Compendium. The primary objective of my research is to enhance the mathematical and scientific foundations of network modeling and system analysis of complex physical systems. The central avenue of my research is a differential geometry-based approach to computational modeling and structure-preserving discretization of distributed-parameter systems. The driving idea behind this work is the need for numerical methods for differential equations that are robust, modular, and globally accurate. Employing the geometric compositional modeling, I strive to enhance the analysis and control of the complex physical systems stemming from mechanics, engineering and systems biology.

1 Overview and Motivation

Hamiltonian systems are at the foundation of many current physical theories, including quantum and relativistic mechanics, electromagnetism, optics, solid and fluid mechanics. Geometry as the study of observable symmetries and dynamical invariants is de facto the lingua franca of the Hamiltonian theories.

The prevailing paradigm in modeling of the complex large-scale physical systems is network modeling. In many problems arising from modern science and engineering, such as multi-body systems, electrical networks and molecular dynamics, the port-based network modeling is a natural strategy of decomposing the overall system into subsystems, which are interconnected to each other through pairs of variables called ports and whose product is the power exchanged between the subsystems.

Physical Networked Systems. The formalism that unifies the geometric Hamiltonian and the port-based network modeling is the port-Hamiltonian, which associates with interconnection structure of the network a geometric structure given by a Poisson, or more generally a Dirac structure [12, 2, 14]. The generalized Hamiltonian dynamic is then defined with respect to this Poisson, or Dirac [1], structure by specifying the Hamiltonian representing the total stored energy, the energy-dissipating elements and the ports of the system. Apart from enunciating a remarkable structural unity, Poisson and Dirac geometry offers a mathematical framework that gives important insights into dynamical systems. Moreover, the geometric formalism transcends the finite-dimensional scenario and has been successfully applied to study of a number of distributed-parameter systems, systems described by a set of partial differential equations.

Motivation. For numerical integration, simulation and control synthesis, it is of paramount interest to have finite approximations of distributed-parameter systems that can be interconnected to one another or via the boundary coupled to other systems, be they finite- or infinite-dimensional. Most of the numerical algorithms for spatial discretization of distributed-parameter systems, 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 Stokes theorem, fail to apply numerically and thus lead to spurious results. Given the overwhelming geometric nature of physical systems, the loss of fidelity to preserve some inherently topological and geometric structures of the continuous models gives a motivation to approach computations from a geometric standpoint.

2 My Contributions

My doctoral research provides a framework for structure-preserving discretization of open distributed-parameter systems with generalized Hamiltonian dynamics.

The underlying structure of distributed-parameter systems I address in my thesis is a Stokes-Dirac structure \([13]\), a type of infinite-dimensional Dirac structure, defined in terms 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. From an interconnection and control viewpoint, such a treatment of boundary conditions is essential for the incorporation of energy exchange through the boundary, since in many applications the interconnection with the environment takes place precisely through the boundary. Well-known examples of distributed-parameter port-Hamiltonian systems a 3-, 2-, and 1-dimensional manifold, for instance, are: Maxwell’s equations on a bounded domain, the two-dimensional wave equation, and the telegraph equations.

Employing the formalism of discrete exterior calculus \([3, 4, 7]\), I have introduced simplicial Dirac structures as discrete analogues of the Stokes-Dirac structure and demonstrated that they provide a natural framework for deriving finite-dimensional port-Hamiltonian systems that emulate the behaviors of their infinite-dimensional counterparts \([18, 19, 20]\). The theory proceeds \textit{ab initio} by mirroring the continuous setting, and as such is not merely tied to the goal of discretization, but rather aims to offer a geometric framework for the analysis and control of physical systems on discrete manifolds.

Structure-Preserving Discretization. The spatial domain, in the continuous theory represented by a finite-dimensional smooth manifold with boundary, is replaced by a homological manifold-like simplicial complex. Familiar examples of such a simplicial manifold are meshes of triangles embedded in \(\mathbb{R}^3\) and tetrahedra obtained by tetrahedrization of a 3-dimensional manifold. The smooth differential forms, in discrete setting, are mirrored by cochains on the primal and dual complexes (Voronoi, i.e., circumcentric dual), while the discrete exterior derivative is defined to be the coboundary operator from algebraic topology \([10]\). This approach of discrete exterior 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, a number of important intrinsically topological and geometric properties of the system are preserved.

The explicit simplicial discretization proposed in \([19, 23]\) leads to the standard input-output port-Hamiltonian systems \textit{without} algebraic constraints, unlike the standard mixed finite element schemes \([6]\), which usually lead to a set of differential and algebraic equations. Thus, the analysis and the control synthesis for the port-Hamiltonian systems on simplicial complexes
belong to the realm of standard finite-dimensional systems.

**Symmetry Reduction.** Although the differential operator in the Stokes-Dirac structure, in the presence of nonzero boundary conditions, is not skew-symmetric, it is possible to associate a Poisson structure to the Stokes-Dirac structure [13]. In the absence of algebraic constraints imposed by boundary conditions, the Stokes-Dirac structure specializes to a Poisson structure [5], and as such it can be derived through symmetry reduction from a canonical Dirac structure on the phase space (symplectic manifold) [25]. How to conduct this reduction for the Stokes-Dirac structure on a manifold with boundary was an open question for quite some time. In order to cope with Dirac structures on a manifold with boundary, I have introduced the notion of a generalized canonical Dirac structure, a type of Dirac structure on an augmented cotangent bundle [22]. Then, the Poisson reduction starting from the generalized canonical Dirac structure leads to the Poisson structure associated with the Stokes-Dirac structure. In the context of dynamics, the canonical port-Hamiltonian systems are the generalized Hamiltonian systems on jet bundles [16], while the reduced systems are exactly port-Hamiltonian systems [13]. Furthermore, I have shown that the Poisson symmetry reduction can be in the similar fashion conducted in the discrete setting on simplicial Dirac structures [22].

**Reaction-Diffusion Systems.** I am very excited by theoretical problems stemming from systems biology. One of those problems is the question of diffusion-driven instability, which constitutes the basis of Turing’s mechanism for pattern formation.

I have introduced a Dirac structure that captures the geometry of reaction-diffusion systems [17]. We start from the fact that the considered reaction systems are defined with respect to a finite Dirac structure on a manifold. This means that the reaction system from a network modeling perspective can be described by a set of energy-storing elements, a set of energy-dissipating (resistive) elements, and a set of ports (by which the interconnections are modeled), all interconnected by power-conserving interconnections [14]. A large class of balanced chemical reaction networks are of this type, reaction networks governed by mass action kinetics, for instance [15]. Here, the port-Hamiltonian perspective permits us to draw immediately some conclusions regarding passivity of reaction-diffusion systems and the existence of attractors. In order to apply the Krasovskii-LaSalle principle, we need the global boundedness of classical solution. For this reason, stability analysis seems to be a very hard problem. Under certain assumptions, I have obtained a result that warrants stability for the asymptotic behavior of the solution of a class of reaction-diffusion systems with Neumann’s boundary conditions [24].

By adopting a discrete differential geometry-based approach and discretizing the reaction-diffusion system in the port-Hamiltonian form, apart from preserving a geometric structure, a compartmental model analogous to the standard one is obtained [24]. In the case of balanced reaction networks, the finite dimensional model exhibits a very interesting spatiotemporal consensus dynamics, which potentially has significant biochemical consequences that remain to be exploited.

### 3 Future Directions

Being excited by both practical and theoretical problems, I plan to explore the emerging connections between geometry, applied analysis, and control theory. My goal is to develop theory and practical algorithms for the systematic construction of geometric structure-preserving numeri-
cal schemes, aiming towards obtaining more robust and accurate numerical implementations of feedback and optimal control laws.

My immediate research plans are:

1. To study discrete Dirac mechanics in the context of constrained and controlled systems.
2. Develop a geometric discretization of interconnected systems using the discrete Dirac framework, that is, to extend variational integrators to open systems.
3. Develop the theory of structural geometric integrators for the systems percolating from fluid dynamics, namely the Euler equations governing inviscid flow, but also the Navier-Stokes equations.
4. To exploit theoretical developments in the field of interconnected and spatially distributed systems in chemistry and biology.

Control of Spatially Distributed Systems. In [23] I have been looking at a simple control strategy for the energy shaping of discretized port-Hamiltonian systems. This attempt has only scratched the surface of a very important problem. Since the discretized model assumes the port-Hamiltonian structure, much more elaborate schemes for the control of port-Hamiltonian systems can be applied. A nontrivial problem in this regard would be to design a controller for the discretized model and then test it on the continuous model and obtain the bounds of the discrepancy norm between the two behaviors. Some initial work has already been done in this vein, however, to my knowledge, mostly pertaining to the systems on a one-dimensional spatial domain (see [6, 8] and references quoted there). In higher dimensions, the interconnection of the finite controller and the infinite-dimensional system (plant) would be naturally realized through the interface of the simplicial triangulation of the boundary.

Optimal Control. An important application of structure-preserving discretization of complex physical systems is in optimal control theory, what also prompts a need for time discretization. For closed Hamiltonian systems, it is well-known that asynchronous variational integrators in general cannot preserve the Hamiltonian exactly; however, these integrators, for small time steps, can preserve a nearby Hamiltonian up to exponentially small errors [9]. An important issue in this context is to study the effects these integrators have on passivity (and losslessness) of open dynamical systems.

Symmetry and Reduction. The idea of Poisson reduction forgoes the analysis conducted in [22], where the configuration space is a space of differential forms and the symmetry group is a gauge group (acts linearly). Furthermore, the main idea behind the construction of the Stokes-Dirac structure considered in [13] applies to a much larger class of systems. How to obtain, for instance, the Lie-Poisson structure of the compressible isentropic fluid with varying boundary condition is an open problem that has been occupying me since the beginning of my postgraduate studies. An important and challenging avenue for future work is to make an explicit relation between multisymplectic and Stokes-Dirac structures, and then to compare their discrete analogues.

Systems Biology. I have provided a geometric formulation of reaction-diffusion systems with a thermodynamical equilibrium. A model obtained by structure-preserving scheme for the spatial discretization is a compartmental model, which exhibits a striking similarity with consensus dynamics [11]. Exploring this resemblance is a very appealing research direction.
References


