Bond-Graph Approach for Computational Fluid Dynamics: a Comparison with other Numerical Methods

Baliño, J. L.
Instituto de Pesquisas Energéticas e Nucleares,
Av. Prof. Lineu Prestes 2242, Cidade Universitária, CEP 05508-000, São Paulo, SP, Brazil
jlbalino@net.ipen.br

Abstract— **This paper shows contributions from a new, Bond-Graph based, formalism for CFD problems, through which the state equations are obtained in terms of nodal vectors of mass, velocity and entropy.**

The resulting state equations are presented for a one-dimensional problem with constant piecewise shape functions. It is shown that there exist contributions coming from the discontinuities; these contributions can be taken into account in the integration process by using distributional derivatives. Although viscous effects cannot be modeled, heat conduction can be rigorously taken into account with the proper choice of the entropy weight functions.

Based on the linearized expressions of the state equations, a comparison is made with a control-volume and with a finite-difference numerical scheme, obtaining an interpretation of the density and entropy weight functions appearing in the Bond-Graph formalism and showing that these popular numerical methods are included as particular cases of this methodology.

Based on the Second Principle of Thermodynamics, it is also shown that the entropy weight functions must decrease as the distance to the corresponding node position increases.

Keywords— **Bond Graphs, Computational Fluid Dynamics, CFD, Control Volume Method, Finite Difference Method.**

I. Introduction

A. The BG-CFD Approach

In recent works [1][2] a theoretical development of a general Bond Graph approach for CFD was presented, which is a result of the right combination of Bond-Graph concepts with elements of numerical methods. The main characteristics of this new methodology, which was called BG-CFD [3], can be summarized as follows:

- Based on the total energy rate per unit volume, a set of independent variables (namely density, velocity and entropy per unit volume) is defined, as well as associated potentials (namely linear momentum per unit volume, kinetic coenergy per unit mass, Gibbs free energy per unit mass and temperature). The potentials are functions of the independent variables through the constitutive relations, which have restrictions due to the equality of the mixed partial derivatives (Maxwell relations).
- The independent variables are discretized in terms of nodal values and interpolation (shape) functions. Since this is the only discretization restriction, it is possible to work with any kind of grids. Nodal vectors are defined as Bond Graph state variables, namely mass, entropy and velocity. The mass and entropy vectors are obtained by integrating the corresponding nodal independent variables in the support of the shape functions. The corresponding integrated potentials also satisfy constitutive, as well as Maxwell relations.
- The system state equations are obtained by systematically volume integrating three balance equations corresponding to each port of the *IC* field representing the total system energy. The balance equations have terms representing the power coupling between the different ports. In this way, the inertial and thermal couplings to the mass conservation equation and the transformation of mechanical energy into thermal energy, as well as the generation of irreversibility, are represented naturally.
- The convective (upwind) nature of the fluid equations is handled through the definition of density and entropy weight functions, which are introduced to satisfy the power interchanged by the system through the boundary conditions, as well as to share the importance of different power terms among neighboring nodes. This concept was successfully applied to convection-diffusion problems [4][5].
- All kind of boundary conditions are handled consistently and can be represented either as generalized modulated effort sources at the inertial port or modulated flow sources at the capacitive ports.

As a consequence, this approach bridges the gap between the continuous formulation of the conservation equations and a discretized numerical scheme framed within the Bond-Graph theory.

B. Discontinuities

The discontinuities present in the description of the flow fields are handled through the use of distributional derivatives [6]. Consider a function χ singular on a fixed surface Γ, as shown in Fig. 1, with derivatives of all orders outside Γ and boundary values of the function and its derivatives from both sides of Γ. The jump across the surface is:

$$[\chi] = \chi_j - \chi_i \tag{1}$$

where χ_i and χ_j are the boundary values of χ from both sides of Γ. If χ is a scalar field, it can be shown that the gradient can be expressed as:

$$\overline{\nabla}\chi = \nabla\chi + [\chi]\,\delta(r - r_\Gamma)\,\check{\mathbf{n}}_{ij} \tag{2}$$

If χ is a vector field, it can be shown that the divergence can be expressed as:

$$\overline{\nabla}.\chi = \nabla.\chi + [\chi]\,\delta(r - r_\Gamma).\check{\mathbf{n}}_{ij} \tag{3}$$

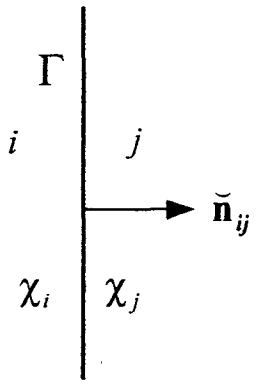

Fig. 1. Function discontinuity in a surface Γ.

where δ is the impulse (Dirac's delta) function, $\breve{\mathbf{n}}_{ij}$ is the normal unity vector (oriented from i to j), $\boldsymbol{r}$ is the position and $\boldsymbol{r}_\Gamma$ is the position of the discontinuity surface. In Eqs. (2) and (3), the bars indicate a distributional operation. In this way, the discontinuities present in the discretized flow fields can be taken into account in the integration procedure by considering all the operators as distributional ones.

II. One-dimensional flow with constant piecewise shape functions

Consider a one-dimensional discretization, as shown in Fig. 2. The volume within the lines located midway between the grid points can be regarded as control volumes. It is interesting to consider also a uniform distribution of the independent variables, because these are the simplest and because the state variables correspond to the mass, entropy and velocity within the control volumes.

A. State equations

The Bond-Graph CFD formalism can be applied to a system with the assumptions made above. For this case, the inertia matrix becomes diagonal and the state equations corresponding to the different nodal state variables can be obtained analytically. The details of the derivation are not given here, but it can be shown that viscous effects cannot be taken into account with a constant velocity shape function, but heat conduction can be modelled with non-constant entropy weight functions. The final expressions are given for an inner node ($1 < i < n$) and for the first and last nodes, in which "half" control volumes result. In these expressions, the following variables are evaluated at different nodes: mass m, velocity V, entropy per unit volume s_v ($s_v = \rho s$, where ρ is the density and s is the entropy per unit mass), Gibbs free energy per unit mass ψ, kinetic coenergy per unit mass $\kappa = \frac{1}{2}V^2$, pressure P, absolute temperature θ, entropy S and thermal conductivity λ. The Gibbs free energy, pressure, temperature and thermal conductivity are functions of the density and entropy per unit volume through the constitutive relations.

In this case, the interpolation functions ($\varphi_{\rho i}$, φ_{Vi}, and φ_{si}) chosen for the independent variables (correspondingly ρ, V and s_v) are, for an inner node ($1 < i < n$):

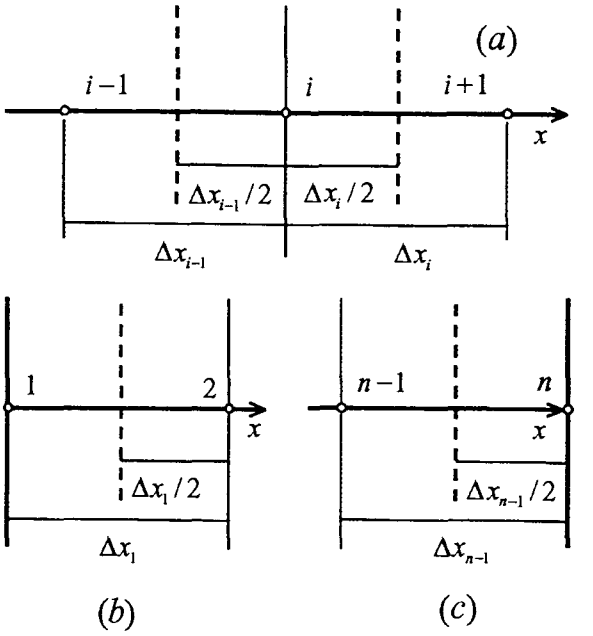

Fig. 2. Discretization for: (*a*) an inner node, (*b*) first node and (*c*) last node.

$$\varphi_{\rho i} = \varphi_{Vi} = \varphi_{si} = \begin{cases} 0 \text{ for } x < -\frac{\Delta x_{i-1}}{2} \\ 1 \text{ for } -\frac{\Delta x_{i-1}}{2} < x < \frac{\Delta x_{i+1}}{2} \\ 0 \text{ for } x > \frac{\Delta x_{i+1}}{2} \end{cases} \tag{4}$$

For the first and last nodes, we have:

$$\varphi_{\rho 1} = \varphi_{V1} = \varphi_{s1} = \begin{cases} 1 \text{ for } 0 \le x < \frac{\Delta x_1}{2} \\ 0 \text{ for } x > \frac{\Delta x_1}{2} \end{cases} \tag{5}$$

$$\varphi_{\rho n} = \varphi_{Vn} = \varphi_{sn} = \begin{cases} 0 \text{ for } x < -\frac{\Delta x_{n-1}}{2} \\ 1 \text{ for } -\frac{\Delta x_{n-1}}{2} < x \le 0 \end{cases} \tag{6}$$

For the density and entropy weight functions the following convention is adopted: $w_{\rho\, i,jk}$ and $w_{s\, i,jk}$ denote weight functions corresponding to node i, evaluated at the face separating nodes j and k. The independent and integrated variables (magnitudes per unit area in the one-dimensional problem) are related as follows:

$$m_i = \rho_i \frac{1}{2}(\Delta x_{i-1} + \Delta x_i) \tag{7}$$

$$m_1 = \rho_1 \frac{1}{2}\Delta x_1 \quad ; \quad m_n = \rho_n \frac{1}{2}\Delta x_{n-1} \tag{8}$$

$$S_i = s_{v\, i} \frac{1}{2}(\Delta x_{i-1} + \Delta x_i) \tag{9}$$

$$S_1 = s_{v\,1}\,\frac{1}{2}\,\Delta x_1 \quad ; \quad S_n = s_{v\,n}\,\frac{1}{2}\,\Delta x_{n-1} \tag{10}$$

For the mass state equations, we have:

$$\begin{aligned}
\dot{m}_i = \frac{1}{(\psi_i + \kappa_i)} \Big\langle & w_{\rho\,i,\,i-1\,i} \Big\{ V_{i-1} \Big[\frac{1}{2} (P_i - P_{i-1}) \\
& - \frac{1}{2}\, s_{v\,i-1} (\theta_i - \theta_{i-1}) + \frac{1}{4} (\rho_{i-1} + \rho_i) (\kappa_i - \kappa_{i-1}) \\
& + \rho_{i-1} (\psi_{i-1} + \kappa_{i-1}) \Big] \\
& + V_i \Big[\frac{1}{2} (P_i - P_{i-1}) - \frac{1}{2}\, s_{v\,i} (\theta_i - \theta_{i-1}) \\
& + \frac{1}{4} (\rho_{i-1} + \rho_i) (\kappa_i - \kappa_{i-1}) - \rho_i (\psi_i + \kappa_i) \Big] \Big\} \\
& + w_{\rho\,i,\,i\,i+1} \Big\{ V_i \Big[\frac{1}{2} (P_{i+1} - P_i) - \frac{1}{2}\, s_{v\,i} (\theta_{i+1} - \theta_i) \\
& + \frac{1}{4} (\rho_i + \rho_{i+1}) (\kappa_{i+1} - \kappa_i) + \rho_i (\psi_i + \kappa_i) \Big] \\
& + V_{i+1} \Big[\frac{1}{2} (P_{i+1} - P_i) - \frac{1}{2}\, s_{v\,i+1} (\theta_{i+1} - \theta_i) \\
& + \frac{1}{4} (\rho_i + \rho_{i+1}) (\kappa_{i+1} - \kappa_i) \\
& - \rho_{i+1} (\psi_{i+1} + \kappa_{i+1}) \Big] \Big\} \Big\rangle
\end{aligned} \tag{11}$$

$$\begin{aligned}
\dot{m}_1 = \frac{1}{(\psi_1 + \kappa_1)} \Big\langle & w_{\rho\,1,\,1\,2} \Big\{ V_1 \Big[\frac{1}{2} (P_2 - P_1) \\
& - \frac{1}{2}\, s_{v\,1} (\theta_2 - \theta_1) \\
& + \frac{1}{4} (\rho_1 + \rho_2) (\kappa_2 - \kappa_1) + \rho_1 (\psi_1 + \kappa_1) \Big] \\
& + V_2 \Big[\frac{1}{2} (P_2 - P_1) - \frac{1}{2}\, s_{v\,2} (\theta_2 - \theta_1) \\
& + \frac{1}{4} (\rho_1 + \rho_2) (\kappa_2 - \kappa_1) - \rho_2 (\psi_2 + \kappa_2) \Big] \Big\} \Big\rangle
\end{aligned} \tag{12}$$

$$\begin{aligned}
\dot{m}_n = \frac{1}{(\psi_n + \kappa_n)} \Big\langle & w_{\rho\,n,\,n-1\,n} \Big\{ V_{n-1} \Big[\frac{1}{2} (P_n - P_{n-1}) \\
& - \frac{1}{2}\, s_{v\,n-1} (\theta_n - \theta_{n-1}) + \frac{1}{4} (\rho_{n-1} + \rho_n) (\kappa_n - \kappa_{n-1}) \\
& + \rho_{n-1} (\psi_{n-1} + \kappa_{n-1}) \Big] + V_n \Big[\frac{1}{2} (P_n - P_{n-1}) \\
& - \frac{1}{2}\, s_{v\,n} (\theta_n - \theta_{n-1}) + \frac{1}{4} (\rho_{n-1} + \rho_n) (\kappa_n - \kappa_{n-1}) \\
& - \rho_n (\psi_n + \kappa_n) \Big] \Big\} \Big\rangle
\end{aligned} \tag{13}$$

For the velocity state equations, neglecting body forces, we get:

$$\begin{aligned}
\dot{V}_i = -\frac{1}{\rho_i (\Delta x_{i-1} + \Delta x_i)} \Big\{ & (P_{i+1} - P_{i-1}) \\
& + \frac{1}{2} \big[(\rho_i - \rho_{i+1}) (\kappa_{i+1} - \kappa_i) \\
& + (\rho_{i-1} + \rho_i) (\kappa_i - \kappa_{i-1}) \big] \Big\}
\end{aligned} \tag{14}$$

$$\dot{V}_1 = -\frac{1}{\rho_1\, \Delta x_1} \Big[(P_2 - P_1) - \frac{1}{2} (\rho_1 + \rho_2) (\kappa_2 - \kappa_1) \Big] \tag{15}$$

$$\begin{aligned}
\dot{V}_n = -\frac{1}{\rho_n\, \Delta x_{n-1}} \Big[& (P_n - P_{n-1}) \\
& + \frac{1}{2} (\rho_{n-1} + \rho_n) (\kappa_n - \kappa_{n-1}) \Big]
\end{aligned} \tag{16}$$

For the entropy state equations, neglecting heat sources, we obtain:

$$\begin{aligned}
\dot{S}_i = -\frac{1}{2\,\theta_i} \Big[& (\lambda_i + \lambda_{i+1}) (\theta_{i+1} - \theta_i) \Big(\frac{\partial w_{s\,i}}{\partial x} \Big)_{i\;i+1} \\
& + (\lambda_{i-1} + \lambda_i) (\theta_i - \theta_{i-1}) \Big(\frac{\partial w_{s\,i}}{\partial x} \Big)_{i-1\;i} \\
& + w_{s\,i,\,i\,i+1} (\theta_i + \theta_{i+1}) (s_{v\,i+1}\, V_{i+1} - s_{v\,i}\, V_i) \\
& + w_{s\,i,\,i-1\,i} (\theta_{i-1} + \theta_i) (s_{v\,i}\, V_i - s_{v\,i-1}\, V_{i-1}) \Big]
\end{aligned} \tag{17}$$

$$\begin{aligned}
\dot{S}_1 = -\frac{1}{2\,\theta_1} \Big[& (\lambda_1 + \lambda_2) (\theta_2 - \theta_1) \Big(\frac{\partial w_{s\,1}}{\partial x} \Big)_{1\;2} \\
& + w_{s\,1,\,1\,2} (\theta_1 + \theta_2) (s_{v\,2}\, V_2 - s_{v\,1}\, V_1) \Big] + \dot{S}_{Q\;1}^{(\Gamma)}
\end{aligned} \tag{18}$$

$$\begin{aligned}
\dot{S}_n = -\frac{1}{2\,\theta_n} \Big[& (\lambda_{n-1} + \lambda_n) (\theta_n - \theta_{n-1}) \Big(\frac{\partial w_{s\,n}}{\partial x} \Big)_{n-1\;n} \\
& + w_{s\,n,\,n-1\,n} (\theta_{n-1} + \theta_n) (s_{v\;n}\, V_n - s_{v\;n-1}\, V_{n-1}) \Big] + \dot{S}_{Q\;n}^{(\Gamma)}
\end{aligned} \tag{19}$$

In the entropy state equations, $\dot{S}_{Q\;1}^{(\Gamma)}$ and $\dot{S}_{Q\;n}^{(\Gamma)}$ are entropy rate sources needed to satisfy the boundary conditions. It can be seen that the state equations are non-linear. The power couplings between the mass and velocity ports are given through the pressure and kinetic coenergy terms, while the power coupling between the mass and thermal ports are given through the entropy terms. Since viscous effects cannot be taken into account with these shape functions, the corresponding power coupling between the velocity and entropy state equations doesn't appear in the resulting expressions.

B. Linearized state equations

It is interesting to write linearized expressions of the state equations obtained in Section II. These will be valid for problems with small space changes of the state variables and can be compared to the resulting expressions obtained by using other numerical schemes. Considering that:

$$\kappa_j - \kappa_i \cong V_i (V_j - V_i) \tag{20}$$

and that, for a pure substance:

$$\psi_j - \psi_i \cong -\frac{s_{v\;i}}{\rho_i} (\theta_j - \theta_i) + \frac{1}{\rho_i} (P_j - P_i) \tag{21}$$

we have, for the linearized mass state equations:

$$\begin{aligned}
\dot{m}_i \cong & -w_{\rho\,i,\,i-1\,i} \big[\rho_i (V_i - V_{i-1}) + V_i (\rho_i - \rho_{i-1}) \big] \\
& - w_{\rho\,i,\,i\,i+1} \big[\rho_i (V_{i+1} - V_i) + V_i (\rho_{i+1} - \rho_i) \big]
\end{aligned} \tag{22}$$

$$\dot{m}_1 \cong -w_{\rho\,1,\,i\,2}\left[\rho_1\left(V_2 - V_1\right) + V_1\left(\rho_2 - \rho_1\right)\right] \tag{23}$$

$$\dot{m}_n \cong -w_{\rho\,n,\,n-1\,n}\left[\rho_n\left(V_n - V_{n-1}\right) + V_n\left(\rho_n - \rho_{n-1}\right)\right] \tag{24}$$

For the linearized velocity state equations, we get:

$$\dot{V}_i \cong -\frac{1}{\rho_i\left(\Delta x_{i-1} + \Delta x_i\right)}\left[\left(P_{i+1} - P_{i-1}\right) + \rho_i V_i\left(V_{i+1} - V_{i-1}\right)\right] \tag{25}$$

$$\dot{V}_1 = -\frac{1}{\rho_1\,\Delta x_1}\left[\left(P_2 - P_1\right) + \rho_1 V_1\left(V_2 - V_1\right)\right] \tag{26}$$

$$\dot{V}_n = -\frac{1}{\rho_n\,\Delta x_{n-1}}\left[\left(P_n - P_{n-1}\right) + \rho_n V_n\left(V_n - V_{n-1}\right)\right] \tag{27}$$

For the linearized entropy state equation, we obtain:

$$\begin{aligned}\dot{S}_i \cong & -w_{s\,i,\,i-1\,i}\left[s_{v\,i}\left(V_i - V_{i-1}\right) + V_i\left(s_{v\,i} - s_{v\,i-1}\right)\right] \\ & -w_{s\,i,\,i\,i+1}\left[s_{v\,i}\left(V_{i+1} - V_i\right) + V_i\left(s_{v\,i+1} - s_{v\,i}\right)\right] \\ & -\left(\frac{\partial w_{s\,i}}{\partial x}\right)_{i-1\,i}\lambda_i\left(1 - \frac{\theta_{i-1}}{\theta_i}\right) \\ & +\left(\frac{\partial w_{s\,i}}{\partial x}\right)_{i\,i+1}\lambda_i\left(\frac{\theta_{i+1}}{\theta_i} - 1\right)\end{aligned} \tag{28}$$

$$\begin{aligned}\dot{S}_1 \cong & -w_{s\,1,\,1\,2}\left[s_{v\,1}\left(V_2 - V_1\right) + V_1\left(s_{v\,2} - s_{v\,1}\right)\right] \\ & -\left(\frac{\partial w_{s\,1}}{\partial x}\right)_{1\,2}\lambda_1\left(\frac{\theta_2}{\theta_1} - 1\right) + \dot{S}_{Q\,1}^{(\Gamma)}\end{aligned} \tag{29}$$

$$\begin{aligned}\dot{S}_n \cong & -w_{s\,n,\,n-1\,n}\left[s_{v\,n}\left(V_n - V_{n-1}\right) + V_n\left(s_{v\,n} - s_{v\,n-1}\right)\right] \\ & -\left(\frac{\partial w_{s\,n}}{\partial x}\right)_{n-1\,n}\lambda_n\left(1 - \frac{\theta_{n-1}}{\theta_n}\right) + \dot{S}_{Q\,n}^{(\Gamma)}\end{aligned} \tag{30}$$

III. Comparison with other numerical schemes

In this Section, a comparison is made between the Bond Graph linearized state equations and the ones obtained by using a control-volume and a finite-difference formulation. We consider as starting differential equations to be discretized by using these formulations the continuity, momentum (inviscid and without body forces) and thermal energy equation (without sources) in terms of the entropy per unit volume:

$$\frac{\partial \rho}{\partial t} = -\nabla.\left(\rho\, V\right) \tag{31}$$

$$\frac{\partial V}{\partial t} = -\frac{1}{\rho}\nabla P - \left(V.\nabla\right)V \tag{32}$$

$$\frac{\partial s_v}{\partial t} = -\frac{1}{\theta}\nabla.q - \nabla.\left(s_v\, V\right) \tag{33}$$

where V is the velocity vector and q is the heat flux.

A. *Control-volume formulation*

In this approach [7], the calculation domain is divided into a number of overlapping control volumes such that there is one control volume surrounding each grid point. The differential equations are then integrated over each control volume, assuming convenient (in general different) profiles for evaluating the flux, source and unsteady terms for the control volumes. Integrating Eq. (31) over an inner control volume, we obtain:

$$\dot{m}_i = -\left(\rho V\right)_{i+\frac{1}{2}} + \left(\rho V\right)_{i-\frac{1}{2}} \tag{34}$$

The mass flux $\rho\, V$, evaluated at both sides of the control volume, can be written as:

$$\begin{aligned}\left(\rho V\right)_{i+\frac{1}{2}} &= \rho_i V_i + w_{\rho\,i+\frac{1}{2}}\left(\rho_{i+1} V_{i+1} - \rho_i V_i\right) \\ &\cong \rho_i V_i + w_{\rho\,i+\frac{1}{2}}\left[\rho_i\left(V_{i+1} - V_i\right) + V_i\left(\rho_{i+1} - \rho_i\right)\right]\end{aligned} \tag{35}$$

$$\begin{aligned}\left(\rho V\right)_{i-\frac{1}{2}} &= \rho_i V_i - w_{\rho\,i-\frac{1}{2}}\left(\rho_i V_i - \rho_{i-1} V_{i-1}\right) \\ &\cong \rho_i V_i - w_{\rho\,i-\frac{1}{2}}\left[\rho_i\left(V_i - V_{i-1}\right) + V_i\left(\rho_i - \rho_{i-1}\right)\right]\end{aligned} \tag{36}$$

where $w_{\rho\,i+\frac{1}{2}}$ and $w_{\rho\,i-\frac{1}{2}}$ are mass flux weight factors. Replacing Eqs. (35) and (36) in Eq. (34) and comparing to Eq. (22), we get:

$$w_{\rho\,i+\frac{1}{2}} = w_{\rho\,i,\,i\,i+1} \;\;;\;\; w_{\rho\,i-\frac{1}{2}} = w_{\rho\,i,\,i-1\,i} \tag{37}$$

This is, the density weight functions evaluated at the discontinuity surfaces can be regarded as mass flux weight factors in a control-volume formulation.

The considerations are also valid for the first and last control volumes, in which a finite volume formulation gives:

$$\dot{m}_1 = -\left(\rho V\right)_{1+\frac{1}{2}} + \left(\rho V\right)_1 \;\;;\;\; \dot{m}_n = -\left(\rho V\right)_n + \left(\rho V\right)_{n-\frac{1}{2}} \tag{38}$$

It is interesting to notice that the mass fluxes calculated in Eqs. (35) and (36) are consistent, since:

$$w_{\rho\,i,\,i\,i+1} + w_{\rho\,i+1,\,i\,i+1} = 1 \tag{39}$$

Eq. (33) can be written in a conservative form by noticing that:

$$\frac{1}{\theta}\nabla.q = \nabla.\left(\frac{q}{\theta}\right) + \frac{q}{\theta^2}.\nabla\theta \tag{40}$$

Since:

$$\left|\frac{\frac{q}{\theta^2}.\nabla\theta}{\nabla.\left(\frac{q}{\theta}\right)}\right| \sim \frac{\left|\theta_j - \theta_i\right|}{\theta_i} \tag{41}$$

it can be written, for $\frac{\left|\theta_j - \theta_i\right|}{\theta_i} \ll 1$:

$$\frac{\partial s_v}{\partial t} \cong -\nabla.\left(\frac{q}{\theta} + s_v\, V\right) \tag{42}$$

Integrating Eq. (42) over an inner control volume, we obtain:

$$\dot{S}_i \cong -\left(\frac{q}{\theta} + s_v V\right)_{i+\frac{1}{2}} + \left(\frac{q}{\theta} + s_v V\right)_{i-\frac{1}{2}} \qquad (43)$$

where $\frac{q}{\theta}$ and $s_v V$ are correspondingly the conductive and convective entropy fluxes. These fluxes can be evaluated at both faces of the control volume as:

$$\left(\frac{q}{\theta}\right)_{i+\frac{1}{2}} = -w_{q\,i+\frac{1}{2}} \frac{2}{\theta_i} \lambda_i \frac{\theta_{i+1} - \theta_i}{\Delta x_i} \qquad (44)$$

$$\left(\frac{q}{\theta}\right)_{i-\frac{1}{2}} = -w_{q\,i-\frac{1}{2}} \frac{2}{\theta_i} \lambda_i \frac{\theta_i - \theta_{i-1}}{\Delta x_{i-1}} \qquad (45)$$

$$\begin{aligned}(s_v V)_{i+\frac{1}{2}} &= s_{v\,i} V_i + w_{s\,i+\frac{1}{2}} (s_{v\,i+1} V_{i+1} - s_{v\,i} V_i) \\ &\cong s_{v\,i} V_i + w_{s\,i+\frac{1}{2}} [s_{v\,i} (V_{i+1} - V_i) + V_i (s_{v\,i+1} - s_{v\,i})]\end{aligned} \qquad (46)$$

$$\begin{aligned}(s_v V)_{i-\frac{1}{2}} &= s_{v\,i} V_i - w_{s\,i-\frac{1}{2}} (s_{v\,i} V_i - s_{v\,i-1} V_{i-1}) \\ &\cong s_{v\,i} V_i - w_{s\,i-\frac{1}{2}} [s_{v\,i} (V_i - V_{i-1}) + V_i (s_{v\,i} - s_{v\,i-1})]\end{aligned} \qquad (47)$$

In Eqs. (44) and (45), $w_{q\,i+\frac{1}{2}}$ and $w_{q\,i-\frac{1}{2}}$ are factors weighting the mean conductive entropy fluxes, while in Eqs. (46) and (47), $w_{s\,i+\frac{1}{2}}$ and $w_{s\,i-\frac{1}{2}}$ are convective flux weight factors. Replacing Eqs. (44) to (47) in Eq. (43) and comparing to Eq. (28), we get:

$$w_{q\,i+\frac{1}{2}} = \frac{1}{2} \Delta x_i \left(\frac{\partial w_{s\,i}}{\partial x}\right)_{i\,i+1} \qquad (48)$$

$$w_{q\,i-\frac{1}{2}} = \frac{1}{2} \Delta x_{i-1} \left(\frac{\partial w_{s\,i}}{\partial x}\right)_{i-1\,i} \qquad (49)$$

$$w_{s\,i-\frac{1}{2}} = w_{s\,i,i-1\,i} \;\; ; \;\; w_{s\,i+\frac{1}{2}} = w_{s\,i,i\,i+1} \qquad (50)$$

This is, the gradients of the entropy weight functions evaluated at the discontinuity surfaces are proportional to the corresponding conductive entropy flux factors. Besides, the entropy weight functions evaluated at the discontinuity surfaces can be regarded as convective entropy flux weight factors.

In [4], a suitable entropy weight function was determined for a one-dimensional convection-diffusion problem with constant velocity. It was shown that the weight function is dependent on the Peclet grid number, with the limit values of $w_{s\,i,i-1\,i} = 1$ and $w_{s\,i,i\,i+1} = 0$ for "full upwind" conditions with positive velocities, while $w_{s\,i,i-1\,i} = 0$ and $w_{s\,i,i\,i+1} = 1$ for full upwind conditions with negative velocities.

For the first and last control volumes, a finite volume formulation gives:

$$\dot{S}_1 \cong -\left(\frac{q}{\theta} + s_v V\right)_{1+\frac{1}{2}} + \frac{q_1}{\theta_1} + s_{v\,1} V_1 \qquad (51)$$

$$\dot{S}_n \cong -\frac{q_n}{\theta_n} - s_{v\,n} V_n + \left(\frac{q}{\theta} + s_v V\right)_{n-\frac{1}{2}} \qquad (52)$$

The considerations are also valid for these control volumes, since:

$$\dot{S}_{Q\,1}^{(\Gamma)} = \frac{q_1}{\theta_1} \;\; ; \;\; \dot{S}_{Q\,n}^{(\Gamma)} = \frac{q_n}{\theta_n} \qquad (53)$$

It is interesting to notice that the convective and conductive entropy fluxes calculated in Eqs. (44) to (47) are consistent, since:

$$w_{s\,i,i\,i+1} + w_{s\,i+1,i\,i+1} = 1 \qquad (54)$$

$$\left(\frac{\partial w_{s\,i}}{\partial x}\right)_{i\,i+1} + \left(\frac{\partial w_{s\,i+1}}{\partial x}\right)_{i\,i+1} = 0 \qquad (55)$$

Integrating Eq. (32) over an inner control volume, considering a constant velocity profile for the unsteady term and a linear profile for the convective term, we obtain:

$$\begin{aligned}\dot{V}_i \frac{1}{2} (\Delta x_{i-1} + \Delta x_i) \cong &-\frac{1}{\rho_i} \frac{1}{2} [(P_i + P_{i+1}) - (P_{i-1} + P_i)] \\ &- V_i \frac{1}{2} [(V_i + V_{i+1}) - (V_{i-1} + V_i)]\end{aligned} \qquad (56)$$

which reduces to Eq. (25).

The considerations are also valid for the first and last control volumes, in which a finite volume formulation gives expressions that reduce to Eq. (26) and (27). It is very interesting to notice that, according to this Bond-Graph formalism, no weight functions result for the velocity state equations.

B. Finite-difference formulation

In this approach [8], the derivatives in the differential equations are replaced by truncated Taylor-series expansions. Expressions coincident with the ones obtained by using this formulation can be obtained with the appropriate choice of the weight functions.

For instance, for $w_{\rho\,i,i\,i+1} = w_{s\,i,i\,i+1} = 1$ and $w_{\rho\,i,i-1\,i} = w_{\,i,i-1\,i} = 0$, we obtain the "forward" approximations for the first derivatives; for $w_{\rho\,i,i\,i+1} = w_{s\,i,i\,i+1} = 0$ and $w_{\rho\,i,i-1\,i} = w_{\,i,i-1\,i} = 1$ we get the "backward" approximations, while for $w_{\rho\,i,i\,i+1} = w_{s\,i,i\,i+1} = w_{\rho\,i,i-1\,i} = w_{s\,i,i-1\,i} = \frac{1}{2}$ the "central" approximations result. The forward and backward approximations correspond to the "full upwind" scheme.

Concerning the heat conduction term in the entropy state equation, it can be easily shown that for $\left(\frac{\partial w_{s\,i}}{\partial x}\right)_{i\,i\,1} = -1$ and $\left(\frac{\partial w_{s\,i}}{\partial x}\right)_{i-1\,i} = 1$, and considering a uniform grid spacing, we obtain the well known "three-point central " approximation to the temperature second derivative. Others approximations can be obtained, of course, with suitable choices of the weight functions and their derivatives.

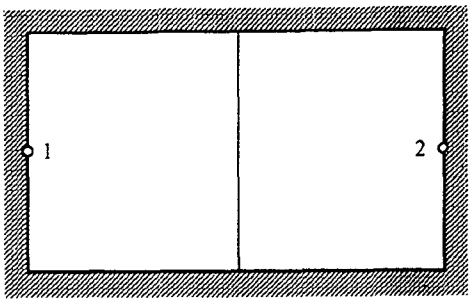

Fig. 3. One-dimensional heat conduction in a reservoir.

IV. Entropy weight functions and the Second Principle of Thermodynamics

Let us consider the simple case of one-dimensional heat conduction shown in Fig. 3. Two reservoirs of thermal energy at absolute temperatures θ_1 and θ_2 are allowed to communicate through a thermal resistance, but are thermally insulated from the surroundings at the rest of the surfaces. The state equations for the reservoirs are:

$$\dot{S}_1 = -\frac{1}{\theta_1}\frac{1}{2}(\lambda_1+\lambda_2)(\theta_2-\theta_1)\left(\frac{\partial w_{s\,1}}{\partial x}\right)_{1\,2} \tag{57}$$

$$\dot{S}_2 = -\frac{1}{\theta_2}\frac{1}{2}(\lambda_1+\lambda_2)(\theta_2-\theta_1)\left(\frac{\partial w_{s\,2}}{\partial x}\right)_{1\,2} \tag{58}$$

Since $w_{s\,1}+w_{s\,2}=1$, we have:

$$\left(\frac{\partial w_{s\,2}}{\partial x}\right)_{1\,2} = -\left(\frac{\partial w_{s\,1}}{\partial x}\right)_{1\,2} \tag{59}$$

The system entropy rate $\dot{S}$ can be written as:

$$\dot{S} = \dot{S}_1+\dot{S}_2 = -\frac{1}{2}(\lambda_1+\lambda_2)\frac{(\theta_2-\theta_1)^2}{\theta_1\,\theta_2}\left(\frac{\partial w_{s\,1}}{\partial x}\right)_{1\,2} \tag{60}$$

Since for the closed system $\dot{S}\geq 0$, the entropy weight functions must be decreasing with respect to the distance to the corresponding entropy node. Although this proof was made for this simple example, this property can be generalized.

V. Conclusions

In this paper the resulting state equations, obtained by using a new Bond-Graph approach for CFD, are presented for a one-dimensional problem with constant piecewise shape functions. This nodalization and the choice of the shape functions allow to perform a closed calculation of the state equations. Since for this case the state variables corresponds to the mass, velocity and entropy in control volumes, it is possible to make a comparison with other numerical schemes.

The existing contributions coming from the discontinuities in the description of the flow fields can be successfully handled in the integration process by using distributional derivatives. Although viscous effects cannot be modeled with a constant piecewise velocity profile, heat conduction can be rigorously taken into account with entropy weight functions with non-zero gradients at the discontinuity surfaces.

The density and entropy weight functions, which are elements of this new approach, are capable of taking into account the upwind nature of the fluid equations. Based on the linearized expressions of the state equations, a comparison is made with a control-volume and with a finite-difference numerical scheme, obtaining an interpretation of the density and entropy weight functions appearing in the Bond-Graph formalism. It is found that the density and entropy weight functions can be regarded as weight factors in the calculation of the corresponding fluxes within a control volume, while the gradient of the entropy weight function come out to be proportional to the weight factors in the calculation of the conductive entropy fluxes.

Based on the Second Principle of Thermodynamics, it is also shown that the entropy weight functions must decrease as the distance to the corresponding node position increases.

As the main conclusion of this work, it is shown that the Bond-Graph methodology provides a powerful tool for discretizing physical distributed-parameter systems. When applied to CFD, the BG-CFD approach includes the Control-Volume and Finite-Difference methods as particular cases.

It is hoped that the findings of this paper encourage other researchers to use this formalism in other problems.

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References

[1] Baliño, J. L., Larreteguy, A. E. & Gandolfo, E. F., "A General Bond Graph Approach for Computational Fluid Dynamics. Part I: Theory", *ICBGM '2001*, The Society for Computer Simulation, pp. 41-46. ISBN 1-56555-221-0, 2001.

[2] Baliño, J. L., Larreteguy, A. E. & Gandolfo, E. F., "A General Bond Graph Approach for Computational Fluid Dynamics", submitted to *Mathematics and Computers in Simulation*.

[3] Gandolfo, E. F., Larreteguy, A. E. & Baliño, J. L., "Bond-Graph Modeling of 1-D Compressible Flows", submitted to this Conference.

[4] Gandolfo, E. F., Larreteguy, A. E. & Baliño, J. L., "A General Bond Graph Approach for Computational Fluid Dynamics. Part II: Applications", *ICBGM '2001*, The Society for Computer Simulation, pp. 47-52. ISBN 1-56555-221-0, 2001.

[5] Gandolfo, E. F., Larreteguy, A. E. & Baliño, J. L., "Bond Graph Modeling of Fluid Convection-Diffusion Problems", submitted to *Mathematics and Computers in Simulation*.

[6] Kanwal, R. P., *Generalized Functions: Theory and Technique*. Birkhäuser, ISBN 0-8176-4006-1, 1998.

[7] Patankar, S. V., *Numerical Heat Transfer and Fluid Flow*, Hemisphere Publishing Corporation, ISBN 0-07-048740-5, 1980.

[8] Tannehill, J. C., Anderson, D. A., Pletcher, R. H., *Computational Fluid Mechanics and Heat Transfer*, Taylor & Francis, ISBN 1-56032-046-X.

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