A discrete exterior approach to structure-preserving discretization of distributed-parameter port-Hamiltonian systems

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A discrete exterior approach to structure-preserving discretization of distributed-parameter port-Hamiltonian systems

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Abstract— **This paper addresses the issue of structure-preserving discretization of open distributed-parameter systems with Hamiltonian dynamics. Employing the formalism of discrete exterior calculus, we introduce simplicial Dirac structures as discrete analogues of the Stokes-Dirac structure and demonstrate that they provide a natural framework for deriving finite-dimensional port-Hamiltonian systems that emulate their infinite-dimensional counterparts. This approach of discrete differential geometry, rather than discretizing the partial differential equations, allows to first discretize the underlying Stokes-Dirac structure and then to impose the corresponding finite-dimensional port-Hamiltonian dynamics. In this manner, we preserve a number of important topological and geometrical properties of the system.**

I. Introduction

The underlying structure of the distributed-parameter port-Hamiltonian systems considered in this paper is a Stokes-Dirac structure [24] and as such is being defined on a certain space of differential forms on a smooth finite-dimensional orientable, usually Riemannian, manifold with a boundary. The Stokes-Dirac structure generalizes the framework of the Poisson and symplectic structures by providing a theoretical account that permits the inclusion of varying boundary variables in the boundary problem for partial differential equations.

For numerical integration, simulation and control synthesis, it is of paramount interest to have finite approximations that can be interconnected to one another or via the boundary coupled to the other systems, be they finite- or infinite-dimensional. Most of the numerical algorithms emanating from the field of numerical analysis and scientific computing, primarily finite difference and finite element methods, fail to capture the intrinsic system structures and properties, such as symplecticity, conservation of momenta and energy, as well as differential gauge symmetry. Furthermore, some important results, including the Stokes theorem, fail to apply numerically and thus lead to spurious results [3], [27].

A notable previous attempt to resolve the problem of structure-preserving discretization of port-Hamiltonian systems is [14], where the authors employ the mixed finite element method. Their treatment is restricted to the one-dimensional telegraph equations and the two-dimensional wave equation. Although it is hinted that the same methodology applies in higher dimensions and to the other distributed-parameter systems, the results are not clear. The discretization scheme proposed in [14] has been successfully used in structure-preserving discretization of one-dimensional distributed port-Hamiltonian systems in [20], [2], [29]. However, the choice of the basis functions can have dramatic consequences on the numerical performance of the mixed finite element method; as the mesh is being refined, it easily may lead to an ill-conditioned finite-dimensional linear system [1]. The other undertaking on discretization of port-Hamiltonian systems can be found in [25], [26], but the treatment is purely topological and is more akin to the graph-theoretical formulation of conservation laws.

Our approach to structure-preserving spatial discretization of port-Hamiltonian systems is based on discrete exterior geometry and as such proceeds *ab initio* by mirroring the continuous setting. Since many of the smooth elements in exterior geometry have discrete analogues formally identical to the continuous models, in this framework it is easy to recognise the coordinate-independent nature of invariants while maintaining a clear distinction between topological and metric-dependent quantities. Discrete exterior calculus [7], [8], [13], [27] has previously been applied to variational problems naturally arising in mechanics and electromagnetism. These problems, however, stem from a Lagrangian rather than Hamiltonian modeling perspective and as such they conform to multisymplectic structure [11], [21], [22], rather than the Stokes-Dirac structure. The discrete exterior literature, furthermore, seems mostly focused on discretization of systems with infinite spatial domains, boundaryless manifolds, and systems with zero boundary conditions. We offer a treatment of the dynamical systems with nonzero energy flow through the boundary.

Contribution and outline. We begin by recalling the definition of the Stokes-Dirac structure and port-Hamiltonian systems. In order to make this paper as self-contained as possible, we present a brief overview of the elementary discrete exterior geometry needed to define discretized Stokes-Dirac structures and impose appropriate port-Hamiltonian dynamics. The third section is a brief summary of the essential definitions and results in discrete exterior calculus as developed in [7], [8], [13]. In this regard, the only novelty this paper brings is a proper treatment of the boundary of the dual cell complex. Namely, in order to allow the inclusion of nonzero boundary conditions on the dual cell complex, we offer a definition of the dual boundary operator that differs from the standard one. Such a construction leads to a discrete analogue of the integration by parts formula, which is a crucial ingredient in establishing discrete (finite-

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dimensional) Stokes-Dirac structures on a primal simplicial complex and its circumcentric dual. The main result is presented in Section IV, where we introduce the notion of simplicial Dirac structures on a primal-dual cell complex, and in the following section define port-Hamiltonian systems with respect to these structures. Finally, we demonstrate how these simplicial Dirac structures relate to spatially discretized telegraph equations on a bounded domain.

II. The Stokes-Dirac structure and port-Hamiltonian dynamics

Dirac structures were originally developed in [4], [5], [10] as a generalization of symplectic and Poisson structures and were employed in modeling interconnected and constrained dynamical systems. The Stokes-Dirac structure is an infinite-dimensional Dirac structure that provides a foundation for port-Hamiltonian formulation of a class of distributed-parameter systems with boundary energy flow [24].

Throughout this paper, let M be an oriented n-dimensional smooth manifold with a smooth $(n-1)$-dimensional boundary ∂M endowed with the induced orientation, representing the space of spatial variables. By $\Omega^k(M)$, $k = 0, 1, \ldots, n$, denote the space of exterior k-forms on M, and by $\Omega^k(\partial M)$, $k = 0, 1, \ldots, n-1$, the space of k-forms on ∂M.

For any pair p, q of positive integers satisfying $p + q = n + 1$, define the flow and effort linear spaces by

$$\begin{aligned} \mathcal{F}_{p,q} &= \Omega^p(M) \times \Omega^q(M) \times \Omega^{n-p}(\partial M) \\ \mathcal{E}_{p,q} &= \Omega^{n-p}(M) \times \Omega^{n-q}(M) \times \Omega^{n-q}(\partial M) \,. \end{aligned}$$

The bilinear form on the product space $\mathcal{F}_{p,q} \times \mathcal{E}_{p,q}$ is

$$\begin{aligned} &\langle\!\langle (\underbrace{f_p^1, f_q^1, f_b^1}_{\in \mathcal{F}_{p,q}}, \underbrace{e_p^1, e_q^1, e_b^1}_{\in \mathcal{E}_{p,q}}), (f_p^2, f_q^2, f_b^2, e_p^2, e_q^2, e_b^2) \rangle\!\rangle \\ &= \int_M e_p^1 \wedge f_p^2 + e_q^1 \wedge f_q^2 + e_p^2 \wedge f_p^1 + e_q^2 \wedge f_q^1 \\ &\quad + \int_{\partial M} e_b^1 \wedge f_b^2 + e_b^2 \wedge f_b^1 \,. \end{aligned} \tag{1}$$

Theorem II.1. *Given linear spaces $\mathcal{F}_{p,q}$ and $\mathcal{E}_{p,q}$, and the bilinear form $\langle\!\langle , \rangle\!\rangle$, define the following linear subspace $\mathcal{D}$ of $\mathcal{F}_{p,q} \times \mathcal{E}_{p,q}$*

$$\begin{aligned} \mathcal{D} = \Big\{ &(f_p, f_q, f_b, e_p, e_q, e_b) \in \mathcal{F}_{p,q} \times \mathcal{E}_{p,q} \Big| \\ &\begin{pmatrix} f_p \\ f_q \end{pmatrix} = \begin{pmatrix} 0 & (-1)^{pq+1}\mathrm{d} \\ \mathrm{d} & 0 \end{pmatrix} \begin{pmatrix} e_p \\ e_q \end{pmatrix}, \\ &\begin{pmatrix} f_b \\ e_b \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -(-1)^{n-q} \end{pmatrix} \begin{pmatrix} e_p|_{\partial K} \\ e_q|_{\partial K} \end{pmatrix} \Big\}, \end{aligned} \tag{2}$$

where d is the exterior derivative and $|_{\partial M}$ stands for a trace on the boundary ∂M. Then $\mathcal{D} = \mathcal{D}^{\perp}$, that is, $\mathcal{D}$ is a Dirac structure.

In order to define Hamiltonian dynamics, consider a Hamiltonian density $\mathcal{H} : \Omega^p(M) \times \Omega^q(M) \to \Omega^n(M)$ resulting with the Hamiltonian $H = \int_M \mathcal{H} \in \mathbb{R}$. Now, consider a time function $t \mapsto (\alpha_p(t), \alpha_q(t)) \in \Omega^p(M) \times \Omega^q(M)$, $t \in \mathbb{R}$, and the Hamiltonian $t \mapsto H(\alpha_p(t), \alpha_q(t))$ evaluated along this trajectory, then at any t

$$\frac{\mathrm{d}H}{\mathrm{d}t} = \int_M \delta_p H \wedge \frac{\partial \alpha_p}{\partial t} + \delta_q H \wedge \frac{\partial \alpha_q}{\partial t} \,,$$

where $(\delta_p H, \delta_q H) \in \Omega^{n-p}(M) \times \Omega^{n-q}(M)$ are the variational derivatives of H at (α_p, α_q).

Setting the flows $f_p = -\frac{\partial \alpha_p}{\partial t}$, $f_q = -\frac{\partial \alpha_q}{\partial t}$ and the efforts $e_p = \delta_p H$, $e_q = \delta_q H$, the distributed-parameter port-Hamiltonian system is defined by the relation

$$\left(-\frac{\partial \alpha_p}{\partial t}, -\frac{\partial \alpha_q}{\partial t}, f_b, \delta_p H, \delta_q H, e_b \right) \in \mathcal{D} \,, \quad t \in \mathbb{R} \,.$$

For such a system, it straightaway follows that $\frac{\mathrm{d}H}{\mathrm{d}t} = \int_{\partial M} e_b \wedge f_b$, expressing the fact that the system is lossless.

III. Discrete exterior calculus

In the discrete setting, the smooth manifold M is replaced by an oriented manifold-like simplicial complex. An n-dimensional simplicial complex K is a simplicial triangulation of an n-dimensional polytope $|K|$ with an $(n-1)$-dimensional boundary. Familiar examples of such a discrete manifold are meshes of triangles embedded in $\mathbb{R}^3$ and tetrahedra obtained by tetrahedrization of a 3-dimensional manifold. It is worth noticing that in practical applications, sometimes the smooth manifold is unknown and can only be sampled by physical measurements. In such situations, it makes sense to model the spatial domain as inherently discrete. This is where discrete port-Hamiltonian theory in the framework of discrete exterior calculus stands in its own right.

A. Chains and cochains

The discrete analogue of a smooth k-form is a k-cochain, a certain type of a function, on a k-chain representing a formal sum of simplices. The role of integration in the discrete theory is replaced by (simple) evaluation of a discrete form on a chain. The discrete exterior derivative is defined by duality to the boundary operator, rendering the Stokes theorem true by definition.

Definition III.1. *Let K be a simplicial complex. We denote the free abelian group generated by a basis consisting of oriented k-simplices by $C_k(K;\mathbb{Z})$. Elements of $C_k(K;\mathbb{Z})$ are called k-chains.*

Definition III.2. *A primal discrete k-form α is a homomorphism from the chain group $C_k(K;\mathbb{Z})$ to $\mathbb{R}$. A discrete k-form is an element of $\Omega_d^k(K) := C^k(K;\mathbb{R}) = \mathrm{Hom}(C_k(K), \mathbb{R})$.*

The natural pairing of a k-form α and a k-chain c is defined as the bilinear pairing $\langle \alpha, c \rangle = \alpha(c)$. As previously pointed out, a differential k-form α^k can be thought of as a linear functional that assigns a real number to each oriented cell $\sigma^k \in K$. In order to understand the process of discretization of the continuous problem consider a smooth k-form $f \in \Omega^k(|K|)$. The discrete counterpart of f on a k-simplex $\sigma^k \in K$ is a discrete form α^k defined as $\alpha(\sigma^k) = \int_{\sigma^k} f$.

Definition III.3. *The discrete exterior derivative* $\mathbf{d} : C^k(K) \to C^{k+1}(K)$ *is defined by duality to the boundary operator* $\partial_{k+1} : C_{k+1}(K;\mathbb{Z}) \to C_k(K;\mathbb{Z})$*, with respect to the natural pairing between discrete forms and chains. For a discrete form* $\alpha^k \in \Omega_d^k(K)$ *and a chain* $c_{k+1} \in C_{k+1}(K;\mathbb{Z})$ *we define* $\mathbf{d}$ *by*

$$\langle \mathbf{d}\alpha^k, c_{k+1} \rangle = \langle \alpha^k, \partial_{k+1} c_{k+1} \rangle \,.$$

Similar to the continuous theory, we drop the index of the boundary operator when its dimension is clear from the context. The discrete exterior derivative $\mathbf{d}$ is constructed in such a manner that the Stokes theorem is satisfied by definition. Thus, given a $(k+1)$-chain c and a discrete k-form α, the *discrete Stokes theorem* states that $\langle \mathbf{d}\alpha, c \rangle = \langle \alpha, \partial c \rangle$.

B. Dual cell complex

An essential constituent of discrete exterior calculus is the dual complex of a manifold-like simplicial complex. The most popular notions of duality are barycentric and circumcentric, also known as Voronoi, duality. In this paper we employ the latter. Furthermore, we shall assume we are always given a so-called well-centered simplicial complex, that is a simplicial complex whose all simplices of all dimensions are well-centered [13].

Given a simplicial well-centered complex K, we define its interior dual cell complex $\star_{\mathrm{i}} K$ (block complex in terminology of algebraic topology [23]) as a circumcentric dual restricted to $|K|$. An important property of the the Voronoi duality is that primal and dual cells are orthogonal to each other. The boundary dual cell complex $\star_{\mathrm{b}} K$ is a dual to ∂K. The dual cell complex $\star K$ is defined as $\star K = \star_{\mathrm{i}} K \cup \star_{\mathrm{b}} K$.

A dual mesh $\star_{\mathrm{i}} K$ is a dual to K in sense of a graph dual, and the dual of the boundary is equal to the boundary of the dual, that is $\partial(\star K) = \star(\partial K) = \star_{\mathrm{b}} K$. This construction of the dual is compatible with [27] and as such is very similar to the use of the ghost cells in finite volume methods in order to account for the duality relation between the Dirichlet and the Neumann boundary conditions. Because of duality, there is a one-to-one correspondence between k-simplices of K and interior $(n-k)$-cells of $\star K$. Likewise, to every k-simplex on ∂K there is a uniquely associated $(n-1-k)$-cell on $\partial(\star K)$. Fig. 1 illustrates the duality on a flat 2-dimensional simplicial complex.

In what follows, we shall abuse notation and use the same symbol $\star\sigma^k$ for both the interior circumcentric and the boundary star operator when the meaning is clear from the context. We adopt the convention that all symbols related to the dual cell complex are labeled by a caret. Everything that has been said about the primal chains and cochains can be extended to dual cells and dual cochains. We do not elaborate on this since it can be found in the literature [13], [8], however, in order to properly account for the behaviours on the boundary, we slightly need to change the definition of the boundary dual operator as presented in [13], [8]. We propose the following definition.

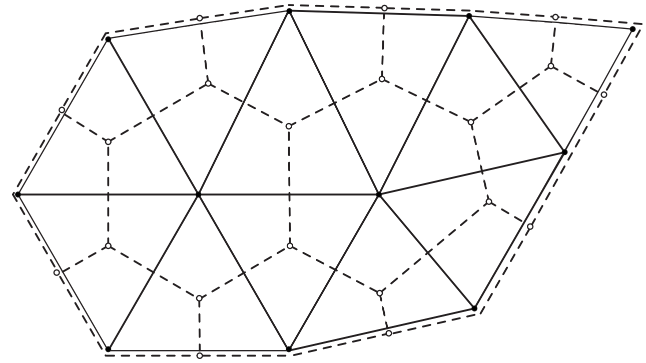

Fig. 1. A 2-dimensional simplicial complex K and its circumcentric dual cell complex $\star K$ indicated by dashed lines. The boundary of $\star K$ is the dual of the boundary of K.

Definition III.4. *The dual boundary operator* $\partial_k : C_k(\star K;\mathbb{Z}) \to C_{k-1}(\star K;\mathbb{Z})$ *is a homomorphism defined by its action on a dual cell* $\hat\sigma^k = \star\sigma^{n-k} = \star[v_0,\ldots,v_{n-k}]$,

$$\begin{aligned}\partial\hat\sigma^k &= \partial \star [v_0,\ldots,v_{n-k}] \\ &= \partial_{\mathrm{i}} \star [v_0,\ldots,v_{n-k}] + \partial_{\mathrm{b}} \star [v_0,\ldots,v_{n-k}]\end{aligned} \tag{3}$$

where the internal boundary operator is $\partial_{\mathrm{i}}\star[v_0,\ldots,v_{n-k}] = \sum_{\sigma^{n-k+1}\succ\sigma^{n-k}} \star(s_{\sigma^{n-k+1}}\sigma^{n-k+1})$ *for* $\star\sigma^{n-k+1} \in \star_{\mathrm{i}} K$ *and the boundary operator associated with* $\partial(\star K)$ *is* $\partial_{\mathrm{b}} \star [v_0,\ldots,v_{n-k}] = \sum_{\sigma^{n-k+1}\succ\sigma^{n-k}} \star(s_{\sigma^{n-k}}\sigma^{n-k+1})$ *for* $\star\sigma^{n-k+1} \in \partial(\star K)$.

The boundary of the dual cell complex as defined in [13] is equal to ∂_{i}. The dual boundary operator ∂_{b} extends the definition from [13] in such a manner that the boundary of the extended dual cell complex $\star K$ is the geometric boundary. The dual exterior derivative $\mathbf{d} : C^k(\star K) \to C^{k+1}(\star K)$ is defined by duality to the dual boundary operator, and as such can be decomposed into the internal $\mathbf{d}_{\mathrm{i}}$ and the boundary part $\mathbf{d}_{\mathrm{b}}$ (see Remak III.1).

C. Discrete wedge and Hodge operator

There exists a natural pairing, via the so-called primal-dual wedge product, between a primal k-cochain and a dual $(n-k)$-cochain. The resulting discrete form is the volume form. In order to insure anticommutativity of the primal-dual wedge product, we take the following definition.

Definition III.5. *Let* $\alpha^k \in \Omega_d^k(K)$ *and* $\hat\beta^{n-k} \in \Omega_d^{n-k}(\star_{\mathrm{i}} K)$*. We define the discrete primal-dual wedge product* $\wedge : \Omega_d^k(K) \times \Omega_d^{n-k}(\star_{\mathrm{i}} K) \to \Omega_d^n(V_k(K))$ *by*

$$\begin{aligned}\langle \alpha^k \wedge \hat\beta^{n-k}, V_{\sigma^k} \rangle &= \binom{n}{k} \frac{|V_{\sigma^k}|}{|\sigma^k||\star\sigma^k|} \langle \alpha^k, \sigma^k \rangle \langle \hat\beta^{n-k}, \star\sigma^k \rangle \\ &= \langle \alpha^k, \sigma^k \rangle \langle \hat\beta^{n-k}, \star\sigma^k \rangle \\ &= (-1)^{k(n-k)} \langle \hat\beta^{n-k} \wedge \alpha^k, V_{\sigma^k} \rangle \,,\end{aligned}$$

where V_{σ^k} *is the* n*-dimensional support volume obtained by taking the convex hull of the simplex* σ^k *and its dual* $\star\sigma^k$.

Here we note the advantage of employing circumcentric dual since one needs to store only volume information about primal and dual cells, and not about the primal-dual convex hulls.

The proposed definition of the dual boundary operator ensures the validity of the evaluation by parts relation that parallels the integration by parts formula for smooth differential forms.

Proposition III.1. *Let K be an oriented well-centered simplicial complex. Given a primal $(k-1)$-form α^{k-1} and a dual $(n-k)$-discrete form $\hat{\beta}^{n-k}$, then*

$$\langle \mathbf{d}\alpha^{k-1} \wedge \hat{\beta}^{n-k}, K\rangle + (-1)^{k-1}\langle \alpha^{k-1} \wedge \mathbf{d}\hat{\beta}^{n-k}, K\rangle = \langle \alpha^{k-1} \wedge \hat{\beta}^{n-k}, \partial K\rangle\,,$$

where in the boundary pairing α^{k-1} is a primal $(k-1)$-form on ∂K, while $\hat{\beta}^{n-k}$ is a dual $(n-k)$-cochain taken on the boundary dual $\star(\partial K)$.

Proof: Follows from direct calculation.

Remark III.1. *Decomposing the dual form $\hat{\beta}^{n-k}$ into the internal and the boundary part as $\hat{\beta}^{n-k} = \begin{cases} \hat{\beta}_{\mathrm{i}} \in \Omega_d^{n-k}(\star_{\mathrm{i}}K) & \text{on } \star_{\mathrm{i}}K \\ \hat{\beta}_{\mathrm{b}} \in \Omega_d^{n-k}(\star_{\mathrm{b}}K) & \text{on } \partial(\star K)\end{cases}$ and decomposing the dual exterior derivative in the same manner, the summation by parts formula can be written as*

$$\langle \mathbf{d}\alpha^{k-1} \wedge \hat{\beta}_{\mathrm{i}}, K\rangle + (-1)^{k-1}\langle \alpha^{k-1} \wedge (\mathbf{d}_{\mathrm{i}}\hat{\beta}_{\mathrm{b}} + \mathbf{d}_{\mathrm{b}}\hat{\beta}_{\mathrm{i}}), K\rangle = \langle \alpha^{k-1} \wedge \hat{\beta}_{\mathrm{b}}, \partial K\rangle\,. \tag{4}$$

The support volumes of a simplex and its dual cell are the same, which suggests that there is a natural identification between primal k-cochains and dual $(n-k)$-cochains. Since the Hodge star operator is metric-dependent, in the discrete theory, it is defined as an equality of averages between primal and their dual forms [16]. The discrete Hodge star maps primal cochains into dual forms, and vice versa [13], [16].

IV. Dirac structures on a simplicial complex

As discrete analogue of the Stokes-Dirac structure, we introduce Dirac structures with respect to the bilinear pairing between primal and duals forms on the underlying discrete manifold. We call these Dirac structures *simplicial Dirac structures*. The flow and the effort spaces will be the spaces of complementary primal and dual forms. The elements of these two spaces are paired via the discrete primal-dual wedge product. One of the two possible choices is

$$\mathcal{F}^d_{p,q} = \Omega^p_d(\star_{\mathrm{i}}K) \times \Omega^q_d(K) \times \Omega^{n-p}_d(\partial(K))\,,$$
$$\mathcal{E}^d_{p,q} = \Omega^{n-p}_d(K) \times \Omega^{n-q}_d(\star_{\mathrm{i}}K) \times \Omega^{n-q}_d(\partial(\star K))\,.$$

The primal-dual wedge product ensures a bijective relation between the primal and dual forms, between the flows and efforts. A natural discrete mirror of the bilinear form (1) is a symmetric pairing on the product space $\mathcal{F}^d_{p,q} \times \mathcal{E}^d_{p,q}$ defined by

$$\begin{aligned}&\langle\!\langle (\underbrace{\hat{f}^1_p, f^1_q, f^1_b}_{\in \mathcal{F}^d_{p,q}}, \underbrace{e^1_p, \hat{e}^1_q, \hat{e}^1_b}_{\in \mathcal{E}^d_{p,q}}), (\hat{f}^2_p, f^2_q, f^2_b, e^2_p, \hat{e}^2_q, \hat{e}^2_b)\rangle\!\rangle_d \\ &= \langle e^1_p \wedge \hat{f}^2_p + \hat{e}^1_q \wedge f^2_q + e^2_p \wedge \hat{f}^1_p + \hat{e}^2_q \wedge f^1_q, K\rangle \\ &\quad + \langle \hat{e}^1_b \wedge f^2_b + \hat{e}^2_b \wedge f^1_b, \partial K\rangle\,.\end{aligned} \tag{5}$$

A discrete analogue of the Stokes-Dirac structure is a finite-dimensional Dirac structure constructed in the following theorem.

Theorem IV.1. *Given linear spaces $\mathcal{F}^d_{p,q}$ and $\mathcal{E}^d_{p,q}$, and the bilinear form $\langle\!\langle , \rangle\!\rangle_d$. The linear subspace $\mathcal{D}_d \subset \mathcal{F}^d_{p,q} \times \mathcal{E}^d_{p,q}$ defined by*

$$\begin{aligned}\mathcal{D}_d = \Big\{ &(\hat{f}_p, f_q, f_b, e_p, \hat{e}_q, \hat{e}_b) \in \mathcal{F}^d_{p,q} \times \mathcal{E}^d_{p,q} \Big| \\ &\begin{pmatrix}\hat{f}_p \\ f_q\end{pmatrix} = \begin{pmatrix} 0 & (-1)^{pq+1}\mathbf{d}_{\mathrm{i}} \\ \mathbf{d} & 0\end{pmatrix}\begin{pmatrix} e_p \\ \hat{e}_q\end{pmatrix} + (-1)^{pq+1}\begin{pmatrix}\mathbf{d}_{\mathrm{b}} \\ 0\end{pmatrix}\hat{e}_b\,, \\ &f_b = (-1)^p e_p|_{\partial K} \Big\}\end{aligned} \tag{6}$$

is a Dirac structure with respect to the pairing $\langle\!\langle , \rangle\!\rangle_d$.

Proof: In order to show that $\mathcal{D}_d \subset \mathcal{D}_d^\perp$, let $(\hat{f}^1_p, f^1_q, f^1_b, e^1_p, \hat{e}^1_q, \hat{e}^1_b) \in \mathcal{D}_d$, and consider any $(\hat{f}^2_p, f^2_q, f^2_b, e^2_p, \hat{e}^2_q, \hat{e}^2_b) \in \mathcal{D}_d$. Substituting (6) into (5) yields

$$\begin{aligned}&\langle (-1)^{pq+1} e^1_p \wedge \big(\mathbf{d}_{\mathrm{i}}\hat{e}^2_q + \mathbf{d}_{\mathrm{b}}\hat{e}^2_b\big) + \hat{e}^1_q \wedge \mathbf{d}e^2_p \\ &+ (-1)^{pq+1} e^2_p \wedge \big(\mathbf{d}_{\mathrm{i}}\hat{e}^1_q + \mathbf{d}_{\mathrm{b}}\hat{e}^1_b\big) + \hat{e}^2_q \wedge \mathbf{d}e^1_p, K\rangle \\ &+ (-1)^p\langle \hat{e}^1_b \wedge e^2_p + \hat{e}^2_b \wedge e^1_p, \partial K\rangle\end{aligned} \tag{7}$$

By the anticommutativity of the primal-dual wedge product on K

$$\langle \hat{e}^1_q \wedge \mathbf{d}e^2_p, K\rangle = (-1)^{q(p-1)}\langle \mathbf{d}e^2_p \wedge \hat{e}^1_q, K\rangle$$
$$\langle \hat{e}^2_q \wedge \mathbf{d}e^1_p, K\rangle = (-1)^{q(p-1)}\langle \mathbf{d}e^1_p \wedge \hat{e}^2_q, K\rangle\,,$$

and on the boundary ∂K

$$\langle \hat{e}^1_b \wedge e^2_p, \partial K\rangle = (-1)^{(p-1)(q-1)}\langle e^2_p \wedge \hat{e}^1_b, \partial K\rangle$$
$$\langle \hat{e}^2_b \wedge e^1_p, \partial K\rangle = (-1)^{(p-1)(q-1)}\langle e^1_p \wedge \hat{e}^2_b, \partial K\rangle\,,$$

the expression (7) can be rewritten as

$$\begin{aligned}&(-1)^{q(p-1)}\langle \mathbf{d}e^2_p \wedge \hat{e}^1_q + (-1)^{n-p} e^2_p \wedge \big(\mathbf{d}_{\mathrm{i}}\hat{e}^1_q + \mathbf{d}_{\mathrm{b}}\hat{e}^1_b\big), K\rangle \\ &+ (-1)^{q(p-1)}\langle \mathbf{d}e^1_p \wedge \hat{e}^2_q + (-1)^{n-p} e^1_p \wedge \big(\mathbf{d}_{\mathrm{i}}\hat{e}^2_q + \mathbf{d}_{\mathrm{b}}\hat{e}^2_b\big), K\rangle \\ &+ (-1)^{p+(p-1)(q-1)}\langle \hat{e}^1_b \wedge e^2_p + \hat{e}^2_b \wedge e^1_p, \partial K\rangle\,.\end{aligned}$$

According to the discrete summation by parts formula (4), the following holds

$$\langle \mathbf{d}e^2_p \wedge \hat{e}^1_q + (-1)^{n-p} e^2_p \wedge \big(\mathbf{d}_{\mathrm{i}}\hat{e}^1_q + \mathbf{d}_{\mathrm{b}}\hat{e}^1_b\big), K\rangle = \langle e^2_p \wedge \hat{e}^1_b, \partial K\rangle$$
$$\langle \mathbf{d}e^1_p \wedge \hat{e}^2_q + (-1)^{n-p} e^1_p \wedge \big(\mathbf{d}_{\mathrm{i}}\hat{e}^2_q + \mathbf{d}_{\mathrm{b}}\hat{e}^2_b\big), K\rangle = \langle e^1_p \wedge \hat{e}^2_b, \partial K\rangle\,.$$

Hence (7) is equal to 0, and thus $\mathcal{D}_d \subset \mathcal{D}_d^\perp$.

Since $\dim \mathcal{F}^d_{p,q} = \dim \mathcal{E}^d_{p,q} = \dim \mathcal{D}_d$, and $\langle\!\langle , \rangle\!\rangle_d$ is a non-degenerate form, $\mathcal{D}_d = \mathcal{D}_d^\perp$. ■

Remark IV.1. *As with the continuous setting [24], the simplicial Dirac structure is spatially compositional. Since the underlying spaces are finite-dimensional linear spaces, the simplicial Dirac structure $\mathcal{D}_d$ is integrable.*

The other possible discrete analogue of the Stokes-Dirac structure is defined on the spaces

$$\tilde{\mathcal{F}}^d_{p,q} = \Omega^p_d(K) \times \Omega^q_d(\star_{\mathrm{i}}K) \times \Omega^{n-p}_d(\partial(\star K))$$
$$\tilde{\mathcal{E}}^d_{p,q} = \Omega^{n-p}_d(\star_{\mathrm{i}}K) \times \Omega^{n-q}_d(K) \times \Omega^{n-q}_d(\partial K)\,.$$

Theorem IV.2. *The linear space $\tilde{\mathcal{D}}_d$ defined by*

$$\begin{aligned}\tilde{\mathcal{D}}_d = \big\{&(f_p, \hat{f}_q, f_b, e_p, e_q, e_b) \in \tilde{\mathcal{F}}^d_{p,q} \times \tilde{\mathcal{E}}^d_{p,q} \,\big|\\ &\begin{pmatrix} f_p \\ f_q \end{pmatrix} = \begin{pmatrix} 0 & (-1)^{pq+1}\mathbf{d} \\ \mathbf{d}_{\mathrm{i}} & 0 \end{pmatrix} \begin{pmatrix} \hat{e}_p \\ e_q \end{pmatrix} + \begin{pmatrix} 0 \\ \mathbf{d}_{\mathrm{b}} \end{pmatrix} \hat{f}_b \,,\\ &e_b \;=\; (-1)^p e_q|_{\partial K} \big\}\end{aligned} \tag{8}$$

is a Dirac structure with respect to the bilinear pairing between $\tilde{\mathcal{F}}^d_{p,q}$ and $\tilde{\mathcal{E}}^d_{p,q}$.

In the following section, the simplicial Dirac structure (6) will be used as *terminus a quo* for the geometric formulation of spatially discrete port-Hamiltonian systems. In the similar manner we can define port-Hamiltonian systems with respect to the Dirac structure (8).

V. Port-Hamiltonian dynamics on a simplicial complex and its circumcentric dual

In the discrete framework one can define an open Hamiltonian system with respect to the simplicial Dirac structure $\mathcal{D}_d$ or the simplicial structure $\tilde{\mathcal{D}}_d$. The choice of the structure has immediate consequence on the open dynamics since it restricts the choice of freely chosen boundary efforts or flows. We define dynamics with respect to (6), and note that in the similar fashion port-Hamiltonian systems can be defined with respect to $\tilde{\mathcal{D}}_d$ what we illustrate by an example in the following section.

Given a discrete Hamiltonian density n-volume form $\mathcal{H}: \Omega^p_d(\star_{\mathrm{i}}K)\times\Omega^q_d(K) \to \Omega_d(V(K))$, the Hamiltonian functional is $H(\hat{\alpha}_p, \alpha_q) = \langle \mathcal{H}(\hat{\alpha}_p, \alpha_q), V(K)\rangle$ for $\hat{\alpha}_p \in \Omega^p_d(\star_{\mathrm{i}}K)$ and $\alpha_q \in \Omega^q_d(K)$. A time derivative of H along an arbitrary trajectory $t \to (\hat{\alpha}_p(t), \alpha_q(t)) \in \Omega^p_d(\star_{\mathrm{i}}K) \times \Omega^q_d(K)$, $t \in \mathbb{R}$, is

$$\frac{\mathrm{d}}{\mathrm{d}t} H(\hat{\alpha}_p, \alpha_q) = \langle \frac{\partial \mathcal{H}}{\partial \hat{\alpha}_p} \wedge \frac{\partial \hat{\alpha}_p}{\partial t} + \frac{\partial \hat{\mathcal{H}}}{\partial \alpha_q} \wedge \frac{\partial \alpha_q}{\partial t}, K\rangle \,. \tag{9}$$

The relations between the simplicial-Dirac structure (6) and time derivatives of the variables are: $\hat{f}_p = -\frac{\partial \hat{\alpha}_p}{\partial t}$, $f_q = -\frac{\partial \alpha_q}{\partial t}$, while the efforts are: $e_p = \frac{\partial \mathcal{H}}{\partial \hat{\alpha}_p}$, $\hat{e}_q = \frac{\partial \hat{\mathcal{H}}}{\partial \alpha_q}$.

This allows us to define time-continuous port-Hamiltonian system on a simplicial complex K (and its dual $\star K$) by

$$\begin{aligned}&\begin{pmatrix} -\frac{\partial \hat{\alpha}_p}{\partial t} \\ -\frac{\partial \alpha_q}{\partial t} \end{pmatrix} = \begin{pmatrix} 0 & (-1)^r \mathbf{d}_{\mathrm{i}} \\ \mathbf{d} & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial \mathcal{H}}{\partial \hat{\alpha}_p} \\ \frac{\partial \hat{\mathcal{H}}}{\partial \alpha_q} \end{pmatrix} + (-1)^r \begin{pmatrix} \mathbf{d}_{\mathrm{b}} \\ 0 \end{pmatrix} \hat{e}_b \,,\\ &f_b \;=\; (-1)^p \frac{\partial \mathcal{H}}{\partial \hat{\alpha}_p}\Big|_{\partial K} \,,\end{aligned} \tag{10}$$

where $r = pq + 1$.

It immediately follows that $\frac{\mathrm{d}H}{\mathrm{d}t} = \langle \hat{e}_b \wedge f_b, \partial K\rangle$, enunciating a fundamental property of the system: the increase in the energy on the domain $|K|$ is equal to the power supplied to the system through the boundary ∂K and $\partial(\star K)$. Due to its structural properties, the system (10) can be called a spatially-discrete time-continuous boundary control system with $\hat{e}_b$ being the boundary control input and f_b being the output.

In contrast to (10), in the case of the port-Hamiltonian formulation with respect to the simplicial Dirac structure (8) the boundary flows $\hat{f}_b$ can be considered to be freely chosen, while the boundary efforts e_b are determined by the dynamics.

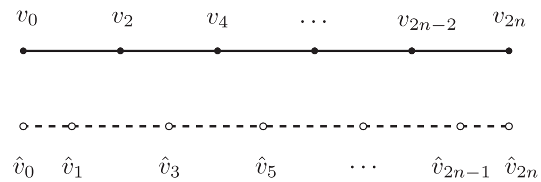

Fig. 2. The primal 1-dimensional simplicaial complex K with even nodes indices and its dual $\star K$ with odd indices, both with conventional orientation of one simplices (from the node with a lower-index to the higher-index node). By construction, the nodes $\hat{v}_0$ and $\hat{v}_{2n}$ are added to the boundary as previously explained to insure that the boundary of the dual is the dual of the boundary, i.e., $\partial(\star K) = \star(\partial K)$.

VI. Example: Telegraph equations

We consider an ideal lossless transmission line on a 1-dimensional simplicial complex. The energy variables are the charge density $q \in \Omega^1_d(K)$, and the flux density $\hat{\phi} \in \Omega^1_d(\star K)$, hence $p = q = 1$. The Hamiltonian representing the total energy stored in the transmission line with distributed capacitance C and distributed inductance L is

$$H = \frac{1}{2}\langle \frac{1}{C} q \wedge * q + \frac{1}{L}\hat{\phi} \wedge *\hat{\phi}, K\rangle \,, \tag{11}$$

where $*$ is the discrete diagonal Hodge operator [13], [16] and the co-energy variables are: $\hat{e}_p = \frac{\partial \hat{\mathcal{H}}}{\partial q} = *\frac{q}{C} = \hat{V}$ representing voltages and $e_q = \frac{\partial \mathcal{H}}{\partial \hat{\phi}} = *\frac{\hat{\phi}}{L} = I$ currents.

Selecting $f_p = -\frac{\partial q}{\partial t}$ and $\hat{f}_q = -\frac{\partial \hat{\phi}}{\partial t}$ leads to the port-Hamiltonian formulation of the telegraph equations

$$\begin{aligned}&\begin{pmatrix} -\frac{\partial q}{\partial t} \\ -\frac{\partial \hat{\phi}}{\partial t} \end{pmatrix} = \begin{pmatrix} 0 & \mathbf{d} \\ \mathbf{d}_{\mathrm{i}} & 0 \end{pmatrix} \begin{pmatrix} *\frac{q}{C} \\ *\frac{\hat{\phi}}{L} \end{pmatrix} + \begin{pmatrix} 0 \\ \mathbf{d}_{\mathrm{b}} \end{pmatrix} \hat{f}_b\\ &e_b \;=\; -*\frac{\hat{\phi}}{L}\Big|_{\partial K} \,,\end{aligned} \tag{12}$$

where the $\hat{f}_b$ are input voltages and the e_b are output currents.

In the case we wanted to have the electrical currents as the inputs, the charge and the flux densities would be defined on the dual mesh and the primal mesh, respectively. Instead of the port-Hamiltonian system in the form (12), the discretized telegraph equations would be in the form (10). The free boundary variables are always defined on the boundary of the dual cell complex.

Note that the structure (12) is in fact a Poisson structure on the state space $\Omega^1_d(K) \times \Omega^1_d(\star K)$. This will become obvious when we present this structure in a matrix representation.

Matrix representation. For the simplicial complex in Fig. 2, a differential form $e_q \in \Omega^0_d(K)$ is uniquely characterized by its coefficient vector $\vec{e}_q \in \mathbb{R}^{n+1}$ since $\dim \Omega^0_d(K) = n + 1$, similarly $\vec{e}_p, \vec{f}_p \in \mathbb{R}^n$, $\vec{f}_q \in \mathbb{R}^{n+1}$, $\vec{e}_b, \vec{f}_b \in \mathbb{R}^2$. Representing discrete forms by their coefficient vectors induces a matrix representation for linear operators (see e.g. [8], [16]). The exterior derivative $\mathbf{d} : \Omega^0_d(K) \to \Omega^1_d(K)$ is represented by a matrix $D \in \mathbb{R}^{n\times(n+1)}$, which is the transpose of the incidence matrix of the primal mesh [8], [9]. The discrete derivative $\mathbf{d} : \Omega^0_d(\star K) \to \Omega^1_d(\star K)$ in the matrix notation is the transpose of the incidence matrix of the dual mesh denoted by $\hat{D} \in \mathbb{R}^{(n+1)\times(n+2)}$, which can be decomposed as $\hat{D} = (D_{\mathrm{i}} \vdots D_{\mathrm{b}})^{\mathrm{T}}$ with $D_{\mathrm{i}} = -D^{\mathrm{T}}$ and D_{b} is the transpose of the boundary incidence matrix, that is,

$$
\begin{aligned}
D &= \begin{pmatrix} -1 & 1 & 0 & \cdots & 0 & 0 \\ 0 & -1 & 1 & \cdots & 0 & 0 \\ & & & \ddots & & \\ 0 & 0 & 0 & \cdots & -1 & 1 \end{pmatrix}, \\
D_b^{\mathrm{T}} &= \begin{pmatrix} -1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 1 \end{pmatrix}.
\end{aligned}
\tag{13}
$$

Implementing the primal-dual wedge product as a scalar multiplication of the coefficient vectors, the simplicial Dirac structure of (12) can be represented by

$$
\begin{pmatrix} \vec{f}_p \\ \vec{f}_q \\ \vec{e}_b \end{pmatrix} = \begin{pmatrix} 0 & D & 0 \\ -D^{\mathrm{T}} & 0 & D_{\mathrm{b}} \\ 0 & -D_{\mathrm{b}}^{\mathrm{T}} & 0 \end{pmatrix} \begin{pmatrix} \vec{e}_p \\ \vec{e}_q \\ \vec{f}_b \end{pmatrix}. \tag{14}
$$

Convergence. Repeating simulation experiments for different parameters we conjecture that the accuracy of the proposed method is $1/n$, what comes as no surprise since we worked with diagonal mass-lumped Hodge operators, which are of first-order accuracy.

VII. Concluding Remarks

A number of interesting topics and open questions still need to be addressed. A major challenge from the numerical analysis standpoint is to offer a careful study of the convergence properties of discrete exterior calculus. In future, in the context of [1], [17], it would be interesting to study structure-preserving discretization of port-Hamiltonian systems in the framework of Hilbert complexes.

An important application of structure-preserving discretization of port-Hamiltonian systems might be in optimal control theory what also prompts a need for time discretization. The issue in this context is to study the effects variational integrators [18], [19] have on passivity (and losslessness) of open dynamical systems.

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