in FV step, as both primitive and conserved variables must be calculated for the flux updates. Not enough.

2.9 Change to Row-Major Ordering

The original GPR papers state the equations for A in column-major order, probably because the authors use Fortran. For C++ and Python implementations it is faster to work in row-major order. ~10% speedup was achieved by implementing this.

The GPR equations are:

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho v_k)}{\partial x_k} = 0 \quad (2.66a)$$

$$\frac{\partial (\rho E)}{\partial t} + \frac{\partial (\rho E v_k + (p \delta_{ik} - \sigma_{ik}) v_i + q_k)}{\partial x_k} = 0 \quad (2.66b)$$

$$\frac{\partial (\rho v_i)}{\partial t} + \frac{\partial (\rho v_i v_k + p \delta_{ik} - \sigma_{ik})}{\partial x_k} = 0 \quad (2.66c)$$

$$\frac{\partial A_{ij}}{\partial t} + \frac{\partial (A_{ik} v_k)}{\partial x_j} + v_k \left(\frac{\partial A_{ij}}{\partial x_k} - \frac{\partial A_{ik}}{\partial x_j} \right) = -\frac{\psi_{ij}}{\theta_1(\tau_1)} \quad (2.66d)$$

$$\frac{\partial (\rho J_i)}{\partial t} + \frac{\partial (\rho J_i v_k + T \delta_{ik})}{\partial x_k} = -\frac{\rho H_i}{\theta_2(\tau_2)} \quad (2.66e)$$

$$\Psi_{ij} = \rho v_i v_j - \sigma_{ij} \quad (2.73a)$$

$$\Phi_{ij}^k = \rho v_k \psi_{ij} - v_m \frac{\partial \sigma_{mk}}{\partial A_{ij}} \quad (2.73b)$$

$$\Omega_i = v_i (E + \rho E_\rho) - \frac{\sigma_{im} v_m}{\rho} + T_\rho H_i \quad (2.73c)$$

$$\Upsilon = \frac{\|\mathbf{v}\|^2 + \mathbf{H} \cdot \mathbf{J} - E - \rho E_\rho}{\rho E_p} \quad (2.73d)$$

$$\tilde{\mathbf{H}} = E_{JJ} \quad (2.73e)$$

$$\mathbf{S}_p = \frac{1}{\theta_1 (\tau_1)} \begin{pmatrix} 0 \\ (\gamma - 1) \rho \|\psi\|_F^2 \\ 0 \\ 0 \\ 0 \\ -\psi_{11} \\ -\psi_{12} \\ -\psi_{13} \\ -\psi_{21} \\ -\psi_{22} \\ -\psi_{23} \\ -\psi_{31} \\ -\psi_{32} \\ -\psi_{33} \\ 0 \\ 0 \\ 0 \end{pmatrix} + \frac{1}{\theta_2 (\tau_2)} \begin{pmatrix} 0 \\ (\gamma - 1) \rho \|\mathbf{H}\|^2 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ -H_1 \\ -H_2 \\ -H_3 \end{pmatrix} \quad (2.82)$$

[illegible]

[illegible]

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Chapter 3

Slow Flow

3.1 Studying numerical smearing with slow flow past a barrier

A checkerboard pattern appears around the corner of the barrier, leading to a crash, using reflective boundary conditions (in velocity) for the barrier. Do we need a staggered grid?

Chapter 4

RGFM

The RGFM does nothing without a temperature fix when applied to the heat conduction test. The linearisation upon which it is based results in a stationary solution when $q_L = q_R$ and $\sigma_L = \sigma_R$ initially. Barton's RGFM is similar. Should q be fixed? Maybe use analytical solution to heat equation at $t = \Delta t$?

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