Modified Roe Flux Function for Perfectly Preconditioned Systems

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1 General Form

Consider a 2D linearized symmetrizable conservation law in the conservative form,

$$\mathbf{U}_t + \mathbf{A}\mathbf{U}_x + \mathbf{B}\mathbf{U}_y = 0. \tag{1}$$

This is transformed into a symmetric form for which a symmetric preconditioning matrix can be constructed, by a matrix \mathbf{T} ,

$$\mathbf{T}(\mathbf{U}_t + \mathbf{A} \mathbf{U}_x + \mathbf{B} \mathbf{U}_y) = 0 \tag{2}$$

$$\rightarrow \qquad \mathbf{U}_t^s + \mathbf{A}^s \mathbf{U}_x^s + \mathbf{B}^s \mathbf{U}_y^s = 0 \tag{3}$$

where the matrix $\mathbf{T} = \mathbf{Q}\mathbf{M}$ is the product of a rotation and a variable transformation matrices, and

$$\mathbf{A}^s = \mathbf{T}\mathbf{A}\mathbf{T}^{-1} \quad \mathbf{B}^s = \mathbf{T}\mathbf{B}\mathbf{T}^{-1}.$$
 (4)

The symmetric form may be written in the streamline coordinates (s, n),

$$\mathbf{U}_t^s + \mathbf{A}_{\parallel}^s \mathbf{U}_s^s + \mathbf{A}_{\perp}^s \mathbf{U}_n^s = 0 \tag{5}$$

where

$$\mathbf{A}_{\parallel}^{s} = \mathbf{A}^{s} \cos \theta + \mathbf{B}^{s} \sin \theta \quad \mathbf{A}_{\perp}^{s} = \mathbf{B}^{s} \cos \theta - \mathbf{A}^{s} \sin \theta \tag{6}$$

and θ is the flow angle.

Note that if \mathbf{P} denotes a symmetric preconditioner to be applied in the form

$$\mathbf{U}_t^s + \mathbf{P}(\mathbf{A}^s \mathbf{U}_x^s + \mathbf{B}^s \mathbf{U}_y^s) = 0, \tag{7}$$

then the corresponding preconditioner for the conservative form to be used in the form

$$\mathbf{U}_t + \mathbf{P}_c(\mathbf{A}\mathbf{U}_x + \mathbf{B}\mathbf{U}_y) = 0 \tag{8}$$

is given by

$$\mathbf{P}_c = \mathbf{T}^{-1} \mathbf{P} \mathbf{T}.$$
 (9)

In finite-volume methods, the Roe scheme is formulated using the Jacobian normal to a cell face, $\vec{\mathbf{n}} = (n_x, n_y) = (\cos \phi, \sin \phi)$,

$$\mathbf{A}_n = \mathbf{A}\,\cos\phi + \mathbf{B}\,\sin\phi,\tag{10}$$

and defines the numerical flux

$$\mathbf{F}_n = \frac{1}{2}(\mathbf{F}_R + \mathbf{F}_L) - \frac{1}{2}|\mathbf{A}_n|\Delta \mathbf{U}.$$
 (11)

The dissipation term must be formulated based on the preconditioned system, and the flux is modified as follows.

$$\mathbf{F}_{n} = \frac{1}{2} (\mathbf{F}_{R} + \mathbf{F}_{L}) - \frac{1}{2} \mathbf{P}_{c}^{-1} |\mathbf{P}_{c} \mathbf{A}_{n}| \Delta \mathbf{U}$$
(12)

where \mathbf{P}_c is a preconditioning matrix in the conservative variable. It is convenient to write the modified version using the matrices associated with the symmetric form. For this purpose, we manipulate the matrix $|\mathbf{P}_c \mathbf{A}_n|$ as follows.

$$|\mathbf{P}_c \mathbf{A}_n| = |\mathbf{T}^{-1} \mathbf{P} \mathbf{T} \mathbf{A}_n| \tag{13}$$

$$= |\mathbf{T}^{-1}\mathbf{PTA}_{n}(\mathbf{T})^{-1}\mathbf{T}|$$
(14)

$$= |\mathbf{T}^{-1}\mathbf{P}\mathbf{T}(\mathbf{A}\,\cos\phi + \mathbf{B}\,\sin\phi)\mathbf{T}^{-1}\mathbf{T}|$$
(15)

$$= |\mathbf{T}^{-1}\mathbf{P}(\mathbf{A}^{s}\cos\phi + \mathbf{B}^{s}\sin\phi)\mathbf{T}|$$
(16)

$$= \mathbf{T}^{-1} |\mathbf{P}(\mathbf{A}^s \cos \phi + \mathbf{B}^s \sin \phi)| \mathbf{T}$$
(17)

$$= \mathbf{T}^{-1} |\mathbf{P}(\mathbf{A}_{\parallel}^{s} \cos(\phi - \theta) + \mathbf{A}_{\perp}^{s} \sin(\phi - \theta))| \mathbf{T}.$$
(18)

In the case of 2D ideal MHD, this matrix is extremely complicated to write down analytically. We may therefore compute this, using some software that returns eigenvalues and eigenvectors numerically. However, we can avoid calling such a routine. Still numerically, but we can evaluate this in a simple way. This is possible if the preconditioner is exact: as it is derived from the theory based on the steady decomposition (no approximation is allowed).

2 Simplification

2.1 Hyperbolic Case

If the subproblem of the steady system is all hyperbolic, the preconditioner is given by

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$$\mathbf{P} = \sum a_k \mathbf{r}_k \mathbf{r}_k^T, \quad a_k = \frac{C}{|\mathbf{r}_k^T \mathbf{A} \mathbf{r}_k| \sqrt{1 + \lambda_k^2}}$$
(19)

Therefore, we have, from equation (18),

$$|\mathbf{P}_{c}\mathbf{A}_{n}| = \mathbf{T}^{-1} \left| \sum a_{k}\mathbf{r}_{k}\mathbf{r}_{k}^{T}(\mathbf{A}_{\parallel}^{s}\cos(\phi-\theta) + \mathbf{A}_{\perp}^{s}\sin(\phi-\theta)) \right| \mathbf{T}.$$
 (20)

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By definition,

$$|\mathbf{P}_{c}\mathbf{A}_{n}| = \mathbf{T}^{-1} \left| \sum a_{k}\mathbf{r}_{k}\mathbf{r}_{k}^{T}\mathbf{A}_{\parallel} \left\{ \cos(\phi - \theta) + \lambda_{k} \sin(\phi - \theta) \right\} \right| \mathbf{T}.$$
 (21)

We write this as

$$|\mathbf{P}_{c}\mathbf{A}_{n}| = \mathbf{T}^{-1} \left| \sum \lambda_{k}^{\star} \frac{\mathbf{r}_{k} \mathbf{r}_{k}^{T} \mathbf{A}_{\parallel}}{|\mathbf{r}_{k}^{T} \mathbf{A} \mathbf{r}_{k}|} \right| \mathbf{T}$$
(22)

where

$$\lambda_k^{\star} = \frac{C\left\{\cos(\phi - \theta) + \lambda_k \sin(\phi - \theta)\right\}}{\sqrt{1 + \lambda_k^2}}$$
(23)

which is exactly the wave speed normal to the cell face of the k-th component of the preconditioned system. Finally, because the matrix

$$\frac{\mathbf{r}_k \mathbf{r}_k^T \mathbf{A}_{\parallel}}{|\mathbf{r}_k^T \mathbf{A} \mathbf{r}_k|} \tag{24}$$

is the k-th orthonormal projection matrix, it has only one nonzero eigenvalue that is unity, and moreover it shares eigenvectors with $\mathbf{A}^{-1}\mathbf{B}$. Therefore, we finally obtain

$$|\mathbf{P}_{c}\mathbf{A}_{n}|\Delta\mathbf{U} = \sum |\lambda_{k}^{\star}| \,\alpha^{\star} \,\mathbf{r}_{k}^{\star}$$
⁽²⁵⁾

where

$$\alpha^{\star} = \ell_k^{\star} \Delta \mathbf{U} = \frac{\mathbf{r}_k^T \mathbf{A}_{\parallel}}{|\mathbf{r}_k^T \mathbf{A} \mathbf{r}_k|} \mathbf{T} \Delta \mathbf{U}$$
(26)

$$\mathbf{r}_k^{\star} = \mathbf{T}^{-1} \mathbf{r}_k. \tag{27}$$

This is an obvious result. The expression above is just straightforward wave decomposition of the preconditioned system *we designed*. The flux function can now be written as

$$\mathbf{F}_{n} = \frac{1}{2} (\mathbf{F}_{R} + \mathbf{F}_{L}) - \frac{1}{2} \mathbf{P}_{c}^{-1} \sum |\lambda_{k}^{\star}| \, \alpha^{\star} \, \mathbf{r}_{k}^{\star}$$
(28)

which does not require any numerical routines to compute eigenvalues and eigenvectors (although it may still be complicated to write down).

2.2 Elliptic Case

If there is an elliptic component, the preconditioner is given by

$$\mathbf{P} = a_e \mathbf{S} \mathbf{S}^T = a_e (\mathbf{r}_R \mathbf{r}_R^T + \mathbf{r}_I \mathbf{r}_I^T)$$
(29)

where $\mathbf{S} = [r_R, r_I]$ and

$$a_{e} = \frac{k_{e}C\sqrt{\frac{1}{2}(1+\lambda_{R}^{2}+\lambda_{I}^{2}-R)}}{|\lambda_{I}|}$$
(30)

$$R = \sqrt{(1 - \lambda_R^2 - \lambda_I^2)^2 + 4\lambda_R^2} \tag{31}$$

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$$k_e = \frac{1}{\sqrt{(\mathbf{r}_R^T \mathbf{A} \mathbf{r}_R)^2 + (\mathbf{r}_R^T \mathbf{A} \mathbf{r}_I)^2}}.$$
(32)

Therefore, we have, from equation (18),

$$|\mathbf{P}_{c}\mathbf{A}_{n}| = \mathbf{T}^{-1} \left| a_{e}\mathbf{S}\mathbf{S}^{T}(\mathbf{A}_{\parallel}^{s}\cos(\phi-\theta) + \mathbf{A}_{\perp}^{s}\sin(\phi-\theta)) \right| \mathbf{T}.$$
 (33)

By definition (real and imaginary parts of $\mathbf{r}^T (\mathbf{A}^s_{\perp} - \lambda \mathbf{A}^s_{\parallel}) = 0$), we have

$$\mathbf{S}^{T}\mathbf{A}_{\perp}^{s} = \begin{bmatrix} \lambda_{R} & -\lambda_{I} \\ \lambda_{I} & \lambda_{R} \end{bmatrix} \mathbf{S}^{T}\mathbf{A}_{\parallel}^{s}, \qquad (34)$$

and so we may write

$$|\mathbf{P}_{c}\mathbf{A}_{n}| = \mathbf{T}^{-1} \left| a_{e}\mathbf{S} \left\{ \cos(\phi - \theta) + \begin{bmatrix} \lambda_{R} & -\lambda_{I} \\ \lambda_{I} & \lambda_{R} \end{bmatrix} \sin(\phi - \theta) \right\} \mathbf{S}^{T}\mathbf{A}_{\parallel}^{s} \right| \mathbf{T}$$
(35)

which can be written also as

$$\begin{aligned} |\mathbf{P}_{c}\mathbf{A}_{n}| &= \mathbf{T}^{-1} \left| a_{e}\mathbf{S}(\mathbf{S}^{T}\mathbf{A}_{\parallel}^{s}\mathbf{S})^{-1}(\mathbf{S}^{T}\mathbf{A}_{\parallel}^{s}\mathbf{S}) \left\{ \cos(\phi-\theta) + \begin{bmatrix} \lambda_{R} & -\lambda_{I} \\ \lambda_{I} & \lambda_{R} \end{bmatrix} \sin(\phi-\theta) \right\} (\mathbf{S}^{T}\mathbf{A}_{\parallel}^{s}) \right| \mathbf{T} \\ &= \mathbf{T}^{-1} \left| a_{e}\mathbf{S}(\mathbf{S}^{T}\mathbf{A}_{\parallel}^{s}\mathbf{S})^{-1} \begin{bmatrix} \mathbf{r}_{R}^{T}\mathbf{A}\mathbf{r}_{R} & \mathbf{r}_{R}^{T}\mathbf{A}\mathbf{r}_{I} \\ \mathbf{r}_{I}^{T}\mathbf{A}\mathbf{r}_{R} & \mathbf{r}_{I}^{T}\mathbf{A}\mathbf{r}_{I} \end{bmatrix} \right\} \left\{ \cos(\phi-\theta) + \begin{bmatrix} \lambda_{R} & -\lambda_{I} \\ \lambda_{I} & \lambda_{R} \end{bmatrix} \sin(\phi-\theta) \right\} (\mathbf{S}^{T}\mathbf{A}_{\parallel}^{s}) \left| \mathbf{T} \\ &= \mathbf{T}^{-1} \left| a_{e}\mathbf{S}(\mathbf{S}^{T}\mathbf{A}_{\parallel}^{s}\mathbf{S})^{-1} \begin{bmatrix} k_{1} & k_{2} \\ k_{2} & -k_{1} \end{bmatrix} \right\} \left\{ \cos(\phi-\theta) + \begin{bmatrix} \lambda_{R} & -\lambda_{I} \\ \lambda_{I} & \lambda_{R} \end{bmatrix} \sin(\phi-\theta) \right\} (\mathbf{S}^{T}\mathbf{A}_{\parallel}^{s}) \left| \mathbf{T} \\ &= \mathbf{T}^{-1} \left| a_{e}\mathbf{S}(\mathbf{S}^{T}\mathbf{A}_{\parallel}^{s}\mathbf{S})^{-1}\mathbf{A}_{en}(\mathbf{S}^{T}\mathbf{A}_{\parallel}^{s}) \right| \mathbf{T} \end{aligned}$$
(36)
$$&= \mathbf{T}^{-1}\mathbf{S}(\mathbf{S}^{T}\mathbf{A}_{\parallel}^{s}\mathbf{S})^{-1} \left| a_{e}\mathbf{A}_{en} \right| \mathbf{S}^{T}\mathbf{A}_{\parallel}^{s}\mathbf{T} \end{aligned}$$

where \mathbf{A}_{en} is a 2x2 matrix whose eigenvalues are

$$\lambda_{en}^{\pm} = \pm a_e \sqrt{\left(k_1^2 + k_2^2\right) \left[\left\{\cos(\phi - \theta) + \lambda_R \sin(\phi - \theta)\right\}^2 + \lambda_I^2 \sin^2(\phi - \theta)\right]}$$
(38)

(See equation (29) in the draft of the AIAA 2003 paper) and the associated eigenvector is given by

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$$\mathbf{r}_{en}^{\pm} = \begin{bmatrix} \sin(\phi - \theta)k_1\lambda_I - \{\cos(\phi - \theta) + \lambda_R\sin(\phi - \theta)\}k_2\\ \sin(\phi - \theta)k_2\lambda_I + \{\cos(\phi - \theta) + \lambda_R\sin(\phi - \theta)\}k_1 - \lambda_{en} \end{bmatrix}.$$
 (39)

Finally, we obtain

$$|\mathbf{P}_{c}\mathbf{A}_{n}|\Delta\mathbf{U} = |\lambda_{en}^{+}|\,\alpha_{e}^{+}\,\mathbf{r}_{e}^{+} + |\lambda_{en}^{-}|\,\alpha_{e}^{-}\,\mathbf{r}_{e}^{-}$$
(40)

where

$$\alpha_e^{\pm} = \ell^{\pm} \Delta \mathbf{U} = (\mathbf{r}_{en}^{\pm})^T \mathbf{S}^T \mathbf{A}_{\parallel}^s \mathbf{T} \Delta \mathbf{U}$$
(41)

$$\mathbf{r}_{e}^{\pm} = \mathbf{T}^{-1} \mathbf{S} (\mathbf{S}^{T} \mathbf{A}_{\parallel}^{s} \mathbf{S})^{-1} \mathbf{r}_{en}^{\pm}.$$

$$\tag{42}$$

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Hence, if there are hyperbolic and elliptic components, the flux is given by

$$\mathbf{F}_{n} = \frac{1}{2} (\mathbf{F}_{R} + \mathbf{F}_{L}) - \frac{1}{2} \mathbf{P}_{c}^{-1} \left\{ \sum_{hyperbolic} |\lambda_{k}^{\star}| \, \alpha^{\star} \, \mathbf{r}_{k}^{\star} + \sum_{elliptic} \left(|\lambda_{en}^{+}| \, \alpha_{e}^{+} \, \mathbf{r}_{e}^{+} + |\lambda_{en}^{-}| \, \alpha_{e}^{-} \, \mathbf{r}_{e}^{-} \right) \right\}.$$

$$(43)$$

Note that by orthogonality of the subspaces, we have been able to consider elliptic parts independently.

3 Euler Equations

3.1 Supersonic Case

In the supersonic case, we obtain

$$\mathbf{F}_{n} = \frac{1}{2} (\mathbf{F}_{R} + \mathbf{F}_{L}) - \frac{1}{2} \mathbf{P}_{c}^{-1} \sum_{k=1}^{4} |\lambda_{k}^{\star}| \, \alpha^{\star} \, \mathbf{r}_{k}^{\star}$$

$$\tag{44}$$

where

$$\lambda_1^{\star} = \cos(\phi - \theta)M \tag{45}$$

$$\lambda_2^{\star} = \cos(\phi - \theta)M \tag{46}$$

$$\lambda_3^{\star} = \cos(\phi - \theta)\sqrt{M^2 - 1 + \sin(\phi - \theta)}$$
(47)

$$\lambda_4^* = \cos(\phi - \theta)\sqrt{M^2 - 1 - \sin(\phi - \theta)}$$
(48)

$$\alpha_1^{\star} = \Delta \rho - \frac{\Delta p}{c^2} \tag{49}$$

$$\alpha_2^{\star} = \frac{\rho q \Delta q + \Delta p}{q} \tag{50}$$

$$\alpha_3^{\star} = \frac{1}{2} \left[\rho q^2 \Delta \theta + \sqrt{M^2 - 1} \Delta p \right] \tag{51}$$

$$\alpha_4^{\star} = \frac{1}{2} \left[\rho q^2 \Delta \theta - \sqrt{M^2 - 1} \Delta p \right]$$
(52)

$$\mathbf{r}_{1}^{\star} = \begin{bmatrix} 1, u, v, q^{2}/2 \end{bmatrix}^{T} \tag{53}$$

$$\mathbf{r}_{2}^{\star} = \begin{bmatrix} 0, \cos\theta, \sin\theta, q \end{bmatrix}^{T}$$
(54)

$$\mathbf{r}_{3}^{\star} = \left[\frac{1}{c^{2}\sqrt{M^{2}-1}}, \frac{\sin\theta + \sqrt{M^{2}-1}\cos\theta}{q}, \frac{\cos\theta + \sqrt{M^{2}-1}\sin\theta}{q}, \frac{-1}{\sqrt{M^{2}-1}}\left(\frac{M^{2}}{2} + \frac{\gamma-2}{\gamma-1}\right)\right]^{T}_{5}$$
$$\mathbf{r}_{4}^{\star} = \left[\frac{-1}{2\sqrt{M^{2}-1}}, \frac{\sin\theta - \sqrt{M^{2}-1}\cos\theta}{q}, \frac{\cos\theta - \sqrt{M^{2}-1}\sin\theta}{q}, \frac{1}{\sqrt{M^{2}-1}}\left(\frac{M^{2}}{2} + \frac{\gamma-2}{\gamma-1}\right)\right]^{T}_{5}_{6}\right]$$

$$\mathbf{r}_{4}^{\star} = \left[\frac{-1}{c^{2}\sqrt{M^{2}-1}}, \frac{\sin b - \sqrt{M^{2}-1}\cos b}{q}, \frac{\cos b - \sqrt{M^{2}-1}\sin b}{q}, \frac{1}{\sqrt{M^{2}-1}}\left(\frac{M}{2} + \frac{\gamma - 2}{\gamma - 1}\right)\right] \mathbf{f}_{4}^{\star}$$

Note that not to mention the case M = 1 some expressions are singular at q = 0.

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3.2 Subsonic Case

$$\mathbf{F}_{n} = \frac{1}{2} (\mathbf{F}_{R} + \mathbf{F}_{L}) - \frac{1}{2} \mathbf{P}_{c}^{-1} \left\{ \sum_{k=1}^{2} |\lambda_{k}^{\star}| \, \alpha^{\star} \, \mathbf{r}_{k}^{\star} + \left(|\lambda_{en}^{+}| \, \alpha_{e}^{+} \, \mathbf{r}_{e}^{+} + |\lambda_{en}^{-}| \, \alpha_{e}^{-} \, \mathbf{r}_{e}^{-} \right) \right\}$$
(57)

where the hyperbolic part is the same as in the supersonic case, and

$$z = \sqrt{(1 - M^2)\cos^2(\phi - \theta) + \sin^2(\phi - \theta)}$$
 (58)

$$\lambda_{en}^+ = Mz \tag{59}$$

$$\lambda_{en}^{-} = -Mz \tag{60}$$

$$\alpha_{e}^{+} = \frac{M\sqrt{1-M^{2}}}{\rho} \left[\sin(\phi-\theta)(1-M^{2})\Delta p - \left\{ z + (1-M^{2})\cos(\phi-\theta) \right\} \rho q^{2}\Delta\theta \right] (61)$$

$$\alpha_e^- = \frac{M\sqrt{1-M^2}}{\rho} \left[\sin(\phi-\theta)(1-M^2)\Delta p + \left\{z - (1-M^2)\cos(\phi-\theta)\right\}\rho q^2\Delta\theta\right] (62)$$

$$\mathbf{r}_{en}^{+} = \begin{bmatrix} \frac{\rho M \sin(\phi - \theta)}{\sqrt{1 - M^2}} \\ \frac{\rho}{M\sqrt{1 - M^2}} \left\{ (1 - M^2) (v \cos(\phi - \theta) - u \sin(\phi - \theta)) + vz \right\} \\ \frac{-\rho}{M\sqrt{1 - M^2}} \left\{ (1 - M^2) (u \cos(\phi - \theta) + v \sin(\phi - \theta)) + uz \right\} \\ \frac{\rho c^2 M \sin(\phi - \theta)}{\sqrt{1 - M^2}} \left(\frac{M^2}{2} - \frac{\gamma - 2}{\gamma - 1} \right) \end{bmatrix}$$
(63)
$$\mathbf{r}_{en}^{-} = \begin{bmatrix} \frac{\rho M \sin(\phi - \theta)}{\sqrt{1 - M^2}} \\ \frac{\rho}{M\sqrt{1 - M^2}} \left\{ (1 - M^2) (v \cos(\phi - \theta) - u \sin(\phi - \theta)) - vz \right\} \\ \frac{-\rho}{M\sqrt{1 - M^2}} \left\{ (1 - M^2) (u \cos(\phi - \theta) + v \sin(\phi - \theta)) - uz \right\} \\ \frac{\rho c^2 M \sin(\phi - \theta)}{\sqrt{1 - M^2}} \left(\frac{M^2}{2} - \frac{\gamma - 2}{\gamma - 1} \right) \end{bmatrix}$$
(64)

Again the eigenvectors are singular at
$$M = 0$$
.

4 Remarks

For the Euler equations, the modified Roe scheme is relatively simple. It is desired that the singularity at M = 0 be removed. Although the step from (36) to (37) has not been proved mathematically, it is found to be true for the Euler equations.

As mentioned before, this modification is valid only for exact preconditioners which may be constructed numerically. For approximate preconditioners, we need to compute eigenvalues and eigenvectors numerically at every face which is very expensive. For this reason, it may turn out that numerically constructed exact preconditioners are more economical than approximate ones.

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