Physical model reduction of interacting, continuous systems

N. E. Ligterink, P. C. Breedveld, and A. J. van der Schaft

***Abstract*— The ab-initio analysis of a continuous system starts with the microscopic theory of the material, usually expressed in terms of partial differential equations, while a system analysis starts with its global properties and interconnections. These two ends must meet for an accurate and effective model of continuous systems. The macroscopic interaction between components is consistently defined by microscopic boundary conditions through conservation of flux defined on the common boundary.**

I. Introduction

Macroscopic modeling, in terms of lumped parameter systems, can be insufficient to recover all the relevant phenomena. Internal dynamics, such as vibrations, deformations, and delays, may spoil the global model. To improve upon such models detailed microscopic theories, of continuous systems, are required. However, many microscopic approaches neglect the global features and interconnections, which have been the main interest.

In this paper, the macroscopic and microscopic approaches are linked together, in more than one way. We show the advantages and disadvantages of a collocated approach and the FEM approach, and show that the microscopic theory of the component can be augmented with a microscopic theory of the boundary, in terms of fluxes. These fluxes are the direct implementation of energy, force, or charge balance, and form the natural link between the global, or macroscopic, modeling, and the microscopic description.

After a general motivation, the link between the macroscopic and microscopic Newton force law is established. Since this is based on general principles, no detailed microscopic theory is required. In the next section the features of microscopic theories which lead to balance laws are investigated, and applied to the inhomogeneous wave equation on a string. In the next section, the interaction with the surrounding through boundary conditions are investigated, first by domain splitting. In the next section by defining appropriate fluxes, the boundary conditions, expressed in the energy flux, yield the core model, which is the microscopic equivalent of the lumped model. The core model may vary with the type of boundary condition and resulting flux. Finally, the leading internal dynamics is discussed. The internal dynamics arises from the coupling with the lumped, or core model, dynamics. We link back to the formal aspects of Hamiltonian dynamics, and we end with some conclusions and an outlook.

Norbert Ligterink and Peter Breedveld are members of the Control Engineering Group at the University Twente, Enschede, The Netherlands, Arjan van der Schaft is professor in Applied Analysis at the Mathematics Department of the University of Groningen, Groningen, The Netherlands, and professor in System and Control Theory at the University Twente.

II. Motivation

Modelling of systems is based on the natural view of the largest independent units of a system. In a human body, for example, we recognize the members separated by joints, although the digits of the hand are much smaller than the upper leg. A medical specialist might, however, see different units, such as muscles, organs, and bones. In principle, units do not need to be spatially distinct. Generally only particular properties, such as electrical, or mechanical, are part of a unit of a model.

Kirchhoff laws and rigid-body dynamics are successful descriptions for lumped parameters of large units. However, for accurate measurement and design of the model units more detailed understanding of the each unit is required. The body, assumed to be rigid, turns out to be elastic, and electrical circuits may have delays and mutual interference between components, which are not present in the dynamics of the Kirchhoff laws. These are both examples of internal dynamics. Instead of a couple of parameters to describe the model, an infinite number, or continuous set, of parameters arise once the unit, or component, no longer acts fully coherently or collectively.

The study and modeling of internal dynamics starts usually with a microscopic theory, expressed in terms of partial differential equations. Successful microscopic theories are consistent with the macroscopic, or lumped results. For example, any theory of elasticity should propagate the force from one end of a free object to another, otherwise the micro-balance law, the basis of the force balance, cannot be satisfied. Similarly, microscopic electromagnetic theories, at the basis of microscopic modeling, should, in practice, satisfy microscopic current conservation in order to satisfy Kirchhoff laws at a macroscopic scale. If a component is size-extensive, like a homogeneous and isotropic block of material, one might split the block into small pieces, and microscopic blocks will inherit the macroscopic laws, yielding a direct link between the integral and the differential version of the same conservation law.

Maxwell equations for the microscopic description of electrodynamics were derived to satisfy conservation laws, such as charge conservation. Maxwell looked toward the theory of hydrodynamics, with divergence-free vector fields, for inspiration of the final displacement current term in the Ampere law, which guaranteed the global conservation of charge. The microscopic formulation in terms of partial

differential equations were only considered complete once the global physical conservation laws were satisfied.

Hence, the microscopic description is connected to the macroscopic description via the physical laws, expressed as conserved macroscopic quantities, such as charge and momentum, on one hand, and, on the other hand, expressed as properties of the fields, like charge, mass, and current densities. In establishing a close connection between the microscopic theory, expressed in partial differential equations or their FEM approximation, and the macroscopic theory, in terms of the lumped parameters, the conservation laws should, and can, play a central role. This is not only for consistency, but also to enable the modeler, or designer, to shift focus smoothly from global system properties to details, which might be critical. Some results, in the more limited context of linear FEM, appeared in [2].

III. Beyond rigid body dynamics

A simple and heuristic example of a bouncing ball should set the mind. In a lumped description of the bounce of a ball, energy is lost at a bounce, to match our observation. However, most balls have a life-span of hundreds of thousands bounces, so it is unrealistic to expect the energy is directly converted to heat via the plasticity of the ball, like with a lump of clay. In a microscopic description energy is converted from the global, or lumped, motion of the ball, to the vibration of the ball, which is again converted into heat and sound. In principle, the whole conversion process is interesting, however, depending on the zeal of the investigator, he or she might wish to truncate the effort at a certain detail. For example, the amount of conversion from kinetic energy to the dominant elastic mode, and the other elastic energy in higher modes, might already be enough information to determine the lost of macroscopic energy within the given accuracy. The dominant elastic mode acts as an ideal spring for the ideal, energy-conserving bounce, while other modes lead to decoherence and the lost of global motion.

Like in the example above, vibrational analysis lies at the core of most efforts to bring to the surface the dominant effects of internal dynamics. This should not be surprising. Vibrational analysis is the physical description of spectral decomposition, which lies at the core of the most powerful mathematical tool for physical systems, namely, functional analysis. However, our mental process might work from the top down: to the macroscopic, or lumped, picture we add a couple of degrees of freedom in the form of low-lying vibrational modes, the mathematical microscopic description starts from the bottom up: from a model with an infinite number of degrees of freedom we should distill a few relevant ones. Spectral decomposition is a hard problem from the bottom up. It is only feasible for discretized FEM models, which truncate wave numbers at the inverse mesh spacing. Therefore, they cannot get into the range of vibrational modes, which, for example, lie at the basis of kinetic energy to heat conversion.

In an appropriate and powerful description of the microscopic details of systems the macroscopic description should meet the microscopic description at some point. We should ask ourselves the question: what are the microscopic equivalents of the macroscopic variables we use? Physical conservation laws should be the guiding principles in such questions. For example, take the motion of an extended object. In the case of a rigid-body description of the extended object the motion of the center-of-mass is a direct consequence of the applied resultant force, also know as Newton force law:

$$\mathbf{F} = M\mathbf{A} \ ,$$

where $\mathbf{A}$ is the acceleration of the center-of-mass.

The corresponding microscopic description is not immediately evident. Starting with the sum, or lumped, mass M, it could easily be derived from the integration over the mass density ρ:

$$M = \int_\Omega \rho(x)dx \ .$$

Furthermore, the acceleration $\mathbf{A}$ can be considered the acceleration of the center-of-mass coordinate $\mathbf{X}$:

$$\mathbf{X} = \frac{1}{M}\int_\Omega \mathbf{x}(x)\rho(x)dx \ ,$$

where the positions are normalized with the mass density, which yields:

$$\mathbf{A} = \ddot{\mathbf{X}} \ ,$$

for a constant mass density $\rho(x)$. The position $\mathbf{X}$ is with respect to a origin $\mathbf{x} = 0$, velocity and acceleration are affine and depend only on the orientation of the coordinate system.

The displacement $\mathbf{x}(x)$ is a function of the reference coordinate x, such that the density $\rho(x)$ is invariant. All fields, such as the forces microscopic forces $\mathbf{f}(x)$, are all functions of the reference coordinates x.

For a rigid body the force law is the direct sum of all the microscopic forces $\mathbf{f}(x)$:

$$\mathbf{F} = \int_\Omega \mathbf{f}(x)dx \ .$$

It is interesting to notice that, unlike the positions $\mathbf{x}$, the forces are not weighted by the mass density. The positions are therefore extensive, while the forces are intensive. In that respect the pair together, which has consequences for the inner-product, as we will see. In the case of a flexible object, forces $\mathbf{f}_\perp(x)$, which sum to zero for the rigid-body force, still contributes to the internal dynamics. The meaning of perpendicular is different from what one expect naively. If the force is applied to a particular point of the rigid body, the, as yet unknown, internal force balance will make the object move coherently; as a whole.

In the case of elasticity, the forces should be separated to two parts: the forces that add up to the force causing the global motion, and the remainder. The global forces should

not cause any deformation hence they should be coherent with the mass distribution in the system:

$$\mathbf{f}(x) = \mathbf{f}_{\parallel}(x) + \mathbf{f}_{\perp}(x) = \mathbf{F}\frac{\rho(x)}{M} + \mathbf{f}_{\perp}(x) \ .$$

The global force $\mathbf{F}$ is defined through the microscopic mass and force distributions.

For the parallel forces, Newton law can be brought inside the integral, to yield an exact microscopic law by definition, for an object without internal stresses. The force yield the corresponding change in momentum, for the collocated inertia $\rho(x)$:

$$\mathbf{f}_{\parallel}(x) = \rho(x)\mathbf{A} = \dot{\mathbf{P}} \ ,$$

while the remaining, perpendicular force does not cause any motion of the center-of-mass, but only deformation. This result is most easily understood if the mass integral is considered a mass-weighted inner product:

$$\langle f(x), \rho(x)g(x)\rangle = \int_{\Omega} f(x)\rho(x)g(x)dx \ .$$

The center-of-mass $\mathbf{X}$ and the parallel force $\mathbf{F}$ are both projections on the constant and orthogonal unit vector fields $\mathbf{e}(x) = (e_x, e_y, e_z)$:

$$\mathbf{X} = \langle \mathbf{e}, \rho\mathbf{x}\rangle \ ,$$

and:

$$\mathbf{F} = \langle \mathbf{f}, \mathbf{e}\rangle \ .$$

Hence the perpendicular force is:

$$\mathbf{f}_{\perp}(x) = \mathbf{f}(x) - \frac{\rho(x)}{M}\langle \mathbf{f}, \mathbf{e}\rangle \ ,$$

which inner-product $\langle \mathbf{f}, \mathbf{f}\rangle$ does not yield an orthogonal decomposition, i.e., $\langle \mathbf{f}_{\perp}, \mathbf{f}_{\parallel}\rangle \neq 0$. The associated decomposition of the displacement $\mathbf{x}(x)$ is

$$\mathbf{x}_{\perp}(x) = \mathbf{x}(x) - \mathbf{X}\mathbf{e}(x) = \mathbf{x}(x) - \frac{1}{M}\langle \mathbf{e}, \rho\mathbf{x}\rangle\mathbf{e}(x) \ ,$$

such that:

$$\langle \mathbf{f}_{\parallel}, \mathbf{x}_{\perp}\rangle = \langle \mathbf{f}_{\perp}, \mathbf{x}_{\parallel}\rangle = 0 \ ,$$

where we used that $\langle e_i, \rho e_j\rangle = M\delta_{ij}$.

Hence it is possible to make a separation between internal dynamics and the rigid dynamics for a microscopic model. The bi-orthogonality is based on the work and energy relations, since, $dE = \mathbf{f}d\mathbf{x}$ is the change in energy density due to the applied force. This work separates into two parts: the rigid-body energy and the internal energy:

$$\int_{\Omega} dE(x)dx = \langle \mathbf{f}, d\mathbf{x}\rangle = \langle \mathbf{f}_{\parallel}, d\mathbf{x}_{\parallel}\rangle + \langle \mathbf{f}_{\perp}, d\mathbf{x}_{\perp}\rangle \ ,$$

since the cross terms vanish.

IV. Microscopic theories

The microscopic theories in terms of partial differential equations, which would for example yield the specific consequences of elasticity in the example above, are more general than only the separation of rigid-body motion and internal deformation. However, the partial differential equations have one particular property, which led to the recognition of rigid-body motion as a specific form of global dynamics. The rigid-body motion has no associated elastic energy, whatever model one chooses for the elastic, or internal dynamics. The fact that any isolated system has rigid-body modes is the consequence of the translation invariance of physical laws.

If we are guided by the microscopic definition of the energy, as defined by the Hamiltonian density H, we find that the elastic energy vanished for any translation combination $T = (t_x, t_y, t_z)$ of the constant displacements $e_i(x)$:

$$V(\mathbf{x} = T\mathbf{e}) = 0 \ ,$$

where V is the potential part of the Hamiltonian. From the equation of motion it follows that, without applied forces or position constraints the translations yield conserved momenta ($\mathbf{P} = \text{constant}$):

$$\dot{\mathbf{P}} = -\frac{\partial H}{\partial T\mathbf{e}} = 0 \ .$$

In many cases, such as Dirichlet boundary conditions, the boundary conditions fix the values of $\mathbf{P} = 0$. In other cases, such as Neumann boundary conditions, the values of $\mathbf{P} = \text{constant}$ are only partly fixed. Even more general boundary conditions exist, expressed in an input function u, such that $\mathbf{P}(u)$. The link between boundary conditions and constants of motion hints at the possibility of separate the direct consequences of the boundary conditions from the internal dynamics.

Since the elastic potential V of the Hamiltonian density H is positive, it can be written as a weighted form:

$$V((D\mathbf{x})^2, \mathbf{x}) \ ,$$

where D is the differential, or moment operator. For example, in the case of elasticity it could be the strain tensor:

$$\epsilon_{ij} = D\mathbf{x} = \frac{1}{2}(\partial_i x_j(x) + \partial_j x_i(x)) \ .$$

In this case the solutions for which the elastic energy vanishes are besides the translations $\mathbf{e}$, also the rotations around an arbitrary axis $\mathbf{n}$:

$$\partial_i(\mathbf{n}\times\mathbf{x})_j + \partial_j(\mathbf{n}\times\mathbf{x})_i = 0 \ .$$

Hence not just the translations but also the rotations are undetermined in the isolated system. The kernel of the differential operator D plays the central role. By introducing the moment variable:

$$q' = D\mathbf{x} \ ,$$

the potential energy of the system has a unique minimum $q' = 0$. The indeterminate part, which is either fixed by

the boundary conditions, or lead to a conserved quantity, is now explicit in the equations of motion, and does no longer depend on the precise details of the potential, now a function of q'.

In the theory of hyperbolic partial differential equations the existence and uniqueness of a solution for given initial and boundary conditions is sought[3] The proper initial conditions are determined by the Cauchy problem, on a infinite space or by local analysis. The boundary conditions might be inconsistent with the initial conditions. One way to avoid this situation is to choose the stationary, or pseudo-stationary solution for the boundary conditions as initial conditions. A pseudo-stationary solution would, for example, be an accelerating solution for a constant force.

The stationary problem for the boundary conditions is called the associated problem. The solutions of the associated problem serve as source to the internal dynamics. Since the solution to the associated problem already satisfies the boundary conditions, the internal dynamics consists of modes with vanishing boundary values. The associated problem, however, is not unique, but may vary with the type of boundary conditions, but as we have seen for the rigid body, a canonical pair of boundary conditions follow from one associated problem. These pairs are called the port variables.

The equations of motion for the moment variables are the equations of motion of the port-Hamiltonian H' [4]:

$$\begin{pmatrix} \dot{q}' \\ \dot{p} \end{pmatrix} = \begin{pmatrix} 0 & D \\ -D^* & 0 \end{pmatrix} \begin{pmatrix} \delta_q H'(q', p) \\ \delta_p H'(q', p) \end{pmatrix} ,$$

where D^* is the formal adjoint of the differential operator D, and p is the canonical momentum for the displacement $\mathbf{x}$. The difference between the port-Hamiltonian and an ordinary Hamiltonian is the use of the moment variable q' instead of the position $\mathbf{x}$ as variable.

The associated stationary problem would be the solution v to:

$$\begin{pmatrix} 0 & D \\ -D^* & 0 \end{pmatrix} v = 0 .$$

The pseudo-stationary problems would be of the type:

$$\begin{pmatrix} q_t \\ p_t \end{pmatrix} = \begin{pmatrix} 0 & D \\ -D^* & 0 \end{pmatrix} v .$$

The corresponding components q', p, q_t, p_t, which are constant in time, yield at most linear time-dependent states, arise from solving the algebraic relations:

$$v = \begin{pmatrix} \delta_{q'} H'(q' + q_t t, p + p_t t) \\ \delta_p H'(q' + q_t t, p + p_t t) \end{pmatrix} ,$$

where q_t and p_t are zero, for the stationary equation.

For example, consider the Hamiltonian of an anisotropic wave equation in one dimension, with a space dependent mass density ρ and stiffness κ:

$$H' = \frac{p^2}{2\rho(x)} + \frac{\kappa(x) q'^2}{2} .$$

The differential operator is $D = -D^* = \partial_x$. Only constant functions vanish for this differential operator. Hence the stationary solution is:

$$v = \begin{pmatrix} F \\ u \end{pmatrix} .$$

which correspond to a constant moving and compressed, or stressed, state with a velocity u and an internal stress F. The states are, almost trivial, solutions to the algebraic equations:

$$\begin{pmatrix} q'(x) \\ p(x) \end{pmatrix} = \begin{pmatrix} \kappa(x)^{-1} F \\ \rho(x) u \end{pmatrix} .$$

The definition of the moment $q' = Dy$ yield the displacement y:

$$y(x) = y(0) + F \int_0^x dx' \frac{1}{\kappa(x')} ,$$

where the the integration constant $y(0) = y_0 + ut$. Hence, a stationary state can be defined through the force F, the velocity u, and the initial displacement y_0 at a point, e.g., $x = 0$ and $t = 0$.

The solution of constant acceleration, discussed above, would be a pseudo-stationary solution:

$$\begin{pmatrix} 0 \\ p_t \end{pmatrix} = \begin{pmatrix} 0 & \partial_x \\ \partial_x & 0 \end{pmatrix} v = \begin{pmatrix} 0 & \partial_x \\ \partial_x & 0 \end{pmatrix} \begin{pmatrix} F(x) \\ u \end{pmatrix}$$
$$= \begin{pmatrix} 0 & \partial_x \\ \partial_x & 0 \end{pmatrix} \begin{pmatrix} \kappa(x) q'(x) \\ \rho(x)^{-1} (p(x) + p_t(x) t) \end{pmatrix} .$$

Hence, from the top row it follows $\rho(x)^{-1} p_t(x) = a$ and $\rho(x)^{-1} p(x) = u$ must both be constant, and therefore:

$$F(x) = F(0) + a \int_0^x \rho(x') dx' ,$$

and the displacement $y(x)$ is given by the same integral, where $F(x)$ is no longer constant:

$$y(x, t) = y_0 + ut + \frac{1}{2} a t^2 + \int_0^x dx' \frac{F(x')}{\kappa(x')} .$$

A pseudo-stationary solution has a polynomial time-dependence of the states and, in the linear case, also of the energy.

V. Boundary conditions

The stationary and pseudo-stationary solutions are not fixed by the equations of motion. They give rise to unknown parameters, such as the force, velocity, and acceleration, which can be seen as the equivalents of constants of motion, in the port-Hamiltonian system. These solutions yield values at the boundary such that the parameters may be fixed by boundary conditions. The boundary-value problem reduces to an algebraic problem.

Decomposition could be an approach to the boundary problems. The integrals of the object domain Ω can be separated in parts $\Omega_1 \cup \Omega_2$:

$$\int_\Omega \to \int_{\Omega_1} + \int_{\Omega_2} .$$

The definitions of the force $\mathbf{F}$ and the center-of-mass $\mathbf{X}$ hold just as well for each part separately, as for the whole. The linearity of the integral yield the linearity of the global, or macroscopic variables. This should not surprise us, as Newton has sought extensive properties of mechanical systems. The work, or power, integral would yield cross-terms between the different domains, related to the power transfer between the domains:

$$\int_\Omega dEdx = \langle \mathbf{f}_1, d\mathbf{x}_1 \rangle + \langle \mathbf{f}_2, d\mathbf{x}_2 \rangle + (\mathbf{f}_1, d\mathbf{x}_2) + (\mathbf{f}_2, d\mathbf{x}_1) \ .$$

where the inner-product $(\cdot, \cdot)$ is defined on the common boundary of Ω_1 and Ω_2. The precise definition of the boundary, or trace, integrals $(\cdot, \cdot)$ depends on the microscopic theory. In the absence of spatial derivatives, the boundary terms vanish. They can be seen as the end terms of partial integration, or the displacement flow along force lines. However, without a microscopic theory we can attach little meaning to these boundary terms. Physical theories, however, must satisfy energy conservation and force balance, which translates in this domain decomposition into a constraint on the separation of rigid-body and internal dynamics:

$$(\mathbf{f}_i, d\mathbf{x}_j) = (\mathbf{f}_{\perp i}, d\mathbf{x}_j) \ ,$$

as the result of the locality of the mass density. Discretization will generally destroy this result, as we will see from the example of a string. If a homogeneous string of length L is discretized in n segments with linear displacement, described by $L+1$ end positions we find a stiffness matrix:

$$\int (\partial_x \cdot)^2 \to K = \frac{n}{L} \begin{pmatrix} -1 & 1 & 0 & \cdots & \\ 1 & -2 & 1 & 0 & \\ 0 & 1 & -2 & 1 & 0 \\ \vdots & & \ddots & \ddots & \ddots \end{pmatrix} \cdot$$

The mass matrix is the integral over the density of the linear displaced string:

$$\int \rho(\cdot)^2 \to M = \frac{n\rho}{6L} \begin{pmatrix} 2 & 1 & 0 & \cdots & \\ 1 & 4 & 1 & 0 & \\ 0 & 1 & 4 & 1 & 0 \\ \vdots & & \ddots & \ddots & \ddots \end{pmatrix} \cdot$$

If the mass matrix would have been diagonal, the principles of the continuum mechanics, for the separation of the rigid-body motion and the internal motion and the corresponding forces, would have carried over to the discrete system. However, for the tri-diagonal mass matrix this is no longer the case. Moreover, for the time simulation the mass matrix must be inverted, which yields a completely filled matrix M^{-1}. As a consequence, the system can no longer be separated while yielding only additional local boundary terms. Each node of the system is connected to each other node, due to the nonlocal mass matrix inverse M^{-1}.

However, if we consider local, or band-diagonal matrices only, it is possible to split the system in different manners. If these tri-diagonal matrices are split into two equivalent matrices, the remainder is part of the diagonal and the complete off-diagonal part across the split:

$$A_{\alpha\beta} = \left(\begin{array}{ccc|ccc} \alpha & \beta & 0 & & & \\ \beta & \alpha & \beta & 0 & & \\ 0 & \beta & \alpha & \beta & 0 & \\ \hline & 0 & \beta & \alpha & \beta & 0 \\ & & 0 & \beta & \alpha & \beta \\ & & & 0 & \beta & \alpha \end{array} \right) \ ,$$

which we denote by the Cartesian product in the two subspaces and the boundary matrix:

$$A_{\alpha\beta} = A^1_{\alpha\beta} \otimes A^2_{\alpha\beta} + \left(\begin{array}{c|c} \alpha' & \beta \\ \hline \beta & \alpha' \end{array} \right)_{12} \ ,$$

where typically the end point yields $\alpha' = \frac{1}{2}\alpha$. This is a so-called force split, as the two boundary points are not collocated, but adjacent, and free to move independently. Their motion is limited by the kinetic and potential energy given by the boundary matrices K_{12} and M_{12}. A film-layer model to connect two systems would be an example of such a force split.

The other method of splitting systems to study boundary dynamics would be the configuration split, which is more common. A configuration split would correspond to a collocation of the boundary points. Rather than a dynamical boundary connection, it is a constraint relation, with partly overlapping mass and stiffness matrices. The boundary matrix A_{12} should be added one of the subspace matrices $A^1_{\alpha\beta}$ or $A^2_{\alpha\beta}$.

In the case of higher-order differential equations, such as the Euler-Bernoulli beam, or higher dimensions, the splitting of systems, and the variety of boundary terms and effects is even greater. In the continuum theory of elasticity it has led to a number of variational principles, such as the three-field method and the four-field method [5] to retain the freedom to match boundaries in different ways. Furthermore, the implementation of such splittings will only be feasible for linear systems, where constant matrices are to be decomposed.

VI. Flux

Clearly, decomposing the linearized and discretized system is hardly unique, or ideal. On the other hand, the rigid-body formulation, with the collocation at the same x of density and displacement is limited. Instead, the boundary integral can be coupled to the volume integrals, through the divergence theorem:

$$\int_\Omega \nabla \cdot \mathbf{J} dx = \int_{\partial\Omega} \mathbf{J} \cdot \mathbf{n} da \ .$$

Therefore, an appropriate formulation should be expressed in terms of fluxes $\mathbf{J}$. The key flux is the energy flux $\mathbf{S}$, since in the case of zero internal energy and zero energy flux the solution, or internal state, is the unique static solution. In general, energy is thus used to determine existence and uniqueness of a solution to a mixed boundary value problem of a hyperbolic equation. The energy flux is derived from the

canonical Hamiltonian $H(q,p)$ of the system, through the differential operator D encountered before in the definition of the elastic energy. However, the Hamiltonian no longer needs to be derived from configuration space. The only link with an underlying continuous reference space, with boundaries, is through the differential operator D.

The energy of the system is given by the Hamiltonian density function: $H(q,p)$, which depends on the canonical position and momentum fields $q(z)$ and $p(z)$. The energy is conserved, hence the Hamiltonian density satisfies the continuity equation:

$$\dot{H} + \nabla \cdot \mathbf{S} = 0 \quad ,$$

where $\mathbf{S}$ is the energy flux [1]. The energy flux is the key guiding principle in the analysis of the interaction between components. The energy function is a positive operator of the state space, or phase space, and zero energy corresponds to the lowest, rest, or ground state. Hence stability analysis and dissipation uses energy and its in- and out-flow.

The energy flux is not uniquely defined. It depends on what quantities are allowed to flow across boundaries. For example, an ideal balloon might change is shape but not its content, while an air pocket can both change shape and content. Constraints on the fields might complicate this matter further. The port-Hamiltonian H' defines the energy-flux. The port-Hamiltonian [4] arises from the Hamiltonian through a variable substitution:

$$H(q,p) = H'(Dq,p) \equiv H'(q',p) \quad ,$$

where D is an appropriate differential operator. The Hamilton-Jacobi equations, the equations of motion, are

$$\begin{pmatrix} \dot{q}' \\ \dot{p} \end{pmatrix} = \begin{pmatrix} 0 & D \\ -D^* & 0 \end{pmatrix} \begin{pmatrix} \delta_{q'} H' \\ \delta_p H' \end{pmatrix} \quad ,$$

where D^* is the formal adjoint of the differential operator D.

The energy flux follows from inserting the equations of motion into the time derivative of the Hamiltonian density:

$$\dot{H} = \delta_{q'} H' D \delta_p H' - \delta_p H' D^* \delta_{q'} H' \equiv -\nabla \cdot \mathbf{S} \quad .$$

The expression on the right-hand side is the divergence of the energy flux, which in many cases can be written as the bilinear product using the boundary operator θ:

$$\delta_{q'} H' \theta(\mathbf{n}) \delta_p H' = \mathbf{S} \quad .$$

Clearly, appropriate boundary conditions are expressed in terms of $\delta_p H'$ and $\delta_{q'} H'$ rather than the normal state variables q and p.

For the linear wave equation the Hamiltonian density is:

$$H = \frac{p(z)^2}{2\rho(z)} + \frac{1}{2}\kappa(z)(\nabla q(z))^2 \quad .$$

The associated differential operator is the gradient $D = \nabla$, the adjoint is the divergence $D^* = -\nabla\cdot$. The directional, or moment, variable is $q' = \nabla q$. Therefore the boundary operator θ is simply the surface normal:

$$\theta = \mathbf{n}$$

and the energy flux follows from the Green identity:

$$\mathbf{S} = \frac{p}{\rho}\mathbf{n} \cdot \kappa \nabla q \quad .$$

More general differential operators appear if there are more that one type of energy flux. For example, take the Euler-Bernoulli beam. The elastic energy is given by the second derivative of the deflection $y(z)$:

$$H_{\text{elastic}} = \frac{1}{2} EI (\partial_z^2 y(z))^2 \quad ,$$

which may seem like a single bending energy. The associated differential operator would be $D = \partial_z^2$ such that $q' = \partial_z^2 y$, however, the boundary operator θ is:

$$f \theta g = g \partial_z f - f \partial_z g \quad .$$

These two terms correspond to the two boundary conditions, which need to be set for an Euler-Bernoulli beam, at each end, which lead to four possible solutions for $\mathbf{S} = 0$, three of those are familiar boundary conditions: free ($\delta_{q'} H = \partial_z \delta_{q'} H' = 0$), clamped ($\delta_p H' = \partial_z \delta_p H' = 0$), and supported ($\delta_p H' = \delta_{q'} H' = 0$), boundary conditions, where in all cases the initial condition $q = 0$, at the boundaries, is used. The fourth boundary condition corresponds to a fixed orientation, but a free displacement ($\partial_z \delta_p H' = \partial_z \delta_{q'} H' = 0$), which is difficult to implement physically. One could think of a clamped beam end moving freely along a rail.

The example of the Euler-Bernoulli beam showed that the physical boundary conditions $\mathbf{S} = 0$ are rather unlike the typical mathematical boundary conditions in terms of the state variables q' and p at the boundary. They are, of course, related through the constitutive relations, expressed in term of variational derivatives of the port-Hamiltonian. In the case of isolated problems, associated with $\mathbf{S} = 0$, such distinction is of little relevance, especially in the linear case. The nonlinear, non-isolated case $\mathbf{S} \neq 0$ the distinction is very important. Not just any boundary condition can be implemented straightforwardly.

The pseudo-stationary states, corresponding to the force $\mathbf{F}$ and the velocity $\mathbf{u}$, are, at one hand, related to physical boundary conditions, and, at the other hand, to states q' and p. They form a bridge between the macroscopic forces and velocities and the internal states. The model with only the degrees of freedom, such determined uniquely by the boundary conditions, we call the core model. In previous papers we referred to this as the "minimal model", but that has led to confusion among system theorists.

VII. Core model

The stationary states are not necessarily static, but they are isolated. For example, a system moving frictionless with constant velocity $\mathbf{u}$ is a stationary state. No energy is transferred in or out of the system, but can be transferred through the system as we will see in the example below. The pseudo-stationary states have a linear time dependence, which may correspond to a complicated energy dependence,

if the Hamiltonian is nonlinear. The energy transfer, or power, can be calculated from the equations of motion:

$$\begin{pmatrix} q_t' \\ p_t \end{pmatrix} = \begin{pmatrix} 0 & D \\ -D^* & 0 \end{pmatrix} \begin{pmatrix} \mathbf{F} \\ \mathbf{u} \end{pmatrix} ,$$

which yields a much simpler flux and boundary operator than in terms of the states:

$$\nabla \cdot \mathbf{S} = \mathbf{u} D\mathbf{F} - \mathbf{F} D^* \mathbf{u}$$

In the case of the differential operator D being the gradient $D = \nabla$, or the divergence $D = \nabla\cdot$, the boundary operators are:

$$\theta = \begin{cases} (\mathbf{n}\cdot\mathbf{u})\mathbf{F}, & D = \nabla\cdot \\ (\mathbf{n}\cdot\mathbf{F})\mathbf{u}, & D = \nabla \end{cases} .$$

In the port-Hamiltonian the canonical variables q' and p are geometrically distinct. As a consequence, depending on the differential operator D, the one of two port variables $\mathbf{u}$ or $\mathbf{F}$ is the boundary-extensive variable; the flux, while the other is the boundary-intensive variable; the potential.

In many cases, the port flux is indeed a conserved flux, besides the energy flux. For example, matter flow and charge flow are conserved fluxes, and so is momentum flow in its peculiar way. It might therefore be important to formulate the microscopic theory such that the port flux corresponds to such conserved flux. In many cases the procedure of recovering a Hamiltonian is therefore reversed. The continuity equation is the first equation of motion, the second equation, the closure relation is of less importance, and contains the material properties. Afterwards, the closure relation is integrated to recover the Hamiltonian, or any other total differential. For example, diffusion equations in physical chemistry arise from such approach. Mass is almost mysteriously conserved for any constitutive relation, relating density to pressure, due to the adjoint pair of the gradient operator and the divergence operator.

VIII. Internal dynamics

The core model, rather than the boundary conditions, are the basis of internal dynamics. Since the boundary conditions are satisfied by the states of the core model, the internal dynamics has vanishing boundary conditions. Therefore, the internal dynamics has gained some of independence of the core model state. In some cases, therefore, the internal dynamics may be linearized, while the core model may not.

Inserting the full model back into the equations of motion, taking into account the time-dependence of the core states $q_0 = (q' + q_t t), p_0 = (p + p_t t)$ which depend of the port-variables $\mathbf{F}(t)$ and $\mathbf{u}(t)$, the internal dynamics appears on the right-hand side of the equation:

$$\begin{pmatrix} \partial_{\mathbf{F}} q_0 \dot{\mathbf{F}} + \partial_{\mathbf{u}} q_0 \dot{\mathbf{u}} \\ \partial_{\mathbf{F}} p_0 \dot{\mathbf{F}} + \partial_{\mathbf{u}} p_0 \dot{\mathbf{u}} \end{pmatrix} = \begin{pmatrix} 0 & D \\ -D^* & 0 \end{pmatrix} \begin{pmatrix} \delta_{q'} H' - \mathbf{F} \\ \delta_p H - \mathbf{u} \end{pmatrix} .$$

Hence, if the input is expanded in terms of polynomials in time, like in a spline approximation, the internal dynamics yield an analogous expansion.

For example, a homogeneous truss of length L, with elasticity κ and mass density ρ, with the velocity u given as input, and the relative distance determined by the external force F, yield a stationary state with a homogeneous compression $q' = F/\kappa$, and a homogeneous momentum $p = \rho u$. Since the stationary state is determined by two quantities F and u, the forces at the ends are equal but opposite $F_1 = -F_2$, and the velocities are equal $u_1 = u_2$. In order to affect a dynamical model in terms of the four port-variables $F_1, F_2, u_1,$ and u_2, we investigate the leading dynamical modes.

The total energy in the truss is:

$$E = \frac{L\rho}{6}(u_1^2 + u_1 u_2 + u_2^2) + \frac{L}{8\kappa}(F_1 - F_2)^2 ,$$

which is similar to the linear finite-element approximation of a truss, expressed in the applied boundary conditions. The power transfer through the truss is $F_1 u_1$, into the truss at end point u_1 and out again at u_2, with $u_1 = u_2$ and $F_2 = -F_1$. The four variables with the two constraints can be seen as the core model, fully determined by the boundary conditions. The micro-balance determines the force constraint, the power balance determines the velocity constraint. However, more appropriately, the model can be extended to include dynamical relations, rather than constraints between the end points, or port, variables (u_1, F_1) and (u_2, F_2).

The energy of the truss, in combination with the constraints, shows that any dynamical model is incomplete. By a change of force or velocity, the power transfer is nonzero, while for the core model, due to the constraints, the power transfer is always zero. The model can be extended, by adding an approximation to the mean, rigid-body inertial force: $F_1 + F_2$ to the overall, or rigid-body, motion approximated by: $u_1 + u_2$, and for the relative motion $u_1 - u_2$ an internal displacement. Instead we proceed, more systematically, by investigating the dynamical effects of time variation of the input.

If we now have a time-varying force difference $F_1 - F_2$ in the truss, the corresponding state q' will vary, yielding inertial effects. The state will vary with time:

$$\begin{pmatrix} q' \\ p \end{pmatrix} = \begin{pmatrix} \frac{F_1(t) - F_2(t)}{2\kappa} \\ \frac{\rho}{2}(u_1 + u_2) + \rho \frac{\dot{F}_1(t) - \dot{F}_2(t)}{\kappa} \frac{x}{L} \end{pmatrix} ,$$

where $x = [-L/2, L/2]$, the reference coordinate along the truss, which is the solution to the differential equation:

$$\partial_x \frac{p}{\rho} = \dot{q}' = \frac{\partial}{\partial t} \frac{F_1(t) - F_2(t)}{2\kappa} .$$

The time-variation of applied force will cause therefore variation in the relative end-point velocity $u_1 - u_2$.

Only at the next order, $\ddot{F}_1 - \ddot{F}_2$ the effect of the inertia will cause a change in the forces at the end points. The boundary flux Fu based analysis yield a polynomial expansion in modes, due to the homogeneous and isotropic nature, rather than a trigonometric expansion typical for $F_i = 0$ or $u_i = 0$ boundary conditions:

$$q'(x) = d_0 + d_1 \frac{2x}{L} ,$$

where the constant deformation is d_0 and space-dependent deformation is d_1. The corresponding the canonical momenta are

$$p(x) = b_0 + b_1 \frac{2x}{L} \ .$$

These four amplitudes d_0, d_1, b_0, and b_1 are directly related to the four port variables:

$$\begin{pmatrix} d_0 \\ d_1 \\ b_0 \\ b_1 \end{pmatrix} = \begin{pmatrix} \frac{F_1 - F_2}{2\kappa} \\ \frac{F_1 + F_2}{2\kappa} \\ \frac{\rho(u_1+u_2)}{2} \\ \frac{\rho(u_2-u_1)}{2} \end{pmatrix} \ .$$

The energy due to the port-Hamiltonian, restricted to the space of these two modes is given by ($D = \partial_x$):

$$E = \int_{-L/2}^{L/2} dx H' = \frac{L b_0^2}{2\rho} + \frac{L b_1^2}{6\rho} + \frac{\kappa L d_0^2}{2} + \frac{\kappa L d_1^2}{6} \ .$$

The equations of motion of the stationary system are:

$$\begin{pmatrix} \dot{d}_0 \\ \dot{d}_1 \\ \dot{b}_0 \\ \dot{b}_1 \end{pmatrix} = \begin{pmatrix} \frac{2b_1}{\rho L} \\ 0 \\ -\frac{2\kappa d_1}{L} \\ 0 \end{pmatrix} \ ,$$

which, once expressed in terms of F_1, F_2, u_1, and u_2, yield two conditions among the four port variables, and two boundary conditions, either for F_1 and u_2, or for F_2 and u_1. The other boundary conditions, like for F_1 and F_2, would arise from the pseudo-stationary state, with, in this case, $p_t \neq 0$.

IX. Pseudo-symplectic operators

From a formal perspective, the conserved energy of a Hamiltonian is not so much the consequence of the Hamiltonian itself, but of the symplectic matrix J in front:

$$\dot{x} = J \nabla_x H \ ,$$

where $J^T = -J$, which in the canonical form reduces to $J = \left(\begin{smallmatrix} 0 & I \\ -I & 0 \end{smallmatrix}\right)$. The port-Hamiltonian changes the symplectic matrix into skew-adjoint differential operator, while the model reduction, based on the core model, changes the differential operator in shift operators $S_\sigma(x_0, x_1, x_2, \cdots) = (x_\sigma, x_{\sigma+1}, x_{\sigma+2}, \cdots)$ acting on vectors $(x_0, x_1, x_2, \cdots)$ in half-infinite spaces:

$$J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \rightarrow \begin{pmatrix} 0 & D \\ -D^* & 0 \end{pmatrix} \rightarrow \begin{pmatrix} 0 & S_\sigma \\ -S_{\sigma'} & 0 \end{pmatrix} \ .$$

The first step is the change of variable from q to $q' = Dq$. The second step is finding the modes for which the differential operators D and D^* reduce to step operators S_σ and $S_{\sigma'}$. The modes, with amplitudes $(x_0, x_1, x_2, \cdots)$, are successively constructed from the core model states.

Depending on the choice of boundary conditions, the values of σ and σ' changes. In the example above, based on the stationary state, $\sigma = \sigma' = 1$. The sum of the two null spaces $\sigma + \sigma'$ is the dimension of the core model; the states not determined by the equations of motion, but either constants of motion, or determined by the port variables.

In the case of $\sigma = 2$ and $\sigma' = 0$ a constant nonzero q_t exists. Likewise, in the case of $\sigma = 0$ and $\sigma' = 2$ a constant nonzero p_t exists. The first case corresponds to u_1 and u_2 given, the second case corresponds to F_1 and F_2 given.

For the homogeneous string they are linear approximations of the states which satisfy the particular boundary conditions. The index σ, σ' yields a classification of boundary conditions.

X. Conclusion and outlook

In this paper we bring out different aspects of macroscopic versus microscopic modeling. Consistent, general, and versatile links between the two approaches are the fluxes, which link micro-balance laws with their global equivalences. Among these fluxes, the energy flux, or power, plays a central role, as the equations of motion are determined by the energy density in canonical form; the Hamiltonian. The internal dynamics, such as vibrations, are no longer a direct consequence of the interaction with the surrounding, but due to the coupling between the core, or lumped, model, and the remainder of the infinite number of degrees of freedom presence in the microscopic model.

Different physical problems and geometries are under investigation. In some cases the core model might have a nontrivial solution, which has it consequences for the internal dynamics. Furthermore, different control problems follow from the core model. For example, for arbitrary dynamics, the pseudo-stationary problem might be a better candidate of an optimal control problem, than the corresponding full dynamical problem.

Acknowledgments

This work was sponsored by Technologiestichting STW through project TWI.6012: "Port-based approach of complex distributed-parameter system models for analysis and simulation." More information on the project can be found at: `http://www.ce.utwente.nl/pacdas`.

References

[1] A. L. Fetter and J. D. Walecka. *Theoretical mechanics of particles and continua*. McGraw-Hill, New York, 1980.

[2] N. E. Ligterink, P. C. Breedveld, and A. J. Van der Schaft. Internal dynamics around operational fem states. *preprint, submitted for publication*, 2006.

[3] R. Sakamoto. *hyperbolic boundary value problems*. Cambridge, Cambridge, 1982.

[4] A. J. van der Schaft and B. M. Maschke. Hamiltonian formulation of distributed-parameter systems with boundary energy fbw. *Journal of Geometry and Physics*, 42:166–194, 2002.

[5] K. Washizu. *Variational methods in elasticity and plasticity*. Pergamon Press, Oxford, 1968.