Thermodynamics Foundations of Mathematical Systems Theory Open Invited Track Code: 51p6d

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Abstract: Contributions on modeling, systems analysis, and control design to complex physical systems are central to the development of automatic control. As a result, techniques for analysis and feedback control design for physical representations based on thermodynamics have emerged in recent years and proved useful in theory and applications alike. In particular, extensions of structure-modeled systems, for example port-Hamiltonian systems, originally developed for electro-mechanical systems, to thermodynamic systems generated novel approaches within the field of automatic control. Moreover, the development of structured-preserving numerical methods for thermodynamic systems shed a light on the the potential interactions between the fields of numerical analysis and feedback control systems analysis for distributed parameters systems. The relation between systems theory, as understood by researchers and practitioners in automatic control, and thermodynamics is an active scientific area. Classical extensions of dissipative systems theory to dynamical systems with inputs and outputs under thermodynamic constraints led, in recent years, to numerous results ranging from investigation son the proper geometric framework for feedback control design to results on stability analysis, both for deterministic and stochastic systems where thermodynamics play a prominent role. Applications where a physically-consistent control theory for thermodynamic systems is needed include sustainable energy production, chemical reaction networks analysis, and quantum systems. The objective of the proposed Open Invited Track is to gather contributions from systems and control practitioners and researchers interested in thermodynamics theory and its extensions in the context of control systems. Contributions are expected to include modeling, analytic and geometric methods, as well as feedback control design methodologies for systems where thermodynamics theory is the fundamental science.

1. HANDLING IFAC TECHNICAL COMMITTEE

Open Invited Track on *Thermodynamics Foundations of Mathematical Systems Theory* will be handled by the **IFAC TC 2.3 — Non-Linear Control Systems**. The Open invited track is organized in collaboration with the following Technical Committees:

- TC 1.1 Modelling, Identification and Signal Processing;
- TC 2.6 Distributed Parameter Systems;
- TC 5.4 Large Scale Complex Systems;
- TC 6.1 Chemical Process Control; and,
- TC 8.4 Biosystems and Bioprocesses.

2. DESCRIPTION OF THE TOPIC

Relations between classical thermodynamics and systems theory were recognized early, and were presented notably in (Willems, 1972) in the context of dissipative systems. On the other hand, a geometric framework for classical thermodynamic systems was presented in (Hermann, 1973). Accordingly, contributions in the literature in the field of *Thermodynamics Foundations of Mathematical Systems Theory* can be organized around these two themes. The recent contribution by (van der Schaft, 2021) presents an overview of the field.

Classical thermodynamics, dissipation and passivity theory are concepts concerned with the study of internal stability of systems and how external actions alter fundamental properties such as energy, momentum, and entropy leading to motion, phase transition and self-organization at the macro-level despite chaotic/random behavior at the micro level (Haddad et al., 2005; Haddad, 2019). Some theoretical developments may draw inspiration for the classical circuit approaches pioneered by Tellegen (Ydstie and Alonso, 1997) and Brayton–Moser (Jeltsema and Scherpen, 2003). Such lines of thought led to a control theory for dissipative systems dealing with applications in mechanics (van der Schaft, 2000). In the same spirit, several research groups initiated programs to connect irreversible thermodynamics with process control. Notable contributions on the analysis of thermodynamic systems include the work by Alonso and Ydstie (1996) where thermodynamic potentials are considered as storage functions for passive systems analysis. Port-Hamiltonian and Brayton–Moser formalisms were considered extensively within this context (Hoang et al., 2011; Ramirez et al., 2013; Ramírez et al., 2016). Recent applications along this line of research, in the context of chemical processes, include (Favache and Dochain, 2009; Hoang and Dochain, 2013; Hoang et al., 2014; Garcia-Sandoval et al., 2016). Stability and passivity analysis for thermodynamic systems is still an active area of research, and new process applications, including observer design (Hoang and Dochain, 2019), multiphase systems, flowing systems (Mora et al., 2020), stochastic systems (Delvenne and Sandberg, 2015; Rajpurohit and Haddad, 2017) and distributed parameter systems (Ramirez et al., 2021).

Borrowing from some of the numerous modern schools of thermodynamics (Muschik, 2007), one aspect of the research relevant to IFAC and the automatic control community is to extend equilibrium thermodynamic to nonequilibrium thermodynamic formalisms, for example the GENERIC formalism (Grmela and Öttinger, 1997; Öttinger and Grmela, 1997) to systems with inputs and outputs (Badlyan et al., 2018). More generally, representations based on bracket formulations (Bloch et al., 1996) and results on dissipation are important aspects for modeling and analysis of nonlinear dynamical systems. Recent contributions relating thermodynamic systems to Lagrangian formulations (Gay-Balmaz and Yoshimura, 2017a,b) Bracket formulations and representations of thermodynamic systems from a variational standpoint are also relevant to the theory (Merker and Krüger, 2013; Gay-Balmaz and Yoshimura, 2018).

Elements of thermodynamic theory turns out to be useful for control design applications of mechanical and process systems and some of these applications and underlying geometric theories were reviewed in the *IFAC Thermodynamic Foundations of Mathematical Systems Theory* workshop series. Following the contribution by Hermann (1973) as well as Mrugala (1996) and Balian and Valentin (2001), control theoretical researchers recognized the central role of contact geometry in the study of thermodynamic systems, notably in (Eberard et al., 2007; Favache et al., 2010; Ramirez et al., 2017; Gromov and Caines, 2015) and the recent contributions relating control theory to contact geometry by van der Schaft and Maschke (2018); Maschke and van der Schaft (2019); Bravetti and Padilla (2019); Schaller et al. (2020).

Relations between thermodynamics and control are also valuable to many applications relevant to the Automatic Control community. Thermodynamics of reaction networks and networks in general were considered for example in the studies provided by Otero-Muras et al. (2008); Lipták et al. (2015). Another area of application, where thermodynamic considerations enable improvements through better controller design is the area of process control design (Hangos et al., 1999; Robinett III and Wilson, 2006).

The objective of this Open Invited Track is to gather contributions from systems and control practitioners and researchers interested in thermodynamic systems and to explore connections between the abstract systems theory and our current understanding for how physical systems behave when they have dynamics constrained by conservation laws and express dissipation that can be related to maximization of entropy like functions. Sought contributions also include complex and networked systems and phenomena occupying a varied range of time and spatial scales. Applications may include, but are not limited to: Energy efficient chemical processes or processes related to the production of smart materials that usually take place in the micro or nano-scale. Biological phenomena from a cell (biochemical) level through a tissue/organism and up to the ecological interactions between organisms. The behavior and control of particulate systems. Emergence of self-organizing behavior in networks of interacting agents where collective dynamics emerge from the consensus among a large number of ensemble members. Applications would cover fields such as ecology, robotics or socio-economy and more generally Cyber-Physical Systems. Control of large scale networked systems, such as chemical plants, integrating financial systems and sociological systems and more generally, modeling and control of irreversible thermodynamic systems.

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