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A General Bond Graph Approach for Computational Fluid Dynamics
Part I: Theory

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Abstract

A theoretical development of a general Bond Graph approach for Computational Fluid Dynamics is presented. Density, entropy per unit volume and velocity are used as discretized variables; in this way, time-dependent nodal values and interpolation functions are introduced to represent the flow field. Nodal vectors are defined as Bond Graph state variables, namely mass, entropy and velocity. It can be shown that the system total energy can be represented as a 3-port IC field. The conservation of linear momentum for the nodal velocity is represented at the inertial port, while mass and entropy conservation equations are represented at the capacitive ports. All kind of boundary conditions are handled consistently and can be represented as generalized modulated effort sources at the inertial port or modulated flow sources at the capacitive ports.

Keywords: Computational Fluid Dynamics, boundary conditions.

1. Introduction

Since the invention of the Bond Graph formalism by Professor Henry Paynter [1] , 40 years ago, this technique has become a powerful tool for modeling and simulating dynamic systems. Used in the beginning in the fields of Electrical and Mechanical Engineering, applications in different areas such as Thermodynamics, Electrodynamics, and even economical systems have been extremely successful. In the field of Fluid Dynamics, however, the potential benefits of Bond Graphs have not yet been exploited. The applications made so far dealt with problem restrictions such as the neglect of inertia terms (which amounts for the major non-linearities), very simple flow geometries, or the use of the so-called "pseudo bond graphs". Once the Bond Graph representation of a system has been obtained, there is a systematic procedure for:

1. Determination of the state variables;
2. Determination of the input variables, which are equivalent to the boundary conditions, by means of generalized effort and flow sources;
3. Assignment of causality, which assures the mathematical well posedness of the state equations; and
4. Determination of the state equations and output variables.

In this way, the Bond Graph formalism can be regarded as a filter through which mathematical inconsistencies can be detected in the modeling process from the very beginning.

An important fraction of the problems in Fluid Mechanics fall within what is called Computational Fluid Dynamics (CFD). This branch of the human knowledge has nurtured the development of various numerical approaches (e.g.: Finite Elements, Finite Volumes, Finite Differences, etc.). In general, all these methods try to solve the problem by discretizing the continua, that is, by replacing the continuous variables by a combination of a finite set of interpolating functions. The result is a (generally nonlinear) algebraic problem, instead of the original differential or integro-differential one.

Although Bond Graphs have been applied to Fluid Mechanics, the applications to fluid dynamic systems were not oriented to a systematic discretization of flow fields, typical of CFD problems. As far as we know, the first attempt to apply Bond Graphs to CFD problems appeared in [2] , although the formulation was restricted to a prescribed nodalization and heat conduction (which lead to convection-diffusion problems) was not modeled. The purpose of this paper is to present a new approach for CFD problems based on the Bond Graph formalism. This approach provides a systematic procedure for volume integrating the power conservation equations in order to get the state equations, which are based on lumped parameters.

The organization of this paper is developed as follows [3] :

1. Based on the total energy rate per unit volume, a set of independent variables (namely entropy per unit volume, density and velocity) 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). From the first derivatives of the total energy per unit volume the constitutive relations are defined, while from the equality of the mixed partial derivatives the Maxwell relations are presented. Finally, the balance equations corresponding to each one of the terms that contributes to the time derivative of the total energy per unit volume are shown.
2. The formalism is extended to a system having a finite volume by defining, for each independent variable, time dependent nodal values and interpolation functions. The nodal vectors of entropy and mass are defined as volume integrals of the corresponding independent variables weighted by the interpolation functions, in such a way that these nodal vectors and the nodal velocity vector are used as Bond Graph state variables. Based on the system total energy, nodal vectors of associated potentials, constitutive relations and Maxwell relations are defined in the same fashion as it was done for the differential volume; in this way, it can be defined an IC field associated to the system total energy.
3. Next, the system state equations are obtained by systematically volume integrating the balance equations corresponding to each port of the IC field.
4. A generic Bond Graph model can be formulated to represent energy storage. 0-elements are used to add entropy rates and mass rates at the field capacitive ports, while a 1-element is used to add all the nodal vector forces. Modulated transformers and a modulated resistance are used to relate generalized variables, whose product gives raise to power terms appearing in more than one port.
5. Finally, modulated flow and effort sources are added to model the different boundary conditions associated correspondingly to the capacitive ports and the inertial port, as well as to represent volumetric sources.

2. Power balance per unit volume

In this section, we present the balance equations and the constitutive and Maxwell relations in terms of a set of independent variables, considering a differential volume. The results obtained in this section will be used in applying the Bond Graph formalism to a system having a finite volume.

2.1 Total Energy

The total energy per unit volume e_v^* is defined as the sum of the internal energy per unit volume u_v and the kinetic coenergy per unit volume t_v^*:

$$e_v^* = u_v(s_v,\, \rho) + t_v^*(\rho, \mathbf{V}) \tag{1}$$

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We assume that the internal energy per unit volume is a function of density ρ and entropy per unit volume $s_v = \rho\, s$, where s is the entropy per unit mass. The kinetic coenergy per unit volume is defined as $t_v^* = \frac{1}{2}\,\rho\,\mathbf{V}^2$, where $\mathbf{V}$ is the velocity. We define the following potentials [5] :

$$\mathbf{p}_v = \left(\frac{\partial t_v^*}{\partial \mathbf{V}}\right)_\rho = \rho\,\mathbf{V} \tag{2}$$

$$\kappa = \left(\frac{\partial t_v^*}{\partial \rho}\right)_{\mathbf{V}} = \frac{1}{2}\,\mathbf{V}^2 \tag{3}$$

$$\theta = \left(\frac{\partial u_v}{\partial s_v}\right)_\rho \tag{4}$$

$$\psi = \frac{1}{\rho}\,(u_v + P - \theta\, s_v) = \left(\frac{\partial u_v}{\partial \rho}\right)_{s_v} \tag{5}$$

where $\mathbf{p}_v$, κ, θ and ψ are correspondingly the linear momentum per unit volume, the kinetic coenergy per unit mass, the temperature and the Gibbs free energy per unit mass. The time derivative of the total energy per unit volume can be written as:

$$\frac{\partial e_v^*}{\partial t} = \theta\,\frac{\partial s_v}{\partial t} + (\psi+\kappa)\,\frac{\partial \rho}{\partial t} + \mathbf{p}_v.\frac{\partial \mathbf{V}}{\partial t} \tag{6}$$

2.2 Constitutive relations

The resulting constitutive relations come from the first derivatives of the total energy per unit volume:

$$\theta = \theta(s_v,\,\rho) \tag{7}$$

$$\psi + \kappa = \psi(s_v,\,\rho) + \kappa(\mathbf{V}) \tag{8}$$

$$\mathbf{p}_v = \mathbf{p}_v(\rho,\,\mathbf{V}) = \rho\,\mathbf{V} \tag{9}$$

2.3 Maxwell relations

The Maxwell relations arise from the equality of the mixed partial derivatives of the total energy per unit volume expressed as a function of the independent variables s_v, ρ and $\mathbf{V}$:

$$\frac{\partial \theta}{\partial \rho} = \frac{\partial}{\partial s_v}\,(\psi+\kappa) = \frac{\partial \psi}{\partial s_v} \tag{10}$$

$$\frac{\partial \theta}{\partial \mathbf{V}} = \frac{\partial \mathbf{p}_v}{\partial s_v} = 0 \tag{11}$$

$$\frac{\partial}{\partial \mathbf{V}}\,(\psi+\kappa) = \frac{\partial \kappa}{\partial \mathbf{V}} = \frac{\partial \mathbf{p}_v}{\partial \rho} = \mathbf{V} \tag{12}$$

2.4 Balance equations

The balance equations are power equations corresponding to each one of the terms that contributes to the time derivative of the total energy per unit volume, namely Eq. (6). They can be obtained starting from the conservation equations [4] and the potentials:

$$\begin{aligned}\mathbf{p}_v\cdot\frac{\partial \mathbf{V}}{\partial t} &= \rho\,\mathbf{G}\,.\,\mathbf{V} + \nabla.\left(\mathbf{V}\,.\,\underline{\underline{\tau}}\right) - \mathbf{V}\,.\,\nabla P \\ &\quad -\rho\,\mathbf{V}\,.\,\nabla\kappa - \nabla\mathbf{V} : \underline{\underline{\tau}}\end{aligned} \tag{13}$$

$$\theta\,\frac{\partial s_v}{\partial t} = -\theta\,\nabla.\,(s_v\,\mathbf{V}) - \nabla.\mathbf{q} + \nabla\mathbf{V} : \underline{\underline{\tau}} + \Phi \tag{14}$$

$$\begin{aligned}(\psi+\kappa)\,\frac{\partial \rho}{\partial t} &= -\nabla.\,[\rho\,(h+\kappa)\,\mathbf{V}] + \mathbf{V}\,.\,\nabla P \\ &\quad +\theta\,\nabla.\,(s_v\,\mathbf{V}) + \rho\,\mathbf{V}\,.\,\nabla\kappa\end{aligned} \tag{15}$$

where t is the time, $\mathbf{q}$ is the heat flux, P is the pressure, $\mathbf{G}$ is the force per unit mass, $\underline{\underline{\tau}}$ is the viscous stress tensor, Φ is the volumetric heat source and $h = \frac{1}{\rho}\,(u_v + P)$ is the enthalpy per unit mass. It is important to notice that all the terms in Eqs. (13), (14) and (15) can be written as a function of the independent variables through the constitutive relations and three independent derivatives [5] , namely:

$$\alpha = -\frac{1}{\rho}\left(\frac{\partial \rho}{\partial \theta}\right)_P \tag{16}$$

$$c_v = \theta\left(\frac{\partial s}{\partial \theta}\right)_\rho \tag{17}$$

$$\kappa_\theta = \frac{1}{\rho}\left(\frac{\partial \rho}{\partial P}\right)_\theta \tag{18}$$

where α, c_v and κ_θ are correspondingly the coefficient of thermal expansion, the constant volume specific heat and the coefficient of isothermal compressibility. In this way, assuming Fourier's law, the heat flux can be calculated as:

$$\mathbf{q} = -\lambda\,\nabla\theta = -\frac{\lambda\,\theta}{\rho\,c_v}\left[\nabla s_v + \frac{1}{\rho}\left(\frac{\alpha}{\kappa_\theta} - s_v\right)\nabla\rho\right] \tag{19}$$

where λ is the thermal conductivity. The pressure gradient can be expressed as:

$$\nabla P = \frac{\theta}{\rho\,c_v}\,\frac{\alpha}{\kappa_\theta}\left[\nabla s_v + \left(\frac{c_v}{\alpha\,\theta} + \frac{\alpha}{\rho\,\kappa_\theta} - \frac{s_v}{\rho}\right)\nabla\rho\right] \tag{20}$$

The viscous stress tensor $\underline{\underline{\tau}}$ can be expressed for a newtonian fluid, assuming Stoke's hypothesis, as:

$$\underline{\underline{\tau}} = \mu\,\left(\nabla\mathbf{V} + \nabla\mathbf{V}^T\right) - \frac{2}{3}\,\mu\,(\nabla.\mathbf{V})\,\underline{\underline{\mathbf{I}}} \tag{21}$$

where μ is the fluid viscosity.

3. Discretization

In order to formulate the discrete model of the fluid continuum in the domain Ω, it is necessary to specify the description of the flow fields. For each discretized variable, the following time-dependent nodal values and interpolation functions are defined:

$$\rho\,(\mathbf{r},t) = \sum_{k=1}^{n_\rho} \rho_k\,(t)\;\varphi_{\rho k}\,(\mathbf{r}) = \underline{\rho}^T\cdot\underline{\varphi_\rho} \tag{22}$$

$$s_v\,(\mathbf{r},t) = \sum_{l=1}^{n_s} s_{vl}\,(t)\;\varphi_{sl}\,(\mathbf{r}) = \underline{s_v}^T\cdot\underline{\varphi_s} \tag{23}$$

$$\mathbf{V}\,(\mathbf{r},t) = \sum_{m=1}^{n_V} \mathbf{V}_m\,(t)\;\varphi_{Vm}\,(\mathbf{r}) = \underline{\mathbf{V}}^T\cdot\underline{\varphi_V} \tag{24}$$

where $\underline{\rho}$, $\underline{s_v}$ and $\underline{\mathbf{V}}$ are time-dependent nodal vectors, while $\underline{\varphi_\rho}$, $\underline{\varphi_s}$ and $\underline{\varphi_V}$ are the corresponding nodal interpolation or shape functions. The interpolation functions have the following properties:

$$\sum_{m=1}^{n_V} \varphi_{Vm}\,(\mathbf{r}) = 1 \qquad \forall\,\mathbf{r}\,\in\,\Omega \tag{25}$$

$$\sum_{k=1}^{n_\rho} \varphi_{\rho k}\,(\mathbf{r}) = 1 \qquad \forall\,\mathbf{r}\,\in\,\Omega \tag{26}$$

$$\sum_{l=1}^{n_s} \varphi_{sl}\,(\mathbf{r}) = 1 \qquad \forall\,\mathbf{r}\,\in\,\Omega \tag{27}$$

For simplicity in the treatment of the boundary conditions, we also require for the interpolation functions the following properties:

$$\varphi_{Vm}\,(\mathbf{r}_n) = \delta_{mn} \tag{28}$$

$$\varphi_{\rho k}\,(\mathbf{r}_n) = \delta_{kn} \tag{29}$$

$$\varphi_{sl}(\mathbf{r}_n) = \delta_{ln} \tag{30}$$

for any velocity, density or entropy node located at position $\mathbf{r}_n$. In Eqs. (28), (29) and (30) δ_{kn} is the Kronecker delta ($\delta_{kn} = 1$ if $k = n$, $\delta = 0$ otherwise).

4. Integrated variables

The system mass, entropy and lineal momentum can be obtained by volume integrating the discretized variables:

$$m = \int_\Omega \rho \, d\Omega = \sum_{k=1}^{n_\rho} m_k \tag{31}$$

$$S = \int_\Omega s_v \, d\Omega = \sum_{l=1}^{n_s} S_l \tag{32}$$

$$\mathbf{p} = \int_\Omega \mathbf{p}_v \, d\Omega = \int_\Omega \rho \mathbf{V} \, d\Omega \tag{33}$$

Based on Eq. (31) and (32) we define nodal vectors of integrated values, related to the discretized ones as:

$$\underline{m} = \underline{\underline{\Omega_\rho}} \cdot \underline{\rho} \tag{34}$$

$$\underline{S} = \underline{\underline{\Omega_s}} \cdot \underline{s_v} \tag{35}$$

where $\underline{\underline{\Omega_\rho}}$ and $\underline{\underline{\Omega_s}}$ are correspondingly diagonal volume matrices associated to the density and entropy per unit volume:

$$\underline{\underline{\Omega_\rho}} = (\Omega_\rho)_{kn} = \int_\Omega \varphi_{\rho k} \, \delta_{kn} \, d\Omega \tag{36}$$

$$\underline{\underline{\Omega_s}} = (\Omega_s)_{ln} = \int_\Omega \varphi_{sl} \, \delta_{ln} \, d\Omega \tag{37}$$

5. System integration

5.1 Total Energy

The system total energy E^* is defined as the sum of the system internal energy U and the system kinetic coenergy T^*:

$$E^* = E^*(\underline{S}, \underline{m}, \underline{\mathbf{V}}) = U(\underline{S}, \underline{m}) + T^*(\underline{m}, \underline{\mathbf{V}}) \tag{38}$$

where:

$$E^* = \int_\Omega e_v^* \, d\Omega \tag{39}$$

$$U = \int_\Omega u_v \, d\Omega = U(\underline{S}, \underline{m}) \tag{40}$$

$$T^* = \int_\Omega t_v^* \, d\Omega = T^*(\underline{m}, \underline{\mathbf{V}}) \tag{41}$$

It can be shown that:

$$T^* = \frac{1}{2} \underline{\mathbf{V}}^T \cdot \underline{\underline{M}} \cdot \underline{\mathbf{V}} \tag{42}$$

where $\underline{\underline{M}}$ is the system inertia matrix (symmetric and regular):

$$\underline{\underline{M}} = (M)_{mn} = \int_\Omega \rho \, \varphi_{Vm} \, \varphi_{Vn} \, d\Omega \tag{43}$$

We define the following potentials:

$$\underline{\mathbf{p}}(\underline{m}, \underline{\mathbf{V}}) = \frac{\partial T^*}{\partial \underline{\mathbf{V}}} = \underline{\underline{M}} \cdot \underline{\mathbf{V}} = \int_\Omega \mathbf{p}_v \, \underline{\varphi_V} \, d\Omega \tag{44}$$

$$\underline{K}(\underline{\mathbf{V}}) = \frac{\partial T^*}{\partial \underline{m}} = \underline{\underline{\Omega_\rho}}^{-1} \cdot \left[\int_\Omega \kappa \, \underline{\varphi_\rho} \, d\Omega \right] \tag{45}$$

$$\underline{\Theta}(\underline{S}, \underline{m}) = \frac{\partial U}{\partial \underline{S}} = \underline{\underline{\Omega_s}}^{-1} \cdot \left[\int_\Omega \theta \, \underline{\varphi_s} \, d\Omega \right] \tag{46}$$

$$\underline{\Psi}(\underline{S}, \underline{m}) = \frac{\partial U}{\partial \underline{m}} = \underline{\underline{\Omega_\rho}}^{-1} \cdot \left[\int_\Omega \psi \, \underline{\varphi_\rho} \, d\Omega \right] \tag{47}$$

where $\underline{\mathbf{p}}$, $\underline{K}$, $\underline{\Theta}$ and $\underline{\Psi}$ are correspondingly nodal vectors of linear momentum, kinetic coenergy per unit mass, temperature and Gibbs free energy per unit mass. It is important to notice that Eq. (44) defines a modulated transformer relating the nodal vectors of velocity and linear momentum. According to the power conservation across the transformer, the generalized effort is given by:

$$\underline{\mathbf{F}} = \underline{\underline{M}} \cdot \dot{\underline{\mathbf{V}}} \tag{48}$$

According to Eqs. (45) to (47), the nodal potential vectors can be regarded as system volume averages of the corresponding local values, weighted by the interpolation functions. Therefore, it is important to realize that the values of the nodal vectors are in general different to the corresponding nodal values calculated with the local variables. The time derivative of the system total energy can be written as:

$$\dot{E}^* = \underline{\Theta}^T \cdot \dot{\underline{S}} + (\underline{\Psi} + \underline{K})^T \cdot \dot{\underline{m}} + \underline{\mathbf{p}}^T \cdot \dot{\underline{\mathbf{V}}} \tag{49}$$

Taking into account Eq. (44) to (47) it can be easily shown that the system linear momentum can be obtained as:

$$\mathbf{p} = \int_\Omega \mathbf{p}_v \, d\Omega = \sum_{m=1}^{n_V} \mathbf{p}_m \tag{50}$$

It can also be shown that the volume integrals of the left side terms of Eqs. (13) to (15) can be calculated as:

$$\int_\Omega \mathbf{p}_v \cdot \frac{\partial \mathbf{V}}{\partial t} \, d\Omega = \underline{\mathbf{p}}^T \cdot \dot{\underline{\mathbf{V}}} \tag{51}$$

$$\int_\Omega \theta \, \frac{\partial s_v}{\partial t} \, d\Omega = \underline{\Theta}^T \cdot \dot{\underline{S}} \tag{52}$$

$$\int_\Omega (\kappa + \psi) \, \frac{\partial \rho}{\partial t} \, d\Omega = (\underline{K} + \underline{\Psi})^T \cdot \dot{\underline{m}} \tag{53}$$

5.2 Constitutive Relations

The system constitutive relations are:

$$\frac{\partial E^*}{\partial \underline{S}} = \frac{\partial U}{\partial \underline{S}} = \underline{\Theta}(\underline{S}, \underline{m}) \tag{54}$$

$$\frac{\partial E^*}{\partial \underline{m}} = \frac{\partial U}{\partial \underline{m}} + \frac{\partial T^*}{\partial \underline{m}} = \underline{\Psi}(\underline{S}, \underline{m}) + \underline{K}(\underline{\mathbf{V}}) \tag{55}$$

$$\frac{\partial E^*}{\partial \underline{\mathbf{V}}} = \frac{\partial T^*}{\partial \underline{\mathbf{V}}} = \underline{\mathbf{p}}(\underline{m}, \underline{\mathbf{V}}) \tag{56}$$

5.3 Maxwell Relations

The Maxwell relations corresponding to the system total energy arise from the equality of the mixed partial derivatives of the system total energy expressed as a function of the independent variables $\underline{S}$, $\underline{m}$ and $\underline{\mathbf{V}}$. These variables are regarded as the state variables for the Bond Graph formalism:

$$\frac{\partial \underline{\Theta}}{\partial \underline{m}} = \frac{\partial}{\partial \underline{S}} (\underline{\Psi} + \underline{K}) = \frac{\partial \underline{\Psi}}{\partial \underline{S}} \tag{57}$$

$$\frac{\partial \underline{\Theta}}{\partial \underline{\mathbf{V}}} = \frac{\partial \mathbf{p}}{\partial \underline{S}} = \underline{\underline{0}} \tag{58}$$

$$\frac{\partial \mathbf{p}}{\partial \underline{m}} = \frac{\partial}{\partial \underline{\mathbf{V}}} \left(\underline{\Psi} + \underline{K}\right) = \frac{\partial \underline{K}}{\partial \underline{\mathbf{V}}} \tag{59}$$

5.4 System *IC* Field

The constitutive relations (namely Eqs. (54), (55) and (56)) and the Maxwell relations (Eqs. (57), (58) and (59)) define an IC field associated to the system total energy. This field has an inertial port ($\underline{\mathbf{p}}^T \,.\, \underline{\dot{\mathbf{V}}}$) and two capacitive ports ($\underline{\Theta}^T \,.\, \underline{\dot{S}}$ and $(\underline{\Psi} + \underline{K})^T \,.\, \underline{\dot{m}}$). The generalized effort variables associated to these ports are $\underline{\dot{\mathbf{V}}}$, $\underline{\Theta}$ and $(\underline{\Psi} + \underline{K})$, while the generalized flow variables are correspondingly $\underline{\mathbf{p}}$, $\underline{\dot{S}}$ and $\underline{\dot{m}}$.

6. System Balance Equations

The system balance equations can be obtained by systematically volume integrating the balance equations corresponding to each port of the IC field.

6.1 Port $\underline{\mathbf{p}}^T \,.\, \underline{\dot{\mathbf{V}}}$

Each term of Eq. (13) is integrated in such a way that the result can be expressed as a product of a corresponding nodal force vector (generalized effort) times the nodal velocity vector $\underline{\mathbf{V}}$ (generalized flow):

$$\underline{\mathbf{p}}^T \,.\, \underline{\dot{\mathbf{V}}} = \left(\underline{\mathbf{F}_G} - \underline{\mathbf{F}_P} - \underline{\mathbf{F}_K} - \underline{\mathbf{F}_D} + \underline{\mathbf{F}_T^{(\Gamma)}}\right)^T \,.\, \underline{\mathbf{V}} \tag{60}$$

where:

$$\underline{\mathbf{F}_G} = \int_\Omega \rho\, \mathbf{G}\, \underline{\varphi_V}\, d\Omega \tag{61}$$

$$\underline{\mathbf{F}_P} = \int_\Omega \nabla P\, \underline{\varphi_V}\, d\Omega \tag{62}$$

$$\underline{\mathbf{F}_K} = \int_\Omega \rho\, \nabla\kappa\, \underline{\varphi_V}\, d\Omega \tag{63}$$

$$\underline{\mathbf{F}_D} = \int_\Omega \left[\nabla.\left(\underline{\varphi_V}\, \underline{\underline{\tau}}\right) - \underline{\varphi_V}\left(\nabla \,.\, \underline{\underline{\tau}}\right)\right] d\Omega \tag{64}$$

$$\underline{\mathbf{F}_T^{(\Gamma)}} = \int_\Gamma \left(\underline{\underline{\tau}} \,.\, \breve{\mathbf{n}}\right) \underline{\varphi_V}\, d\Gamma \tag{65}$$

6.2 Port $\underline{\Theta}^T \,.\, \underline{\dot{S}}$

We define a diagonal temperature matrix, whose diagonal elements are the components of the nodal temperature vector $\underline{\Theta}$:

$$\underline{\underline{\Theta}} = (\Theta)_{ln} = \Theta_l\, \delta_{ln} \tag{66}$$

We also introduce nodal entropy weight functions w_{sl} with the following properties:

$$\sum_{l=1}^{n_s} w_{sl}(\mathbf{r}, t) = 1 \qquad \forall\, t,\ \forall\, \mathbf{r} \in \Omega \tag{67}$$

$$w_{sl}(\mathbf{r}_n, t) = \delta_{ln} \tag{68}$$

for an entropy node located at position $\mathbf{r}_n$. Each term of Eq. (14) is integrated in such a way that the result can be expressed as a product of the nodal temperature vector $\underline{\Theta}$ (generalized effort) times a corresponding nodal entropy rate vector (generalized flow):

$$\underline{\Theta}^T \,.\, \underline{\dot{S}} = \underline{\Theta}^T \,.\, \left(\underline{\dot{S}_{QF}} + \underline{\dot{S}_Q^{(\Gamma)}} - \underline{\dot{S}_C} + \underline{\dot{S}_D} + \underline{\dot{S}_F}\right) \tag{69}$$

where:

$$\underline{\dot{S}_{QF}} = \underline{\underline{\Theta}}^{-1} \,.\, \left[\int_\Omega \mathbf{q} \,.\, \nabla \underline{w_s}\, d\Omega\right] \tag{70}$$

$$\underline{\dot{S}_Q^{(\Gamma)}} = -\,\underline{\underline{\Theta}}^{-1} \,.\, \left[\int_\Gamma \underline{w_s}\, \mathbf{q} \,.\, \breve{\mathbf{n}}\, d\Gamma\right] \tag{71}$$

$$\underline{\dot{S}_C} = \underline{\underline{\Theta}}^{-1} \,.\, \left[\int_\Omega \underline{w_s}\, \theta\, \nabla.\left(s_v\, \mathbf{V}\right)\, d\Omega\right] \tag{72}$$

$$\underline{\dot{S}_D} = \underline{\underline{\Theta}}^{-1} \,.\, \left[\int_\Omega \underline{w_s}\left(\nabla\mathbf{V} : \underline{\underline{\tau}}\right) d\Omega\right] \tag{73}$$

$$\underline{\dot{S}_F} = \underline{\underline{\Theta}}^{-1} \,.\, \left[\int_\Omega \underline{w_s}\, \Phi\, d\Omega\right] \tag{74}$$

6.3 Port $(\underline{\Psi} + \underline{K})^T \,.\, \underline{\dot{m}}$

We define diagonal matrices, whose diagonal elements are correspondingly the components of the nodal Gibbs free energy per unit mass vector and the nodal coenergy per unit mass vector:

$$\underline{\underline{\Psi}} = (\Psi)_{kn} = \Psi_k\, \delta_{kn} \tag{75}$$

$$\underline{\underline{K}} = (K)_{kn} = K_k\, \delta_{kn} \tag{76}$$

We also introduce nodal density weight functions $w_{\rho l}$ with the following properties:

$$\sum_{l=1}^{n_s} w_{\rho l}(\mathbf{r}, t) = 1 \qquad \forall\, t,\ \forall\, \mathbf{r} \in \Omega \tag{77}$$

$$w_{\rho k}(\mathbf{r}_n, t) = \delta_{kn} \tag{78}$$

for a density node located at position $\mathbf{r}_n$. Each term of Eq. (15) is integrated in such a way that the result can be expressed as a product of the nodal vector $(\underline{\Psi} + \underline{K})$ (generalized effort) times a corresponding nodal mass rate vector (generalized flow):

$$(\underline{\Psi} + \underline{K})^T \,.\, \underline{\dot{m}} = (\underline{\Psi} + \underline{K})^T \,.\, \left(-\underline{\dot{m}_{WF}} - \underline{\dot{m}_W^{(\Gamma)}} + \underline{\dot{m}_P} + \underline{\dot{m}_C} + \underline{\dot{m}_K}\right) \tag{79}$$

where:

$$\underline{\dot{m}_{WF}} = -\left(\underline{\underline{\Psi}} + \underline{\underline{K}}\right)^{-1} \,.\, \left[\int_\Omega \rho\, (h + \kappa)\, \mathbf{V} \,.\, \nabla \underline{w_\rho}\, d\Omega\right] \tag{80}$$

$$\underline{\dot{m}_W^{(\Gamma)}} = \left(\underline{\underline{\Psi}} + \underline{\underline{K}}\right)^{-1} \,.\, \left\{\int_\Gamma \left[\underline{w_\rho}\, \rho\, (h + \kappa)\, \mathbf{V}\right] .\, \breve{\mathbf{n}}\, d\Gamma\right\} \tag{81}$$

$$\underline{\dot{m}_P} = \left(\underline{\underline{\Psi}} + \underline{\underline{K}}\right)^{-1} \,.\, \left[\int_\Omega \underline{w_\rho}\, \mathbf{V} \,.\, \nabla P\, d\Omega\right] \tag{82}$$

$$\underline{\dot{m}_C} = \left(\underline{\underline{\Psi}} + \underline{\underline{K}}\right)^{-1} \,.\, \left[\int_\Omega \underline{w_\rho}\, \theta\, \nabla.\left(s_v\, \mathbf{V}\right)\, d\Omega\right] \tag{83}$$

$$\underline{\dot{m}_K} = \left(\underline{\underline{\Psi}} + \underline{\underline{K}}\right)^{-1} \,.\, \left[\int_\Omega \underline{w_\rho}\, \rho\, \mathbf{V} \,.\, \nabla\kappa\, d\Omega\right] \tag{84}$$

7. System Bond Graph

The resulting system Bond Graph is shown in Fig. 1. A modulated transformer with transformation matrix $\underline{\underline{M}}$ is connected to the port

$\underline{\mathbf{p}}^T \cdot \dot{\underline{\mathbf{V}}}$. At the 1-element with common $\underline{\mathbf{V}}$ we add all the nodal vector forces; in this way, the effort balance represents the linear momentum conservation equation for the nodal velocity values. At the 0-element with common $(\underline{\Psi} + \underline{K})$ we add all the nodal mass changes per unit time; in this way, the flow balance represents the mass conservation equations for the nodal mass values. At the 0-element with common $\underline{\Theta}$ we add all the nodal entropy changes per unit time; in this way, the flow balance represents the thermal energy conservation equation for the nodal entropy values. The modulated sources are needed to represent the different boundary conditions established in the problem, as well as to represent volumetric sources. The modulated transformers and the modulated resistance field connect power terms that appear in the conservation equations corresponding to more than one IC port. It can be shown [3] that:

$$\underline{\dot{m}_P} + \underline{\dot{m}_K} = \left[\left(\underline{\Psi} + \underline{K} \right)^{-1} \cdot \underline{\underline{M_{PK}}} \right] \cdot \underline{\mathbf{V}} \tag{85}$$

$$\underline{\mathbf{F}_P} + \underline{\mathbf{F}_K} = \left[\left(\underline{\Psi} + \underline{K} \right)^{-1} \cdot \underline{\underline{M_{PK}}} \right]^T \cdot \left(\underline{\Psi} + \underline{K} \right) \tag{86}$$

$$\underline{\dot{m}_C} = \left[\left(\underline{\Psi} + \underline{K} \right)^{-1} \cdot \underline{\underline{M_\theta}} \cdot \underline{\underline{\Theta}}^{-1} \right] \cdot \underline{\Theta} \tag{87}$$

$$\underline{\dot{S}_C} = \left[\left(\underline{\Psi} + \underline{K} \right)^{-1} \cdot \underline{\underline{M_\theta}} \cdot \underline{\underline{\Theta}}^{-1} \right]^T \cdot \left(\underline{\Psi} + \underline{K} \right) \tag{88}$$

$$\underline{\mathbf{F}_D} = \left[\underline{\underline{M_S}} \cdot \underline{\underline{\Theta}}^{-1} \right] \cdot \underline{\Theta} \tag{89}$$

$$\underline{\dot{S}_D} = \left[\underline{\underline{M_S}} \cdot \underline{\underline{\Theta}}^{-1} \right]^T \cdot \underline{\mathbf{V}} \tag{90}$$

where the rectangular matrices $\underline{\underline{M_{PK}}}$ (n_ρ rows x n_V columns), $\underline{\underline{M_\theta}}$ (n_ρ x n_s) and $\underline{\underline{M_S}}$ (n_V x n_s) are correspondingly defined as:

$$\left(M_{PK} \right)_{km} = \int_\Omega w_{\rho k}\, \varphi_{Vm}\, \left(\nabla P + \rho\, \nabla \kappa \right)\, d\Omega \tag{91}$$

$$\left(M_\theta \right)_{kl} = \int_\Omega w_{\rho k}\, w_{sl}\, \theta\, \nabla . \left(s_v\, \mathbf{V} \right)\, d\Omega \tag{92}$$

$$\left(M_S \right)_{ml} = \int_\Omega w_{sl} \left[\nabla . \left(\varphi_{Vm}\, \underline{\underline{\tau}} \right) - \varphi_{Vm} \left(\nabla . \underline{\underline{\tau}} \right) \right] d\Omega \tag{93}$$

Since the transformation matrices are in general not inversible, it means that there exist restrictions in the allowable causalities.

8. State Equations

The system state equations are:

$$\dot{\underline{\mathbf{V}}} = \underline{\underline{M}}^{-1} \cdot \left(\underline{\mathbf{F}_G} - \underline{\mathbf{F}_P} - \underline{\mathbf{F}_K} - \underline{\mathbf{F}_D} + \underline{\mathbf{F}_T^{(\Gamma)}} \right) \tag{94}$$

$$\underline{\dot{S}} = \underline{\dot{S}_{QF}} + \underline{\dot{S}_Q^{(\Gamma)}} - \underline{\dot{S}_C} + \underline{\dot{S}_D} + \underline{\dot{S}_F} \tag{95}$$

$$\underline{\dot{m}} = -\underline{\dot{m}_{WF}} - \underline{\dot{m}_W^{(\Gamma)}} + \underline{\dot{m}_P} + \underline{\dot{m}_C} + \underline{\dot{m}_K} \tag{96}$$

In order to solve the state equations, we need to set initial and boundary conditions.

9. Initial Conditions

Initial conditions can be written as:

$$\underline{S}\,(t=0) = \underline{S_0} \tag{97}$$

$$\underline{m}\,(t=0) = \underline{m_0} \tag{98}$$

$$\underline{\mathbf{V}}\,(t=0) = \underline{\mathbf{V}_0} \tag{99}$$

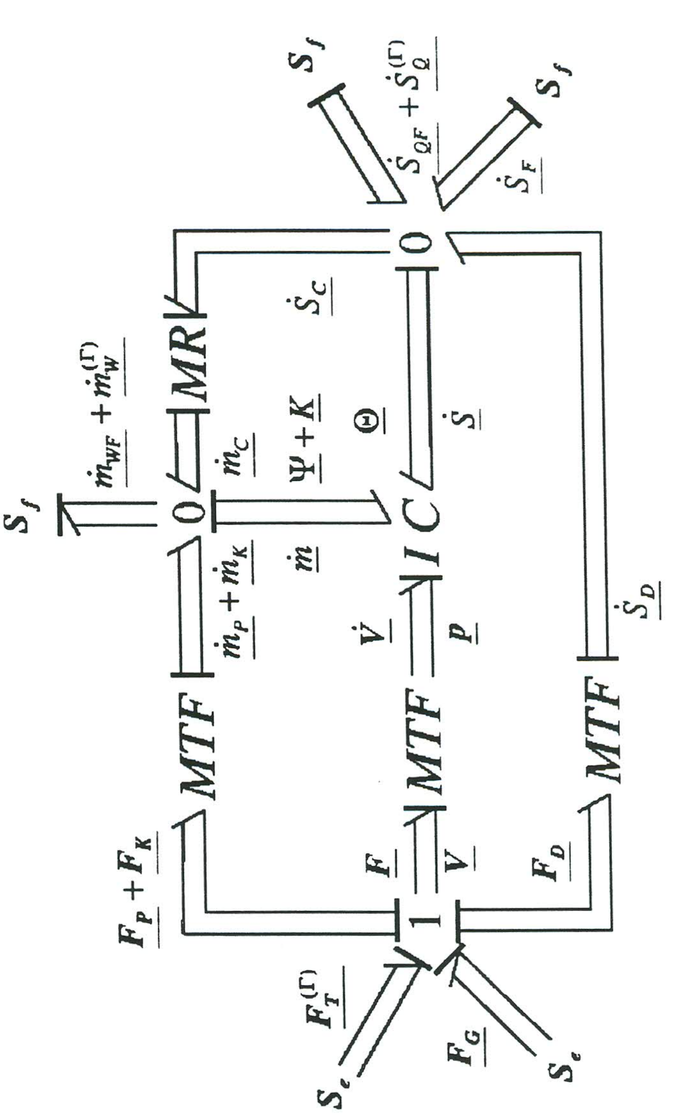

Figure 1: System Bond Graph.

10. Boundary Conditions

The boundary conditions establish relationships among the variables corresponding to the nodes related to the system surface. All possible boundary conditions can be modeled in terms of generalized sources connected to the ports $\underline{\Theta}^T \cdot \underline{\dot{S}_Q^{(\Gamma)}}$, $(\underline{\Psi} + \underline{K})^T \cdot \underline{\dot{m}_W^{(\Gamma)}}$ and $\underline{\mathbf{F}_T^{(\Gamma)}}^T \cdot \underline{\mathbf{V}}$.

10.1 Imposed Surface Heat Flux (Neumann)

The Neumann boundary condition can be stated as:

$$\mathbf{q}\,(\mathbf{r}_{\Gamma_N},\, t)\ .\, \breve{\mathbf{n}} = q_{\Gamma_N}\,(\mathbf{r}_{\Gamma_N},\, t) \tag{100}$$

Introducing the weight functions w_{sl} and integrating over the surface Γ_N with Neumann boundary condition, we finally get:

$$\underline{\dot{S}_Q^{(\Gamma_N)}} = -\,\underline{\underline{\Theta}}^{-1} \cdot \left[\int_{\Gamma_N} \underline{w_s}\, q_{\Gamma_N}\, d\Gamma \right] \tag{101}$$

10.2 Imposed Surface Temperature (Dirichlet)

The Dirichlet boundary condition can be stated as:

$$\theta\,(\mathbf{r}_{\Gamma_D},\, t) = \theta_{\Gamma_D}\,(\mathbf{r}_{\Gamma_D},\, t) \tag{102}$$

Considering a functional dependence through the discretized variables, we have:

$$\theta(\mathbf{r},t)=\theta(s_v(\mathbf{r},t),\rho(\mathbf{r},t)) = \theta\left(\sum_{l=1}^{n_s} s_{vl}(t)\,\varphi_{sl}(\mathbf{r}),\ \sum_{k=1}^{n_\rho}\rho_k(t)\,\varphi_{\rho k}(\mathbf{r})\right) \quad (103)$$

Let us consider the set of n_{Γ_D} entropy nodes located at the positions $\mathbf{r}_i$ $(i=1,...,n_{\Gamma_D})$ in which the Dirichlet boundary condition is established. For these positions, only the interpolating function for the corresponding node takes the value 1 and the rest take the value 0, so we can write:

$$\theta_i(t)=\theta(\mathbf{r}_i,t)=\theta\left(\frac{S_i(t)}{(\Omega_s)_{ii}},\ \sum_{k=1}^{n_\rho}\frac{m_k(t)}{(\Omega_\rho)_{kk}}\varphi_{\rho k}(\mathbf{r}_i)\right) \quad (104)$$

From Eq. (104) it is possible to obtain $S_i(t)$ as a function of the boundary condition $\theta_i(t)$. Derivating Eq. (104) with respect to time we get:

$$\frac{d\theta_i}{dt}=\left[\frac{\theta}{\rho\, c_v}\right](\mathbf{r}_i,t)\left\{\frac{\dot S_i(t)}{(\Omega_s)_{ii}} + \left[\frac{1}{\rho}\left(\frac{\alpha}{\kappa_\theta}-s_v\right)\right](\mathbf{r}_i,t)\sum_{k=1}^{n_\rho}\frac{\dot m_k(t)}{(\Omega_\rho)_{kk}}\varphi_{\rho k}(\mathbf{r}_i)\right\} \quad (105)$$

Replacing $\dot S_i$ and $\dot m_k$ from the state equations, namely Eq. (95) for node i and Eq. (96) for nodes k, we get the nodal entropy rate vector $\underline{\dot S_Q^{(\Gamma_D)}}$ due to the heat power flowing through the surface Γ_D with Dirichlet boundary conditions as a function of the boundary conditions θ_i, $\frac{d\theta_i}{dt}$ and the state variables. In practice, the state equation corresponding to node i are replaced by the expression for $\dot S_i$ obtained from Eq. (105), in which $\dot m_k$ is substituted from the state equations (96).

10.3 Convection (mixed)

The mixed boundary condition can be stated as:

$$\mathbf{q}(\mathbf{r}_{\Gamma_C},t)\,.\,\breve{\mathbf{n}}=H\,(\theta_{\Gamma_C}-\theta_{\Gamma\infty}) \quad (106)$$

where H is the heat transfer coefficient and $\theta_{\Gamma\infty}$ is a reference local surface temperature. Introducing the weight functions w_{sl} and integrating over the surface Γ_C with mixed boundary condition, we finally get:

$$\underline{\dot S_Q^{(\Gamma_C)}}=-\underline{\underline{\Theta}}^{-1}\cdot\left[\int_{\Gamma_C}\underline{w_s}\,H\,(\theta_{\Gamma_C}-\theta_{\Gamma\infty})\,d\Gamma\right] \quad (107)$$

10.4 Imposed velocity field (mass flow port)

In order to calculate Eq. (81) it is necessary to impose at the system surface the velocity field, as well as two independent variables needed to determine the thermodynamic state of the fluid; normally, pressure and temperature are used as boundary conditions, from which density and enthalpy can be calculated. The velocity boundary condition can be stated as:

$$\mathbf{V}(\mathbf{r}_{\Gamma_V},t)=\mathbf{V}_{\Gamma_V} \quad (108)$$

$$\kappa(\mathbf{r}_{\Gamma_V},t)=\kappa_{\Gamma_V} \quad (109)$$

We get, from Eq. (81):

$$\underline{\dot m_W^{(\Gamma_V)}}=\left(\underline{\underline{\Psi}}+\underline{\underline{K}}\right)^{-1}\cdot\left[\int_{\Gamma_V}\left[\underline{w_\rho}\,\rho_{\Gamma_V}\,(h_{\Gamma_V}+\kappa_{\Gamma_V})\,\mathbf{V}_{\Gamma_V}\right].\,\breve{\mathbf{n}}\,d\Gamma\right] \quad (110)$$

10.5 Imposed stress force

The stress force boundary condition can be stated as:

$$\underline{\underline{\tau}}(\mathbf{r}_{\Gamma_\tau},t)\,.\,\breve{\mathbf{n}}=\tau_{\Gamma_\tau} \quad (111)$$

From Eq. (65) the stress force can be written as:

$$\underline{\mathbf{F}_T^{(\Gamma_\tau)}}=\int_{\Gamma_\tau}\tau_{\Gamma_\tau}\,\underline{\varphi_V}\,d\Gamma \quad (112)$$

10.6 Imposed velocity field (force port)

Let us consider the set of n_{Γ_V} velocity nodes located at the positions $\mathbf{r}_j$ $(j=1,...,n_{\Gamma_V})$ in which the velocity boundary condition is established. For these positions we can write:

$$\mathbf{V}_j(t)=\mathbf{V}(\mathbf{r}_j,t) \quad (113)$$

Derivating Eq. (113) with respect to time we get:

$$\dot{\mathbf{V}}_j=\frac{\partial\mathbf{V}}{\partial t}(\mathbf{r}_j,t) \quad (114)$$

Replacing $\dot{\mathbf{V}}_j$ in the state equations, namely Eq. (94) for nodes j, we get the stress force $\underline{\mathbf{F}_T^{(\Gamma_V)}}$ due to the stress power flowing through the surface Γ_V with velocity boundary conditions as a function of the boundary conditions $\mathbf{V}_j$ and the state variables. In practice, the state equation corresponding to node j is replaced by the expression for $\dot{\mathbf{V}}_j$ from Eq. (114).

10.7 Flow and effort sources

It can be observed that any boundary condition related to the port $\underline{\underline{\Theta}}^T\,.\,\underline{\dot S_Q^{(\Gamma)}}$ or $(\underline{\underline{\Psi}}+\underline{\underline{K}})^T\,.\,\underline{\dot m_W^{(\Gamma)}}$ can be regarded as a flow source, while any boundary condition related to the port $\underline{\mathbf{F}_T^{(\Gamma)}}^T\,.\,\underline{\mathbf{V}}$ can be regarded as an effort source. These sources are modulated by the state variables.

11. Conclusions

The present paper addresses the theoretical development of a general Bond Graph approach for Computational Fluid Dynamics. The system state equations are obtained in terms of the state variables, namely nodal values of mass, entropy and velocity. Since the formulation is based on the definition of nodal discretized variables, different numerical schemes can be obtained by means of the appropriate choice of the interpolation and weight functions. This work represents a new approach to CFD and an extension of the Bond Graph methodology to general Fluid Dynamic problems. Examples of application of this formalism are presented in a companion paper [6] .

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