ACURA: Acoustics Convection Upstream Resolution Algorithm

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A novel multi-dimensional upwind bias formulation is presented. Designed to solve accurately the Euler and Navier-Stokes conservation-law systems on arbitrary grids, this new formulation is developed within the continuous conservation-law systems ahead of any discretization in space and time. This formulation utilizes shock-jump surface integrals, which emerge within integral weak statements for these conservation laws. The mean value theorem is then applied to express these surface integrals in terms of differences of gradients of differentiable entropy solutions. In the continuum, this process yields shock-capturing entropy weak statements with embedded upwind bias that are consistent with the theory of characteristics. These entropy weak statements are then discretized in space through a Galerkin finite element method, an inherently centered dissipation-free discretization. This automatically generates an intrinsically multi-dimensional upstreamed discrete system on any grid without the need for any further upwinding within the discrete equations. The computational solutions crisply capture shocks and reflect available exact solutions.

I. Introduction

Computational Fluid Dynamics (CFD) is routinely applied to support aerospace designs [1, 2]. As aerospace structural analyses utilize the finite element method, it is also beneficial to expand robust CFD finite element formulations, as these formulations readily support fluid-structure interaction studies. Critical to the success of CFD applications in the aerospace industry, is the reliability of the attendant algorithms, most of which depend on upwind schemes that have incorporated the various flux vector splittings developed over the past four decades [3–7]. Emerging from one-dimensional formulations, these schemes have been generalized to multi-dimensional flows by applying a flux vector splitting along each Cartesian axis. These schemes share the foundational concept [6–9] that the inviscid flux vector should be discretized with a bias in the direction from which information arrives at each discretization point, reflecting the theory of characteristics.

Provided the eigenvalues of the Jacobian matrix of the flux vector along a direction have the same sign, an upwind discretization along that direction typically yields a stable discrete scheme. When the eigenvalues have mixed signs, the flux vector is split into components with uniform-sign Jacobian eigenvalues. These components are then discretized in opposite upwind directions with the expectation that the resulting discretization will be stable. In this connection, the partial differential equations that correspond to this opposite-direction upwind discretization always incorporate an upwind-signature matrix [6]. This matrix consists of the difference of the positive- and negative-eigenvalue flux vector Jacobian matrices. Hence, the intrinsic assumption for the stability of all flux vector splitting algorithms is that the eigenvalues of the upwind-signature matrix have become positive, thereby generating dissipation.

However, it cannot be mathematically guaranteed [10] that an upwind-signature matrix will always have positive eigenvalues, as examples exist of matrices that exhibit mixed-sign eigenvalues, which may be complex, even though such matrices result from the difference of matrices respectively with strictly positive and strictly negative eigenvalues. Accordingly, the need for positive eigenvalues for the upwind-signature matrix provides an additional mathematical

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criterion for developing novel upwind algorithms as well as analyzing existing ones. The strictest realization of this criterion is that all the eigenvalues of the upwind-signature matrix be real, not complex conjugate, to promote non-oscillatory solutions, and positive for all geometric directions emanating from any flow-field point.

Many successful flux vector splittings satisfy this criterion to some degree. For the Euler and Navier-Stokes equations, this is arguably the case for those splittings that are based on the physical convection and acoustics wave propagation modes [11, 12]. A precursor prototypical splitting of this kind [13] separated the convection divergence and pressure gradient within the inviscid flux vector from each other. It was then followed by the popular advection upstream splitting method [14, 15] and its sequels, e.g. [16–19], which introduced a variety of fixes to cure the challenges emerged during applications of the method to increasingly complex flows and also tackle slow convergence rates to steady state for low-speed subsonic flows. Developed at the discrete level, the method employs heuristic Mach number splittings, pressure partitions, and numerical speed of sound approximations.

A theoretically separate approach for calculating flow fields with embedded shocks involves the solution of parabolically perturbed Euler conservation-law systems [20] for compressible flows. The parabolic perturbation in these systems embeds within the physical conservation laws a non-linear dissipation matrix that leads to solutions satisfying an entropy condition and approaching a shocked flow field, as the magnitude of the perturbation becomes vanishingly small. This approach resembles traditional artificial viscosity methods [4] that are introduced as mathematical devices to generate a stable solution.

In this paper, these traditional methods and upwind flux-vector splitting algorithms are unified. This is accomplished by constructing a multi-dimensional parabolic perturbation that yields an upwind-biased integral weak statement for the conservation-law convection and pressure fluxes. This parabolic perturbation is entirely developed in the continuum, at the partial differential equation level [22–24], before any discretization in space and time. This feature is particularly important for generating consistent upwind discretizations on arbitrary grids. This approach contributes a new theoretical foundation for developing multi-dimensional shock-capturing weak statements.

Rather than appearing as an ad-hoc addition, this parabolic perturbation resolves shock jumps, which naturally appear in integral weak statements of the conservation laws. This resolution applies the multi-dimensional Rankine-Hugoniot shock conditions [21] and decomposes the shock jumps in the Euler fluxes into convection and pressure flux components. The jumps in these components are then modelled through the mean-value theorem, via differences of gradients of differentiable entropy solutions. By construction, the resulting parabolic perturbation remains consistent with the theory of characteristics. Expressed in terms of intrinsically multi-dimensional fluxes, this parabolic perturbation yields an upwind-signature matrix that consists of a difference of positive- and negative-eigenvalue flux vector Jacobian matrices. The perturbation remains continuous for all subsonic and supersonic Mach parameters and induces an upwinding bias on the divergence of the entire flux vector, for supersonic flows. The parameters of the perturbation are then constrained by imposing the previously mentioned strict eigenvalue-positivity criterion on the upwind-signature matrix. Accordingly, the eigenvalues of the upwind-signature matrix remain real and positive along all geometric directions emanating from any flow field point.

This study emphasizes shock jump conditions because these conditions naturally emerge in surface integrals within a weak statement formulation of the Euler equations of gas dynamics. This emphasis also shows why instabilities can develop within classical Galerkin weak statements. This is because these classical formulations have implicitly discarded these surface integrals [25]. The dissipative parabolic perturbation obtained from retaining and modelling these terms through entropy-solution gradients naturally stabilizes the Galerkin weak statements. In this study, these integral statements are named entropy weak statements. Since it utilizes acoustic and convection components, the overall algorithm is termed the Acoustics Convection Upstream Resolution Algorithm (ACURA). A forthcoming journal article will provide detailed derivations.

A Galerkin finite element discretization [26–29] of the entropy weak statement, which produces a central dissipation-free discretization, then automatically generates an intrinsically multi-dimensional upstreamed discrete system without the need for further upwinding within the discretized equations. The theoretical and numerical results show that the parabolic perturbation consistently remains dissipative for all Mach numbers and geometric directions and the overall algorithm crisply captures shocks within solutions that reflect available exact solutions.

II. Governing System

The developments in this study are presented for both the quasi one-dimensional and multi-dimensional Euler gas dynamics system, expressed as

$$\frac{\partial q}{\partial t} + \frac{\partial f(q)}{\partial x} + s(q, x) = 0, \quad \frac{\partial q}{\partial t} + \frac{\partial f_j(q)}{\partial x_j} = 0, \quad 1 \leq j \leq n \quad (1)$$

with $n = 2, 3$ for two- and three-dimensional flows; implied summation on twice repeated indices is used throughout this paper. The source term $s(q, x)$ within the one-dimensional system partially models multi-dimensional effects through the varying cross-sectional area A of a flow channel. This source term separates the quasi one-dimensional and multi-dimensional systems. With a decomposition of the total flux into convection and pressure components as $f(q) \equiv f^q(q) + f^p(q)$, the various arrays in the quasi one-dimensional system are defined as

$$q \equiv \begin{pmatrix} \rho \\ m \\ E \end{pmatrix}, \quad f^q(q) \equiv \begin{pmatrix} m \\ \frac{m^2}{\rho} \\ \frac{m}{\rho}(E + p) \end{pmatrix}, \quad f^p(q) \equiv \begin{pmatrix} 0 \\ p \\ 0 \end{pmatrix}, \quad s \equiv - \begin{pmatrix} \frac{m}{A} \frac{\partial A}{\partial x} \\ \frac{m^2}{\rho A} \frac{\partial A}{\partial x} \\ \frac{m(E + p)}{\rho A} \frac{\partial A}{\partial x} \end{pmatrix}. \quad (2)$$

With $f_j(q) \equiv f_j^q(q) + f_j^p(q)$, the corresponding arrays for multi-dimensional flows are expressed as

$$q \equiv \begin{pmatrix} \rho \\ \mathbf{m} \\ E \end{pmatrix}, \quad f_j^q(q) \equiv \begin{pmatrix} m_j \\ \frac{m_j}{\rho} \mathbf{m} \\ \frac{m_j}{\rho}(E + p) \end{pmatrix}, \quad f_j^p(q) \equiv \begin{pmatrix} 0 \\ p \delta_j \\ 0 \end{pmatrix}. \quad (3)$$

The array $f_j^q(q)$ may be termed the convection array and $f_j^p(q)$ the acoustics array. In these arrays, $\rho, \mathbf{m}, E$ respectively denote the flow density and volume-specific linear momentum and total energy. The flow velocity then results as $\mathbf{u} = \mathbf{m}/\rho$. Additionally, δ_j for each j indicates the n components of the Kronecker delta and p is the static pressure. To close the system, the pressure is expressed through the perfect-gas equation of state $p = (\gamma - 1)(E - \|\mathbf{m}\|^2/2\rho^2)$, where $\gamma > 1$ is the constant specific-heat ratio.

III. Shock and Rankine-Hugoniot Jump Conditions

As this paper utilizes the multi-dimensional Rankine-Hugoniot jump conditions, they are summarized in this section. These jump conditions connect the jump in the state variable q with the jump in the flux components $f_j(q)$ across shocks that may exist for weak solutions of the partial differential equation system (1).

These multi-dimensional jump conditions have been stated in [30] and proven for the one-dimensional case. Other authors have similarly provided proofs for one-dimensional flows [21, 24]. For one- and multi-dimensional flows, these conditions may be expressed as

$$(q^+ - q^-)v^s = (f^+ - f^-), \quad (q^+ - q^-)\mathbf{v}^s \cdot \mathbf{n}^s = (f_j^+ - f_j^-)n_j^s \quad (4)$$

where $\mathbf{n}^s$ denotes a unit vector that is perpendicular to a shock front within the spatial domain of (1) and $v^s \equiv \mathbf{v}^s \cdot \mathbf{n}^s \geq 0$ corresponds to the shock speed.

These expressions become the gas dynamics Rankine-Hugoniot jump conditions for q and f_j the state and flux vectors in (2)-(3). In this case $\mathbf{v}^s$ denotes the propagation velocity of the shock into the region of higher pressure across the shock. For an ideal gas, the corresponding speed v^s along $\mathbf{n}^s$ is expressed in terms of the flow speed u^- approaching the shock, the corresponding sound speed c^- , and the pressure ratio p^+/p^- across the shock [21]. The resulting expression is

$$v^s = u^- + \bar{c}, \quad \bar{c} \equiv c^- \sqrt{1 + \frac{\gamma + 1}{\gamma} \left(\frac{p^+}{p^-} - 1 \right)}. \quad (5)$$

For the case of a vanishing flow speed u^- , as may be the case during the initial instants subsequent to the rupture of a diaphragm separating two chambers with different pressures, e.g. a shock-tube flow, the shock speed v^s approaches the sound speed $\bar{c}$. In these conditions, the jump in the pressure flux $f_j^p(q)$ approaches the jump in q multiplied by the sound speed $\bar{c}$. This observation leads to a robust resolution of the variation of the pressure flux within low-speed flows region. A similar resolution is applied to model the propagation of acoustic waves in any cross-flow direction. Any jumps in the total flux $f_j(q)$ are then cast through gradients of differentiable fluxes of entropy solutions modeling the solution of system (1).

IV. Modelling of Jump Conditions in Weak Statements

Within an integral weak statement, the presence of a shock-induced discontinuity generates a jump-condition term, which is implicitly discarded in many traditional weak statement formulations, e.g. Galerkin finite element methods [25]. The elimination of this term induces an instability of classical finite-element and central-difference spatial discretizations. In this paper, a stabilization contribution is thus developed by retaining and modelling this jump-condition term that naturally emerges from an integration-by-parts of the continuous equations.

This term is derived by multiplying (1) by a differentiable test function ϕ with compact support within the spatial domain Ω of (1) and integrating by parts the resulting expression in Ω . Let $\Omega \equiv \Omega_I \cup \Omega_{II}$, with Ω_I and Ω_{II} denoting regions of space that are separated by a shock $\mathcal{S}$ and within each of which q is a classical solution of (1).

For quasi one-dimensional flows, with $\Omega_I \equiv [-\varepsilon, 0)$, $\Omega_{II} \equiv (0, \varepsilon]$, and $\mathcal{S}$ at $x = 0$, this transformation yields the following integral statements

$$\int_{\Omega_I} \phi \left(\frac{\partial q}{\partial t} + \frac{\partial f(q)}{\partial x} + s(q, x) \right) dx = \int_{\Omega_I} \left(\phi \frac{\partial q}{\partial t} - \frac{\partial \phi}{\partial x} f(q) + \phi s(q, x) \right) dx + \left[\phi f^-(q) \right]_{-\varepsilon}^{0_-} \quad (6)$$

$$\int_{\Omega_{II}} \phi \left(\frac{\partial q}{\partial t} + \frac{\partial f(q)}{\partial x} + s(q, x) \right) dx = \int_{\Omega_{II}} \left(\phi \frac{\partial q}{\partial t} - \frac{\partial \phi}{\partial x} f(q) + \phi s(q, x) \right) dx + \left[\phi f^+(q) \right]_{0_+}^{\varepsilon} \quad (7)$$

Summing these two integrals and recognizing that, on either side of the shock, the flow field is a classical solution of (1) generate

$$\int_{\Omega} \left(\phi \frac{\partial q}{\partial t} - \frac{\partial \phi}{\partial x} f(q) + \phi s(q, x) \right) dx - \phi(0) \left[f^+ - f^- \right] = 0 \quad (8)$$

which naturally includes a shock-jump term. The corresponding results for multi-dimensional flows are as follows:

$$\int_{\Omega_I} \phi \left(\frac{\partial q}{\partial t} + \frac{\partial f_j(q)}{\partial x_j} \right) d\Omega = \int_{\Omega_I} \left(\phi \frac{\partial q}{\partial t} - \frac{\partial \phi}{\partial x_j} f_j(q) \right) d\Omega + \oint_{\partial\Omega_I} \phi f_j^-(q) n_j^I d\Gamma \quad (9)$$

$$\int_{\Omega_{II}} \phi \left(\frac{\partial q}{\partial t} + \frac{\partial f_j(q)}{\partial x_j} \right) d\Omega = \int_{\Omega_{II}} \left(\phi \frac{\partial q}{\partial t} - \frac{\partial \phi}{\partial x_j} f_j(q) \right) d\Omega + \oint_{\partial\Omega_{II}} \phi f_j^+(q) n_j^{II} d\Gamma. \quad (10)$$

Summing these two integrals and recognizing again that, on either side of the shock, the flow field is a classical solution of (1) yield

$$\int_{\Omega} \left(\phi \frac{\partial q}{\partial t} - \frac{\partial \phi}{\partial x_j} f_j(q) \right) d\Omega - \int_{\mathcal{S}} \phi \left[f_j^+ - f_j^- \right] n_j^s d\Gamma = 0 \quad (11)$$

which includes a shock-jump term within a surface integral over the shock surface $\mathcal{S}$. In this result, $n_j^s \equiv n_j^I = -n_j^{II}$ points into the region of f_j^+ .

A discretization of (8) or (11) without the shock-jump terms typically yields traditional Galerkin finite element and centered differencing algorithms, which are well known to be inadequate for convection dominated flow, unless stabilizing mechanisms are added to these algorithms [25]. Expressions (8) and (11) with the shock-jump terms may be interpreted as a prototypical statement for Discontinuous Galerkin (DG) methods [32], which require numerical fluxes within discrete models of the shock jump terms in (8) and (11). Incidentally, the considerations in the next section identify one- and multi-dimensional fluxes that may be used within DG methods. Rather than modelling the jump terms in (8) and (11) within a discrete algorithm through either a Riemann solver, numerical fluxes, or other discrete stabilizing mechanisms, in the present algorithm the one- and multi-dimensional shock-jump terms are modelled directly at the partial differential equation level before any spatial discretization.

V. Synopsis of the Algorithm

This section provides a condensed overview of the phases that lead to a multi-dimensional Acoustics-Convection Upstream Resolution Algorithm (ACURA) for the conservation law system of gas dynamics. Complete details on the methodology and derivation of the algorithm and its technical components will be provided in a forthcoming article.

As stated in Section IV, a chief feature of ACURA is that it is an inherently multi-dimensional upwind formulation developed on the continuous level, where operations such as the chain rule or integration-by-parts remain valid. The terms that necessitate careful treatment are the flux jump terms in (8), for one spatial dimension, or (11), for multiple spatial dimensions. These terms arise naturally in the context of Rankine-Hugoniot conditions for shock formation / propagation. From a practical standpoint, such flux discontinuities are commonplace in the context of discontinuous Galerkin (DG) methods where such jumps are resolved with a symmetric numerical flux function, e.g., that of Harten, Lax, and van Leer [31]. For numerical fluxes of this type, dissipation proportional to the full eigenstructure of the flux Jacobian is added locally at each interface.

It is at this stage where the ACURA methodology differs from DG methods. Instead of being developed as two-point numerical flux functions, which typically belong to the broader class of so-called Riemann solvers, these flux jump conditions are modelled in terms of an entropy regularisation. In doing so, the solution quantities of interest q are replaced with an entropy solution q^ε . As a result, this approach intrinsically induces global dissipation that is controlled by the dissipation variable $\psi\|\Delta\mathcal{E}\|$, which is taken to be small. In the limit of vanishing dissipation we recover the original weak solution q from the entropy solution under consideration. Working on the continuous level, the entropy solution q^ε is differentiable in the classical sense on either side of a discontinuity. This facilitates the development of ACURA.

The physical flux vectors are evaluated in terms of an entropy solution, i.e., $f^\varepsilon \equiv f(q^\varepsilon)$ in one dimension or in each component $f_j^\varepsilon \equiv f_j(q^\varepsilon)$ in multiple dimensions. From there, the flux jumps evaluated at an entropy solution are carefully modelled, taking care to respect the positive, negative, or mixed sign-signature of the flux Jacobian on either side of the shock. This is crucial to ensure that dissipation is correctly induced in the shocked region and anti-dissipation is avoided. This helps to ensure that the modelled flux jumps remain stable as, for example, unphysical transfer of kinetic and inner energies are expressly forbidden.

The flux jumps evaluated at an entropy solution within a shocked region are then reinterpreted into the form of flux gradients, via the mean value theorem. This is done in order to generate a dissipative parabolic perturbation near the shock assumed to be present within a region of width $[-\varepsilon, \varepsilon]$. We note here that as the dissipation control $\psi\|\Delta\mathcal{E}\| \rightarrow 0$, the width of this shock region shrinks until one recovers the true flux discontinuity present in the purely hyperbolic form of the PDE system. The analysis and estimation of these slopes is performed in a general, multi-dimensional fashion.

With the flux slope estimates established, the next phase in the derivation uses a Taylor expansion to rewrite the test function ϕ on either side of an interface. Here, the fact that the test functions are smooth with compact support is repeatedly used to simplify terms. Such expansions, which are truncated at terms proportional to $\mathcal{O}(\varepsilon^2)$, generate second order flux derivative terms along the interfaces. This explicitly highlights the mixed hyperbolic-parabolic character of the entropy regularised PDE system. Furthermore, these derivations grant us a greater degree of control as to the impact of these regularising parabolic expressions, through the $\psi\|\Delta\mathcal{E}\|$ term.

A particular strength of ACURA is its ability to capture and model flow configurations at any Mach number across the sub-, trans- and supersonic regimes. This property and handling of the Mach number is explicitly built into ACURA by subdividing the estimated flux slopes, and their corresponding Jacobian matrix contributions, into acoustic (involving pressure) and convective (involving momenta) components, along the streamline and in the cross-flow plane. This corresponds to subdividing the flux components as $f_j(q^\varepsilon) = f_j^q(q^\varepsilon) + f_j^p(q^\varepsilon)$ and is done to avoid degeneracies and other difficulties that one can encounter, particularly for low speed, subsonic flows [17]. Effectively, this amounts to a splitting of the flux Jacobian and introduces three partition parameters: α and α^N for the acoustics term, respectively in the streamline direction and on the cross-flow plane, and δ for the pressure gradient. Significantly, α , α^N , and δ smoothly depend on the Mach number of the flow configuration. More details on these partition parameters and how they influence the size of the eigenvalues, across a range of sub-, trans- and supersonic Mach numbers, in the multi-dimensional flux Jacobian are provided in Section VI.

In non-discrete integral weak statement form, the complete ACURA formulation is expressed as

$$\int_{\Omega} \left(\phi \frac{\partial q^\varepsilon}{\partial t} + \left(\phi \alpha \frac{\partial f_j^p}{\partial x_j} + \frac{\partial \phi}{\partial x_i} \psi \|\Delta\mathcal{E}\| \bar{c} \left(\alpha a_i a_j + \alpha^N \left(a_i^{N_1} a_j^{N_1} + a_i^{N_2} a_j^{N_2} \right) \right) \frac{\partial q^\varepsilon}{\partial x_j} \right) \right) d\Omega +$$

$$\begin{aligned}
& \int_{\Omega} \left(\phi - \psi \|\Delta \mathbf{e}\| a_i \frac{\partial \phi}{\partial x_i} \right) \left(\frac{(1 - \alpha - \delta)}{2} \frac{\partial f_j^{p\epsilon}}{\partial x_j} \right) d\Omega + \\
& \int_{\Omega} \left(\phi + \psi \|\Delta \mathbf{e}\| a_i \frac{\partial \phi}{\partial x_i} \right) \left(\frac{\partial f_j^{q\epsilon}}{\partial x_j} + \frac{(1 - \alpha + \delta)}{2} \frac{\partial f_j^{p\epsilon}}{\partial x_j} \right) d\Omega - \\
& \oint_{\partial\Omega} \phi \left(f_j n_j + \psi \|\Delta \mathbf{e}\| \bar{c} \left(n_i \alpha a_i a_j + \alpha^N \left(n_i a_i^{N_1} a_j^{N_1} + n_i a_i^{N_2} a_j^{N_2} \right) \right) \frac{\partial q^\epsilon}{\partial x_j} \right) d\Gamma - \\
& \oint_{\partial\Omega} \phi \left(\psi \|\Delta \mathbf{e}\| \left(n_i a_i \frac{\partial f_j^{q\epsilon}}{\partial x_j} + n_i a_i \delta \frac{\partial f_j^{p\epsilon}}{\partial x_j} \right) \right) d\Gamma = 0
\end{aligned} \tag{12}$$

In this statement, q^ϵ is a differential entropy solution that models and approaches a weak solution of (1), with $f_j^{q\epsilon}$ and $f_j^{p\epsilon}$ denoting flux components evaluated at q^ϵ . The ψ term denotes a shock controller that remains constant in a neighborhood of a shock, with $0 < \psi \leq 1$ and $\psi = 1$ for non-weak shocks. The reference speed of sound $\bar{c}$ corresponds to the expression in (5). For $\|\Delta \mathbf{e}\| = 0$, these statements revert to the classical results without shock terms. The $\|\Delta \mathbf{e}\|$ term is a positive length scale, uniquely identified within a discrete statement with the radius of an inscribed ellipse or ellipsoid within each computational cell. As $\|\Delta \mathbf{e}\|$ is thus set equal to a computational cell measure, q is accurately rendered by q^ϵ as a solution that models the actual shock jumps and leads to a physically admissible solution that satisfies the entropy condition through the parabolic perturbation.

The subscripted terms, $\{a_i\}$, $\{a_i^{N_1}\}$, and $\{a_i^{N_2}\}$ denote the components of three mutually orthogonal unit vectors. The first points in the streamline direction, as it provides the unit vector of the local flow velocity $\mathbf{u}$; the other two unit vectors point in any two directions in the cross-flow plane. Together with α^N , they control cross-flow dissipation. Also, $\{n_j\}$ denote the components of the outward pointing normal unit vector on the $\partial\Omega$ boundary of Ω .

The parabolic-perturbation modelling of the jump conditions produces domain integrals with test function expressions that are biased in the upstream and downstream directions. This induces an upstream bias in the divergence of the convection flux and a portion of the pressure gradient and a downstream bias of the balance of the pressure gradient. These biases correspond to an intrinsically multi-dimensional non discrete upwind fluxes, which may also be used in DG methods. As the local Mach number increases and upstream wave propagation weakens, an increasingly smaller portion of the pressure gradient is downwinded while a greater portion is upwinded. As shown in Section VI, $\alpha \rightarrow 0$ and $\delta \rightarrow 1$, for flows that approach the supersonic state. In this flow regime, the upstream bias in the test function applies to the entire divergence of the flux vector, as expected, and ACURA induces an upwinding on the entire multi-dimensional flux divergence.

The surface integrals in (12) provide an optimal venue to enforce non-Dirichlet boundary conditions effectively. At solid walls, for instance, where a flow-tangency boundary condition is needed for inviscid flow calculations, this boundary condition is expressed through the dot products $u_i n_i = 0$ and $a_i n_i = 0$, which are directly inserted in the corresponding expressions in the surface integrals to enforce this boundary condition.

The weak statement (12) is then discretized in space by way of a traditional Galerkin finite element method [25–29], with test and trial functions selected from the same function space. This process produces a central discretization of the entropy weak statement, which automatically generates an upstream-bias discrete statement without the need for further upwind corrections at the discrete level. At this level, within each computational cells, ψ , $\bar{c}$, α , α^N , δ , $\{a_i\}$, $\{a_i^{N_1}\}$, and $\{a_i^{N_2}\}$ are set equal to their respective centroidal values. The finite-element generated system of coupled non-linear ordinary differential equations are then numerically integrated in time through an unconditionally non-linearly (algebraically) stable and rapidly converging implicit 2nd-order Runge-Kutta procedure [33–35]. The corresponding sequence of banded linear systems is then efficiently solved through FGMRES [36, 37], which is a GMRES procedure [38] that uses GMRES itself to precondition the systems.

VI. ACURA Eigenvalue Analysis

Integrating (12) by parts on the $\frac{\partial \phi}{\partial x_i}$ terms and moving the result to the right-hand side, lead to the ACURA parabolic-perturbation integral

$$\mathcal{P} \equiv \int_{\Omega} \phi \frac{\partial}{\partial x_i} \left[\psi \|\Delta \mathbf{e}\| \left(\bar{c} \left(\alpha a_i a_j + \alpha^N \left(a_i^{N_1} a_j^{N_1} + a_i^{N_2} a_j^{N_2} \right) \right) \frac{\partial q^\epsilon}{\partial x_j} + a_i \frac{\partial f_j^{q\epsilon}}{\partial x_j} + a_i \delta \frac{\partial f_j^{p\epsilon}}{\partial x_j} \right) \right] d\Omega. \tag{13}$$

When q^ε is expressed in the travelling plane-wave form $q^\varepsilon = q^\varepsilon(\mathbf{x} \cdot \mathbf{n} - \lambda t)$, the partial derivatives with respect to x_j of the flux vectors $f_j^{q^\varepsilon}$ and $f_j^{p^\varepsilon}$ are calculated through the chain rule, and the resulting Jacobians of these vectors, as well as all the other terms between brackets, are frozen within subdomains of Ω , the following stability matrices are identified within (13) for one- and multi-dimensional flows

$$\mathcal{A} \equiv \bar{c}\alpha \mathcal{I} + \frac{\partial f_j^{q^\varepsilon}}{\partial q} + \delta \frac{\partial f_j^{p^\varepsilon}}{\partial q}$$

$$\mathcal{A} \equiv n_i \left(\bar{c} \left(\alpha a_i a_j + \alpha^N \left(a_i^{N_1} a_j^{N_1} + a_i^{N_2} a_j^{N_2} \right) \right) \mathcal{I} + a_i \frac{\partial f_j^{q^\varepsilon}}{\partial q} + a_i \delta \frac{\partial f_j^{p^\varepsilon}}{\partial q} \right) n_j \quad (14)$$

which incorporate the Jacobian matrices of $f_j^{q^\varepsilon}$ and $f_j^{p^\varepsilon}$. In (14), $\mathcal{I}$ denotes the identity matrix and $\{n_j\}$ the components of a unit vector $\mathbf{n}$, which may point in any geometric direction issuing from any flow field point, given that ϕ represents any smooth test function with compact support in Ω . The developed parabolic perturbation (13) is dissipative, hence stable, since all the eigenvalues of matrices (14) have been constrained to remain real and positive for any magnitude of the flow speed $\|\mathbf{u}\|$ and directions $\mathbf{n}$, which corresponds to upwinding along every geometric direction in space. This requirement on all these eigenvalues determines the stability functions α , δ , and α^N .

All the eigenvalues of $\mathcal{A}$, have been analytically determined exactly in closed form for three-dimensional flows, hence $n = 3$. After dividing them by the local speed of sound c , these eigenvalues are expressed in non-dimensional form as

$$\lambda_{3,2+n} = n_i \left(\alpha a_i a_j + \alpha^N \left(a_i^{N_1} a_j^{N_1} + a_i^{N_2} a_j^{N_2} \right) \right) n_j + n_i a_i \frac{u_j}{\|\mathbf{u}\|} n_j M$$

$$\lambda_{1,2} = n_i \left(\alpha a_i a_j + \alpha^N \left(a_i^{N_1} a_j^{N_1} + a_i^{N_2} a_j^{N_2} \right) \right) n_j +$$

$$+ n_i a_i \left(1 + \frac{1-\delta}{2} p_E \right) \frac{u_j}{\|\mathbf{u}\|} n_j M \pm n_i a_i \sqrt{\left(\frac{1-\delta}{2} p_E \frac{u_j}{\|\mathbf{u}\|} n_j M \right)^2 + \delta} \quad (15)$$

where $1 \leq i, j \leq n$, $a_i a_i^{N_\ell} = 0$, $\ell = 1, 2$, $a_i^{N_1} a_i^{N_2} = 0$, and $p_E \equiv \partial p / \partial E = (\gamma - 1)$, from the equation of state for (3). The eigenvalues for two-dimensional flows follow from (15) for $n = 2$ and $a_i^{N_2} = a_j^{N_2} = 0, \forall i, j$. Those for one-dimensional flows are obtained for $n = 1$, $a_i^{N_\ell} = a_i^{N_\ell} = 0, \forall \ell$, and $a_1 = 1$.

The stability functions α , δ , and α^N have been determined, as stated, under the requirement that all these eigenvalues be real and positive for any flow dimensionality and for any direction $\mathbf{n}$. These functions have been exactly determined in closed form. They remain bounded and non-negative, satisfy the constraints $0 \leq \alpha, \delta, \alpha^N \leq 1$, and depend on the local flow Mach number $M \equiv \|\mathbf{u}\|/\bar{c}$ as $\alpha = \alpha(M)$, $\delta = \delta(M)$, and $\alpha^N = \alpha^N(M)$.

For any direction $\mathbf{n}$, hence any propagating wave, $\lambda_{3,2+n} \geq 0$, as long as $\alpha \geq 0$, $\alpha^N \geq 0$, $\mathbf{a}$ is a unit vector in the streamline direction, $a_i \equiv u_i/\mathbf{u}$, and $\mathbf{a}^{N_1}$ and $\mathbf{a}^{N_2}$ are two mutually orthogonal unit vectors in any two cross-flow directions. For $\mathbf{n}$ in the cross-flow plane, hence $n_i a_i = 0$ and $n_i \left(a_i^{N_1} a_j^{N_1} + a_i^{N_2} a_j^{N_2} \right) n_j = 1$, all the eigenvalues (15) equal α^N , which becomes the cross-flow eigenvalue. Figure 1 presents the variations of the stability functions and dissipation eigenvalues (15) in the streamline direction. All these variations remain smooth for all Mach numbers. The dissipation eigenvalues remain positive and coincide with the inviscid-flux eigenvalues ($M, M \pm 1$) for supersonic flows. The stability functions remain non-negative, with α rapidly decreasing and δ rapidly increasing for rising Mach numbers. For stagnation flows, $\alpha \rightarrow 1$, $\alpha^N \rightarrow 1$, and $\delta \rightarrow 0$. Hence (14) generates upwinding on acoustic waves. For increasing M , $\alpha \rightarrow 0$, $0 < \alpha^N \leq 1$, and $\delta \rightarrow 1$. In this case, (14) generates upwinding both inside and outside a conical region that has its vertex at each flow-field point and its axis along a streamline arc at that point. The α^N term induces upwinding outside this conical region, through its two cross-flow principal directions, while the $\{a_i\}$ terms induce upwinding inside this conical region, within which the eigenvalues are both positive and distinct. Eventually, $\alpha \equiv 0$ and $\delta \equiv 1$ for supersonic flows, which implies that (14) induces upwinding on the entire diverge of the inviscid flux f_j .

Fig. 1 Eigenvalues and Stability Parameters

VII. Computational Results

The ACURA formulation has generated essentially non-oscillatory results for representative shocked flows. Owing to its consistent multi-dimensional upwinding, the formulation updates the upstream directions continuously as the computational solutions evolve, while exhibiting a high rate of convergence of the residual norm to machine zero. The calculations proceeded with a prescribed constant maximum Courant number, set equal to 100, and corresponding variable Δt computed as as

$$C_{\max} = \max\{\|\mathbf{u}\| + c, \|\mathbf{u}\| - c, c\} \frac{\Delta t}{(\Delta \ell)_e} \Rightarrow \Delta t = \frac{C_{\max}(\Delta \ell)_e}{\max\{\|\mathbf{u}\| + c, \|\mathbf{u}\| - c, c\}} \quad (16)$$

In this expression, $(\Delta \ell)_e$ denotes the minimum element size within each grid. The steady state was defined as the state at which the Euclidean norm of the total residual fell below 1×10^{-14} .

Figure 2 presents quasi-one dimensional results that correspond to the calculation of an off-design flow within a nozzle, with $0 \leq x \leq 1$. For this flow, the inlet and outlet area ratios of the nozzle are $A_{\text{in}}/A_{\text{throat}} = 2.5$ and $A_{\text{out}}/A_{\text{throat}} = 1.5$. The initial conditions correspond to a uniform $M = 0.25$ subsonic flow. The inlet Dirichlet boundary conditions are prescribed density ρ and energy E , corresponding to the inlet Mach number; the outlet boundary condition is static pressure corresponding to a $M = 0.6$ subsonic flow. This steady-state solution was rapidly achieved from the initial conditions in about 40 time cycles. The solution in the figure corresponds to a uniform grid with 401 nodes and 200 Lagrange quadratic elements. For the same number of computational nodes within a uniform grid, the solution was also calculated with 400 linear elements and 134 cubic elements, for 402 nodes. All of these computational solutions remained non-oscillatory and reflected the exact solution. These solutions crisply captured the shock and related jumps, which are accurately computed at the exact shock location, $x_s = 0.79$. There is one data point within the shock. This is expected because this entropy solution mimics a viscous shock structure.

Fig. 2 Nozzle Flow: Pressure and Mach Number

Another measure of solution quality is the ACURA capability of preserving the Rankine-Hogoniot jump conditions. According to these conditions, the mass flow rate is conserved across a shock. This physical quantity is indeed conserved by the computational solution, as illustrated in Figure 3 in terms of the liner momentum distribution. Figure 3 also documents the convergence rate of the computational solution towards the exact solution, as the grid is refined. This convergence rate is expressed in terms of the H^1 and H^2 norms of the total error in the entire solution q from quadratic elements; the H^2 norm was obtained by excluding from the calculation the shock interval, defined as $(x_s - \Delta x, x_s + \Delta x)$, with Δx the width of one element on either side of the shock. Both norms decrease as anticipated, particularly the H^1 norm, the calculation of which included the shock interval.

Fig. 3 Nozzle Flow: Linear Momentum and Error Norms

Figures 4-5 present the results of a two-dimensional supersonic intake flow with an embedded shock reflection.

Fig. 4 $M_{\infty} = 2.40$ Shock Reflection, Computational Grid

The essentially uniform and relatively coarse grid consists of 40×40 Lagrange bilinear, square isoparametric finite elements. Hence, this grid consists of 1,681 nodes for a total of 6,724 degrees of freedom.

At the inlet, the flow is supersonic, with a free-stream Mach number $M_{\infty} = 2.40$. At this location, the boundary conditions are fixed density ρ , longitudinal and transversal linear momentum components m_1 and m_2 , and total energy E . Since the outlet remains supersonic, no boundary condition is enforced at that location. At the solid upper and lower walls, the inviscid wall-tangency boundary condition $\mathbf{u} \cdot \mathbf{n} = 0$ is enforced through the surface integrals in (12).

The initial conditions correspond to a uniform supersonic $M = 2.40$ flow. The initially uniform supersonic flow at the inlet is deflected by a 10° ramp and the final steady state is computationally achieved by advancing the solution in time. On the grid in Figure 5, the solution converged to steady state in 40 iterations. Reflecting the exact solution, the computational solution in Figure 5 juxtaposes three plateaus with correct local Mach numbers.

Fig. 5 $M_{\infty} = 2.40$ Shock Reflection, Mach Number Contours

The plateaus are separated by sharply captured oblique shocks at the correct position and with correct inclinations angles. The reflected shock is able to cross the outlet boundary without any spurious distortions.

The third benchmark involves an asymmetric two-dimensional interaction and reflection of two oblique shocks, with computational results presented in Figures 6 and 7.

Fig. 6 $M_\infty = 2.40$ Shock-on-Shock Interaction, Computational Grid

Consisting of the same number and type of elements as in the previous test case, this benchmark used an adapted body-fitted grid. The clustering of elements towards the wall has generated a grid that features a large spread of element sizes, which has increased the stiffness of the system of fully discrete equations.

The supersonic inlet corresponds to a free-stream Mach number $M_\infty = 2.40$, hence the inlet boundary conditions constrain density ρ , longitudinal and transversal linear momentum components m_1 and m_2 and total energy E . The total outlet remains supersonic, hence no boundary conditions are enforced at this boundary. At the solid upper and lower walls, the inviscid-flow wall-tangency boundary condition is enforced via surface integrals. This solid-wall specification only extends to half of the horizontal length of the computational domain; beyond this station, the upper and lower boundaries correspond to supersonic outlets, to allow the reflected shocks to cross the computational boundaries. Also in this case are the initial conditions those that correspond to a uniform $M_\infty = 2.40$ supersonic flow.

The initially uniform supersonic flow is subject to an upward 5° deflection by the lower wall and a downward 3° deflection by the upper wall. On the chosen grid, a final steady state is computationally achieved within 40 time cycles. The wall-tangency boundary conditions on the upper and lower boundary walls generate two separate oblique shocks that propagate toward each other with different strengths, interact, and reflect away from each other, towards the outlet as displayed in Figure 7

Fig. 7 $M_\infty = 2.40$ Shock-on-Shock Interaction, Mach Number Contours

The final steady state remains essentially non-oscillatory with crisply calculated incident and reflected shocks. This computational solution mirrors the available exact solution, with four juxtaposed plateaus connected by four oblique shocks. Since the ramp deflection angles remain somewhat moderate and close to each other, the velocity magnitudes and Mach numbers remain essentially constant across the slip line that originates at the reflected-shock intersection point. The reflected-shock interaction rotates the emerging velocity vector to the equilibrium angle of 2° with respect to the horizontal direction. The calculated Mach numbers in the plateaus downstream of the interacting shocks are $M_2 = 2.20$, $M_3 = 2.28$, $M_4 \approx M_5 = 2.08$; the shock inclination angles are $\theta_2 = 28.53^\circ$, $\theta_3 = -26.90^\circ$, $\theta_4 = 29.52^\circ$ and $\theta_5 = -30.15^\circ$. All of these calculated quantities coincide with the exact values. In particular, the algorithm allows the reflected shocks to cross the outflow boundaries without any alterations.

Concluding Remarks

A new theoretical foundation based on shock-jump resolutions has been established to develop upstream resolution algorithms for solving conservation-law systems computationally. These developments express the shock-jump surface integrals that naturally arise in integral weak statements in terms of differences of gradients of entropy functions through the mean-value theorem. The resulting expressions become parabolic perturbations to the original systems, perturbations that are made stable by imposing that all the eigenvalues of the perturbation stability matrix remain real and positive along every geometric direction emanating from any point in the computational domain. Under these conditions, an entropy principle is satisfied and the weak statement on the perturbed system is termed an entropy weak statement. Since these parabolic perturbations emerge from a resolution in the jumps of the hyperbolic flux, the developments unify artificial dissipation methods and upwind flux vector splitting schemes in that the entropy weak statement on the perturbed system is shown to be equivalent to an upstream biased formulation of the hyperbolic fluxes.

All the developments take place in the continuum, at the partial differential equation level, before any discretization in space. This is important because a subsequent discretization of the perturbed system automatically generates consistent upwind discrete equations on arbitrary grids. In this work, the entropy weak statement is discretized by a Galerkin finite element method, which is stabilized by the parabolic perturbation and naturally generates discrete equations that are free of any additional discretization-induced dissipation.

Applied to the gas dynamics equations systems, these developments resolve the shock jumps in the inviscid flux through a decomposition of the flux vector in terms of convection and acoustic components. In the low-speed regime, the acoustic components are expressed through the Rankine-Hugoniot jump conditions, in order to preserve computational stability for vanishing Mach numbers. The resulting parabolic perturbation smoothly and structurally varies from an upstream resolution of acoustic components for low subsonic flows, to an upstream bias on the entire flux divergence for supersonic flows. Correspondingly, the eigenvalues of the perturbation stability matrix smoothly vary from the speed of sound to the convection velocity superimposed to this speed. Furthermore, the parabolic perturbation is shown to correspond to an inherently multi-dimensional upwind formulation, with the streamline and two mutually orthogonal cross-flow directions becoming the principal directions of the perturbation. A forthcoming article will provide exhaustive details on the overall continuous modelling and discretization.

The benefits of unifying artificial viscosity methods with upwind flux vector splitting algorithms and establishing the upstream formulation at the partial differential equation level ahead of any spatial discretization are reflected in the efficiency and accuracy of the computational solutions presented in this work. Steady state solutions for mixed subsonic-supersonic flows and supersonic flows featuring shock reflections and interactions rapidly converge to steady states, feature sharply captured shocks, and reflect available exact solutions.

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