# Towards a port-Hamiltonian approach to study Stirling-cycle devices

**Markus Lohmayer**

Supervisors: Prof. Dr.-Ing. habil. Sigrid Leyendecker
PD Dr.-Ing. habil. Paul Kotyczka
M.Sc. Tobias Scheuermann

Department of Mechanical Engineering
Friedrich-Alexander-Universität Erlangen-Nürnberg

This thesis is submitted for the degree of
*Master of Science*

December 2019

## Abstract

Energy conversion devices which are based on a practical Stirling cycle comprise 'engines' which can use low-temperature heat sources such as solar thermal energy and industrial waste heat as well as 'refrigerators' which can be used for air-conditioning. Currently, these devices are not very popular but they could play an important role in dealing with global challenges such as pollution and climate change. Port-Hamiltonian systems theory provides a modular approach to modeling physical systems. These systems are defined based on a geometric object called Dirac structure which encodes the exchange of power between different aspects of the system. Port-Hamiltonian systems are naturally passive making them attractive representations of complex systems arising from network modeling as well as modeling of distributed parameter systems. Their structural properties turn out to be useful for accurate numerical computations, model generation, model simplification, optimization and control. In order to apply this theory to nonequilibrium thermodynamic systems such as Stirling-cycle devices, a previously mentioned connection to the GENERIC framework is explored in this thesis. By using the total exergy as a Hamiltonian function, irreversible and reversible processes can be modeled on an equal footing. The structure of GENERIC port-Hamiltonian systems ensures that the reversible dynamics conserve the exchanged exergy and the irreversible dynamics destroy some of the exchanged exergy. A simple lumped-parameter example shows how the graphical modeling language of bond graphs can be used to represent GENERIC port-Hamiltonian systems. Simulation results are obtained based on a software implementation which automatically turns equations into results. Manually writing problem-specific code is avoided by leveraging symbolic computation and code generation.

# Contents

## Declaration

Ich versichere, dass ich die Arbeit ohne fremde Hilfe und ohne Benutzung anderer als der angegebenen Quellen angefertigt habe und dass die Arbeit in gleicher oder ähnlicher Form noch keiner anderen Prüfungsbehörde vorgelegen hat und von dieser als Teil einer Prüfungsleistung angenommen wurde. Alle Ausführungen, die wörtlich oder sinngemäß übernommen wurden, sind als solche gekennzeichnet.

Markus Lohmayer
December 2019

# Acknowledgements

I would like to thank professor Sigrid Leyendecker from the Chair of Applied Dynamics at FAU for supporting me with my thesis. She made it possible to work in collaboration with Paul Kotyczka and Tobias Scheuermann from the Chair of Automatic Control at the Technical University of Munich (TUM). I would like to thank them for welcoming me at TUM and for supporting me with my wish to write a thesis about port-Hamiltonian modeling of thermodynamical systems. I further wish to thank them for co-organizing a spring school on port-Hamiltonian systems earlier this year. For me, those days on Frauenchiemsee were a great way to get started in this field and overall a really enjoyable experience. I am very grateful that you three gave me the chance to work on this project! Without your trust it would have been impossible to pursue my goal.

I also would like to thank Guillaume Penelet from the Laboratoire d'Acoustique de l'Université du Mans for welcoming me as a guest last winter. During my two-month stay in Le Mans, I had the chance to learn more about thermoacoustic engines and explore some ideas which eventually inspired this thesis.

Last but not least, I would like to thank my friends and my girlfriend for their moral support.

# 1

# Introduction

This thesis tries to make a first step towards using port-Hamiltonian systems theory to model, simulate and optimize energy conversion devices such as (thermoacoustic) Stirling engines.

## 1.1 Stirling-cycle devices

Devices based on the Stirling cycle can operate in two modes: As prime movers (or engines) they can use any heat source such as solar thermal power, waste heat or external combustion to produce mechanical power. As heat pumps (or refrigerators) they use mechanical power to move thermal energy from a colder to a warmer space.

The Stirling cycle is a closed thermodynamic cycle. A compressible working fluid such as air, argon, helium or nitrogen is periodically compressed and expanded at different temperature levels to either produce mechanical power or to pump heat. The working fluid remains in the device indefinitely and needs to be replenished only if there is some leakage.

Figure 1.1 shows a schematic drawing of a Stirling engine. Thermal energy is supplied to the hot compartment via the hot heat exchanger and taken from the cold compartment via the ambient heat exchanger. The displacer piston is actuated by some drive mechanism causing the volumes of the two compartments to change periodically.

When the displacer piston moves to the left, the hot working fluid is pushed through the regenerator into the cold compartment where it is cooled by the ambient heat exchanger. As the hot gas moves through the regenerator, some of its thermal energy is temporarily stored there. Hence, the ambient heat exchanger has to do less cooling.

When the displacer piston moves back to the right, the cold working fluid is pushed trough the regenerator into the hot compartment where it is heated by the hot heat ex-

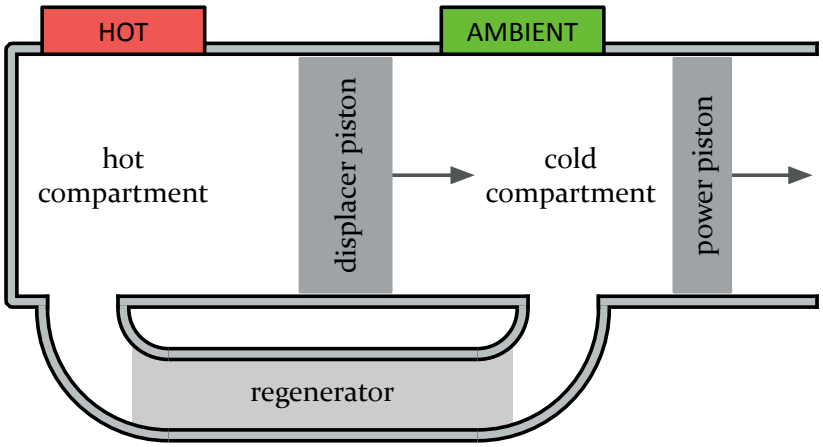



Fig. 1.1 Schematic drawing of a Stirling engine. HOT represents a hot heat exchanger and AMBIENT represents a heat exchanger which has a temperature slightly above ambient temperature. The displacer piston is actuated by a controlled force input (not depicted). Further, the load which is attached to the power piston is not shown. For a traditional Stirling engine, the power piston and the displacer piston are kinematically linked to a flywheel and their phase angle is chosen as 90°.

changer. As the cold gas moves through the regenerator, it already warms up. Hence, the hot heat exchanger has to do less heating.

The design of the regenerator involves a trade-off between a high heat capacity and a low heat conductivity and another trade-off between a large surface area for heat exchange and low viscous losses. If viscous losses are low, little force is required to drive the displacer piston because the pressure in both compartments is nearly the same.

If the displacer piston is on the left then most of the working fluid is in the cold compartment and the average temperature is low. Likewise, if the displacer piston is on the right then most working fluid is in the hot compartment and the average temperature is high. Hence, a periodic movement of the displacer piston causes an oscillation of the average temperature of the working fluid. This oscillation is accompanied by an oscillation of the average pressure. This pressure oscillation drives the power piston which in turn drives a load.

The limit cycle and consequently also the performance of the engine are strongly influenced by the movement of the displacer piston. Traditionally, a mechanical mechanism is used as a simple physical feedback controller: Some of the extracted mechanical power is fed back to the engine to drive the displacer piston. The mechanism links

the linear motion of the pistons and the rotrary motion of a shaft. This drive mechanism determines the (usually fixed) phase difference between the (usually harmonic) motions of the different pistons. Numerous variants of such engines exist differing for instance in their arrangement of the pistons, the number of cylinders and the type of drive mechanism. Unfortunately, traditional Stirling devices require lubrication and dynamic seals which can withstand pressure. Further, traditional Stirling engines are not self-starting.

Over time, various other kinds of Stirling-cycle devices have been developed:

Free-piston devices use (gas) springs attached to the pistons to eliminate the drive mechanism. This reduces the need for lubrication and dynamic seals. Further, these engines are self-starting.

Actively controlled Stirling devices use some actuator to drive the displacer piston. This leads to greater flexibility in shaping the limit cycle of the engine. The idea of designing limit cycles by solving an optimal periodic control problem has been explored in [36].

Liquid-piston devices use oscillating liquid columns as pistons. These engines are simple, cheap, reliable and often self-starting. Unfortunately, they tend to have low efficiencies because they usually operate at atmospheric pressure (as mean pressure). Nevertheless, a cost-effective and robust design can still lead to a great product for certain use cases. For instance, these engines can be used for pumping water even if electricity is not available.

### 1.1.1 Thermoacoustic devices

In travelling-wave thermoacoustic devices the working fluid also approximately executes a Stirling cycle [3, 12, 14]. Acoustic waves involve periodic compression and expansion of the fluid and therefore they are accompanied by temperature oscillations. In thermoacoustic devices, an acoustic wave in a sense replaces the pistons and the drive mechanism.

As prime movers, these devices convert thermal energy into acoustic power and as heat pumps (or refrigerators) they consume acoustic power. The conversion process takes place inside so-called thermoacoustic cores which consist of two heat exchangers and a regenerator (i.e. a porous medium) placed between them. A core which is operating as a prime mover can be seen as an acoustic amplifier. Tubes are con-

nected to both ends of a core to create a feedback loop. This feedback loop essentially serves as the drive mechanism. There are various possible configurations for building thermoacoustic systems. These differ for instance in the number of cores and the topology and dimensions of the feedback network which connects the cores. These systems usually have no moving parts (at high temperatures). As a consequence, they are rather easy to fabricate at low cost, require no lubrication and they are expected to be reliable systems. Thermoacoustic engines are self-starting.

### 1.1.2 Why these devices?

During the last century, the use of fossil fuels has become extremely prominent. As a consequence, problems related to pollution now affect the lives of most people and other species on the globe in various ways. Nowadays, many of us hope that we will soon be able to satisfy our energy demand using clean renewable sources.

At the same time, industrial processes reject large amounts of low and moderate temperature heat into the atmosphere. Cheap heat engines which can utilize this waste heat seem to be an attractive technology to mitigate the negative impact of industrial processes on the environment and the climate.

In many places, solar thermal energy is an abundant resource which is barely tapped. Among the technologies which are able to use solar energy, photovoltaics (PV) is by far the most popular one. It is well known that the production of PV panels is expensive. Further, PV panels eventually turn into electronic waste which is hard to recycle. Due to these factors, regenerative heat engines may be a superior alternative for cetrain applications.

**Example 1.1** (solar cooling systems)**.**
By combining thermoacoustic prime movers and heat pumps, a refrigeration system powered by solar thermal energy can be realized. The idea is illustrated in Fig. 1.2 and a possible setup is shown schematically in Fig. 1.3.

A thermoacoustic cooling system (consisting of vacuum tube solar thermal collectors, tubes and heat exchangers) seems to be a promising, simple and durable solution. Its components are easy to recycle.

In comparison, a cooling system consisiting of PV panels, PV inverters and a traditional air-conditioning device is much more expensive to fabricate in theory. Further,

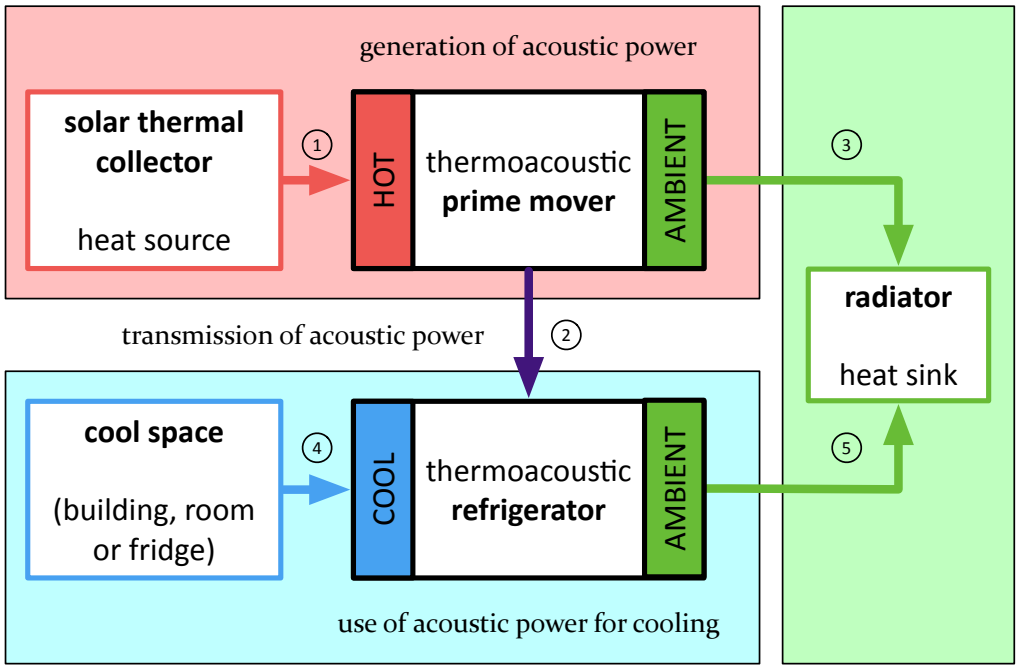



Fig. 1.2 In a thermoacoustic cooling system, the solar thermal collector supplies heat at a relatively high temperature level to the thermoacoustic cores running as prime movers (1). The prime movers generate acoustic power which is then used by the cores running as refrigerators (2). The remaining heat at the cold end of the prime movers is released to the environment (3). The refrigerators are using the acoustic power to extract heat from a cool space (4). This heat is then released to the environment which is at a higher temperature level (5).

these components have a rather limited lifetime and recycling them is much more difficult. ◇

More information about Stirling-cycle devices can for instance be found in the review article [39] and the references therein.

## 1.2 Port-Hamiltonian systems

The port-Hamiltonian approach [8] combines the systems-theoretic perspective which is known for example from control and information engineering with Hamiltonian mechanics.

Hamiltonian mechanics developed as a reformulation of Lagrangian mechanics which in turn was born as a reformulation of Newtonian mechanics. These three perspec-

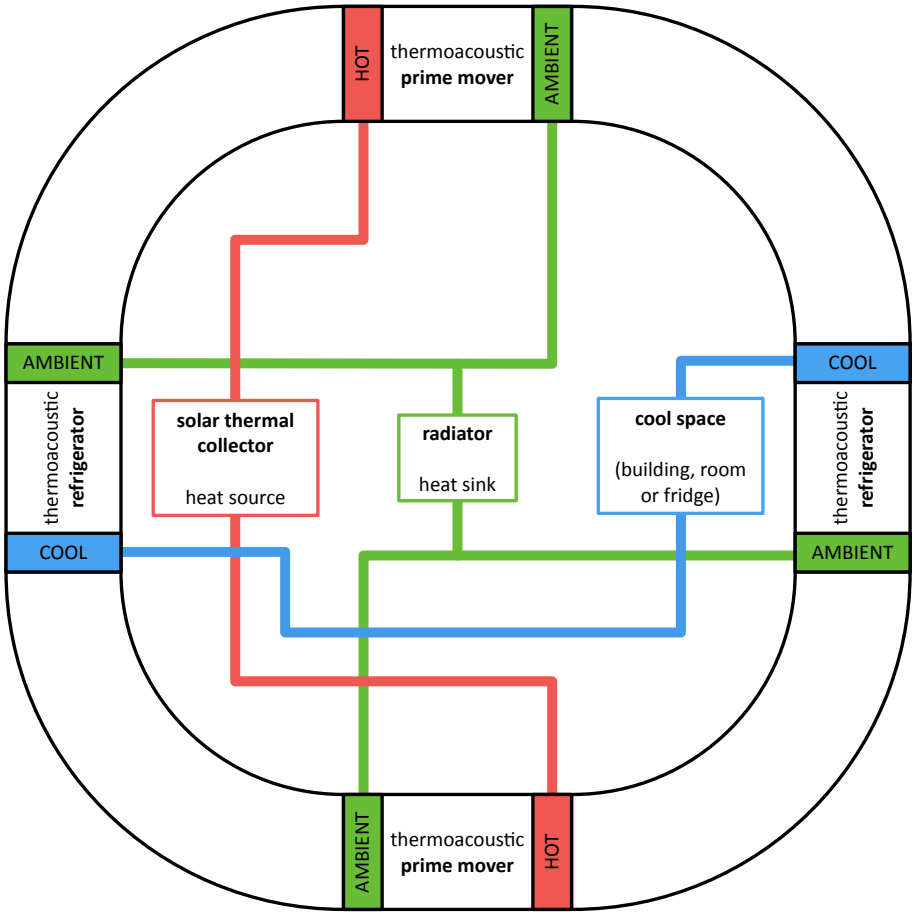



Fig. 1.3 Four thermoacoustic cores are connected with tubes to form a thermoacoustic cooling system. The two cores operating as prime movers generate acoustic power which is consumed by the two cores running as refrigerators. An acoustic wave is travelling around the loop. It transports mechanical power and lets the fluid inside the cores execute approximately a Stirling cycle.

tives on the phenomenon of motion of macroscopic objects lead to the same predictions. Lagrangian mechanics derives balance laws from a variational principle. A Hamiltonian system can (usually) be obtained from a Lagrangian system by means of the Legendre transformation. The time-evolution of a Hamiltonian system is 'driven' by the differential of the total energy in the system. A geometric structure describes the reversible exchange of energy between different forms of energy storage.

Systems theory developed as a general theory of signals and systems in the context of electrical, electronic and information engineering. These systems interact by exchanging signals. In contrast, the port-based approach [2] to modeling physical sys-

tems is a more constrained theory of systems which is closer to physics. These systems interact by exchanging power.

Port-Hamiltonian systems are Hamiltonian systems which can interact with other (port-Hamiltonian) systems through ports. Further, irreversible dynamics can be modeled by terminating a port with a resistive relation.

### 1.2.1 Why port-Hamiltonian modeling?

Today, computer-aided engineering (CAE) tools are widely used in industry for simulation and optimization tasks. By now, there also exist various software packages for the simulation of multiphysics systems. Unfortunately, most tools are not suited to model complex systems by interconnecting simpler subsystems in a systems-theoretic sense. Yet, many systems (e.g. thermoacoustic cooling systems) are best modeled as interconnected (multiphysics) systems. It should be possible to replace one subsystem model with another one if both models interact with their environment in a sufficiently similar way. For instance, it is often desirable to replace a high-fidelity model of a subsystem with a less complex surrogate model to make optimization tasks faster or even practically feasible. Different models for the same subsystem can be evaluated by comparing simulation results before and after changing the model. Optimization algorithms could then adaptively switch between models of different complexity / fidelity. Similarly, a systems-theoretic approach to simulation software would help to bridge the gap between plant design and control design.

Compared to traditional systems theory, port-Hamiltonian systems theory is based on a more structured *representation* of systems and subsystems which is based on the exchange of energy. The port-Hamiltonian approach focuses on the flow of power between the components of the system. Since energy is a quantity common to all areas of physics, this approach can help to systematically formulate the coupling between different physical domains. Further, a more structured representation should facilitate the automated generation of correct equations and algorithms based on high-level descriptions.

Port-Hamiltonian systems are based on a geometric structure which describes the power-conserving interconnection of different parts of the system. This stucture is useful for analysis tasks. In particular, it makes it much easier to find conserved quantities (so-called Casimirs [13]) which can be used to simplify the model or to design

control laws. Further, the abstract formulation based on concepts from differential geometry often makes reasoning independent of a particular choice of coordinates.

Discretization in space and time should be guided by an attempt to find a discrete analogue of the underlying continuous structure. When successful, unphysical artifacts such as numerical damping and spurious modes are avoided. Research on geometric numerical integration shows that awareness of the geometrical structure can be beneficial for developing numerical methods for time integration [19, 25]. Geometric integrators preserve in some sense the geometrical structure in the discrete setting. Information about structure-preserving space discretization methods for distributed-parameter port-Hamiltonian systems based on Discrete Exterior Calculus (DEC) [20] as well as Finite Element Exterior Calculus (FEEC) [30, 41] can for instance be found in the recent monograph [46].

Similarly, model-order reduction should preserve as much structure as possible to retain basic physical properties such as passivity. The recent preprint [45] is concerned with structure-preserving model reduction for linear differential-algebraic systems. Model reduction for nonlinear port-Hamiltonian systems is for instance the topic of article [38].

The port-Hamiltonian setting is also well suited for applying energy-based (nonlinear) control methods [15, 16, 17, 22, 27, 40]. The Passivity–Based Control (PBC) technique of Control by Interconnection (CbI) assumes the controller as another port-Hamiltonian system. I think that Stirling-cycle devices could be an application where the energy-based viewpoint and in particular the control by interconnection paradigm might be superior to the classical signal-processing paradigm where input and output causalities are fixed by assuming sensors and actuators. The CbI method allows for a physical interpretation of the controller which could possibly inspire new engineering solutions.

Energy-based modeling of physical systems using port-Hamiltonian systems theory seems to be a promising direction for further research and could easily lead to a revolution in the world of CAE tools. In particular, using this approach to study and optimize regenerative heat engines seems to be an interesting field for future research. The possible benefits of this setting could help researchers to bring forth more sustainable solutions.

### 1.2.2 Irreversible thermodynamical systems

The Hamiltonian approach to classical mechanics is concerned with formalizing the reversible exchange of energy between different forms of storage in a geometric way. The time evolution of a Hamiltonian system is 'driven' by the differential of the Hamiltonian function. This function is sometimes called energy function because it maps the system state to the total energy stored in the system.

Hamiltonian systems have reversible dynamics. Therefore, it is not possible to model thermodynamic systems which feature irreversible heat transfer as Hamiltonian systems. In contrast, port-Hamiltonian systems can incorporate irreversible dynamics. This is achieved by terminating a port with a resistive relation. The system dynamics can then be seen as a superposition of a reversible (Hamiltonian) contribution and an irreversible contribution.

A port-Hamiltonian formulation of heat conduction has been presented in [21] by using the total internal energy as the Hamiltonian function. Other approaches for modeling irreversible thermodynamical systems as (quasi) port-Hamiltonian systems have been suggested: For instance, a class of quasi-port Hamiltonian systems called Irreversible Port-Hamiltonian Systems has been presented in [34]. These systems are called quasi-port Hamiltonian because an additional modulating function is used to ensure that the total energy (which is expressed by the Hamiltonian function) is conserved by the irreversible dynamics. More recently, an approach based on the symplectization of contact manifolds has been presented in [44].

The idea of splitting the system dynamics into a reversible and an irreversible contribution also lies at the heart of the *General Equation for the nonequilibrium reversible-irreversible coupling* (GENERIC) [9, 10, 24]. The GENERIC can be seen as a general framework for modeling thermodynamical systems. The reversible contribution is modeled by a Hamiltonian system whose dynamics is generated by the total energy function. A condition ensures that the reversible dynamics conserve the total entropy. The irreversible contribution is modeled by a gradient system whose dynamics is generated by the total entropy function. A condition ensures that the irreversible dynamics conserve the total energy. The GENERIC framework can be extended to open thermodynamical systems [26].

Most (quasi) port-Hamiltonian approaches for modeling thermodynamic systems use the total energy in the system as the Hamiltonian function generating the dynamics. In contrast, the GENERIC relies on two different functions, namely the total energy

and the total entropy functions. The preprint [42] shows a connection between the GENERIC framework and port-Hamiltonian systems theory. The central idea is to use the total exergy of the system as the Hamiltonian function. This approach is explored in the present thesis.

## 1.3 Scope of this work

In the following chapter, important aspects of equilibrium and nonequilibrium thermodynamics are reviewed. This is followed by an introduction to port-Hamiltonian modeling in Chapter 3: After a short section about traditional Hamiltonian systems, the port-based approach is introduced alongside the graphical modeling language of bond graphs. Lumped-parameter systems are used as simple examples illustrating the ideas. Attention is paid in particular to systems with irreversible dynamics. Finally, the structure-preserving time integration of port-Hamiltonian systems based on continuous collocation methods is reviewed and then applied to examples. Chapter 4 introduces the GENERIC approach to modeling irreversible non-equilibrium thermodynamical systems. A lumped-parameter system is used as an example illustrating the main idea. Chapter 5 explores the connection between the GENERIC framework and port-Hamiltonian systems theory. This leads to a class of irreversible port-Hamiltonian systems which use the total exergy as their Hamiltonian function. The simple but physically relevant example of the previous chapter is revisited to illustrate the idea of exergy-based port-Hamiltonian systems. It is shown that these systems can be visualized as bond graphs: Power bonds are used to express the exergy exchange between the system components and irreversible processes such as heat conduction and friction are expressed by components which destroy exergy. Chapter 6 draws conclusions and discusses possible directions for future work. Appendix A gives a high-level low-threshold introduction to differential geometry basics for people who are unfamilar with the subject. In Appendix B, a thermodynamic potential for an ideal gas is derived from the Sackur-Tetrode equation.

# 2

# Thermodynamics

This chapter shall give a self-contained introduction to those aspects of thermodynamics which are important in later chapters. Thermodynamics aims at describing physical systems at the *macroscopic* level. The microscopic configuration (which is considered for instance in statistical mechanics) is not taken into account in a thermodynamical system model.

Equilibrium thermodynamics is actually concerned with 'thermostatics': The systems of interest are assumed to be in an equilibrium state. In fact, thermodynamic equilibrium is an axiomatic concept. The theory focuses on fundamental properties of the constitutive relations linking the different thermodynamic variables of a system. Nonequilibrium thermodynamics on the other hand is concerned with dynamical systems which may undergo reversible and irreversible processes such as work interaction and heat conduction.

**Definition 2.1.**
Thermodynamic systems may be classified according to how they can interact with their environment [37]: A system is said to be

- *closed* if it does not exchange matter (i.e. mass or particles).
- *adiabatically closed* if it is closed and there there is no heat flux across the system boundary.
- *isolated* if it is adiabatically closed and there is no exchange of mechanical power.

△

## 2.1 Equilibrium Thermodynamics

This section shall give a short overview of some of the most important fundamentals of equilibrium thermodynamics. The textbook [4] shall serve as a reference for this section.

**Definition 2.2** (types of variables)**.**
Thermodynamic variables can be divided into different categories:

1. The magnitude of an *intensive variable* does not depend on the system's size.
2. On the other hand, the magnitude of an *extensive variable* depends homogeneously (of degree 1) on the system size: If a system is divided into subsystems, the sum of the values for each subsystem is equal to the value for the whole system.
   (a) Dividing an extensive variable by the mass of the system yields a so-called *specific variable*. The magnitude of a mass-specific variable does not depend on the system's size. In this sense, specific variables are intensive variables.
   (b) Similarly, an extensive variable can be divided by the system's volume resulting in a (volumetric) *density*. The magnitude of a density does also not depend on the size of the system.

△

**Remark 2.3** (notation for different types of variables)**.**
In this thesis, extensive variables, specific variables and densities are referred to as variables with *extensive character*. These variables are denoted by lowercase Latin letters. Intensive variables which are not specific variables or densities are referred to as variables with *intensive character*. These variables are denoted by lowercase Greek letters.

For instance, $s$ denotes entropy (density), $v$ denotes volume and $m$ denotes mass (density). The corresponding intensive variables are the temperature $\theta$, the pressure $\pi$ and the chemical potential $\mu$, respectively. Similarly, $p$ denotes the linear momentum (density) and the corresponding velocity is denoted by $\upsilon$ (upsilon).

To avoid confusion, the ratio of a circle's circumference to its diameter is denoted by $\mathring{\pi}$ throughout. △

A widely accepted postulational formulation of equilibrium thermodynamics is presented in [4, p. 283f.] (using a slightly different notation):

"**Postulate I.** There exist particular states (called equilibrium states) that, macroscopically, are characterized completely by the specification of the internal energy $u$ and a set of parameters $x_1, x_2, \ldots, x_n$ later to be specifically enumerated."

It can often be observed that isolated systems approach an equilibrium state which is independent of the history of the system. Postulate I says that such an equilibrium state is fully determined (on the macroscopic level) by a finite set of extensive state variables $u, x_1, \ldots, x_n$. Here, $u$ is the internal energy of a system and $x_1$ could for example be its volume.

"**Postulate II.** There exists a function (called the entropy) of the extensive parameters, defined for all equilibrium states, and having the following property. The values assumed by the extensive parameters in the absence of a constraint are those that maximize the entropy over the manifold of constrained equilibrium states."

Postulate II essentially assures the existence of a *fundamental equation*

$$s = S(u, x_1, \ldots, x_n).$$

The function $S$ contains all the thermodynamically relevant information about the system.

"**Postulate III.** The entropy of a composite system is additive over the constituent subsystems (whence the entropy of each constituent system is a homogeneous first-order function of the extensive parameters). The entropy is continuous and differentiable and is a monotonically increasing function of the energy."

Postulate III says that $S$ is a homogeneous first-order function of the extensive parameters, i.e.

$$\forall\, c \in \mathbb{R}^+ : S(c\,u, c\,x_1, \ldots, c\,x_n) = c\,S(u, x_1, \ldots, x_n).$$

The latter part of the postulate implies that $s = S(u, x_1, \ldots, x_n)$ can be solved for $u$ and hence

$$u = U(s, x_1, \ldots, x_n)$$

is also a fundamental equation. The function $U$ is called a *thermodynamic potential* of the system. It is a smooth function on the $(1+n)$-dimensional manifold of equilibrium

states with coordinates $(s,\, x_1,\, \ldots,\, x_n)$. Its differential is

$$\mathrm{d}U \;=\; \underbrace{\frac{\partial U(s,\, x_1,\, \ldots,\, x_n)}{\partial s}}_{\theta(s,\, x_1,\, \ldots,\, x_n)} \mathrm{d}s \;+\; \underbrace{\frac{\partial U(s,\, x_1,\, \ldots,\, x_n)}{\partial x_1}}_{\pi_1(s,\, x_1,\, \ldots,\, x_n)} \mathrm{d}x_1 \;+\; \ldots \;+\; \underbrace{\frac{\partial U(s,\, x_1,\, \ldots,\, x_n)}{\partial x_n}}_{\pi_n(s,\, x_1,\, \ldots,\, x_n)} \mathrm{d}x_n \,.$$

The component functions of the differential are called *thermodynamic equations of state*. In paricular, $\theta$ is called thermodynamic (equilibrium) temperature and the quantities $\pi_i$ are called *thermodynamic forces*.

The temperature and the thermodynamic forces are intensive variables. If $U$ is chosen as a potential then the intensive variables are not independent variables but rather functions of the state.

"**Postulate IV.** The entropy of any system vanishes in the state for which $\theta = \frac{\partial U}{\partial s} = 0$."

**Example 2.4.**
A more concrete example of a thermodynamic system is a gas contained in a volume $v = x_1$. If it is possible to add or remove some amount of gas from the system then the mass $m = x_2$ is another extensive state variable. There exists a function $U(s,\, v,\, m)$ which is the thermodynamic potential of the system. Since all parameters are extensive variables, $U$ must be a homogeneous first-order function, i.e.

$$\forall\, c \in \mathbb{R}^+ \,:\, U(c\, s,\, c\, v,\, c\, m) \;=\; c\, U(s,\, v,\, m) \,. \tag{2.1}$$

From this it follows that

$$\frac{\partial U(c\, s,\, c\, v,\, c\, m)}{\partial c} \;=\; \frac{\partial \big(c\, U(s,\, v,\, m)\big)}{\partial c} \;=\; U(s,\, v,\, m) \tag{2.2}$$

and therefore

$$\begin{aligned} U(s,\, v,\, m) &\overset{(2.2)}{=} \frac{\partial U(c\, s,\, c\, v,\, c\, m)}{\partial (c\, s)} \frac{\partial (c\, s)}{\partial c} \;+\; \frac{\partial U(c\, s,\, c\, v,\, c\, m)}{\partial (c\, v)} \frac{\partial (c\, v)}{\partial c} \;+\; \ldots \\ &= \underbrace{\frac{\partial U(s,\, v,\, m)}{\partial s}}_{\theta(s,\, v,\, m)} s \;+\; \underbrace{\frac{\partial U(s,\, v,\, m)}{\partial v}}_{-\pi(s,\, v,\, m)} v \;+\; \underbrace{\frac{\partial U(s,\, v,\, m)}{\partial m}}_{\mu(s,\, v,\, m)} m \,. \end{aligned} \tag{2.3}$$

Here, $\theta$ is the thermodynamic equilibrium temperature, $\pi$ is the thermodynamic equilibrium pressure and $\mu$ is the chemical potential per unit mass.

An infinitesimal change in internal energy can be written as the sum of energy-conjugate pairs formed by a (dependent) intensive variable and an infinitesimal change of the corresponding extensive variable:

$$\mathrm{d}U(s,\, v,\, m) \;=\; \theta(s,\, v,\, m)\,\mathrm{d}s \;-\; \pi(s,\, v,\, m)\,\mathrm{d}v \;+\; \mu(s,\, v,\, m)\,\mathrm{d}m$$

A fundamental equation of the form $u = U(s,\, v,\, m)$ for an ideal gas can for example be derived from the Sackur-Tetrode equation, see Section B.2.

If alternatively $s = S(u,\, v,\, m)$ is used as a fundamental equation then a tuple $(u,\, v,\, m)$ fully characterizes a thermodynamic equilibrium state of the system. Analogously to Eq. (2.3), it can be shown that

$$S(u,\, v,\, m) \;=\; \left(\frac{1}{\theta}\right)(u,\, v,\, m)\,u \;+\; \left(\frac{\pi}{\theta}\right)(u,\, v,\, m)\,v \;-\; \left(\frac{\mu}{\theta}\right)(u,\, v,\, m)\,m\,.$$

where for instance $\left(\frac{1}{\theta}\right)$ is in fact one symbol representing a single function.

An infinitesimal change in entropy can be written as the sum of entropy-conjugate pairs formed by a (dependent) intensive variable and an infinitesimal change of the corresponding extensive variable, i.e.

$$\mathrm{d}S(u,\, v,\, m) \;=\; \left(\frac{1}{\theta}\right)(u,\, v,\, m)\,\mathrm{d}u \;+\; \left(\frac{\pi}{\theta}\right)(u,\, v,\, m)\,\mathrm{d}v \;-\; \left(\frac{\mu}{\theta}\right)(u,\, v,\, m)\,\mathrm{d}m\,.$$

A fundamental equation of the form $s = S(u,\, v,\, m)$ for an ideal gas is for example given by the Sackur-Tetrode equation, see Section B.1.

If the system would contain only solid material then assuming a fixed mass and a fixed volume would turn $m$ and $v$ into constants. Consequently, a fundamental equation of the form $u = U(s)$ or $s = S(u)$ would suffice. ◇

Throughout this thesis, the internal energy will be used as a thermodynamic potential.

Since equilibrium thermodynamics is limited to describing equilibrium states of a system, only those changes of the system can be considered which happen so slowly that the system always remains in some equilibrium state. These so-called *quasi-static* processes can be seen as curves on the $(1 + n)$-dimensional manifold of equilibrium states. A quasi-static process is an idealized concept which is of limited practical use in many engineering applications, see also [4, p. 95].

The internal energy $u$ of a system can change due to exchange of energy with the environment. This exchange can happen in two forms, namely work and heat. It is expressed by the balance equation

$$\mathrm{d}u \;=\; đW \;+\; đQ\,.$$

Here, $đW$ and $đQ$ represent infinitesimal amounts of transferred energy in the form of work and heat, respectively. Note that $W$ and $Q$ are not thermodynamic variables and hence $đW$ and $đQ$ are not differentials but *process-dependent* quantities (in the general case).

For a quasi-static process however, it holds that $đQ = \theta\,\mathrm{d}s$ and that $đW = -\pi\,\mathrm{d}v + \mu\,\mathrm{d}m$. It can be shown that this follows from the principle of maximum entropy stated in Postulate II. Further, the thermodynamic equilibrium pressure $\pi$ can be identified with the external mechanical pressure.

**Remark 2.5** (Carnot engine)**.**
The Carnot cycle is a theoretical thermodynamic cycle [4, p. 118]. It describes an idealized heat engine called the Carnot engine. The Carnot cycle is entirely reversible and hence generates no entropy. It achieves the highest efficiency which is possible for any heat engine operating betwen two given reservoirs. This theoretical limit for achievable efficiency is called the Carnot efficiency.

Figure 2.1 shows a Carnot engine which extracts mechanical work from a hot reservoir with constant temperature $\theta_h$. The heat intake per cycle $Q_{\mathrm{in}} > 0$ from this reservoir is associated with an entropy intake $s_{\mathrm{in}} > 0$. Since the Carnot engine is executing a thermodynamic cycle, entropy cannot accumulate inside the engine. Further, no entropy is generated inside the engine because the Carnot cycle is perfectly reversible. Consequently, the intake of entropy $s_{\mathrm{in}}$ has to be balanced by a discharge of entropy to the ambient reservoir implying that $s_{\mathrm{out}} = s_{\mathrm{in}}$. This is associated with a discharge of heat $Q_{\mathrm{out}} > 0$ to the ambient reservoir at constant temperature $\theta_0$.

The entropy balance equation $s_{\mathrm{out}} = s_{\mathrm{in}}$ can be written as

$$\frac{1}{\theta_h}\,Q_{\mathrm{in}} \;=\; \frac{1}{\theta_0}\,Q_{\mathrm{out}}\,. \tag{2.4}$$

This yields the energy balance equation

$$W_{\mathrm{out}} \;=\; Q_{\mathrm{in}} \;-\; Q_{\mathrm{out}} \overset{(2.4)}{=} Q_{\mathrm{in}} \;-\; \frac{\theta_0}{\theta_h}\,Q_{\mathrm{in}} \;=\; \frac{\theta_h - \theta_0}{\theta_h}\,Q_{\mathrm{in}}\,, \tag{2.5}$$

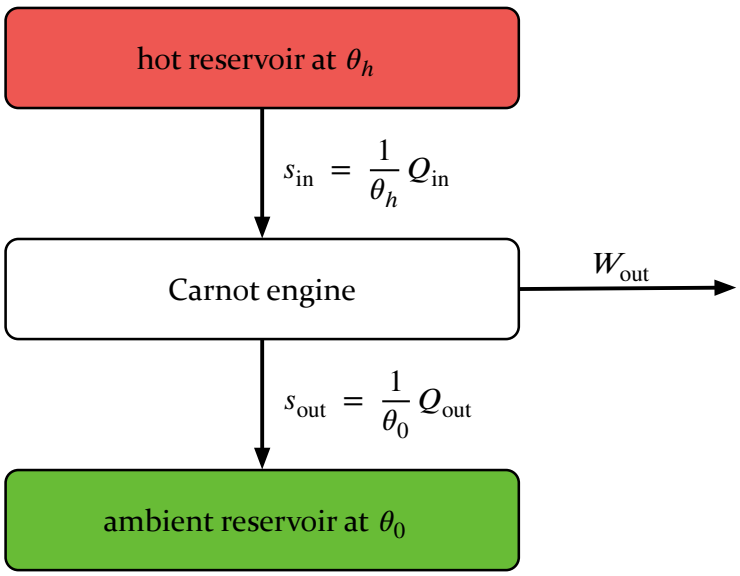



Fig. 2.1 A Carnot engine operating between two isothermal heat reservoirs. In each cycle, the fictitious engine consumes the heat $Q_{\text{in}}$ at the temperature level $\theta_h$ and rejects the heat $Q_{\text{out}}$ at the temperature level $\theta_0$ to produce the work output $W_{\text{out}}$.

expressing how much work $W_{\text{out}}$ is obtained for a given heat intake $Q_{\text{in}}$.
The temperature ratio

$$\eta_{\text{Carnot}} = \frac{\theta_h - \theta_0}{\theta_h} \tag{2.6}$$

is the efficiency of the Carnot engine and hence called the Carnot efficiency. △

**Remark 2.6** (exergy)**.**
Work can be turned into heat but heat cannot fully be turned into work. Therefore, it is important to differentiate between exchange of work (mechanical power, electrical power, etc.) and exchange of thermal energy (heat power). Exchange of work is reversible whereas (non-convective) exchange of heat is irreversible.

Based on the concept of a Carnot engine, irreversible exchange of heat power $\dot{Q}$ at a temperature level $\theta$ can be associated with an exchange of 'value'. This value is the amount of mechanical (or electrical) power $\dot{W}$ that could be extracted from the heat power by a hypothetical engine which achieves Carnot efficiency and rejects heat at the reference temperature $\theta_0$. The value is given by

$$\dot{W} = \frac{\theta - \theta_0}{\theta} \dot{Q} \,.$$

The exchanged value is called exergy exchange rate, see [1]. It is measured relative to a fixed reference temperature $\theta_0$.

If heat is exchanged at a higher temperature it carries more exergy and at the same time less entropy is produced. Only reversible work interaction carries 100% exergy and produces no entropy. Even though irreversible exchange of heat has a different nature than reversible exchange of work, the concept of exergy makes it possible to directly compare the two forms of energy exchange.

Heat conduction is caused by temperature differences. When heat leaves one subsystem at a higher temperature level and arrives at another subsystem at a lower temperature level then the exergy that is removed from the first subsystem is larger than the exergy added to the second subsystem. Irreversible processes such as non-isothermal heat conduction destroy exergy and create entropy.

Throughout this thesis, the word 'power' is used for 'energy exchange rate' as well as for 'exergy exchange rate'. If not stated, the precise meaning can be inferred from the context.

The exergy of a system is the amount of work which can theoretically be extracted from it by a perfectly reversible process until it is in equilibrium with a given reference environment. In the absence of chemical reactions, the exergy of a system with thermodynamic potential $U(s, \ldots)$ is given by

$$U(s, \ldots) \; - \; \theta_0 \, s \, . \tag{2.7}$$

The derivative of this exergy with respect to entropy is $\theta(s, \ldots) - \theta_0$. If exergy is considered as a potential (to do work) then an infinitesimal change of exergy caused by an infinitesimal change of entropy can be written as $\big(\theta(s, \ldots) - \theta_0\big) \, \mathrm{d}s$. An exchange of heat power $\dot{Q}$ at temperature $\theta$ is associated with an entropy exchange rate $\dot{s} = \frac{1}{\theta} \dot{Q}$. Consequently, the exergy exchange rate is given as $\big(\theta(s, \ldots) - \theta_0\big)\dot{s} = \frac{\theta - \theta_0}{\theta} \dot{Q}$, see Eq. (2.6).

△

## 2.2 Nonequilibrium Thermodynamics

It can often be observed that isolated thermodynamic systems which are not at equilibrium approach an equilibrium state which is independent of the system's history.

But equilibrium thermodynamics doesn't have anything to say about the time evolution towards this state. This is the task that nonequilibrium thermodynamics tries to solve. Of course, a macroscopic description of time evolution is not only interesting for isolated systems. Especially in engineering, it is much more interesting to consider systems which can interact with their environment.

A very common approach is to consider spatially-distributed thermodynamical systems which are locally assumed to be in a (time-dependent) equilibrium state. This *local equilibrium assumption* allows for instance to define a temperature field for a heat-conducting fluid or rigid body [24, p. 39].

Every point in the spatial domain of a system is considered as an infinitesimally small thermodynamic system. Yet, from the microscopic perspective this infinitesimally small system ought to contain a big number of atoms or molecules such that averaging over its microstructure makes sense.

This may sound paradoxical but one has to remember that the balance laws for the state variables are obtained in integral form and partial differential equations are then derived using a localization argument. Therefore it is argued that the integral form of the balance laws is physically more meaningful.

Numerical computations rely on finite spatial resolution and many discretization methods such as finite volume methods, finite element methods as well as discrete exterior calculus methods are based on precisely the integral form of the balance laws. If for instance all finite volumes are big enough to contain enough matter to justify the macroscopic viewpoint yet small enough to justify the assumption that the contained matter is in (or at least sufficiently close to) a thermodynamic equilibrium state then the paradox is resolved.

**Example 2.7.**
Similar to Example 2.4, a gas contained in a volume shall serve as an example of a thermodynamic system. But this time, the gas is considered as a spatially-distributed system on a spatial domain $\mathscr{R}$ and no global equilibrium state is assumed.

To differentiate between the distributed case here and the lumped case from Example 2.4, in this example all lumped quantities are denoted with an extra bar on top.

A particular equilibrium state of the gas in Example 2.4 is defined by a tuple $(\bar{s},\ \bar{v}, \bar{m})$. In contrast, the macroscopic state of the gas in this example is given by a tuple $(s,\ m)$, i.e. the entropy and mass density fields. For instance, the entropy density field (at a

fixed point in time) is a map

$$\begin{aligned} s : \mathscr{R} &\to \mathbb{R}^+ \\ r &\mapsto s(r)\,. \end{aligned}$$

This choice of (infinite-dimensional) state variables assumes that the internal energy density serves as the local thermodynamic potential.

The task here is to convert a fundamental equation of the form $\bar{u} = \bar{U}(\bar{s},\, \bar{v},\, \bar{m})$ to a local fundamental equation of the form $u = U(s,\, m)$. Since the volume density $v$ is always 1, only the entropy density $s$ and the mass density $m$ remain as (infinite-dimensional) state variables. The local thermodynamic potential $U$ contains all thermodynamic information except for the system's size.

Let $C \subset \mathscr{R}$ be a control volume and define $\bar{v} = \mathrm{Vol}(C)$. If the gas inside $C$ is at equilibrium then $s$ and $m$ are constant fields. Hence, $u = U(s,\, m)$ is also constant throughout $C$. Consequently, it must hold that

$$\begin{aligned} \bar{s} &= s\,\bar{v} \\ \bar{m} &= m\,\bar{v} \\ \bar{u} &= \bar{U}(\bar{s},\, \bar{v},\, \bar{m}) = U(s,\, m)\,\bar{v} = U\left(\frac{\bar{s}}{\bar{v}},\, \frac{\bar{m}}{\bar{v}}\right)\bar{v} = u\,\bar{v}\,. \end{aligned} \tag{2.8}$$

According to Eq. (2.8), $U$ is defined as

$$U(s,\, m) = \frac{\bar{U}(\bar{s},\, \bar{v},\, \bar{m})}{\bar{v}} = \frac{\bar{U}(s\,\bar{v},\, 1\,\bar{v},\, m\,\bar{v})}{\bar{v}} = \frac{\bar{U}\left(s\,\mathrm{m}^3,\, 1\,\mathrm{m}^3,\, m\,\mathrm{m}^3\right)}{1\,\mathrm{m}^3} \tag{2.9}$$

expressing the internal energy per unit volume. The last equality in Eq. (2.9) is a consequence of the homogeneity of $\bar{U}$, see Eq. (2.1).

The intensive quantities can equivalently be expressed as functions of $s$ and $m$. For the temperature it holds that

$$\begin{aligned} \bar{\theta}(\bar{s},\, \bar{v},\, \bar{m}) &= \frac{\partial \bar{U}(\bar{s},\, \bar{v},\, \bar{m})}{\partial \bar{s}} \\ &= \frac{\partial\left(U\left(\frac{\bar{s}}{\bar{v}},\, \frac{\bar{m}}{\bar{v}}\right)\bar{v}\right)}{\partial \bar{s}} = \frac{\partial U(s,\, m)}{\partial s}\,\frac{1}{\bar{v}}\,\bar{v} = \frac{\partial U(s,\, m)}{\partial s} = \theta(s,\, m) \end{aligned} \tag{2.10a}$$

and similarly for the chemical potential per unit mass it holds that

$$\bar{\mu}(\bar{s},\, \bar{v},\, \bar{m}) \;=\; \frac{\partial \bar{U}(\bar{s},\, \bar{v},\, \bar{m})}{\partial \bar{m}} \;=\; \frac{\partial U(s,\, m)}{\partial m} \;=\; \mu(s,\, m)\,. \tag{2.10b}$$

For the pressure it holds that

$$\begin{aligned}
\bar{\pi}(\bar{s},\, \bar{v},\, \bar{m}) \;&=\; -\frac{\partial \bar{U}(\bar{s},\, \bar{v},\, \bar{m})}{\partial \bar{v}} \\
&=\; -\frac{\partial \left( U\left(\frac{\bar{s}}{\bar{v}},\, \frac{\bar{m}}{\bar{v}}\right) \bar{v} \right)}{\partial \bar{v}} \\
&=\; -\frac{\partial U(s,\, m)}{\partial s} \left(-\frac{s}{\bar{v}}\right) \bar{v} \;-\; \frac{\partial U(s,\, m)}{\partial m} \left(-\frac{m}{\bar{v}}\right) \bar{v} \;-\; U(s,\, m) \\
&=\; \frac{\partial U(s,\, m)}{\partial s}\, s \;+\; \frac{\partial U(s,\, m)}{\partial m}\, m \;-\; U(s,\, m) \;=\; \pi(s,\, m)\,.
\end{aligned} \tag{2.10c}$$

Clearly, the function $U$ in Eq. (2.9) is independent of $\bar{v} = \mathrm{Vol}(C)$ and hence the above equations for $u$, $\theta$, $\mu$ and $\pi$ also hold in the limit $\mathrm{Vol}(C) \to 0$.

If a local potential function $U$ is known then an entropy density field $s : \mathscr{R} \to \mathbb{R}^+$ and a mass density field $m : \mathscr{R} \to \mathbb{R}^+$ fully determine the internal energy density field $u$, the temperature field $\theta$, the chemical potential field $\mu$ and the pressure field $\pi$.

A local fundamental equation of the form $u = U(s,\, m)$ for an ideal gas can for example be derived from the Sackur-Tetrode equation, see Section B.3. ⋄

Chapter 4 continues to discuss nonequilibrium thermodynamics.

# 3

# Port-Hamiltonian systems

Section 1.2 already motivated port-Hamiltonian systems (PHS) theory. This chapter shall give a short introduction to modeling physical systems using this approach. The first section presents the idea of Hamiltonian systems based on two simple examples. In the second section, the port-based approach which originated in the works of Paynter [2] is introduced. First and foremost, attention is given to the concept of bond graphs. Section 3.3 then hints at the connection between bond graph modeling and Hamiltonian mechanics. To make the connection precise, the concept of Dirac structures is formally introduced in Section 3.4. A Dirac structure is a geometric structure which is associated with the power-conserving interconnection structure of the physical system. Based on this, Section 3.5 continues with the explicit representation of finite-dimensional port-Hamiltonian systems. Section 3.6 looks more closely at the port concept and how it allows to model irreversible dynamics in this generalized Hamiltonian setting. Finally, structure-preserving time integration of port-Hamiltonian systems using continuous (Gauss-Legendre) collocation methods is reviewed in Section 3.7.

Further introductory reading material can be found for instance in [28, 35].

## 3.1 Hamiltonian systems

**Example 3.1** (simple mass-spring harmonic oscillator)**.**
Usually, the differential equation describing the free vibration of a mass-spring harmonic oscillator is written as

$$m\,\ddot{q} \;+\; k\,q \;=\; 0\,, \tag{3.1}$$

i.e. as a second-order ordinary differential equation (ODE). This equation is derived based on Newton's second law and expresses a balance of forces.

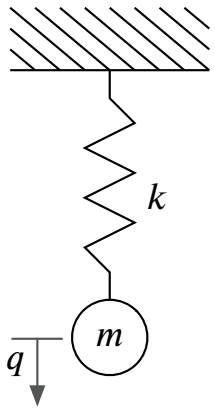



Fig. 3.1 A simple harmonic oscillator with mass $m$ and stiffness of the linear spring $k$.

It is well known that a higher-order ODE can be converted to a system of first-order ODEs. By introducting the velocity $v = \dot{q}$ as a new state variable, Eq. (3.1) can be rewritten as

$$\begin{bmatrix} 1 & 0 \\ 0 & m \end{bmatrix} \begin{bmatrix} \dot{q} \\ \dot{v} \end{bmatrix} = \begin{bmatrix} v \\ -k\,q \end{bmatrix} . \tag{3.2}$$

In systems theory, state-space representations are very popular. A linear time-invariant system without inputs is written as an equation of the form $\dot{x} = A\,x$ where $x$ is the state and $A$ is a linear operator.

If the linear momentum of the mass $p = m\,v$ is chosen as a new state variable instead of the velocity $v$ then Eq. (3.2) can be rewritten in state-space representation as

$$\begin{bmatrix} \dot{q} \\ \dot{p} \end{bmatrix} = \begin{bmatrix} \frac{1}{m}\,p \\ -k\,q \end{bmatrix} . \tag{3.3}$$

The system comprises two energy-storing elements, namely the mass which stores kinetic energy and the spring which stores potential energy.

The Hamiltonian $H$ is a function that maps the system state to the total energy stored in the system:

$$H(q,p) = H_q(q) + H_p(p) = \frac{1}{2}\,q\,k\,q + \frac{1}{2}\,p\,\frac{1}{m}\,p$$

The right-hand side of Eq. (3.3) contains the derivatives of the Hamiltonian function with respect to the state variables $q$ and $p$:

$$\begin{bmatrix} \dot{q} \\ \dot{p} \end{bmatrix} = \begin{bmatrix} \frac{1}{m}\, p \\ -k\, q \end{bmatrix} = \begin{bmatrix} \frac{\partial H}{\partial p}(p) \\ -\frac{\partial H}{\partial q}(q) \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} \frac{\partial H}{\partial q}(q) \\ \frac{\partial H}{\partial p}(p) \end{bmatrix} \tag{3.4}$$

The skew-symmetric matrix is called structure matrix. The extra structure of Eq. (3.4) (in comparison to Eq. (3.1)) helps to show that the system conserves energy. ◇

A more general class of finite-dimensional Hamiltonian systems contains systems of the form

$$\dot{x} = J\, \frac{\partial H}{\partial x}(x)\,. \tag{3.5}$$

These systems are defined on a vector space called state space $\mathscr{X} \ni x$ by specifying a smooth Hamiltonian function $H : \mathscr{X} \to \mathbb{R}$ and a skew-symmetric structure matrix $J$.

Since $J + J^{\mathrm{T}} = 0$, it follows that every system of the form (3.5) conserves energy:

$$\begin{aligned} \frac{\mathrm{d}H}{\mathrm{d}t} &= \frac{\partial H}{\partial x}^{\mathrm{T}}(x)\, \frac{\mathrm{d}x}{\mathrm{d}t} = \frac{\partial H}{\partial x}^{\mathrm{T}}(x)\, J\, \frac{\partial H}{\partial x}(x) \\ &= \frac{\partial H}{\partial x}^{\mathrm{T}}(x)\, J^{\mathrm{T}}\, \frac{\partial H}{\partial x}(x) = -\frac{\partial H}{\partial x}^{\mathrm{T}}(x)\, J\, \frac{\partial H}{\partial x}(x) = 0 \end{aligned}$$

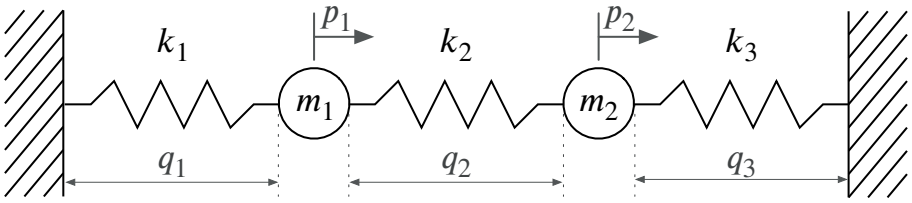



Fig. 3.2 Spring-mass system.

**Example 3.2** (spring-mass system)**.**
The spring-mass system depicted in Fig. 3.2 can be seen as an interconnection of energy-storage components. The *interconnection structure* can be represented by the incidence matrix $G$ of a graph which has the masses as its nodes and the springs as its edges:

$$G = \begin{bmatrix} 1 & -1 & 0 \\ 0 & 1 & -1 \end{bmatrix}$$

The second column of $G$ for instance says that the second edge goes from the first node to the second node.

The state of the system can be identified with a vector of the form

$$x = \begin{bmatrix} q_1 & q_2 & q_3 & p_1 & p_2 \end{bmatrix}^{\mathrm{T}} = \begin{bmatrix} q & p \end{bmatrix}^{\mathrm{T}} \in \mathcal{X}\,.$$

The Hamiltonian function of the system is

$$H(x) = \frac{1}{2}\, q^{\mathrm{T}} \operatorname{diag}\bigl(k_1,\, k_2,\, k_3\bigr)\, q + \frac{1}{2}\, p^{\mathrm{T}} \operatorname{diag}\left(\frac{1}{m_1},\, \frac{1}{m_2}\right) p\,.$$

The spring-mass system can then be modeled by the Hamiltonian system

$$\underbrace{\begin{bmatrix} \dot{q} \\ \dot{p} \end{bmatrix}}_{\dot{x}} = \underbrace{\begin{bmatrix} 0 & G^{\mathrm{T}} \\ -G & 0 \end{bmatrix}}_{J} \underbrace{\begin{bmatrix} \frac{\partial H}{\partial q}(q) \\ \frac{\partial H}{\partial p}(p) \end{bmatrix}}_{\frac{\partial H}{\partial x}(x)}.$$

This example shows that the skew-symmetric structure matrix $J$ encodes how energy is exchanged between the different components of the system. If the Hamiltonian system is interpreted as a network model, then $J$ encodes the topology of the "energy-exchange network". ◇

Many more details about Hamiltonian mechanics can for instance be found in [13, 29].

## 3.2 Bond graphs

A bond graph is a graphical representation of a (multi-domain) physical system model. Such models are called *port-based network models* [2].

The nodes of a bond graph are called components. A component can be a storage element, a source, a dissipative element or a component used to interconnect other components. The edges of a bond graph are called *power bonds*. A power bond represents an interaction or more precisely an exchange of power between two components.

Block diagrams which are often used as a graphical representation in systems theory and control engineering feature unidirectional links: The arrow of an edge indicates

the direction of the signal flow. In contrast, power bonds represent *bilateral relations*: The half-arrow of an edge merely indicates the direction in which an exchange of energy is counted positive.

A power bond is associated with a pair of conjugated quantities: The pairing $\langle e \mid f \rangle$ of the *flow variable* $f$ and the *effort variable* $e$ has the dimension of power.

The half-arrow notation is used to graphically distinguish between the two sides of the arrow: The flow variable is written on the side with the arrowhead and the effort variable is written on the opposite side.

**Example 3.3.**

$$\text{prime mover} \xrightarrow[f]{e} \text{heat pump}$$

In the above bond graph, if the pairing between effort and flow variable is positive, i.e. if

$$\langle e \mid f \rangle > 0\,,$$

then the prime mover is supplying mechanical power to the heat pump. ◇

Optionally, a power bond may be annotated with a so-called *causal stroke*. The position of the causal stroke indicates which end of the bond defines which variable: The *end with the stroke defines the flow variable* and the opposite end defines the effort variable.

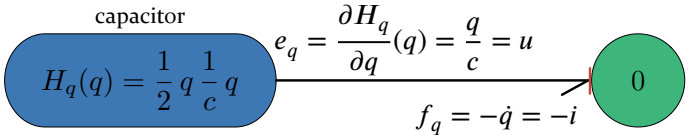



Fig. 3.3 Part of a bond graph showing an ideal capacitor with capacity $c$ and charge $q$ connected to a 0-junction.

In Fig. 3.3 the causal stroke is shown in red and indicates that the capacitor on the left side is defining the effort (voltage) and the 0-junction on the right side is defining the flow (current).

The position of the arrowhead and the position of the causal stoke are independent of each other. The former is always an arbitrary assignment whereas the latter is not: Storage is naturally associated with integration with respect to time. For example, the

effort and flow variables at the capacitor are related as follows:

$$e_q(t) = \frac{1}{c}\left(q(0) - \int_0^t f_q(\tau)\,\mathrm{d}\tau\right)$$

Hence, a capacitor determines the effort (voltage) according to a flow (current) which is imposed by what sits at the other end of the bond.

## 3.3 From bond graphs to port-Hamiltonian systems

Port-Hamiltonian systems (PHS) theory [8] recognizes that port-based network models are generalized Hamiltonian systems called port-Hamiltonian systems.

The storage components of a PHS are characterized by their additive contribution to the Hamiltonian function. This implies the constitutive relations of the system. For example, the capacitor in Fig. 3.3 is characterized by the contribution $H_q$ which expresses the electric energy stored inside the capacitor as a function of the capacitor's charge. Since energy is expressed in terms of charge, $q$ is called an energy variable. The time derivative of an energy variable is called a (storage) flow. In the case of a capacitor, the flow variable is the current flowing out of the capacitor. The derivative of the energy with respect to a energy variable is called (storage) effort. For the capacitor, the effort variable is the voltage across its terminals.

The power-conserving interconnection of components has a geometric structure which is formalized by the notion of a Dirac structure. The capacitor is connected to a so-called 0-junction. All flows at a 0-junction must sum to zero and all efforts must have the same value. A 0-junction thus generalizes Kirchhoff's current law and is a special type of a Dirac structure.

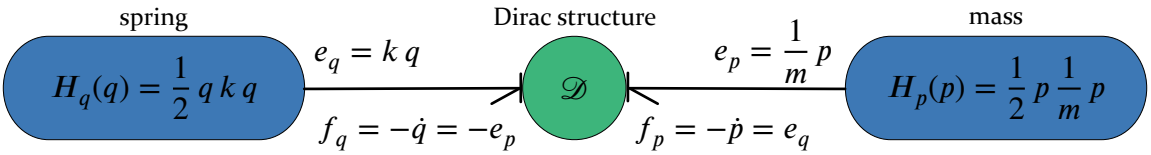



Fig. 3.4 Bond-graph representation of the simple mass-spring harmonic oscillator.

**Example 3.4** (simple mass-spring harmonic oscillator)**.**
The Hamiltonian system describing the harmonic oscillator from Example 3.1 can be represented as a bond graph, see Fig. 3.4.

The two storage components are characterized by their contribution to the Hamiltonian function, i.e. $H = H_q + H_p$. They are connected via another component $\mathscr{D}$ which is characterized by the structure matrix $J$: The Hamiltonian system

$$\underbrace{\begin{bmatrix}\dot{q}\\ \dot{p}\end{bmatrix}}_{-f} = \underbrace{\begin{bmatrix}0 & 1\\ -1 & 0\end{bmatrix}}_{J} \underbrace{\begin{bmatrix}\frac{\partial H}{\partial q}(q)\\ \frac{\partial H}{\partial p}(p)\end{bmatrix}}_{e}$$

can also be written as

$$f + J\,e = 0\,.$$

This equation expresses the relation between flows and efforts at the component $\mathscr{D}$. In this cannonical case, $\mathscr{D}$ generalizes the concept of a *gyrator* from electrical network theory.

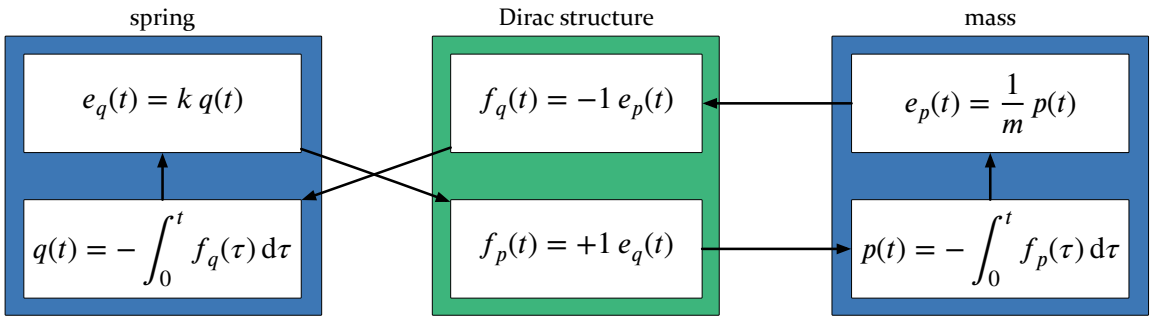



Fig. 3.5 Block-diagram representation of the simple mass-spring harmonic oscillator. The initial values $q(0)$ and $p(0)$ are taken to be zero.

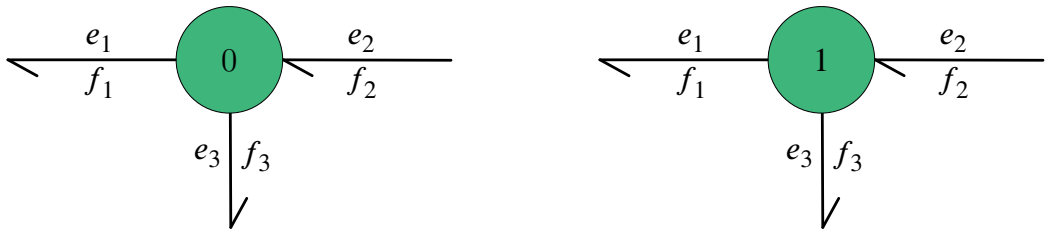
In contrast, traditional systems theory uses block diagrams to graphically represent models. Figure 3.5 shows a direct translation of the bond graph in Fig. 3.4 into a block diagram. It can be observed that a bilateral relation specified by a power-bond indeed translates to a pair of unidirectional signal flows. ◇

A general block diagram can model arbitrary signal flows between arbitrary mathematical operators and therefore has no implicit connection to physics. In contrast, the bond-graph modeling languange is quite restricted since it automatically implies certain structural properties (of the corresponding block-diagram) which are intimately linked to physics.

## 3.4 Dirac structures

Port-Hamiltonian systems have rich structural properties. Their definition is based on Dirac structures which formalize the concept of a power-conserving interconnection of different system components. Further, Dirac structures allow the definition of so-called *ports* through which a port-Hamiltonian system can interact with its environment. Usually, this either means interconnecting a PHS with another PHS to form a larger PHS or terminating a port with a dissipative relation to incorporate irreversible dynamics. Dirac structures further allow to define systems with algebraic constraint equations.

A constant Dirac structure, i.e. an interconnection structure which does not depend on the state of the system, is a linear subspace.




(a) 0-junction with 3 ports.

(b) 1-junction with 3 ports.

Fig. 3.6 Junctions express a power balance.

**Example 3.5** (0-junction and 1-junction)**.**
A 0-junction is a multi-port component and a particularly simple type of Dirac structure. Figure 3.6a shows a 0-junction with 3 ports. Let $\mathscr{F} \ni (f_1, f_2, f_3)$ and $\mathscr{E} \ni (e_1, e_2, e_3)$ denote the linear spaces of flow and effort variables.

Then the Dirac structure $\mathscr{D}_0$ characterizing the 0-junction is a subspace of the so-called bond space $\mathscr{B} = \mathscr{F} \times \mathscr{E}$ defined as

$$\mathscr{D}_0 = \left\{(f_1, f_2, f_3, e_1, e_2, e_3) \in \mathscr{B} \mid -f_1 + f_2 - f_3 = 0\,,\ e_1 = e_2 = e_3\right\} \subset_{\text{vec}} \mathscr{B}\,.$$

For electical systems, flows correspond to currents, efforts correspond to voltages and a 0-junction corresponds to Kirchhoff's current law.

A 1-junction is defined in a dual manner: Figure 3.6b shows a 1-junction with 3 ports. The Dirac structure $\mathscr{D}_1$ characterizing the 1-junction is defined as

$$\mathscr{D}_1 \;=\; \left\{ \left( f_1,\, f_2,\, f_3,\, e_1,\, e_2,\, e_3 \right) \in \mathscr{B} \;\middle|\; f_1 = f_2 = f_3\,,\; -e_1 + e_2 - e_3 = 0 \right\} \subset_{\text{vec}} \mathscr{B}\,.$$

◇

**Definition 3.6** (finite-dimensional constant Dirac structure)**.**
Let $\mathscr{F}$ be the finite-dimensional linear space of flow variables and let $\mathscr{E} = \mathscr{F}^*$ be the corresponding dual space containing the effort variables. Further, let

$$\begin{aligned} \langle \cdot \mid \cdot \rangle \;:\; \mathscr{E} \times \mathscr{F} &\xrightarrow{\sim} \mathbb{R} \\ (e, f) &\mapsto \langle e \mid f \rangle \;=\; e(f) \end{aligned}$$

denote the natural pairing between efforts (covectors) and flows (vectors).

Then, a constant Dirac structure is a subspace $\mathscr{D} \subset_{\text{vec}} \mathscr{B}$
of the bond space $\mathscr{B} = \mathscr{F} \times \mathscr{E}$ which satisfies the following two conditions:

(i)

$$\forall\, (f,\, e) \in \mathscr{D} \,:\, \langle e \mid f \rangle \;=\; 0 \tag{3.6a}$$

(ii)

$$\dim(\mathscr{D}) \;=\; \dim(\mathscr{F}) \;=\; \dim(\mathscr{E}) \tag{3.6b}$$

△

Equation (3.6a) says that the net inflow of power at the interconnection is zero, i.e. the interconnection is power-conserving. Equation (3.6b) states that the subspace of power-conserving flows and efforts has half the dimension of the bond space. If Eq. (3.6a) is satisfied then it is not possible to have $\dim(\mathscr{D}) > \dim(\mathscr{F})$. Hence, Eq. (3.6b) is a maximality condition.

**Example 3.7.**
A Dirac structure $\mathscr{D}$ which is defined as the graph of a skew-symmetric linear operator $J : \mathscr{F}^* \xrightarrow{\sim} \mathscr{F}$, i.e.

$$\mathscr{D} \;=\; \operatorname{graph}(J) \;=\; \left\{ (f,\, e) \in \mathscr{B} \;\middle|\; f + J\, e = 0 \right\}$$

clearly satisfies Definition 3.6. ◇

A more general characterization of constant Dirac structures also applies to infinite-dimensional vector spaces $\mathscr{E}$ and $\mathscr{F}$:

**Definition 3.8** (constant Dirac structure [6, 7])**.**
Let $\mathscr{F}$ be the linear space of flow variables and let $\mathscr{E} = \mathscr{F}^*$ be the corresponding dual space of effort variables. Further, let

$$\begin{aligned} \langle \cdot \mid \cdot \rangle \,:\; \mathscr{E} \times \mathscr{F} &\xrightarrow{\sim} \mathbb{R} \\ (e, f) &\mapsto \langle e \mid f \rangle \;=\; e(f) \end{aligned}$$

denote the natural pairing between efforts (covectors) and flows (vectors).

A non-degenerate symmetric indefinite bilinear form on the bond space $\mathscr{B} = \mathscr{F} \times \mathscr{E}$ is defined by symmetrizing the natural pairing:

$$\begin{aligned} &\langle\!\langle \cdot, \cdot \rangle\!\rangle \,:\; \mathscr{B} \times \mathscr{B} \xrightarrow{\sim} \mathbb{R} \\ &\left((f, e),\, \left(\hat{f}, \hat{e}\right)\right) \mapsto \langle e \mid \hat{f} \rangle \,+\, \langle \hat{e} \mid f \rangle \end{aligned}$$

Then, a Dirac structure $\mathscr{D} \subset_{\text{vec}} \mathscr{B}$ satisfies $\mathscr{D} = \mathscr{D}^\perp$ where

$$\mathscr{D}^\perp \;=\; \left\{(f, e) \in \mathscr{B} \;\middle|\; \forall \left(\hat{f}, \hat{e}\right) \in \mathscr{D} : \langle\!\langle (f, e),\, \left(\hat{f}, \hat{e}\right) \rangle\!\rangle \;=\; 0\right\}$$

is the orthogonal complement of $\mathscr{D} \subset_{\text{vec}} \mathscr{B}$ with respect to $\langle\!\langle \cdot, \cdot \rangle\!\rangle$. △

The subspace $\mathscr{D} \subset_{\text{vec}} \mathscr{B}$ is called an *isotropic* subspace because it is required that for any pair of elements of $\mathscr{D}$ the bilinear form $\langle\!\langle \cdot, \cdot \rangle\!\rangle$ vanishes, i.e.

$$\forall\, (f, e) \in \mathscr{D}\,,\; \forall \left(\hat{f}, \hat{e}\right) \in \mathscr{D} : \langle\!\langle (f, e),\, \left(\hat{f}, \hat{e}\right) \rangle\!\rangle \;=\; 0\,.$$

This is equivalent to the condition $\mathscr{D} \subseteq_{\text{vec}} \mathscr{D}^\perp$.

Further, $\mathscr{D}$ is called a *maximal* isotropic subspace because it is required to have maximal dimension, i.e.

$$\forall \left(\hat{f}, \hat{e}\right) \in \mathscr{D} : \nexists\, (f, e) \notin \mathscr{D} : \langle\!\langle (f, e,),\, \left(\hat{f}, \hat{e}\right) \rangle\!\rangle \;=\; 0\,.$$

This is equivalent to the condition $\mathscr{D}^\perp \subseteq_{\text{vec}} \mathscr{D}$.

Since $\mathscr{D} \subseteq_{\text{vec}} \mathscr{D}^\perp$ and $\mathscr{D}^\perp \subseteq_{\text{vec}} \mathscr{D} \iff \mathscr{D} = \mathscr{D}^\perp$, a constant Dirac structure is a maximal isotropic subspace.

A formal proof showing the equivalence of Definition 3.6 and Definition 3.8 for the finite-dimensional (lumped-parameter) case can for instance be found in [35, Appendix A.1].

A non-constant (or modulated) Dirac structure is an interconnection structure which depends on the state of the system. To make this precise, the notion of a linear state space is replaced by the more abstract notion of a smooth manifold. If $\mathscr{X} \ni x$ denotes the *state manifold* of a PHS then the flow[1] $f_S$ at time $t$ is a vector in the tangent space at $x(t)$, i.e. $f_S(t) = -\dot{x}(t) \in T_{x(t)}\mathscr{X}$. The coresponding effort $e_S$ is a covector (or 1-form) in the cotangent space at the same point, i.e. $e_S(t) = \mathrm{d}H\big(x(t)\big) \in T^*_{x(t)}\mathscr{X}$ where $H \in C^\infty(\mathscr{X})$ is the Hamiltonian function of the system. The flow $f_S$ and the effort $e_S$ are associated with the storage components of the system. It holds that

$$\big(f_S,\, e_S\big) \;=\; \big(-\dot{x},\, \mathrm{d}H(x)\big) \;\in\; \big(T\mathscr{X} \oplus T^*\mathscr{X}\big)\,. \tag{3.7}$$

This sum of two vector bundles is the vector bundle over $\mathscr{X}$ which has at every point $x \in \mathscr{X}$ the fiber $T_x\mathscr{X} \times T^*_x\mathscr{X}$.

If the system has further ports for interacting with its environment or for incorporating irreversible dynamics, there is another set of flows and efforts $\big(f_P,\, e_P\big) \in \mathscr{F}_P \times \mathscr{E}_P$ associated with the system's interaction over these ports. Here, $\mathscr{F}_P$ and $\mathscr{E}_P = \mathscr{F}_P^*$ are linear spaces and hence flat manifods. Thus, it holds that

$$\big(f_S, f_P, e_S, e_P\big) \;\in\; T\mathscr{X} \oplus \mathscr{F}_P \oplus T^*\mathscr{X} \oplus \mathscr{F}_P^* \;=\; \mathscr{B}\,. \tag{3.8}$$

A (generalized) Dirac sturcture is a vector subbundle $\mathscr{D} \subset_{\text{bundle}} \mathscr{B}$. This means that for every point $x \in \mathscr{X}$ some subspace $\mathscr{D}(x) \subset_{\text{vec}} \mathscr{B}(x) = T_x\mathscr{X} \times \mathscr{F}_P \times T^*_x\mathscr{X} \times \mathscr{F}_P^*$ is chosen.

**Definition 3.9** (non-constant generalized Dirac structure)**.**
Let $\mathscr{X}$ denote the state manifold of a port-Hamiltonian system with tangent bundle $T\mathscr{X} \ni f_S$ and cotangent bundle $T^*\mathscr{X} \ni e_S$.

Further, let $\mathscr{F}_P \ni f_P$ and $\mathscr{E}_P = \mathscr{F}_P^* \ni e_P$ be the linear spaces containing the port variables.

[1] In the context of differential equations, the mapping which advances initial conditions in time (solution operator) is called flow. In the context of port-based modeling, a flow is simply a vector which is tangent to the solution at a particular instant in time.

Let $\mathscr{B} = T\mathscr{X} \oplus \mathscr{F}_P \oplus T^*\mathscr{X} \oplus \mathscr{F}_P^*$ be the smooth vector bundle over $\mathscr{X}$ with fiber $T_x\mathscr{X} \times \mathscr{F}_P \times T_x^*\mathscr{X} \times \mathscr{F}_P^*$ for every point $x \in \mathscr{X}$. This means that there is a *copy* of $\mathscr{F}_P$ and $\mathscr{F}_P^*$ over every point $x \in \mathscr{X}$.

For some smooth vector subbundle $\mathscr{D} \subset_{\text{bundle}} \mathscr{B}$, the notation $\left(f_S,\, f_P,\, e_S,\, e_P\right) \in \mathscr{D}$ means that $\forall x \in \mathscr{X} : \left(f_S(x),\, f_P(x),\, e_S(x),\, e_P(x)\right) \in \mathscr{D}(x) \subset_{\text{vec}} \mathscr{B}(x)$.

Define the smooth vector subbundle

$$\mathscr{D}^\perp \;=\; \left\{(f,e) \in \mathscr{B} \;\middle|\; \forall \left(\hat{f},\hat{e}\right) \in \mathscr{D} : \langle e \mid \hat{f}\rangle \;+\; \langle \hat{e} \mid f\rangle \;=\; 0\right\}$$

where

$$\begin{aligned}\langle \cdot \mid \cdot \rangle :\; \left(T^*\mathscr{X} \oplus \mathscr{F}_P^*\right) \oplus \left(T\mathscr{X} \oplus \mathscr{F}_P\right) &\xrightarrow{\sim} C^\infty(\mathscr{X}) \\ \left(\left(e_S, e_P\right), \left(f_S, f_P\right)\right) &\mapsto e_S(f_S) + e_P(f_P)\end{aligned}$$

is the natural pairing between covector and vector fields and $0 \in C^\infty(\mathscr{X})$ is the function that takes the value zero everywhere on $\mathscr{X}$.

Then $\mathscr{D} \subset_{\text{bundle}} \mathscr{B}$ is a generalized Dirac structure on $\mathscr{X}$ if $\mathscr{D}^\perp = \mathscr{D}$. △

In particular, the graph of a skew-symmetric vector bundle map $\left(T^*\mathscr{X} \oplus \mathscr{E}_P\right) \xrightarrow{\sim} \left(T\mathscr{X} \oplus \mathscr{F}_P\right)$ defines a generalized Dirac structure.

For systems defined with a non-constant Dirac structure *integrability* (or closedness) becomes an issue. This is closely related to the topic of holonomic vs. nonholonomic constraints and to the existence of cannonical coordinates. If a certain integrability condition is satisfied then the predicate 'generalized' is dropped. More information about (generalized) Dirac structures and their integrability can for instance be found in [11].

## 3.5 Finite-dimensional port-Hamiltonian systems

A finite-dimensional port-Hamiltonian system (in explicit[2] input-state-output representation) is a dynamical system of the form

$$\begin{aligned} \dot{x} &= J(x)\big[\mathrm{d}H(x)\big] + B(x)\big[u\big] \\ y &= B^{\mathrm{T}}(x)\big[\mathrm{d}H(x)\big]\,. \end{aligned} \tag{3.9}$$

Here, $\mathcal{X} \ni x$ is the state manifold and $H \in C^\infty(\mathcal{X})$ is the Hamiltonian function of the system. The flows $f_S = -\dot{x} \in T_x\mathcal{X}$ and the corresponding efforts $e_S = \mathrm{d}H(x) \in T_x^*\mathcal{X}$ define the storage port $\big(f_S, e_S\big)$ of the port-Hamiltonian system. The family of linear maps

$$\begin{aligned} J :\ \mathcal{X} &\to \mathrm{Hom}(T_x^*\mathcal{X}, T_x\mathcal{X}) \\ x &\mapsto J(x) \end{aligned}$$

has to satisfy

$$\forall\, x \in \mathcal{X}\ :\ \forall \tilde{e}_S \in T_x^*\mathcal{X}\ :\ J(x)\big[\tilde{e}_S\big] + J^{\mathrm{T}}(x)\big[\tilde{e}_S\big] = 0 \in T_x\mathcal{X}$$

where $J^{\mathrm{T}}(x)$ is the dual (or transpose) map of $J(x)$.

The outputs $y = f_P \in \mathcal{F}_P = \mathbb{R}^m$ and the corresponding inputs $u = e_P \in \mathcal{E}_P = \mathcal{F}_P^* = \big(\mathbb{R}^m\big)^*$ together define the port $\big(f_P, e_P\big)$ through which the system can interact with its environment. The family of linear maps

$$\begin{aligned} B :\ \mathcal{X} &\to \mathrm{Hom}(\mathcal{F}_P^*, T_x\mathcal{X}) \\ x &\mapsto B(x) \end{aligned}$$

defines how the inputs affect the system and the corresponding family of dual maps

$$\begin{aligned} B^{\mathrm{T}} :\ \mathcal{X} &\to \mathrm{Hom}(T_x^*\mathcal{X}, \mathcal{F}_P) \\ x &\mapsto B^{\mathrm{T}}(x) \end{aligned}$$

[2] A PHS may also be stated in an implicit representation. Network modeling of physical systems generally leads to systems of differential-algebraic equations (DAEs) since connecting the subsystems amounts to imposing constraints, see for instance [32, 48].

defines the outputs of the port-Hamiltonian system.

**Remark 3.10** (differential vs. gradient)**.**
Instead of $\mathrm{d}H(x)$ often the symbol $\frac{\partial H}{\partial x}(x)$ is used to denote the differential of $H$ in matrix notation. This should not be called a gradient since gradients are vectors and $\mathrm{d}H(x) \in T_x^*\mathcal{X}$ is a covector. Gradients are not intrinsically defined since additionally a Riemannian metric on $\mathcal{X}$ would be required to speak of a gradient. △

The energy balance for this system is

$$\begin{aligned}\frac{\mathrm{d}H}{\mathrm{d}t} &= \frac{\partial H}{\partial x}^{\mathrm{T}}(x)\,\frac{\mathrm{d}x}{\mathrm{d}t} = \underbrace{\frac{\partial H}{\partial x}^{\mathrm{T}}(x)\,J(x)\,\frac{\partial H}{\partial x}(x)}_{0} + \frac{\partial H}{\partial x}^{\mathrm{T}}(x)\,B(x)\,u \\ &= \left(B^{\mathrm{T}}(x)\,\frac{\partial H}{\partial x}(x)\right)^{\mathrm{T}} u = y^{\mathrm{T}}\,u\,.\end{aligned}$$

Since the output map is the dual of the input map, inputs and outputs come in pairs. The outputs and inputs are said to be *collocated* and their pairing yields the power that is exchanged across the respective port.

Equation (3.9) can also be written as

$$\underbrace{\begin{bmatrix}\dot{x}\\ -y\end{bmatrix}}_{-f} = \underbrace{\begin{bmatrix}J(x) & B(x)\\ -B^{\mathrm{T}}(x) & 0\end{bmatrix}}_{N(x)} \underbrace{\begin{bmatrix}\mathrm{d}H(x)\\ u\end{bmatrix}}_{e}. \tag{3.10}$$

For every fixed $x \in \mathcal{X}$, the linear map $N(x)\colon \left(T^*\mathcal{X} \oplus \mathcal{F}_P^*\right) \xrightarrow{\sim} \left(T\mathcal{X} \oplus \mathcal{F}_P\right)$ is skew-symmetric and hence the family of maps $N$ defines the (generalized) Dirac structure

$$\mathcal{D} = \left\{\left(f, e\right) \in \left(T\mathcal{X} \oplus \mathcal{F}_P\right) \oplus \left(T^*\mathcal{X} \oplus \mathcal{F}_P^*\right) \mid \forall\, x \in \mathcal{X}\colon\ f(x) + N(x)\,e(x) = 0\right\}.$$

This geometic structure encodes how power can be reversibly exchanged among the different storage components and the environment.

## 3.6 Port-Hamiltonian systems with irreversible dynamics

Exchange of energy across system boundaries is not only necessary for modelling larger systems by interconnecting different subsystems but also to incorporate dissipation of energy. Hamiltonian systems have reversible dynamics and therefore irreversible dynamics need to be generated 'externally'. This is achieved by terminating a port with a *resistive relation*.

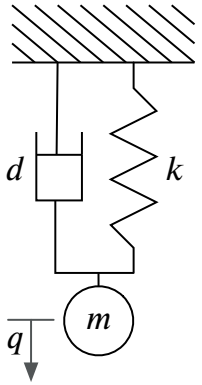



Fig. 3.7 A damped harmonic oscialltor with mass $m$, stiffness of the linear spring $k$ and coefficient of the linear damper $d$.

**Example 3.11** (damped harmonic oscillator)**.**
The differential equation describing the free vibration of the damped harmonic oscillator is usually written as

$$m\,\ddot{q} \;+\; d\,\dot{q} \;+\; k\,q \;=\; 0\,.$$

The damped harmonic oscillator can be modeled as a port-Hamiltonian system by considering the damping as an external forcing:

$$\begin{aligned}\begin{bmatrix}\dot{q}\\ \dot{p}\end{bmatrix} &= \begin{bmatrix}0 & 1\\ -1 & 0\end{bmatrix}\begin{bmatrix}\frac{\partial H}{\partial q}(q)\\ \frac{\partial H}{\partial p}(p)\end{bmatrix} + \begin{bmatrix}0\\ 1\end{bmatrix} u\\ y &= \begin{bmatrix}0 & 1\end{bmatrix}\begin{bmatrix}\frac{\partial H}{\partial q}(q)\\ \frac{\partial H}{\partial p}(p)\end{bmatrix}\end{aligned} \tag{3.11}$$

The force input $u = e_R$ and the velocity output $y = f_R = v$ together define the port $(f_R, e_R)$ which is terminated by the resistive relation

$$u = -d\,y \iff e_R + d\,f_R = 0\,. \tag{3.12}$$

This yields the energy balance

$$\frac{\mathrm{d}H}{\mathrm{d}t} = y^{\mathrm{T}} u = -v\,d\,v < 0\,.$$

By combining differential and algebraic equations, Eq. (3.11) can be written as

$$\left[\begin{array}{c} \dot{q} \\ \dot{p} \\ \hline -y \end{array}\right] = \left[\begin{array}{cc|c} 0 & 1 & 0 \\ -1 & 0 & 1 \\ \hline 0 & -1 & 0 \end{array}\right] \left[\begin{array}{c} \frac{\partial H}{\partial q}(q) \\ \frac{\partial H}{\partial p}(p) \\ \hline u \end{array}\right].$$

This shows the (extended) skew-symmetric structure matrix which defines the Dirac structure of the system. ◇

Generalizing Example 3.11 yields the following class of port-Hamiltonian systems:

$$\underbrace{\begin{bmatrix} \dot{x} \\ -y_B \\ -y_R \end{bmatrix}}_{-f} = \underbrace{\begin{bmatrix} J(x) & B(x) & C(x) \\ -B^{\mathrm{T}}(x) & 0 & 0 \\ -C^{\mathrm{T}}(x) & 0 & 0 \end{bmatrix}}_{N(x)} \underbrace{\begin{bmatrix} \mathrm{d}H(x) \\ u_B \\ u_R \end{bmatrix}}_{e} \tag{3.13a}$$

$$u_R = -D(x)\,y_R \tag{3.13b}$$

The flow vector and the effort covector are partitioned into storage, boundary and resistive parts, i.e.

$$f = \begin{bmatrix} f_S \\ f_B \\ f_R \end{bmatrix} = \begin{bmatrix} -\dot{x} \\ y_B \\ y_R \end{bmatrix} \in T_x\mathcal{X} \oplus \mathcal{F}_B \oplus \mathcal{F}_R = \mathcal{F}(x)$$
$$e = \begin{bmatrix} e_S \\ e_B \\ e_R \end{bmatrix} = \begin{bmatrix} \mathrm{d}H(x) \\ u_B \\ u_R \end{bmatrix} \in T_x^* \oplus \mathcal{F}_B^* \oplus \mathcal{F}_R^* = \mathcal{E}(x)\,.$$

The families of linear maps $B$ and $C$ define the boundary and resistive ports, repectively. The resistive port $(f_R, e_R)$ is terminated by the resisitve relation

$$\mathfrak{R}(f_R, e_R) = e_R + D\,f_R = 0\,.$$

The family of linear maps

$$\begin{aligned} N : \mathcal{X} &\to \mathrm{Hom}\big(\mathcal{E}(x), \mathcal{F}(x)\big) \\ x &\mapsto N(x) \end{aligned}$$

satisfies

$$\forall\, x \in \mathcal{X} \;:\; \forall \tilde{e} \in \mathcal{E}(x) \;:\; N(x)\big[\tilde{e}\big] + N^{\mathrm{T}}(x)\big[\tilde{e}\big] = 0 \in \mathcal{F}(x)\,.$$

and defines the (generalized) Dirac structure

$$\mathcal{D} = \Big\{ (f, e) \in \big(T\mathcal{X} \oplus \mathcal{F}_B \oplus \mathcal{F}_R\big) \oplus \big(T^*\mathcal{X} \oplus \mathcal{F}_B^* \oplus \mathcal{F}_R^*\big) \mid \forall\, x \in \mathcal{X} : f(x) + N(x)\,e(x) = 0 \Big\}\,.$$

Figure 3.8 shows system (3.13) as a bond graph.

The power balance equation

$$\begin{aligned} \langle e \mid f \rangle &= e^{\mathrm{T}} f = e^{\mathrm{T}}\big(-N(x)\,e\big) = -e^{\mathrm{T}} N^{\mathrm{T}}(x)\,e = 0 \\ &= \underbrace{\langle e_S \mid f_S \rangle}_{-\frac{\mathrm{d}H}{\mathrm{d}t}} + \underbrace{\langle e_B \mid f_B \rangle}_{u_B^{\mathrm{T}} y_B} + \underbrace{\langle e_R \mid f_R \rangle}_{\leq 0} \end{aligned} \tag{3.14}$$

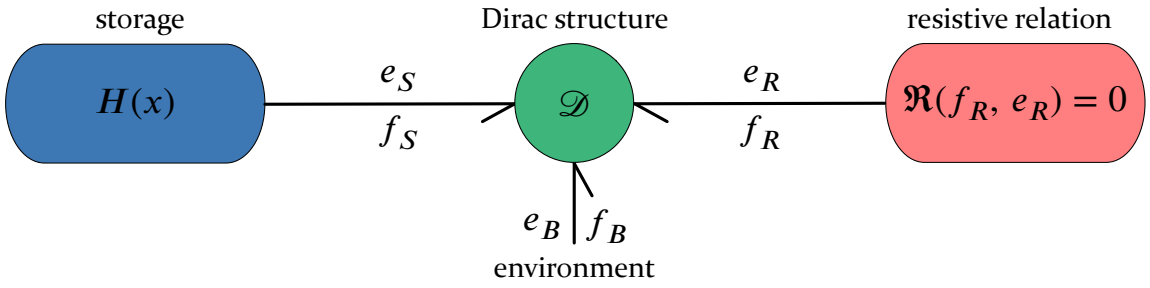



Fig. 3.8 Bond graph representation of a general port-Hamiltonian system incorporating irreversible dynamics and exchange of energy with the environment.

which says that

$$\text{stored power} \;+\; \text{dissipated power} \;=\; \text{supplied power}$$

might be called the most important structural property of port-Hamiltonian systems. An immediate consequence is the so-called *passivity property*

$$\frac{\mathrm{d}H}{\mathrm{d}t} \;\leq\; u_B^{\mathrm{T}}\, y_B \tag{3.15}$$

which says that

$$\text{stored power} \;\leq\; \text{supplied power}\,.$$

**Remark 3.12** (thermodynamic meaning of the Hamiltonian function)**.**
In Example 3.11, the damper converts kinetic energy into internal energy.

Since the Hamiltonian function $H$ does not include internal energy and the Hamiltonian is not conserved it cannot be the total energy of the system.

In fact, $H$ is the total exergy of the system, i.e. the maximum amount of work which can possibly be extracted from it, see Remark 2.6. The common assumption was made that the system is *isothermal*. This means it is in equilibrium with an unlimited heat reservoir at a constant temperature $\theta_0$. The exergy of the system is defined with $\theta_0$ as the reference temperature.

Since internal energy $u$ and entropy $s$ are both extensive variables,

$$u \;=\; U(s) \;=\; \theta_0\, s$$

is a fundamental equation for an isothermal system at temperature $\theta_0$ which has no further state variables. The isothermal assumption renders the state variable $s$ basi-

cally meaningless because $U$ describes a heat reservoir whose dynamics can be neglected.

If $K(p)$ is the kinetic energy and $V(q)$ is the potential energy of the damped harmonic oscillator then its exergy $H$ is

$$H(q, p) = K(p) + V(q) + \cancel{U(s)} - \cancel{\theta_0 s},$$

see Eq. (2.7).

Hence, the passivity property (3.15) asserts that no exergy is created inside a port-Hamiltonian system. △

## 3.7 Geometric numerical integration

The field of geometric numerical integration [19, 23, 25] deals with the design and analysis of numerical integrators for time integration of ODE systems. The goal is to preserve geometric properties of the flow of a differential equation by finding a discrete formulation which shares important properties with the continuous formulation. In particular, this results in good long-time behavior of the discrete dynamics in the sense that errors don't grow unbounded as time approaches infinity. Ideally the discrete-time system would conserve (within machine precision) all quantities which are conserved for the continuous-time system.

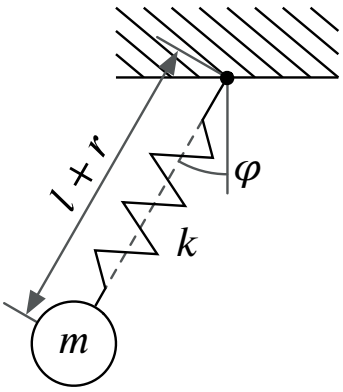



Fig. 3.9 A simple pendulum with an integrated spring.

**Example 3.13** (simple pendulum with spring)**.**
Figure 3.9 shows a simple pendulum with an integrated spring. The mass $m$ is attached

to the pendulum rod which has length $l$ if the spring is relaxed. The gravitational constant is $g$. The configuration is given by the angular displacement of the pendulum rod $\varphi$ and the spring's extension $r$. The corresponding conjugate momenta $p_\varphi$ and $p_r$ determine the kinetic energy of the mass. Hence,

$$x = \begin{bmatrix} \varphi & r & p_\varphi & p_r \end{bmatrix}^{\mathrm{T}}$$

determines the state of the system. Its total energy (or exergy for that matter) is

$$H(x) = \underbrace{\frac{p_\varphi^2}{2\,m\,(l+r)^2} + \frac{p_r^2}{2\,m}}_{K} \underbrace{- m\,g\,(l+r)\cos(\varphi) + \frac{k\,r^2}{2}}_{V}.$$

The reversible process is modeled by the Hamiltonian system

$$\underbrace{\begin{bmatrix} \dot{\varphi} \\ \dot{r} \\ \dot{p}_\varphi \\ \dot{p}_r \end{bmatrix}}_{-f(t)} = \underbrace{\begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix}}_{J} \underbrace{\begin{bmatrix} m\,g\,(l+r)\sin(\varphi) \\ -m\,g\,\cos(\varphi) + k\,r - \frac{p_\varphi^2}{m(l+r)^3} \\ \frac{p_\varphi}{m(l+r)^2} \\ \frac{p_r}{m} \end{bmatrix}}_{e(t) = \frac{\partial H}{\partial x}\left(x(t)\right)}.$$

The variables $\varphi$ and $r$ correspond to two different forms of storing potential energy inside the system. The system is nonlinear due to the coupling between the gravitational potential and the spring and due to the trigonometric functions describing the pendulum kinematics.

The fourth-order Gauss-Legendre collocation method is a geometric integrator. The simulated dynamics for this example show a nice (but not perfect) result: The error oscillates inside an interval with fixed bounds. The size of the interval depends on the time step: $\sim 10^{-5}$ for a time step of 0.1 seconds and $\sim 10^{-9}$ for a time step of 0.01 seconds, see Fig. 3.10. For linear dynamics, the quadratic Hamiltonian is conserved by this method nearly up to machine precision ($\sim 10^{-14}$) given that the time step is not too large to capture the dynamical behavior. ◇

This section introduces continuous collocation methods and in particular Gauss-Legendre methods. More details can be found in the articles[47, 48].

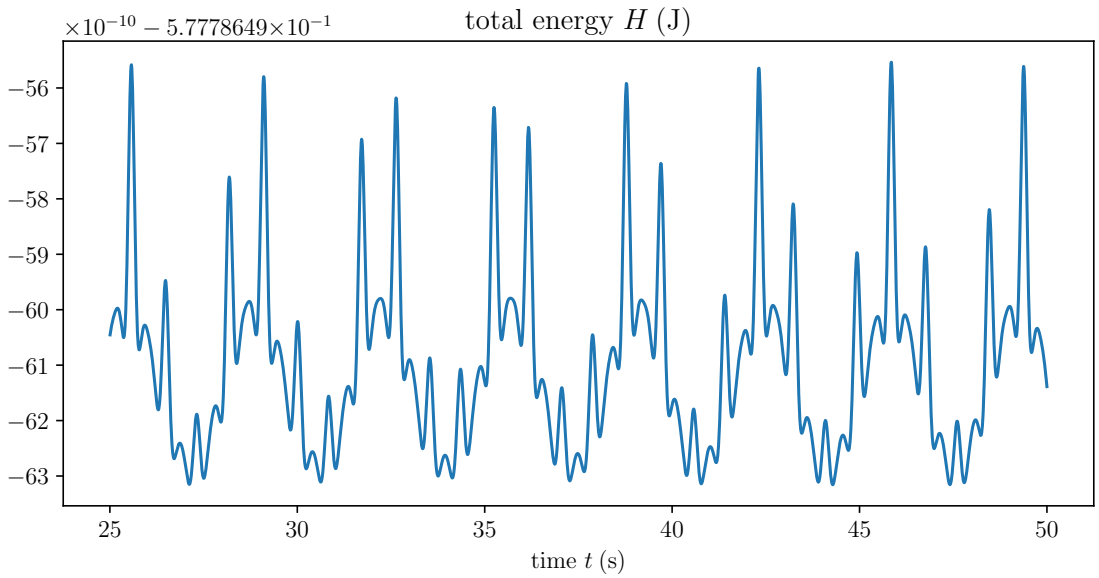



Fig. 3.10 A geometrical integrator simulating a nonlinear Hamiltonian system: The total energy is conserved well. The error remains bounded in time.

### 3.7.1 Continuous collocation methods

Let a port-Hamiltonian system of the form

$$\underbrace{\dot{x}(t)}_{-f(t)} = J\big(x(t)\big) \underbrace{\frac{\partial H}{\partial x}\big(x(t)\big)}_{e(t)} + B\big(x(t)\big)\, u(t) \tag{3.16a}$$

$$y(t) = B^{\mathrm{T}}\big(x(t)\big)\, e(t) \tag{3.16b}$$

be given.

Solving the initial value problem

$$\dot{x}(t) = J\big(x(t)\big)\, e(t) + B\big(x(t)\big)\, u(t) \tag{3.17a}$$

$$x(0) = x_0 \tag{3.17b}$$

on some time interval $I = t \in [0, t_f]$ is in general not possible analytically.

The problem can be solved numerically by splitting the time interval $I$ into $K$ subintervals

$$I^k = [(k-1)\,h,\ kh] \ .$$

The index $k = 1, 2, \dots, K$ identifies a paricular subinterval. The length of the subintervals has to be prescribed by chosing a time step $h$ such that $t_f = hK$.

The true solution $x(t)$ (with $t \in I$) is then approximated by the numerical solution $\tilde{x}(t)$ which is defined picewise: On each subinterval, $\tilde{x}(t)$ (with $t \in I^k$) is a polynomial of degree $s$ in the variable $t$. More precisely, if $x(t) \in \mathbb{R}^N$ then $\tilde{x}(t)$ is a vector of $N$ polynomials.

Like the time step $h$, the oder of the polynomial approximation is a parameter that has to be chosen by the user to control the fidelity of the numerical method.

Since a polynomial of degree $s$ is determined by $s+1$ coefficients there are $s+1$ (vectorial) unknowns per interval. The continuity of the solution between two intervals determines one (vectorial) unknown. For the first interval $I^1$, this unknown is determined by the initial condition (3.17b).

The remaining $s$ unknowns are fixed by requiring that the differential equation has to hold at $s$ collocation points $t_1^k, \dots, t_s^k \in I^k$. The choice of these points within each subinterval is important for obtaining a good numerical approximation.

By defining $t_0^k = (k-1)\,h$ and $t_{s+1}^k = hk$, each subinterval can be written as

$$I_k \;=\; \left[t_0^k, t_{s+1}^k\right] .$$

Then, the collocation points $t_1^k, \dots, t_s^k$ can be written as $t_i^k = t_0^k + c_i\,h$ with coefficients $c_1, \dots, c_s$ satisfying

$$\begin{aligned} &\forall\, i \in \{1, \dots, s\} \;:\; 0 \le c_i \le 1 \\ &\forall\, i \in \{1, \dots, s-1\} \;:\; c_i < c_{i+1} . \end{aligned}$$

Since on each subinterval the numerical solution $\tilde{x}(t)$ is given as a vector of polynomials of degree $s$, the time derivative $\dot{\tilde{x}}(t)$ is a vector of polynomials of degree $s-1$.

The numerical solution $\tilde{x}(t)$ with $t \in I^k$ can be written as

$$\tilde{x}(t) \;=\; \tilde{x}(t_0^k) \;+\; \int_{t_0^k}^{t} \dot{\tilde{x}}(z)\,\mathrm{d}z\,. \tag{3.18}$$

To make life easier, a local time coordinate $\tau^k \in [0,1]$ is defined on each subinterval $I^k$ by requiring that $t = \big((k-1) + \tau^k\big)h$. Hence, $\tau^k = 0$ corresponds to $t_0^k$ and $\tau^k = 1$ corresponds to $t_{s+1}^k$.

Based on this normalized time, the polynomial approximation of $\dot{\tilde{x}}$ can be defined in a unified manner for all $k$: On each subinterval, the vector $\dot{\tilde{x}}$ can be written as a linear combination

$$\dot{\tilde{x}}(\tau^k) \;=\; \sum_{i=1}^{s} \Big( -f_i^k \, l_i(\tau^k) \Big) \,.$$

More precisely, the $n$-th component of $\dot{\tilde{x}}$ is a vector in the vector space that is spanned by the $s$ basis functions $l_1, \dots, l_s$. Given such a basis, this vector is determined by the tuple consisting of the $n$-th component of each of the vectors $f_1, \dots, f_s$.

With this change of time coordinate and a choice of basis, Eq. (3.18) can be written as

$$\begin{aligned} \tilde{x}(t_0^k + \tau^k \, h) \;&=\; \tilde{x}(t_0^k) \;+\; \int_0^\tau \sum_{j=1}^{s} \Big( -f_j^k \, l_j(\mu) \Big) \, h \, \mathrm{d}\mu \\ &=\; \tilde{x}(t_0^k) \;-\; h \sum_{j=1}^{s} \Big( f_j^k \int_0^\tau l_j(\mu) \, \mathrm{d}\mu \Big) \,. \end{aligned}$$

The collocation method is based on relating $\dot{\tilde{x}}$ and $\tilde{x}$ at the $s$ collocation points $c_1, \dots, c_s$. Hence, it is convenient to chose the basis polynomials such that the $n$-th component of $f_i$ expresses the value of the $n$-th component of $\dot{\tilde{x}}$ at $\tau = c_i$, i.e. $-f_i \overset{!}{=} \dot{\tilde{x}}(c_i)$.

These basis polynomials are the Lagrange polynomials

$$l_i(\tau) \;=\; \prod_{\substack{j=1 \\ j \neq i}}^{s} \frac{\tau - c_j}{c_i - c_j}$$

which have the desired property $l_i(c_j) = \delta_{ij}$ where $\delta_{ij}$ is the Kronecker delta.

The value of the numerical solution $\tilde{x}$ at the beginning of each subinterval $I^k$ shall be denoted by $x_0^k = \tilde{x}(t_0^k)$. This value is known because of the continuity of the solution between subintervals or because of the initial condition (3.17b), i.e. $x_0^1 = x_0$ and $x_0^k = x_{s+1}^{k-1}$ for $k > 1$.

By defining

$$b_j \;=\; \int_0^1 l_j(\mu)\,\mathrm{d}\mu$$

the numerical solution at the endpoint of a subinterval can be written as

$$x_{s+1}^k \;=\; \tilde{x}(t_{s+1}^k) \;=\; x_0^k \;-\; h\sum_{j=1}^{s}\left(b_j\, f_j^k\right).$$

It is the final goal of all computations done for a particular step $k$ to obtain the value $x_{s+1}^k$ which is determined by the result $x_{s+1}^{k-1} = x_0^k$ of the previous step and the coefficients $f_1^k, \ldots, f_s^k$.

These coefficients have to be determined by solving a (nonlinear) system of equations: Equation (3.17a) has to hold at the collocation points $t_1^k, \ldots, t_s^k$. Hence, the system of equations defines a relationship between the values of the derivative of the numerical solution at the collocation points given by the the unknowns $f_1^k, \ldots, f_s^k$ and the values of the numerical solution at the collocation points $\tilde{x}(t_1^k), \ldots, \tilde{x}(t_s^k)$ which in turn also depend on $f_1^k, \ldots, f_s^k$.

By defining

$$a_{ij} \;=\; \int_0^{c_i} l_j(\mu)\,\mathrm{d}\mu$$

the numerical solution $\tilde{x}$ can conveniently be expressed at the collocation points:

$$x_i^k \;=\; \tilde{x}(t_i^k) \;=\; x_0^k \;-\; h\sum_{j=1}^{s}\left(a_{ij}\, f_j^k\right)$$

for $i = 1, \ldots, s$.

The following definitions are introduced for convenience:

$$\begin{aligned}
\boldsymbol{J}_i^k &= \boldsymbol{J}(x_i^k)\\
e_i^k &= \left.\frac{\partial H}{\partial x}\right|_{x=x_i^k}\\
\boldsymbol{B}_i^k &= \boldsymbol{B}(x_i^k)\\
u_i^k &= u(t_i^k)
\end{aligned}$$

Then, the system of equations, which has to be solved at the $k$-th step, can be written as

$$f_i^k + J_i^k e_i^k + B_i^k u_i^k = 0 \quad \text{for } i = 1, \dots, s\,. \tag{3.20}$$

In the general case, every term of the above equation, except for $u_i^k$, depends on the unknowns $f_1^k, \dots, f_s^k$.

By introducing the block vectors and matrices

$$\begin{aligned} f^k &= \left[ \left(f_1^k\right)^{\mathrm{T}}, \dots, \left(f_s^k\right)^{\mathrm{T}} \right]^{\mathrm{T}} \\ J^k &= \mathrm{blockdiag}(J_1^k, \dots, J_s^k) \\ e^k &= \left[ \left(e_1^k\right)^{\mathrm{T}}, \dots, \left(e_s^k\right)^{\mathrm{T}} \right]^{\mathrm{T}} \\ B^k &= \mathrm{blockdiag}(B_1^k, \dots, B_s^k) \\ u^k &= \left[ \left(u_1^k\right)^{\mathrm{T}}, \dots, \left(u_s^k\right)^{\mathrm{T}} \right]^{\mathrm{T}} \end{aligned}$$

the system of equations (3.20) can be written as

$$f^k + J^k e^k + B^k u^k = 0\,.$$

### 3.7.2 Gauss-Legendre collocation

Gauss-Legendre collocation methods use the roots of the shifted Legendre polynomial

$$\frac{1}{s!} \frac{\mathrm{d}^s}{\mathrm{d}x^s} \Big( \big( x\,(x-1) \big)^s \Big)$$

as coefficients $c_1, \dots, c_s$.

A $s$-stage Gauss-Legendre collocation method has *accuracy order* $2\,s$, i.e.

$$\int_0^1 f(t_0 + h\,\tau)\,\mathrm{d}\tau = \sum_{i=1}^{s} b_i\, f(t_0 + h\,c_i) + \mathcal{O}(h^{2s+1})\,.$$

The choice $s = 1$ yields the implicit midpoint rule which is second-order accurate.

Gauss-Legendre collocation methods applied to port-Hamiltonian systems with quadratic Hamiltonian are the only numerical integrators which yield an exact discrete energy balance [47].

# 4

# GENERIC

This chapter shall summarize some important aspects of the GENERIC approach to nonequilibrium thermodynamics which was introduced in [9, 10]. The textbook [24] explains the *General Equation for the NonEquilibrium Reversible-Irreversible Coupling* (GENERIC) in greater detail.

The fundamental idea behind the GENERIC approach is the additive splitting of the time evolution of a thermodynamical system into reversible and irreversible contributions. If $x \in \mathcal{X}$ describes the macroscopic state of a system then the time evolution $\dot{x}$ is given by

$$\dot{x} = \dot{x}_{\text{rev}} + \dot{x}_{\text{irr}} \tag{4.1}$$

where $\dot{x}_{\text{rev}}$ is the reversible and $\dot{x}_{\text{irr}}$ is the irreversible contribution.

Reversible processes are modeled by a Hamiltonian system and conserve both energy and entropy. Irreversible processes are modeled by a gradient system. They conserve energy and generate entropy.

The GENERIC framework can be defined using a Poisson bracket together with a dissipation bracket. Alternatively, it can be defined as a state-space formalism using (families of) linear operators. In either case, the "state space" is a smooth manifold which of course includes the case of a linear space.

The literature about GENERIC focuses on distributed parameter systems and in particular (complex) fluids. The following section introduces the GENERIC framework as a state-space formalism. To highlight the central thermodynamic aspects of the GENERIC, the framework is introduced using a simple lumped parameter system as an example. Section 4.2 touches upon the extension of the framework to open thermodynamical systems.

## 4.1 Operator-GENERIC formulation

In the distributed-parameter setting, the state space is infinite-dimensional and consequently various functional-analytical intricacies arise. Unfortunately, no attention is paid to such details in this thesis. More information can be found in the preprint [43] which also coined the term "Operator-GENERIC formulation". Here, a finite-dimensional setting is assumed.

Let $\mathscr{X} \ni x$ be the smooth state manifold of an isolated thermodynamical system.

The GENERIC can be written as

$$\dot{x} = \underbrace{J(x)\big[\mathrm{d}E(x)\big]}_{\dot{x}_{\mathrm{rev}}} + \underbrace{R(x)\big[\mathrm{d}S(x)\big]}_{\dot{x}_{\mathrm{irr}}} . \tag{4.2}$$

The time evolution $\dot{x} \in T\mathscr{X}$ is the sum of the reversible contribution $\dot{x}_{\mathrm{rev}} \in T\mathscr{X}$ and the irrevesible contribution $\dot{x}_{\mathrm{irr}} \in T\mathscr{X}$. Further, $E \in C^\infty(\mathscr{X})$ is the energy function expressing the total energy in the system and $S \in C^\infty(\mathscr{X})$ is the entropy function expressing the total entropy in the system. The families of linear maps

$$\begin{aligned} J :\ \mathscr{X} &\to \mathrm{Hom}(T_x^*\mathscr{X},\, T_x\mathscr{X}) \\ x &\mapsto J(x) \end{aligned}$$

$$\text{and} \quad \begin{aligned} R :\ \mathscr{X} &\to \mathrm{Hom}(T_x^*\mathscr{X},\, T_x\mathscr{X}) \\ x &\mapsto R(x) \end{aligned}$$

have to satisfy certain conditions which give physical meaning to Eq. (4.2).

For any fixed $x \in \mathscr{X}$, the Poisson operator $J(x) : T_x^*\mathscr{X} \xrightarrow{\sim} T_x\mathscr{X}$ maps the differential of the total energy $\mathrm{d}E(x) \in T_x^*\mathscr{X}$ to the reversible contribution $\dot{x}_{\mathrm{rev}} \in T_x\mathscr{X}$. This operator is skew-symmetric, i.e.

$$\forall x \in \mathscr{X} \ :\ \forall \alpha \in T_x^*\mathscr{X} \ :\ J(x)\big[\alpha\big] + J^{\mathrm{T}}(x)\big[\alpha\big] = 0 \in T_x\mathscr{X} . \tag{4.3}$$

Similarly, for any fixed $x \in \mathscr{X}$, the dissipation operator $R(x) : T_x^*\mathscr{X} \xrightarrow{\sim} T_x\mathscr{X}$ maps the differential of the total entropy $\mathrm{d}S(x) \in T_x^*\mathscr{X}$ to the irreversible contribution

$\dot{x}_{\mathrm{irr}} \in T_x\mathscr{X}$. This operator is symmetric and positive semi-definite, i.e.

$$\forall x \in \mathscr{X} \,:\, \forall \alpha,\, \beta \in T_x^*\mathscr{X} \,:\, \alpha\Big(R(x)\big[\beta\big]\Big) = \alpha\Big(R^{\mathrm{T}}(x)\big[\beta\big]\Big) \equiv \beta\Big(R(x)\big[\alpha\big]\Big) \tag{4.4a}$$

$$\alpha\Big(R(x)\big[\alpha\big]\Big) \geq 0\,. \tag{4.4b}$$

It can be said that the energy function 'generates' the Hamiltonian dynamics and that the entropy function generates the irreverisble dynamics. Since the dissipation operator is positive semi-definite, irreversible contributions lead to an increase in entropy. The irreversible contribution is sometimes called a 'gradient system'.

The following two conditions express the thermodynamical nature of the reversible and the irreversible contributions:

1. Any reversible contribution $\dot{\tilde{x}}_{\mathrm{rev}}$ (generated by some energy function $\tilde{E}$) has to leave the total entropy $S$ invariant. This yields to the following *degeneracy condition* for the Poisson operator:

$$\forall\, \tilde{E} \in C^\infty(\mathscr{X}) \,:\, \forall\, x \in \mathscr{X} \,:\, \mathrm{d}S(x)\Big(\dot{\tilde{x}}_{\mathrm{rev}}\Big) = \mathrm{d}S(x)\Big(J(x)\big[\mathrm{d}\tilde{E}(x)\big]\Big) \overset{!}{=} 0 \tag{4.5}$$

Since

$$\mathrm{d}S(x)\Big(J(x)\big[\mathrm{d}\tilde{E}(x)\big]\Big) = \mathrm{d}\tilde{E}(x)\Big(J^{\mathrm{T}}(x)\big[\mathrm{d}S(x)\big]\Big) \overset{(4.3)}{=} -\mathrm{d}\tilde{E}(x)\Big(J(x)\big[\mathrm{d}S(x)\big]\Big)\,,$$

it holds that for all $x \in \mathscr{X}$, the linear operator $J(x)$ must be defined in a way such that the differential of $S$ at $x$ lies in its kernel.

2. Any irreversible contribution $\dot{\tilde{x}}_{\mathrm{irr}}$ (generated by some entropy function $\tilde{S}$) has to leave the total energy $E$ invariant. This yields to the following degeneracy condition for the dissipation operator:

$$\forall\, \tilde{S} \in C^\infty(\mathscr{X}) \,:\, \forall\, x \in \mathscr{X} \,:\, \mathrm{d}E(x)\Big(\dot{\tilde{x}}_{\mathrm{irr}}\Big) = \mathrm{d}E(x)\Big(R(x)\big[\mathrm{d}\tilde{S}(x)\big]\Big) \overset{!}{=} 0 \tag{4.6}$$

Since

$$\mathrm{d}E(x)\Big(R(x)\big[\mathrm{d}\tilde{S}(x)\big]\Big) = \mathrm{d}\tilde{S}(x)\Big(R^{\mathrm{T}}(x)\big[\mathrm{d}E(x)\big]\Big) \overset{(4.4a)}{=} \mathrm{d}\tilde{S}(x)\Big(R(x)\big[\mathrm{d}E(x)\big]\Big)\,,$$

it holds that for all $x \in \mathscr{X}$, the linear operator $R(x)$ must be defined in way such that the differential of $E$ at $x$ lies in its kernel.

The GENERIC (4.2) and the conditions given in Eqs. (4.3), (4.4a), (4.4b), (4.5) and (4.6) together imply the following balance equations for $E$ and $S$:

The total energy $E$ of an isolated system is conserved:

$$\begin{aligned}\frac{\mathrm{d}E}{\mathrm{d}t} = \mathrm{d}E(x)\big(\dot{x}\big) &= \mathrm{d}E(x)\Big(J(x)\big[\mathrm{d}E(x)\big]\Big) + \mathrm{d}E(x)\Big(R(x)\big[\mathrm{d}S(x)\big]\Big) \\ &= \underbrace{-\mathrm{d}E(x)\Big(J(x)\big[\mathrm{d}E(x)\big]\Big)}_{=0} + \mathrm{d}S(x)\Big(\underbrace{R(x)\big[\mathrm{d}E(x)\big]}_{=0}\Big) = 0 \end{aligned} \tag{4.7}$$

The total entropy $S$ of an isolated system is non-decreasing over time:

$$\begin{aligned}\frac{\mathrm{d}S}{\mathrm{d}t} = \mathrm{d}S(x)\big(\dot{x}\big) &= \mathrm{d}S(x)\Big(J(x)\big[\mathrm{d}E(x)\big]\Big) + \mathrm{d}S(x)\Big(R(x)\big[\mathrm{d}S(x)\big]\Big) \\ &= -\mathrm{d}E(x)\Big(\underbrace{J(x)\big[\mathrm{d}S(x)\big]}_{=0}\Big) + \underbrace{\mathrm{d}S(x)\Big(R(x)\big[\mathrm{d}S(x)\big]\Big)}_{\geq 0} \geq 0 \end{aligned} \tag{4.8}$$

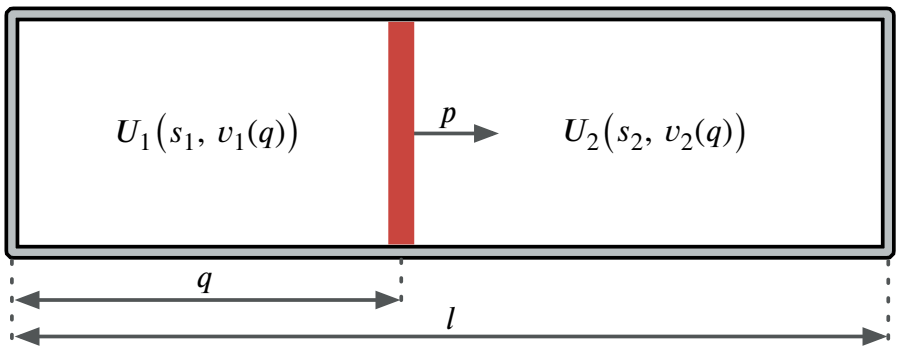



Fig. 4.1 A heat-conducting piston moving inside an isolated cyclinder.

**Example 4.1** (heat conduction through a moving piston)**.**
Figure 4.1 shows a piston inside an adiabatically isolated cylinder of length $l$ and cross-sectional area $A$. The piston has mass $m$, wall thickness $w$, heat conductivity $\kappa$ and linear momentum $p$. Its cross-sectional area is also assumed to be $A$. The volumes $v_1$ and $v_2$ at each side of the piston are filled with an ideal gas of fixed mass $m_1$ and $m_2$, respectively. At all times, the gas within each volume is assumed to be at equilibrium.

It is assumed that the model comprises only three storage components, namely the two lumped volumes filled with an ideal gas which has only internal energy and a piston which seperates the two volumes and stores only kinetic energy. To keep the

example simple, the kinetic energy of the gas as well as the internal energy of the piston and the cylinder wall are neglected.

The volumes $v_1$ and $v_2$ of the compartments can be expressed as a function of the cylinder's position $q$, i.e.

$$\begin{aligned} v_1(q) &= \left(q - \frac{w}{2}\right) A \\ v_2(q) &= \left(l - \frac{w}{2} - q\right) A \,. \end{aligned}$$

The entropies $s_1$ and $s_2$ are the thermal state variables for the two compartments. The macroscopic state of the system can thus be expressed by

$$x = \begin{bmatrix} q & p & s_1 & s_2 \end{bmatrix}^{\mathrm{T}} \in \mathcal{X} \subset \mathbb{R}^4 \,.$$

The enery function is

$$E(x) = \frac{1}{2}\, p\, \frac{1}{m}\, p + U_1\big(s_1,\, v_1(q)\big) + U_2\big(s_2,\, v_2(q)\big) \tag{4.9}$$

where the thermodynamic potentials $U_1$ and $U_2$ are given according to Eq. (B.3) with the fixed masses $m_1$ and $m_2$ taken into account. The differential of $E$ (expressed in matrix notation) is

$$\begin{aligned} \frac{\partial E}{\partial x}(x) &= \begin{bmatrix} \frac{\partial U_1}{\partial v_1}(x)\, \frac{\partial v_1}{\partial q} + \frac{\partial U_2}{\partial v_2}(x)\, \frac{\partial v_2}{\partial q} & \frac{1}{m}\, p & \frac{\partial U_1}{\partial s_1}(x) & \frac{\partial U_2}{\partial s_2}(x) \end{bmatrix}^{\mathrm{T}} \\ &= \begin{bmatrix} \Big(-\pi_1\big(s_1,\, v_1(q)\big) + \pi_2\big(s_2,\, v_2(q)\big)\Big) A & v(p) & \theta_1\big(s_1,\, v_1(q)\big) & \theta_2\big(s_2,\, v_2(q)\big) \end{bmatrix}^{\mathrm{T}} . \end{aligned} \tag{4.10}$$

Here, the functions $\pi_1$ and $\pi_2$ yield the (equilibrium) pressure and the functions $\theta_1$ and $\theta_2$ yield the (equilibrium) temperature of the gas inside the two compartments, see Eqs. (B.4a) and (B.4b).

The entropy function is

$$S(x) = s_1 + s_2 \tag{4.11}$$

and its differential (expressed in matrix notation) is

$$\frac{\partial S}{\partial x} = \begin{bmatrix} 0 & 0 & 1 & 1 \end{bmatrix}^{\mathrm{T}} . \tag{4.12}$$

The dynamics of the system can then be expressed in the form of Eq. (4.2) as

$$\underbrace{\begin{bmatrix}\dot{q}\\ \dot{p}\\ \dot{s}_1\\ \dot{s}_2\end{bmatrix}}_{\dot{x}} = \underbrace{\begin{bmatrix}0 & 1 & 0 & 0\\ -1 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\end{bmatrix}}_{J} \underbrace{\begin{bmatrix}\left(\pi_2(x)-\pi_1(x)\right) A\\ v(x)\\ \theta_1(x)\\ \theta_2(x)\end{bmatrix}}_{\frac{\partial E}{\partial x}(x)} + \underbrace{\begin{bmatrix}0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & \alpha\frac{\theta_2(x)}{\theta_1(x)} & -\alpha\\ 0 & 0 & -\alpha & \alpha\frac{\theta_1(x)}{\theta_2(x)}\end{bmatrix}}_{R(x)} \underbrace{\begin{bmatrix}0\\0\\1\\1\end{bmatrix}}_{\frac{\partial S}{\partial x}} \tag{4.13}$$

where $\alpha = \kappa \frac{A}{w}$ is a heat transfer coefficient.

In the above model, the heat transfer between the two compartments is the only irreversible effect. To extend the example, friction between the piston and the cyclinder wall shall be included in the model. This irreversible process converts kinetic energy of the piston into internal energy. Since the model does not consider the internal energy of the piston and the cylinder wall, the simplest way of taking the friction into account is by assuming that it increases the internal energy in each volume by the same amount regardless of the direction in which the piston moves.

The dissipation operator $R(x)$ in Eq. (4.13) models the irreversible heat conduction through the piston and shall be renamed to $R_\alpha(x)$. A further contribution $R_d(x)$ shall model the friction effect and it shall hold that $R(x) = R_\alpha(x) + R_d(x)$. Both contributions must individually satisfy the conditions stated in Eqs. (4.4a), (4.4b) and (4.6).

By assumption, the friction effect leads to a velocity-proportional force on the piston given by $-d\,v$ where $d$ is the friction coefficient. The dissipated power $d\,v^2$ reappears as heat. It is assumed that half of this heat power is entering the first volume and the other half is entering the second volume. The damping force $-d\,v$ determines the third and fourth column of the second row of the operator written in matrix notation. Both entries are the same because it is assumed that the dissipated energy increases the internal energy in each volume by the same ammount. The degeneracy condition then determines the second column of this row. Further, the symmetry condition determines the third and fourth row of the second column. Then the degeneracy condition determines the third and fourth columns of the third and fourth row. This

yields

$$R_d(x) = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} d \left(\theta_1 + \theta_2\right) & -\frac{1}{2} d\, v & -\frac{1}{2} d\, v \\ 0 & -\frac{1}{2} d\, v & \frac{1}{\theta_1} \frac{1}{2} d\, v^2 & 0 \\ 0 & -\frac{1}{2} d\, v & 0 & \frac{1}{\theta_2} \frac{1}{2} d\, v^2 \end{bmatrix}. \tag{4.14}$$

◇

The GENERIC structure can be seen as a guide throughout the modeling process which ensures that the balance equations are formulated in a thermodynamically consistent manner.

## 4.2 Open GENERIC systems

To consider open thermodynamic systems, the GENERIC (4.2) has to be extended by a boundary contribution which is defined by the boundary operator $B(x)$ and the input vector $u_B$:

$$\dot{x} = \underbrace{J(x)\left[\mathrm{d}E(x)\right]}_{\dot{x}_{\mathrm{rev}}} + \underbrace{R(x)\left[\mathrm{d}S(x)\right]}_{\dot{x}_{\mathrm{irr}}} + B(x)\left[u_B\right] \tag{4.15}$$

In [26], it is shown that distributed-parameter GENERIC systems can be considered as open thermodynamic systems by using an approach sharing "the spirit of Stokes-Dirac structures". Stokes-Dirac structures were introduced in [18] to define distributed parameter port-Hamiltonian systems.

# 5

# GENERIC port-Hamiltonian systems

This chapter discusses port-Hamiltonian systems which can directly be related to the GENERIC framework. Other approaches to modeling nonequilibrium thermodynamical systems as (quasi) port-Hamiltonian systems use the total energy as the Hamiltonian function, see Section 1.2.2. This entails the need for a modulating function leading to a quasi-Hamiltonian formulation [34]. In contrast, the class of port-Hamiltonian systems which is introduced in this chapter uses the total exergy as the Hamiltonian function. In Remark 3.12 it has been argued that the Hamiltonian function of systems which neglect thermal dynamics (isothermal systems) is indeed an exergy function. Hence, it can be said that the approach to modeling thermodynamical systems taken in this chapter fits well to the established theory of isothermal port-Hamiltonian systems. This chapter is inspired by the preprint [42].

The dynamics of a GENERIC system are generated by its energy function $E \in C^\infty(\mathcal{X})$ and its entropy function $S \in C^\infty(\mathcal{X})$. These two functions can be combined into one exergy function

$$H = E - \theta_0 S \in C^\infty(\mathcal{X}). \tag{5.1}$$

where $\theta_0 \in \mathbb{R}^+$ is a constant defining the *reference temperature*, see Eq. (2.7). The choice of a *fixed* reference temperature leads to an exergy function for the system which is considered as a state function. Its differential is

$$\mathrm{d}H(x) = \mathrm{d}E(x) - \theta_0 \,\mathrm{d}S(x).$$

Further, for every $x \in \mathcal{X}$ the dissipation operator $R(x)$ is factorized according to

$$R(x) = \theta_0 \, C(x) \, D(x) \, C^{\mathrm{T}}(x). \tag{5.2}$$

For distributed parameter systems it may be physically meaningful to diagonalize $R(x)$. In this case, $C$ and $C^{\mathrm{T}}$ are spatial differential operators and $D$ contains the

transport coefficients, see [24, p. 67]. For lumped-parameter systems, like the system of Example 4.1, it makes more sense to consider $C$ and $C^{\mathrm{T}}$ as identity operators.

In particular in view of Remark 3.12, the GERNERIC system Eq. (4.15) is closely related to the irreversible port-Hamiltonian system

$$\underbrace{\begin{bmatrix} \dot{x} \\ -y_B \\ -y_R \end{bmatrix}}_{-f} = \underbrace{\begin{bmatrix} J(x) & B(x) & C(x) \\ -B^{\mathrm{T}}(x) & 0 & 0 \\ -C^{\mathrm{T}}(x) & 0 & 0 \end{bmatrix}}_{N(x)} \underbrace{\begin{bmatrix} \mathrm{d}H(x) \\ u_B \\ u_R \end{bmatrix}}_{e}$$

$$u_R = -D(x)\, y_R$$

introduced in Section 3.6 since it holds that

$$\begin{aligned} \dot{x} &= J(x)\big[\mathrm{d}E(x) - \theta_0\, \mathrm{d}S(x)\big] + B(x)\big[u_B\big] + C(x)\big[u_R\big] \\ &= J(x)\big[\mathrm{d}E(x)\big] + B(x)\big[u_B\big] - \big(C(x)\, D(x)\big)\big[y_R\big] \\ &= J(x)\big[\mathrm{d}E(x)\big] + B(x)\big[u_B\big] - \big(C(x)\, D(x)\, C^{\mathrm{T}}(x)\big)\big[\mathrm{d}E(x) - \theta_0\, \mathrm{d}S(x)\big] \\ &= J(x)\big[\mathrm{d}E(x)\big] + B(x)\big[u_B\big] + \big(\theta_0\, C(x)\, D(x)\, C^{\mathrm{T}}(x)\big)\big[\mathrm{d}S(x)\big] \\ &= J(x)\big[\mathrm{d}E(x)\big] + R(x)\big[\mathrm{d}S(x)\big] + B(x)\big[u_B\big]\,. \end{aligned}$$

The family of linear maps $N$ defines a (generalized) Dirac structure. The conditions on $J$ and $R$ which are imposed by the GENERIC framework provide guidance for modeling thermodynamic systems and in particular they ensure that for isolated systems the total energy is conserved and the total entropy is non-decreasing, see Eqs. (4.7) and (4.8). This implies that for an isolated GENERIC port-Hamiltonian system, the total exergy is non-increasing. An open GENERIC port-Hamitonian system with boundary ports defined through the boundary operator $B(x)$ is passive with respect to the output $y_B$, i.e.

$$\frac{\mathrm{d}H}{\mathrm{d}t} \leq \langle u_B \mid y_B \rangle\,. \tag{5.3}$$

Just like Eq. (3.15), this says that

$$\text{stored power} \leq \text{supplied power}$$

but here power clearly means rate of exergy exchange.

Using this approach, it is possible to model irreversible thermodynamical systems as port-Hamiltonian systems in a relatively straightforward way. In particular, it is not necessary to adapt the existing theory. Only the physical meaning of the Hamiltonian function needs to be rethought if the storage of internal energy is taken into account. The exergy concept allows to describe the exchange of heat on an equal footing with the exchange of work by measuring the value of the exchanged heat with respect to a given reference temperature.

Even though the Hamiltonian function, the resulting efforts and the resistive relations all depend on the reference temperature, the predections of the resulting model are independent of the chosen reference temperature.

**Example 5.1** (heat conduction through a moving piston)**.**
This example shows a reformulation of Example 4.1 as a port-Hamiltonian system. According to Eqs. (4.9), (4.11) and (5.1), the Hamiltonian is defined as the exergy function

$$H(x) \;=\; \frac{1}{2}\, p\, \frac{1}{m}\, p \;+\; U_1\big(s_1,\, v_1(q)\big) - \theta_0\, s_1 \;+\; U_2\big(s_2,\, v_2(q)\big) - \theta_0\, s_2$$

where $\theta_0 \in \mathbb{R}^+$ is the reference temperature. The differential of the exergy function (in matrix notation) is

$$\frac{\partial H}{\partial x}(x) \;=\; \begin{bmatrix} \Big(\pi_2\big(s_2,\, v_2(q)\big) \;-\; \pi_1\big(s_1,\, v_1(q)\big)\Big)\, A \\ v(p) \\ \theta_1\big(s_1,\, v_1(q)\big) \;-\; \theta_0 \\ \theta_2\big(s_2,\, v_2(q)\big) \;-\; \theta_0 \end{bmatrix}.$$

The operator $R_\alpha(x)$ is factorized by taking $C$ and $C^{\mathrm{T}}$ to be identity operators and defining $D_\alpha(x) = \frac{1}{\theta_0}\, R_\alpha(x)$. The operator $R_d(x)$ is factorized in the same manner.

This leads to the port-Hamiltonian system

$$\underbrace{\begin{bmatrix} \dot{x} \\ -y_\alpha \\ -y_d \end{bmatrix}}_{-f} = \underbrace{\begin{bmatrix} J & I & I \\ -I & 0 & 0 \\ -I & 0 & 0 \end{bmatrix}}_{N} \underbrace{\begin{bmatrix} \frac{\partial H}{\partial x}(x) \\ u_\alpha \\ u_d \end{bmatrix}}_{e} \tag{5.4a}$$

$$u_\alpha \;=\; -D_\alpha(x)\, y_\alpha \tag{5.4b}$$

$$u_d \;=\; -D_d(x)\, y_d \tag{5.4c}$$

Hence, the reversible contribution to the time evolution is given by

$$\dot{x}_{\mathrm{rev}} = J \frac{\partial H}{\partial x} = \begin{bmatrix} v(p) & \left(\pi_1\left(s_1, v_1(q)\right) - \pi_2\left(s_2, v_2(q)\right)\right) A & 0 & 0 \end{bmatrix}^{\mathrm{T}}$$

and the irreversible contribution is given by $\dot{x}_{\mathrm{irr}} = u_\alpha + u_d$ where

$$u_\alpha = \begin{bmatrix} 0 & 0 & \frac{1}{\theta_1}\alpha\left(\theta_2 - \theta_1\right) & \frac{1}{\theta_2}\alpha\left(\theta_1 - \theta_2\right) \end{bmatrix}^{\mathrm{T}}$$

$$u_d = \begin{bmatrix} 0 & -d\,v & \frac{1}{\theta_1}\frac{d\,v^2}{2} & \frac{1}{\theta_2}\frac{d\,v^2}{2} \end{bmatrix}^{\mathrm{T}}.$$

It is important to note that the reference temperature $\theta_0$ eventually canceled out.

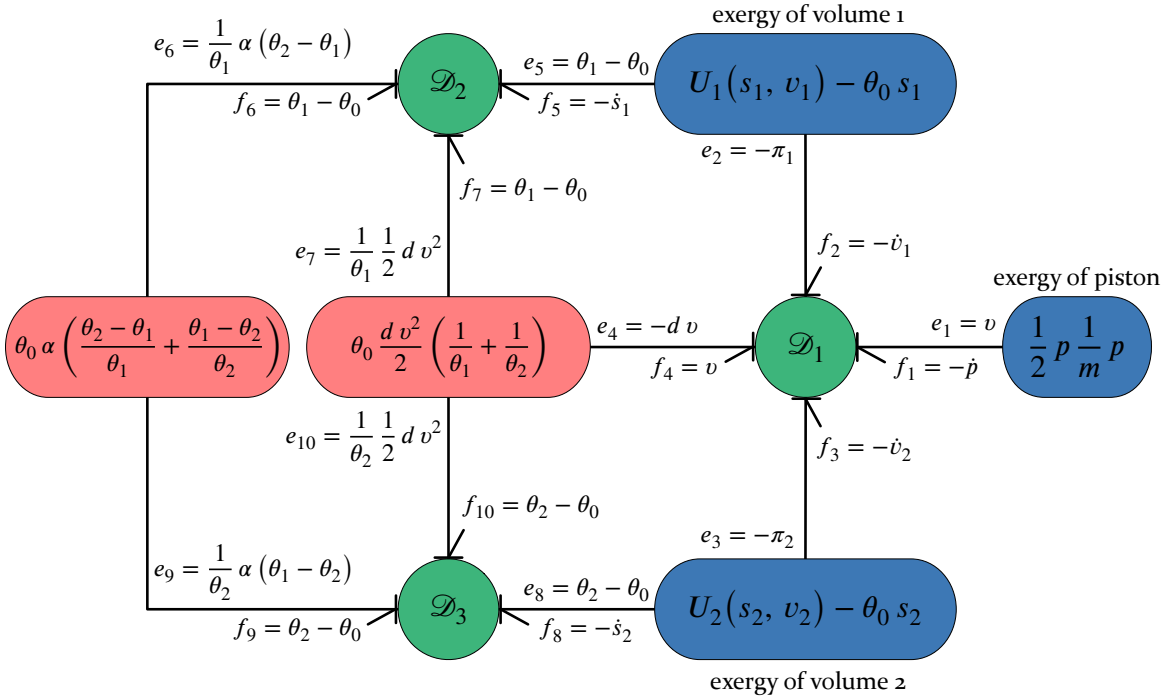



Fig. 5.1 Bond graph representation of a GENERIC port-Hamiltonian system: The exergy storage components are shown in blue. The underlying Dirac structure is represented by the green components. At these green components, the net exergy exchange rate is zero. The red components represent irreversible processes, namely heat conduction and friction. The respective exergy destruction rate is written inside those dissipative components.

The system comprises three interconnected exergy storage components, namely the piston's kinetic energy which is pure exergy and each compartment's exergy which is

less than the internal energy. The gas compartments are two-port components having one port for the exchange of mechanical exergy (i.e. pressure-volume work) and another port for the exchange of thermal exergy (i.e. heat). From this interconnection perspective it is perhaps more natural to express the system state in terms of the five exergy variables

$$x = \begin{bmatrix} p & s_1 & v_1 & s_2 & v_2 \end{bmatrix}^{\mathrm{T}} \in \mathcal{X} \subset \mathbb{R}^5 .$$

The interconnection of the three storage components yields the holonomic constraint

$$v_1 + v_2 = A\,(l - w) \tag{5.5}$$

relating the two state variables $v_1$ and $v_2$. In the previously presented descriptions of this example system, the constraint is eliminated by replacing the two variables $v_1$ and $v_2$ with the single variable $q$. This corresponds to finding coordinates for the four-dimensional constraint manifold itself. Figure 5.1 shows a bond graph representing the model as a GENERIC PHS. The skew-symmetric map

$$\left[\begin{array}{c} -f_1 \\ -f_2 \\ -f_3 \\ -f_4 \\ \hline -f_5 \\ -f_6 \\ -f_7 \\ \hline -f_8 \\ -f_9 \\ -f_{10} \end{array}\right] = \left[\begin{array}{cccc|ccc|ccc} & -A & A & 1 & & & & & \\ A & & & & & & & & \\ -A & & & & & & & & \\ -1 & & & & & & & & \\ \hline & & & & & 1 & 1 & & \\ & & & & -1 & & & & \\ & & & & -1 & & & & \\ \hline & & & & & & & & 1 \quad 1 \\ & & & & & & & -1 & \\ & & & & & & & -1 & \end{array}\right] \left[\begin{array}{c} e_1 \\ e_2 \\ e_3 \\ e_4 \\ \hline e_5 \\ e_6 \\ e_7 \\ \hline e_8 \\ e_9 \\ e_{10} \end{array}\right] \tag{5.6}$$

defines the Dirac structure of this system. Zeros have been omitted for readability. This map has a block-diagonal structure. The first block defines $\mathscr{D}_1$ and expresses the exchange of mechanical exergy between the piston, the two gas compartments and the friction effect. The two remaining blocks define $\mathscr{D}_2$ and $\mathscr{D}_3$. They express the exchange of thermal exergy between the compartments, the heat conduction effect and the friction effect. The flow variables related to the storage port define the time evolution of the system state:

$$-\dot{x} = f_S = \begin{bmatrix} f_1 & f_5 & f_2 & f_8 & f_3 \end{bmatrix}^{\mathrm{T}} . \tag{5.7}$$

Since the system is isolated, all remaining flow variables are associated with the irreversible dynamics modeled by the red components. The component representing the heat conduction effect is defined by

$$e_6 = \frac{1}{\theta_0 + f_6}\,\alpha\left(f_9 - f_6\right) \tag{5.8a}$$

$$e_9 = \frac{1}{\theta_0 + f_9}\,\alpha\left(f_6 - f_9\right)\,. \tag{5.8b}$$

It holds that

$$\langle e_6 \mid f_6\rangle + \langle e_9 \mid f_9\rangle = \underbrace{-\theta_0\,\alpha\left(\frac{\theta_2 - \theta_1}{\theta_1} + \frac{\theta_1 - \theta_2}{\theta_2}\right)}_{\text{exergy destruction rate}} \leq 0\,.$$

The component representing the friction effect is defined by

$$e_4 = -d\,f_4 \tag{5.9a}$$

$$e_7 = \frac{1}{\theta_0 + f_7}\,\frac{1}{2}\,d\,f_4^2 \tag{5.9b}$$

$$e_{10} = \frac{1}{\theta_0 + f_{10}}\,\frac{1}{2}\,d\,f_4^2\,. \tag{5.9c}$$

It holds that

$$\langle e_4 \mid f_4\rangle + \langle e_7 \mid f_7\rangle + \langle e_{10} \mid f_{10}\rangle = \underbrace{-\theta_0\,\frac{d\,v^2}{2}\left(\frac{1}{\theta_1} + \frac{1}{\theta_2}\right)}_{\text{exergy destruction rate}} \leq 0\,.$$

At those dissipative components, the net outflow of exergy is always nonpositive. This nonnegative net inflow is equal to the exergy which is destroyed by the respective irreversible process. The exergy destruction rate may also be called 'dissipated power'. In Fig. 5.1, the rate of exergy destruction associated to a particular irreversible process is written on the corresponding red component.

Equations (5.5) to (5.9) form a system of Differential-Algebraic Equations (DAEs) which can for instance be integrated by a Gauss-Legendre collocation method. By requiring that not only the differential but also the algebraic equations hold at every collocation point, it can be guaranteed that the discrete trajectory remains on the four-dimensional constraint manifold. Simulation results are shown in Fig. 5.2.

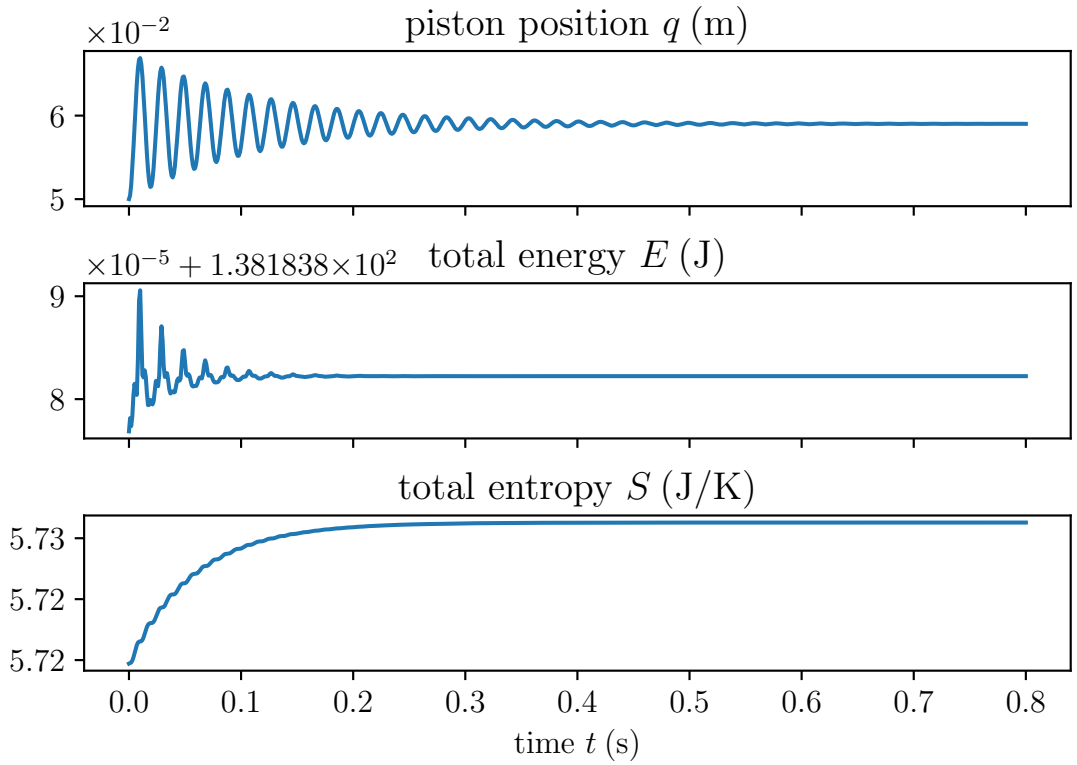



Fig. 5.2 Simulation results for the system shown in Fig. 5.1: Different pressure and temperature values in the two compartments have been set as initial conditions. A transient steers the system into its equilibrium state, thereby maximizing the total entropy. A time step of one millisecond was used which in total corresponds to 800 steps. The fourth-order ($s = 2$) Gauss-Legendre collocation method was used to integrate the DAE system. The total energy $E$ is conserved quite well (with a relative error of $3.9 \times 10^{-8}$) even though the system is highly nonlinear. The constraint equation (5.5) is conserved up to machine precision.

A more realistic model of the physical system would include the exergy associated to the piston's internal energy. This would lead to another term in the Hamiltonian function, namely $U_3(s_3) - \theta_0 s_3$. The modified example is shown as a bond graph in Fig. 5.3.

Unfortunately, no simulation results for this modified case are included in the present thesis since I could not find a suitable expression for the potential $U_3$ which should approximately characterize the constitutive relations of internal energy storage for a solid metal or some other relevant solid material. ◇

**Example 5.2** (Carnot engine)**.**
Figure 5.4 shows a bond graph representation of a hypothetical Carnot engine operating between two isothermal heat reservoirs, see Remark 2.5. The hot reservoir always

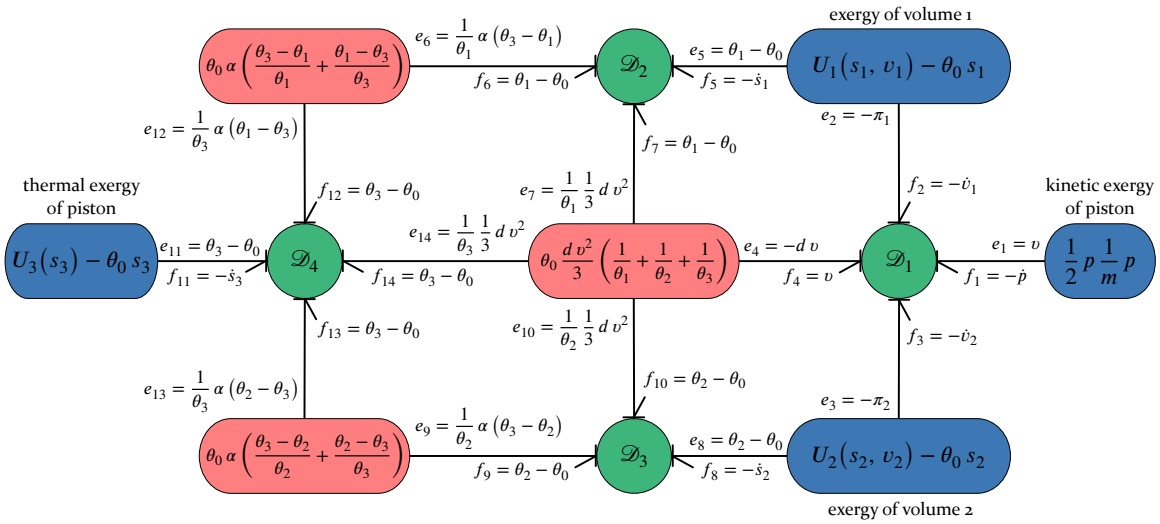



Fig. 5.3 Bond graph representation of the modified example which also includes the storage of thermal exergy inside the piston.

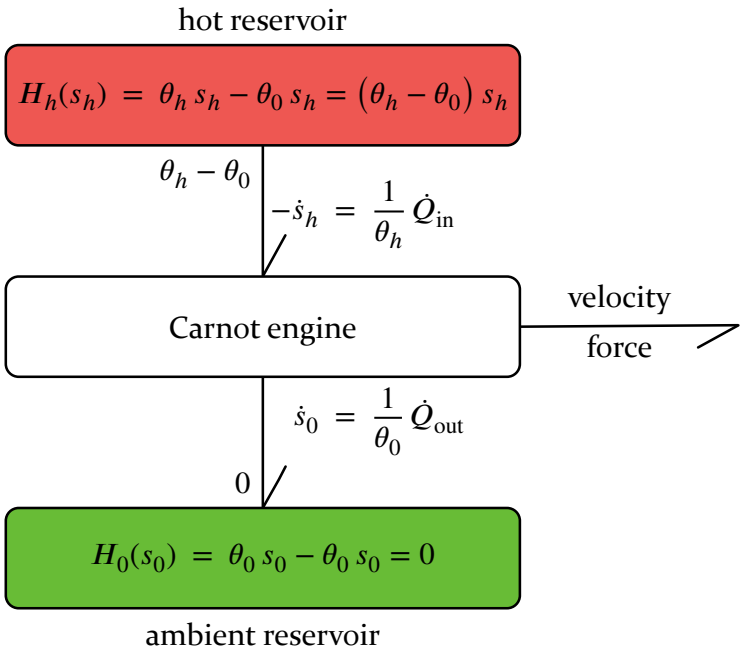



Fig. 5.4 Bond graph representation of a Carnot engine.

stays at the temperature $\theta_h$ and acts like an infinitely large source of entropy. The ambient reservoir always stays at the temperature $\theta_0$ and acts like an infinitely large sink of entropy. The ambient temperature $\theta_0$ is used as the reference temperature of the system which is necessary to define the exergy storage functions $H_h$ and $H_0$. Consequently, the ambient reservoir stores no exergy, i.e. $H_0 = 0$. Further, the pairing

between effort and flow variable for the bond which connects the hot reservoir and the engine is equal to

$$\frac{\partial H_h(s_h)}{\partial s_h}\left(-\dot{s}_h\right) \;=\; \left(\theta_h - \theta_0\right)\frac{1}{\theta_h}\,\dot{Q}_{\text{in}} \;=\; \eta_{\text{Carnot}}\,\dot{Q}_{\text{in}}$$

and hence equal to the exergy provided to the engine per unit of time. The pairing for the bond which connects the engine and the ambient reservoir is equal to zero because the Carnot engine rejects heat at the temperature $\theta_0$. This leads to the effort variable being zero. The entropy flow through this bond is nonzero, though. The work output of the engine is equal to the exergy intake since, due to its reversible nature, no exergy is destroyed within the engine. ◇

# 6

# Conclusion and future directions

## 6.1 Summary and discussion

This thesis is motivated by an urge to learn more about regenerative heat engines and in particular thermoacoustic engines. The motivation is ultimately rooted in the hope that technological advances and entrepreneurial initiative in this field will contribute to mitigate problems related to pollution, scarcity of natural resources and anthropogenic climate change. The future will tell how successful these devices will be in serving humanity in a sustainable way. At the same time, we will have to find out to what extent (optimization- and control-oriented) modeling of these systems will play a role in driving the desired developments.

Fig. 6.1 According to an article which is part of the World Economic Forum Annual meeting 2019 in Davos-Klosters, Switzerland, "Air conditioners alone could account for up to 40% of the world's remaining global carbon budget by 2050." Image by REUTERS/Vivek Prakash.

So far, Stirling-cycle devices such as thermoacoustic engines are usually modeled in the frequency domain based on linear acoustic wave equations which take heat transfer and fluid viscosity into account. This approach is limited to stability analysis based on the assumption of a sinusoidal steady state. In real systems, and in particular when trying to push the frontier towards higher power-density and performance, the dynamics of these devices can become highly nonlinear. Furthermore, transient effects can also play an important role in practice. This poses a demand for nonlinear time-domain models. It is only natural to expect such models to be composable: A complex system is split into subsystems which are interacting with each other. The modeling framework of port-Hamiltonian systems seems to be well suited for this task.

Chapter 2 provides an introduction to some fundamental aspects of thermodynamics. The following chapter first covers the basics for reversible lumped-parameter port-Hamiltonian systems. Then, systems with irreversible dynamics are discussed also from a thermodynamic perspective. This leads to the conclusion that for isothermal systems the physical meaning of the Hamiltonian function is the total exergy, i.e. the maximum amount of work which can theoretically be extracted from the system. Port-Hamiltonian systems are naturally passive because their stucture ensures that no exergy is created. This makes them attractive representations of complex physical systems arising from network modeling and discretization of distributed-parameter systems. The structural properties of port-Hamiltonian systems are not only beneficial for accurate numerical computations but can also help for model generation, model simplification, as well as optimization and control. The graphical modeling language of bond graphs [2] which predates port-Hamiltonian systems theory [8] is used in combination with simple examples to illustrate the main ideas. Chapter 3 also deals with structure-preserving time discretization which is used to present some simulation results.

Chapter 4 introduces the most important aspects of the GENERIC framework [9, 10] which constitutes a geometric approach to modeling nonequilibrium thermodynamic systems. Compared to port-Hamiltonian systems theory, this framework is perhaps less suited for network modeling. The GENERIC framework was discovered while studying the dynamics of complex fluids and therefore the literature is focused predominantly on isolated distributed-parameter systems. Later, an extension to open GENERIC systems has been established in [26] using essentially the same approach that is used for capturing boundary interaction in distributed-parameter port-Hamiltonian systems.

Chapter 5 presents the main contribution of this thesis which is to help clarifying the relationship between the GENERIC framework and port-Hamiltonian sytems theory. This connection has already been discussed in the preprint [42]. The article suggests a straightforward way for representing GENERIC systems as port-Hamiltonian systems. This is achieved by combining the energy and the entropy functions employed by the GENERIC framework into a single exergy function which serves as the Hamiltonian function of the corresponding port-Hamiltonian system. This function characterizes the constitutive nature of the system's storage components. The Dirac structure models the power-conserving interconnection of different aspects of the system. Having the system's total exergy as a Hamiltonian function implies that the meaning of 'power' is 'exergy exchange rate'. The name 'GENERIC port-Hamiltonian systems' is used to refer to port-Hamiltonian systems which use the total exergy as their Hamiltonian function and inherit basic structural properties of the GENERIC framework. In particular, this means that the Dirac structure of a GENERIC port-Hamiltonian system is defined in such a way that the reversible exchange of exergy conserves both energy and entropy and therefore also exergy. In addition, the resistive relations which are part of the definition of a GENERIC port-Hamiltonian system are defined in a way that the irreversible exchange of exergy conserves energy, produces entropy and therefore destroys some of the exchanged exergy. A lumped-parameter GENERIC system which is already introduced as an example in Chapter 4 to illustrate the GENERIC approach is represented as a GENERIC port-Hamiltonian system. Furthermore, it is shown how the graphical modeling language of bond graphs can be adapted to represent GENERIC port-Hamiltonian systems. Simulation results suggest that Gauss-Legendre collocation methods are well suited for the time-integration of nonlinear GENERIC port-Hamiltonian systems. In particular, the total energy is conserved well.

Simulations are carried out using a software implementation which automatically turns the equations describing the port-Hamiltonian system into problem-specific code and executes it. The SymPy library is used to represent equations as Python code and to perform symbolic computations and code generation. The software is available on my personal research website[1] where I also plan to post updates about my future works in this field.

[1] https://MarkusLohmayer.github.io/research

The present work just made a small step towards modeling Stirling-cycle devices as port-Hamiltonian systems. In particular, modeling the Stirling engine shown in Fig. 1.1 as a GENERIC port-Hamiltonian system remains an unreached milestone.

## 6.2 Outlook

Future research will focus on modeling distributed-parameter systems and in particular on modeling a Navier-Stokes-Fourier fluid. Theory concerning this has already been presented in [42, 43].

To model a regenerator component, the heat-exchange between the fluid and the solid material has to be taken into account. Among other things, this requires finding an expression for the internal energy of the solid material as a function of entropy. So far, I have not found such thermodynamic potentials for relevant solid materials and consequently I could not simulate the system shown in Fig. 5.3.

Once the formulation is completely worked out for a simple (one-dimensional) spatial domain, a structure-preserving spatial discretization method, presumably using mixed finite elements, needs to be implemented.

It will also be interesting to see how the bond graph language can be used to represent the interconnection of (distributed-parameter) models and how such representations can be used as input for code generation pipelines.

I hope that this thesis can serve as a stepping stone for future work following this direction. I further hope that I can continue on this path. I also hope to find other people who are interested in this topic. Plese feel free to reach out to me at any time if you are!

# A

# Mathematical background

This appendix shall give a bird's eye view on some mathematical preliminaries. The main goal is to build an intuitive understanding of core concepts in differential geometry. To this end, the exposition shall focus on definitions. Proofs and remarks about mathematical technicalities are entirely omitted.

Section A.6 is included as the last section even though it is not directly relevant for this thesis. This material becomes particularly relevant when discussing distributed parameter systems.

A much more thorough presentation of the material is given in the books [5] and [31]. Together with the "Lectures on the Geometric Anatomy of Theoretical Physics" [1] given by Dr. Frederic Schuller, these two books shall serve as references for this appendix.

## A.1 Groups

Groups are an ubiquitous algebraic structure.

**Definition A.1** (group)**.**
A group $(G, \odot)$ is a set $G$ together with a binary operation

$$\odot : G \times G \to G$$

that satisfies the *group axioms*

(i) *closure*: $\forall\, a, b \in G : a \odot b \in G$

(ii) *associativity*: $\forall\, a, b, c \in G : (a \odot b) \odot c = a \odot (b \odot c)$

(iii) existence of a unique *identity element*: $\exists\, e \in G : \forall\, a \in G : e \odot a = a$

(iv) *inverse elements*: $\forall\, a \in G : \exists\, a^{-1} : a^{-1} \odot a = e$

[1] https://www.video.uni-erlangen.de/course/id/242

△

Axioms (iii) and (iv) talk about a left-identity and left-inverse elements. Additionally or alternatively, existence of a right-identity and right-inverse elements can be demanded.

If a group $(G, \odot)$ further satisfies the *commutativity* property $\forall\, a,\, b \in G :\ a \odot b = b \odot a$ then the group is called an *abelian group*. In this case there is no distinction between left- and right-identity and -inverse elements.

If $+$ denotes the group operation, the inverse element of $a$ is usually denoted by $-a$.

A group homomorphism is a map between two groups that respects the group structure:

**Definition A.2** (group homomorphism)**.**
Let $(G, \cdot)$ and $(H, +)$ be two groups. Then a group homomorphism $h : G \to H$ is a map for which it holds that

$$\forall\, g_1,\, g_2 \in G :\ h(g_1 \cdot g_2) = h(g_1) + h(g_2)\,.$$

△

In particular, a group homomorphism maps the identity element of $G$ (denoted by $1$) to the identity element of $H$ (denoted by $0$), i.e. $h(1) = 0$ and it maps inverse elements to inverse elements, i.e. $\forall\, g \in G :\ h(g^{-1}) = -h(g)$.

**Example A.3** (symmetric group / permutation group)**.**
Let $M$ be a set with cardinality $|M| = n$. Then the symmetric group (or permutation group) over $M$ is the set

$$S_M \ = \ \big\{\pi :\ M \to M \mid \pi \text{ is bijective}\big\}$$

(with cardinality $n!$) together with composition of these bijections as the group operation.

If $M = \{1, \ldots, n\}$ then $S_M$ is also denoted by $S_n$.

A *transposition* is a permutation that swaps exactly two elements. Every permutation $\pi$ can be written as a combination of transpositions. If the number of transpositions is odd then $\operatorname{sgn}(\pi) = -1$ and if it is even then $\operatorname{sgn}(\pi) = +1$. In fact, $\operatorname{sgn} :\ S_M \to \{-1, +1\}$ is a group homeomorphism that maps a permutation group to the group $(\{-1, +1\}, \cdot)$ (with neutral element $+1$). ◇

## A.2 Vector spaces

Since differentiation and integration are built on the concept of infinitesimal quantities, the mathematical description of nonlinear objects and effects can locally still be accomplished using linear spaces and maps between them.

Vector spaces (sometimes also called linear spaces) require another underlying algebraic structure:

**Definition A.4** (field)**.**
An (algebraic) field $(K, +, \cdot)$ is a set $K$ together with two maps

$$\begin{aligned} + &: K \times K \to K \\ \cdot &: K \times K \to K \end{aligned}$$

called addition and multiplication which have the following properties:

(i) $(K, +)$ is an abelian group (with the identity element denoted by 0)

(ii) $(K \setminus \{0\}, \cdot)$ is an abelian group (with the identity element denoted by 1)

(iii) distributivity of $\cdot$ w.r.t. $+$: $\forall\, a, b, c \in K : a \cdot (b + c) = a \cdot b + a \cdot c$

△

The most relevant example here is of course the field of real numbers $(\mathbb{R}, +, \cdot)$.

A vector space is a slightly more complicated algebraic structure:

**Definition A.5** (vector space)**.**
A $K$-vector space $(V, \oplus, \odot)$ over a field $(K, +, \cdot)$ is a set $V$ together with two maps

$$\begin{aligned} \oplus &: V \times V \to V \\ \odot &: K \times V \to V \end{aligned}$$

called vector addition and scalar multiplication that satisfy the following axioms:

(i) $(V, \oplus)$ is an abelian group (where the identity element is called zero vector and the inverse element of $a \in V$ is denoted by $-a$)

(ii) compatibility of scalar multiplication $\odot$ with field multiplication $\cdot$:
$\forall\, k_1, k_2 \in K : \forall\, v \in V : \left(k_1 \cdot k_2\right) \odot v = k_1 \odot \left(k_2 \odot v\right)$

(iii) existence of a multiplicative identity: $\exists\, 1 \in K : \forall\, v \in V : 1 \odot v = v$

(iv) distributivity of $\odot$ with respect to $\oplus$:
$\forall\, k \in K : \forall\, v_1, v_2 \in V : k \odot \left(v_1 \oplus v_2\right) = k \odot v_1 \oplus k \odot v_2$

(v) distributivity of $\odot$ with respect to. $+$:
$\forall\, k_1, k_2 \in K : \forall\, v \in V : \left(k_1 + k_2\right) \odot v = k_1 \odot v \oplus k_2 \odot v$

△

**Definition A.6** (linear map)**.**
Let $(V, \oplus, \odot)$ and $(W, \boxplus, \boxdot)$ be two K-vector spaces. A map $f : V \to W$ is called linear if it has the following properties:

(i) additivity: $\forall\, v_1, v_2 \in V : f(v_1 \oplus v_2) = f(v_1) \boxplus f(v_2)$

(ii) homogeneity (of degree 1): $\forall\, k \in K : \forall\, v \in V : f(k \odot v) = k \boxdot f(v)$

△

In the sequel, the symbol "$\sim$" above the arrow in "$f : V \xrightarrow{\sim} W$" shall indicate the linearity of the map $f$.

The linear maps between two linear spaces form again a linear space:

**Definition A.7** (vector space homomorphisms)**.**
Let $(V, +, \cdot)$ and $(W, \oplus, \odot)$ be two $K$-vector spaces. The set of all linear maps

$$\mathrm{Hom}(V, W) = \left\{ f : V \xrightarrow{\sim} W \right\}$$

together with the operations

$$\begin{aligned} \boxplus : \mathrm{Hom}(V, W) \times \mathrm{Hom}(V, W) &\xrightarrow{\sim} \mathrm{Hom}(V, W) \\ (f, g) &\mapsto f \boxplus g \end{aligned}$$

where

$$\begin{aligned} f \boxplus g : V &\xrightarrow{\sim} W \\ v &\mapsto f(v) \oplus g(v) \end{aligned}$$

and

$$\begin{aligned} \boxdot : K \times \mathrm{Hom}(V, W) &\xrightarrow{\sim} \mathrm{Hom}(V, W) \\ (k, f) &\mapsto k \boxdot f \end{aligned}$$

where

$$\begin{aligned} k \boxdot f : V &\xrightarrow{\sim} W \\ v &\mapsto k \odot f(v) \end{aligned}$$

is a $K$-vector space called the vector space homomorphisms from $V$ to $W$. △

**Definition A.8** (vector space endomorphisms)**.**
The set of all linear maps from a vector space $V$ to itself are called the endomorphisms on $V$:

$$\mathrm{End}(V) \;=\; \mathrm{Hom}(V, V)$$

△

**Definition A.9** (vector space isomorphism)**.**
A bijective linear map is called a vector space isomorphism. △

The vector space isomorphisms are the bijective homomorphisms and the structure-preserving maps between vector spaces, i.e. they preserve the vector space structure. Two $K$-vector spaces $V$ and $W$ are called isomorphic if there exists a vector space isomorphism between them. This is denoted by $V \cong_{\mathrm{vec}} W$.

The dual space of a $K$-vector space $V$ is the $K$-vector space containing all $K$-valued linear maps on $V$:

**Definition A.10** (dual vector space)**.**
The field $(K, +, \cdot)$ can itself be considered as a $K$-vector space. Then

$$V^* \;=\; \mathrm{Hom}(V, K)\,,$$

i.e. the vector space of all linear functionals on $V$, is called the dual vector space of $V$.
△

Elements of the dual space are often called *covectors*.

**Definition A.11** (dual basis)**.**
Let $V$ be a $n$-dimensional vector space with ordered basis $\{e_1, \ldots, e_n\}$. Then there exists a unique ordered basis $\{e^1, \ldots, e^n\}$ of the dual space $V^*$ called the *dual basis* such that

$$\forall\, i, j \in \{1, \ldots, n\} \;:\; e^j(e_i) \;=\; \delta_i^j$$

where $\delta_i^j = 1$ if $i = j$ and $\delta_i^j = 0$ if $i \neq j$ (Kronecker delta). △

For finite-dimensional spaces it follows that $\dim(V) = \dim(V^*)$ and $V \cong_{\text{vec}} V^*$.

**Definition A.12** (orientation)**.**
Let $V$ be a $n$-dimensional vector space. Let $e = \{e_1, \ldots, e_n\}$ and $f = \{f_1, \ldots, f_n\}$ be two ordered bases of $V$. Then there exists a unique endomorphism $A : V \xrightarrow{\sim} V$ for which it holds that $\forall\, i \in \{1, \ldots, n\} : A(e_i) = f_i$.

The bases $e$ and $f$ are said to have the same orientation if $\det(A) > 0$. Otherwise they are said to have opposite orientations. Hence, there are two equivalence classes of bases.

An *orientation* on $V$ is the (arbitrary) assignment of $+1$ to one class and $-1$ to the other. △

## A.3 Tensors

Tensors are multi-linear maps related to a vector space and its dual space.

In differential geometry, this vector space is usually a tangent space on a manifold, see Section A.5.3. This and the fact that the definition of a tensor does not ask for a choice of basis makes a tensor a (coordinate-free) geometric object. In this sense, tensors are much more than merely multidimensional arrays.

**Definition A.13** (tensor)**.**
Let $V$ be a $K$-vector space and let $V^*$ denote its dual space. Then a $(p, q)$-tensor $t$ on $V$ (*contravariant* of order $p$ and *covariant* of order $q$) is a multilinear map

$$t : \underbrace{V^* \times \cdots \times V^*}_{p \text{ copies}} \times \underbrace{V \times \cdots \times V}_{q \text{ copies}} \xrightarrow{\sim} K$$

△

A map is called multilinear if it is linear in each argument separately (with the other arguments held constant).

The set of all $(p, q)$-tensors can be understood as a vector space:

**Definition A.14** (tensor space)**.**
Let $V$ be a vector space over a field $(K, +, \cdot)$ and let $V^*$ be its dual space. Then the set

$$\begin{aligned} T_q^p(V) &\equiv \underbrace{V \otimes \cdots \otimes V}_{p \text{ copies}} \otimes \underbrace{V^* \otimes \cdots \otimes V^*}_{q \text{ copies}} \qquad \text{(only notation)} \\ &= \left\{ t : \underbrace{V^* \times \cdots \times V^*}_{p \text{ copies}} \times \underbrace{V \times \cdots \times V}_{q \text{ copies}} \xrightarrow{\sim} K \right\} \end{aligned}$$

equipped with the maps

$$\begin{aligned} \oplus : T_q^p(V) \times T_q^p(V) &\xrightarrow{\sim} T_q^p(V) \\ (t_1, t_2) &\mapsto t_1 \oplus t_2 \end{aligned}$$

where

$$(t_1 \oplus t_2)(\alpha_1, \ldots, \alpha_p, v_1, \ldots, v_q) = t_1(\alpha_1, \ldots, \alpha_p, v_1, \ldots, v_q) + t_2(\alpha_1, \ldots, \alpha_p, v_1, \ldots, v_q)$$

and

$$\begin{aligned} \odot : K \times T_q^p(V) &\xrightarrow{\sim} T_q^p(V) \\ (k, t) &\mapsto k \odot t \end{aligned}$$

where

$$(k \odot t)(\alpha_1, \ldots, \alpha_p, v_1, \ldots, v_q) = k \cdot t(\alpha_1, \ldots, \alpha_p, v_1, \ldots, v_q)$$

forms a $K$-vector space called the $(p, q)$-tensor space on $V$. △

**Example A.15** (two tensor spaces)**.**

1. $T_1^0(V) \equiv V^* = \left\{ t : V \xrightarrow{\sim} K \right\} = \mathrm{Hom}(V, K)$ is the dual space of $V$.
2. The space of $(1,1)$-tensors on $V$ is isomorphic to the endomorphisms on $V^*$, i.e.

$$T_1^1(V) \equiv V \otimes V^* = \left\{ t : V^* \times V \xrightarrow{\sim} K \right\} \cong_{\mathrm{vec}} \mathrm{End}(V^*) .$$

| | components | basis |
|---|---|---|
| contravariant (vectors) | up | down |
| covariant (covectors) | down | up |

Table A.1 placement of indices according to Einstein's notation

The isomorphism is given by:

$$\begin{aligned} T^1_1(V) &\xrightarrow{\sim} \mathrm{End}(V^*) & \mathrm{End}(V^*) &\xrightarrow{\sim} T^1_1(V) \\ t &\mapsto m & m &\mapsto t \end{aligned}$$

where

$$\begin{aligned} m :\ V^* &\xrightarrow{\sim} V^* & t :\ V^* \times V &\xrightarrow{\sim} K \\ \alpha &\mapsto t(\alpha, \bullet) & (\alpha, v) &\mapsto m(\alpha)(v) \end{aligned}$$

◇

**Definition A.16** (tensor product)**.**
Let $t_1 \in T^{p_1}_{q_1}(V)$ and $t_2 \in T^{p_2}_{q_2}(V)$.

Then the tensor product $t_1 \otimes t_2 \in T^{p_1+p_2}_{q_1+q_2}(V)$ is defined as

$$\begin{aligned} &(t_1 \otimes t_2)(\alpha_1, \ldots, \alpha_{p_1}, \alpha_{p_1+1}, \ldots, \alpha_{p_1+p_2}, v_1, \ldots, v_{q_1}, v_{q_1+1}, \ldots, v_{q_1+q_2}) \\ &\qquad = t_1(\alpha_1, \ldots, \alpha_{p_1}, v_1, \ldots, v_{q_1}) \cdot t_2(\alpha_{p_1+1}, \ldots, \alpha_{p_1+p_2}, v_{q_1+1}, \ldots, v_{q_1+q_2}) \end{aligned}$$

△

The multiplication operation $\cdot$ above is the field multiplication, i.e. the $\cdot$ in $(K, +, \cdot)$.

**Remark A.17** (Einstein's notation)**.**
Indices are placed either up or down according to the type of quantity, cf. Table A.1.

Einstein's summation convention mandates that the sum symbol is omitted for sums over an index that appears twice (once as subscript and once as superscript) within a term. △

## A.4 Topological spaces

A set can be equipped with a structure called topology turning the set into a so-called topological space. This makes it possible to speak about neighborhoods of points and to define what it means for a function to be continuous.

A topology $\mathcal{O}$ on a set $M$ declares which subsets of $M$ are the so-called open sets. Any topology must contain the empty set and the entire set. It must further hold that finite intersections and arbitrary unions of open sets are again open sets.

The power set $\mathcal{P}(M)$ is the set of all possible subsets of $M$ (including the empty set $\varnothing$ and the entire set $M$ itself).

**Definition A.18** (topology and topological space)**.**
Let $M$ be some set. Then a choice $\mathcal{O} \subseteq \mathcal{P}(M)$ is called a topology on $M$ if

(i) $\varnothing \in \mathcal{O}$ and $M \in \mathcal{O}$

(ii) $U, V \in \mathcal{O} \Rightarrow (U \cap V) \in \mathcal{O}$

(iii) $S \subseteq \mathcal{O} \Rightarrow \left(\bigcup S\right) \in \mathcal{O}$

The pair $(M, \mathcal{O})$ is called a topological space. △

The standard topology on $\mathbb{R}^n$ is induced by the Euclidian metric of the space. It is *generated* by the open balls (with non-zero radius). This means that any open set (in the standard topology) can be represented as the union of a (possibly infinite) set of open balls.

**Theorem A.19** (subspace topology)**.**
Let $(M, \mathcal{O})$ be a topological space. Let $N \subseteq M$. Then

$$\mathcal{O}\Big|_N = \{U \cap N \mid U \in \mathcal{O}\} \subseteq \mathcal{P}(N)$$

is a (natural) topology on $N$ called the subspace topology (induced from the topology on $M$). △

A topology is the minimal structure that needs to be defined on a set to establish the notion of continuity:

**Definition A.20** (continuous map)**.**
Let $\left(M, \mathcal{O}_M\right)$ and $\left(N, \mathcal{O}_N\right)$ be two topological spaces. Let $\phi\colon M \to N$ be a map.

Then $\phi$ is called continuous if

$$\forall\, B \in \mathcal{O}_N : \ \mathrm{preim}_\phi(B) \in \mathcal{O}_M \,.$$

△

Hence, a map $\phi : M \to N$ is continuous if the preimage

$$\mathrm{preim}_\phi(B) \ = \ \{m \in M \mid \phi(m) \in B\}$$

of any open set $B \in \mathcal{O}_N$ is open (with respect to $\mathcal{O}_M$).

**Definition A.21** (homeomorphism)**.**
Let $\left(M, \mathcal{O}_M\right)$ and $\left(N, \mathcal{O}_N\right)$ be two topological spaces. Let $\phi : M \to N$ be a bijection. Then $\phi$ is called a homeomorphism if $\phi : M \to N$ and $\phi^{-1} : N \to M$ are continuous.

△

Homeomorphisms are the structure-preserving maps between topological spaces, because they preserve topological properties. In particular, if $\phi : M \to N$ is a homeomorphism it holds that $U \in \mathcal{O}_M$ is a neighborhood of $p \in M$ if and only if $\phi(U) \in \mathcal{O}_N$ is a neighborhood of $\phi(p) \in N$. Two topological spaces $\left(M, \mathcal{O}_M\right)$ and $\left(N, \mathcal{O}_N\right)$ are called homeomorphic if there exists a homeomorphism between them. This is denoted by $M \cong_{\mathrm{hom}} N$ or more precisely $\left(M, \mathcal{O}_M\right) \cong_{\mathrm{hom}} \left(N, \mathcal{O}_N\right)$.

## A.5 Manifolds

A Manifold is a special kind of topological space: Every point of a $n$-manifold has a neighborhood that is homeomorphic to the Euclidean space of dimension $n$. For example, a sphere is a two-dimensional manifold because locally it looks like $\mathbb{R}^2$ but globally it is certainly not a linear space.

### A.5.1 Topological manifolds

Topological manifolds are the simplest kind of manifolds.

**Definition A.22** (topological manifold)**.**
A paracompact Hausdorff topological space $(M, \mathcal{O})$ is called a $n$-dimensional topolog-

ical real manifold if

$$\forall\, p \in M :\ \left(\exists\, U \in \mathcal{O} \text{ with } U \ni p \text{ and } \exists \text{ homeomorphism } x :\ U \to x(U) \subseteq \mathbb{R}^n\right)$$

△

**Definition A.23** (submanifold)**.**
Let $(M,\ \mathcal{O})$ be a topological manifold. Let $N \subseteq M$. Then $\left(N,\ \mathcal{O}\big|_N\right)$ is called a submanifold of $(M,\ \mathcal{O})$ if it is a manifold in its own right. △

**Definition A.24** (bundle)**.**
A bundle is a triple $(E,\ \pi,\ M)$ (also denoted by $E \xrightarrow{\pi} M$) where $E$ is a topological manifold called the *total space* and $M$ is also a topological manifold called the *base space*. The *projection* $\pi :\ E \to M$ is a surjective continuous map. For any $p \in M$ the set $E_p = \text{preim}_\pi\left(\{p\}\right)$ is called the *fiber* over $p$. △

A vector-bundle $E \xrightarrow{\pi} M$ is a special kind of bundle: For any two points on the base space $M$, the corresponding fibers are isomorphic vector spaces. It can be imagined that there is a vector space "attached" to every point on the base space. The tangent bundle (cf. Section A.5.4) is an important example of a vector bundle.

**Definition A.25** (section)**.**
Let $E \xrightarrow{\pi} M$ be a bundle. Then a map $\sigma :\ M \to E$ is called a section of the bundle if $\pi \circ \sigma = id_M$. △

A section $\sigma$ of a bundle $E \xrightarrow{\pi} M$ maps every point $p \in M$ to a point $\sigma(p) \in E_p$.

If the bundle $E \xrightarrow{\pi} M$ is a vector bundle, then a section $\sigma$ maps every point $p \in M$ to a vector $\sigma(p)$ in the vector space $E_p$.

Manifolds are geometric objects which can be defined independently from a certain choice of coordinates. In fact, many different coordinate systems can coexist on one manifold. A chart defines a local coordinate system for some part of a manifold:

**Definition A.26** (chart)**.**
Let $(M,\ \mathcal{O})$ be a $n$-dimensional topological manifold. Then a pair $(U,\ x)$ of an open set $U \in \mathcal{O}$ and a homeomorphism $x :\ U \to x(U) \subseteq \mathbb{R}^n$ is called a chart of the manifold.

The component functions $x^i :\ U \to \mathbb{R},\ p \mapsto \text{proj}_i\left(x(p)\right)$ are called the coordinates of the point $p \in U$ with respect to the chart $(U,\ x)$. △

A transition maps formalizes the idea of "patching together" two charts:

**Definition A.27** ($C^0$-compatibility of charts and transition maps)**.**
Two charts $(U,\ x)$ and $(V,\ y)$ are called $C^0$-compatible if *either*

(i) $U \cap V = \varnothing$

(ii) $U \cap V \neq \varnothing$ and $y \circ x^{-1}$ is continuous

The map $y \circ x^{-1}$ is called a coordinate change map or a transition map. △

Any two charts of a topological manifold are by definition $C^0$-compatible because composition of homeomorphisms yields a homeomorphism.

**Remark.**
From this it also follows that for example a curve $\gamma : \mathbb{R} \supseteq \mathbb{I} \to M$ on a manifold $M$ is continuous at a point $p \in M$ iff. for some chart $(U,\ x)$ with $U \ni p$ it holds that $x \circ \gamma$ is continuous as a map from $\mathbb{R} \supseteq \mathbb{I} \supseteq \mathrm{preim}_\gamma(U) \to x(U) \subseteq \mathbb{R}^{\dim(M)}$. △

An atlas is a collection of charts covering the entire manifold:

**Definition A.28** (atlas)**.**
A set $\mathscr{A}$ of charts such that

$$\bigcup_{(U,x)\in\mathscr{A}} U \;=\; M$$

is called an atlas of the manifold. △

**Definition A.29** ($C^0$-atlas)**.**
An atlas whose charts are pairwise $C^0$-compatible is called a $C^0$-atlas. △

Again by definition, every atlas is a $C^0$-atlas.

**Definition A.30** (maximal $C^0$-atlas)**.**
A $C^0$-atlas $\mathscr{A}$ is called maximal if any chart $(U,\ x)$ which is $C^0$-compatible with any chart $(V,\ y) \in \mathscr{A}$ is already contained in $\mathscr{A}$. △

### A.5.2 Differentiable manifolds

Admittedly, definitions A.27 and A.29 are not too meaningful as such. But if we change definitions A.27, A.29 and A.30 slightly by demanding that the transition maps $y \circ x^{-1}$ between pairs of overlapping charts are not only continuous but $k$ times or infinitely

often differentiable, we obtain definitions for $C^k$- and $C^\infty$-compatibility of charts and consequently also definitions for a (maximal) $C^k$- and $C^\infty$-atlas. This way, differential calculus can be "lifted" from $\mathbb{R}^{\dim(M)}$ (i.e. from the chart level) to a manifold $M$.

**Definition A.31** ($C^k$-manifold)**.**
If $(M, \mathcal{O})$ is a topological manifold and $\mathcal{A}$ is a maximal $C^k$-atlas then $(M, \mathcal{O}, \mathcal{A})$ is a $C^k$-manifold. △

**Remark A.32** (smooth manifold)**.**
A result obtained by Whitney in 1936 shows that any maximal $C^k$-atlas ($k \geq 1$) contains a $C^\infty$-atlas and therefore can be uniquely turned into a $C^\infty$-atlas by removing charts. In this sense, it is not necessary to distinguish between differentiable manifolds and smooth manifolds. △

**Remark A.33** (oriented manifold)**.**
A differentiable manifold is called *orientable* if the determinant of the Jacobian matrix of any chart transition map is always positive. The choice of a maximal atlas with this property is called an *orientation*. △

The *differentiability* of a map between manifolds is defined on the chart level but the definition is independent of the choice of a particular chart:

**Definition A.34** ($C^k$-map)**.**
Let $\left(M, \mathcal{O}_M, \mathcal{A}_M\right)$ and $\left(N, \mathcal{O}_N, \mathcal{A}_N\right)$ be two $C^k$-manifolds and let $\phi : M \to N$ be a map between them. Then $\phi$ is called $k$ times differentiable at $p \in M$ if, for some $(U, x) \in \mathcal{A}_M$ with $U \ni p$ and some some $(V, y) \in \mathcal{A}_N$ with $V \ni \phi(p)$, the map $y \circ \phi \circ x^{-1}$ is $k$ times differentiable as a map from $x(U) \to y(V)$, see Fig. A.1. △

This definition rests on the fact that the composition of $C^k$-maps yields a $C^k$-map.

$$\begin{array}{ccc} M \supseteq U & \xrightarrow{\quad\phi\quad} & V \subseteq N \\ \downarrow x & & \downarrow y \\ \mathbb{R}^{\dim(M)} \supseteq x(U) & \xrightarrow{\; y \circ \phi \circ x^{-1} \;} & y(V) \subseteq \mathbb{R}^{\dim(N)} \end{array}$$

Fig. A.1 A differentiable map between manifolds is defined by "lifting" the concept of differentiability from the chart representation to the manifold.

**Remark A.35** (differentiable real-valued function)**.**
Definition A.34 also includes the case of a differentiable function $f : M \to \mathbb{R}$: If

$N = \mathbb{R}^1$ then $y$ is just the identity map on $\mathbb{R}^1$ and hence $f$ is $k$ times differentiable at a point $p \in M$ if for any chart $(U, x) \in \mathscr{A}_M$ with $U \ni p$ it holds that $f \circ x^{-1} : \mathbb{R}^{\dim(M)} \supseteq x(U) \to \mathbb{R}$ is $k$ times differentiable at the point $x(p)$. △

**Definition A.36** ($C^k$-diffeomorphism)**.**
If a map between two $C^k$-manifolds $\phi : M \to N$ is bijective and both $\phi$ and $\phi^{-1}$ are $C^k$-maps, then $\phi$ is called a $C^k$-diffeomorphism. △

Diffeomorphisms are the structure-preserving maps between differentiable manifolds because they preserve the differential structure. Two differentiable manifolds $\left(M, \mathscr{O}_M, \mathscr{A}_M\right)$ and $\left(N, \mathscr{O}_N, \mathscr{A}_N\right)$ are called diffeomorphic if there exists a diffeomorphism between them. This is denoted by $M \cong_{\text{diff}} N$ or more precisely $\left(M, \mathscr{O}_M, \mathscr{A}_M\right) \cong_{\text{diff}} \left(N, \mathscr{O}_N, \mathscr{A}_N\right)$.

### A.5.3 Tangent and cotangent spaces

The most basic derivative that can be defined on a manifold is the the directional derivative of a function.

**Definition A.37** (space of smooth functions)**.**
Let $M$ be a smooth manifold. Then the set of smooth functions on $M$

$$C^\infty(M) = \left\{ f : M \to \mathbb{R} \mid f \text{ is smooth} \right\}$$

forms a $\mathbb{R}$-vector space $(C^\infty, +, \cdot)$ with vector addition and scalar multiplication defined point-wise, i.e. for $f, g \in C^\infty(M)$ and $a \in \mathbb{R}$ it holds that $(f + g)(p) = f(p) + g(p)$ and $(a \cdot f)(p) = a \cdot f(p)$. △

In general, a manifold doesn't have a vector space structure and hence defining the derivative by subtracting two points (vectors) to form a difference quotient (like in Euclidian space) makes no sense. Instead, the change of a function is evaluated along a curve:

**Definition A.38** (directional derivative operator)**.**
Let $\gamma : \mathbb{R} \supseteq \mathbb{I} \to M$ be a smooth curve through some point $p \in M$. Without loss of generality, let $\gamma(0) = p$. Then the directional derivative operator at $p$ along $\gamma$ is the linear map

$$\begin{aligned} X_{\gamma,p} : C^\infty(M) &\xrightarrow{\sim} \mathbb{R} \\ f &\mapsto \left(f \circ \gamma\right)'(0) \end{aligned}$$

where the prime denotes the derivative of the map from $\mathbb{I} \subseteq \mathbb{R}$ to $\mathbb{R}$. △

The directional derivative of a function $f$ along $\gamma$ at $p$ depends only on the curve's tangent vector at $p$ (and obviously $f$ itself). Therefore, the directional derivative operator $X_{\gamma,p}$ is called the *tangent vector* to the curve $\gamma$ at $p$. It can be thought of as the velocity vector of the curve $\gamma$ at $p$.

Due to the absence of a global linear structure on manifolds, the concept of curve for measuring the change of a function is necessary to define the directional derivative operator. But due to the local nature of the directional derivative operator, it can be understood as an element of a vector space (called tangent space) which 'belongs to' a particular point $p$ on the manifold.

**Definition A.39** (tangent vector space)**.**
The set of all directional derivative operators at a point $p \in M$

$$T_pM \;=\; \left\{ X_{\gamma,p} \mid \gamma \text{ is a smooth curve with } \gamma(0) = p \right\}$$

together with the maps

$$\begin{array}{rccccc} \oplus: & T_pM & \times & T_pM & \xrightarrow{\sim} & T_pM \\ \odot: & \mathbb{R} & \times & T_pM & \xrightarrow{\sim} & T_pM \end{array}$$

forms a $\mathbb{R}$-vector space called the tangent space at $p$. Vector addition and scalar multiplication are defined point-wise, i.e. for $f \in C^\infty(M)$ and $a \in \mathbb{R}$

$$\begin{aligned} \left(X_{\gamma,p} \oplus X_{\delta,p}\right)(f) \;&=\; X_{\gamma,p}(f) + X_{\delta,p}(f) \\ \left(a \odot X_{\gamma,p}\right)(f) \;&=\; a \cdot X_{\gamma,p}(f) \end{aligned}$$

△

Given two smooth curves $\gamma$ and $\delta$ on $M$ with $\gamma(0) = \delta(0) = p$, it can be shown that there exists a smooth curve $\epsilon$ with $\epsilon(0) = p$ such that $X_{\gamma,p}(f) + X_{\delta,p}(f) = X_{\epsilon,p}(f)$. Hence, it can be shown that $T_pM$ is closed under $\oplus$ and $\odot$.

The following theorem should not come as a surprise, given Definition A.22:

**Theorem A.40** (dimension of the tangent space)**.**

$$\forall\, p \in M:\; \dim(T_pM) \;=\; \dim(M)$$

△

**Remark A.41** (chart-induced basis)**.**
Any tangent vector $X \in T_pM$ can be represented as

$$X \;=\; X^i \left.\frac{\partial}{\partial x^i}\right|_p .$$

The components $X^1, \ldots, X^{\dim(M)} \in \mathbb{R}$ encode an infinitesimal displacement (i.e. the direction and magnitude of a tangent vector). The change of a function can then be evaluated along this tangent. The maps

$$\left.\frac{\partial}{\partial x^i}\right|_p : C^\infty(M) \xrightarrow{\sim} \mathbb{R}$$

with $1 \leq i \leq \dim(M)$ form a basis of $T_pM$. This basis is induced from a chart$(U, x)$ with $p \in U$: For some $f \in C^\infty(M)$ it holds that

$$\left.\frac{\partial}{\partial x^i}\right|_p (f) \;\equiv\; \left(\frac{\partial}{\partial x^i} f\right)(p) \;=\; \partial_i\big(f \circ x^{-1}\big)\big(x(p)\big)$$

where $\partial_i$ denotes the $i$-th partial derivative of the map from $\mathbb{R}^{\dim(M)}$ to $\mathbb{R}$. △

For every fixed function $f \in C^\infty(M)$, the map

$$\begin{aligned} T_pM &\xrightarrow{\sim} \mathbb{R} \\ X &\mapsto X(f) \end{aligned}$$

is a linear functional[2] on the tangent space. These functionals are elements of the so-called cotangent space:

**Definition A.42** (cotangent space)**.**
Let $M$ be a smooth manifold. The cotangent space $T_p^*M$ of $M$ at the point $p \in M$ is the dual space of the tangent space of $M$ at $p$, i.e. $T_p^*M = \big(T_pM\big)^*$. △

For $\dim(M) < \infty$ it holds that $\dim(T_p^*M) = \dim(T_pM) = \dim(M)$ and $T_p^*M \cong_{\text{vec}} T_pM$.

The differential of a function $f$ at point $p$ is a *covector* (or 1-form) 'living' in the cotangent space $T_p^*M$:

[2] In linear algebra, elements of the dual space (i.e. linear maps from the 'primal' space to its field) are called functionals.

**Definition A.43** (differential)**.**
At every point $p \in M$ there exists a $\mathbb{R}$-linear map (differential operator)

$$\begin{aligned} \mathrm{d}_p : C^\infty(M) &\xrightarrow{\sim} T_p^* M \\ f &\mapsto \mathrm{d}_p f \end{aligned}$$

yielding a linear functional $\mathrm{d}_p f$ called the *differential* of $f$ at $p$. It is defined by

$$\big(\mathrm{d}_p f\big)(X) \;=\; X(f)$$

for any $X \in T_p M$. △

The basis of $T_p^* M$ is also induced from a chart $(U,\, x)$ with $U \ni p$: The basis covectors are the differentials of the component functions $x^j : U \to \mathbb{R}$, $p \mapsto \mathrm{proj}_j\big(x(p)\big)$, i.e.

$$\big\{\mathrm{d}_p x^1,\, \ldots,\, \mathrm{d}_p x^{\dim(M)}\big\}$$

forms a basis of $T_p^* M$. In fact, this is also the dual basis of $\big(T_p M\big)^*$:
For $i,\, j \in \big\{1,\, \ldots,\, \dim(T_p M)\big\}$:

$$\mathrm{d}_p x^j \left( \left.\frac{\partial}{\partial x^i}\right|_p \right) \;=\; \left.\frac{\partial}{\partial x^i}\right|_p (x^j) \;=\; \partial_i\big(x^j \circ x^{-1}\big)'\big(x(p)\big) \;=\; \delta_i^j$$

**Remark A.44** (nonrigorous metaphor)**.**
If one would imagine to draw on the manifold the local coordinate system which is assigned by some chart $(U,\, x)$ with $U \ni p$, then $\mathrm{d}_p x^j$ could be interpreted as the "density of ticks" on the $j$-th coordinate axis at point $p$ (i.e. the number of ticks between two points on the manifold). In contrast, the components $g_i \in \mathbb{R}$ of the differential $\mathrm{d}_p f \;=\; g_j\, \mathrm{d}_p x^j$ can be interpreted as the "density of level curves" when moving along the $j$-th coordinate axis at point $p$ (i.e. the number of crossed level curves when moving between two ticks). △

### A.5.4 Tangent bundle and vector fields

A manifold $M$ together with all its tangent spaces $\big\{T_p M \mid p \in M\big\}$ can be turned into a vector bundle (with base space $M$):

**Definition A.45** (tangent bundle)**.**
Let $M$ be a smooth manifold. Then the tangent bundle $TM$ of $M$ is the disjoint union

of all tangent spaces:

$$TM = \bigsqcup_{p \in M} T_p M = \bigcup_{p \in M} \{(p, X) \mid X \in T_p M\}$$

The bundle projection is a smooth map defined as

$$\begin{aligned} \pi : TM &\to M \\ X &\mapsto p \end{aligned}$$

where $p \in M$ is the point for which $X \in T_p M$. △

The tangent bundle $TM$ is a smooth manifold of dimension $2\dim(M)$ since a smooth atlas $\mathscr{A}_{TM}$ of $TM$ can be constructed from a given smooth atlas $\mathscr{A}_M$ of $M$:
For $(U, x) \in \mathscr{A}_M$, the corresponding chart in $\mathscr{A}_{TM}$ is given by $\big(\mathrm{preim}_\pi(U), y\big)$ with

$$\begin{aligned} y : \ \mathrm{preim}_\pi(U) &\to y\big(\mathrm{preim}_\pi(U)\big) \subseteq \mathbb{R}^{2\dim(M)} \\ X &\mapsto \Big(x^1\big(\pi(X)\big), \ldots, x^{\dim(M)}\big(\pi(X)\big), X^1, \ldots, X^{\dim(M)}\Big). \end{aligned}$$

where $X^1, \ldots, X^{\dim(M)}$ are the components of $X$ with respect to the basis of $T_{\pi(X)}M \ni X$ (which is induced by the same chart). It can be shown that any two charts in $\mathscr{A}_{TM}$ are $C^\infty$-compatible.

A *vector field* on a manifold $M$ assigns to each point $p \in M$ a tangent vector $X \in T_p M$:

**Definition A.46** (vector field)**.**
Let $M$ be a smooth manifold and let $TM \xrightarrow{\pi} M$ be its tangent bundle. Then a vector field is a smooth section of $TM$. △

The set of all vector fields is denoted by

$$\Gamma(TM) = \big\{\sigma : M \to TM \mid \pi \circ \sigma = id_M\big\} .$$

This set has a structure that is similar but not quite like a vector space: It is a $C^\infty(M)$-module (if addition and multiplication operations are defined accordingly).

A module (over a ring) is essentially the same kind of structure as a vector space (over a field). What makes a module different from a vector space is merely its underlying ring structure: In contrast to a field, a ring $(R, +, \cdot)$ does *not* have the property

that $(R \setminus \{0\}, \cdot)$ is an abelian group. The multiplication operation is only required to be associative and to distribute over the addition operation. In case the multiplication operation is commutative, the ring is called a commutative ring. If there exists a unique neutral element with respect to multiplication, the ring is called a unital ring. Further, if there exists an inverse element for every element in the ring, the ring is called a division ring.

Hence, $(C^\infty(M), +, \cdot)$ with $+$ and $\cdot$ defined point-wise is a ring. Due to its point-wise definition, $\cdot$ inherits the commutative property of multiplication on $\mathbb{R}$ making this a commutative ring. The function in $C^\infty(M)$ that takes the value 1 everywhere on $M$ makes this a unital ring. But since there exists no inverse for functions that take the value 0 at some point on $M$ this is *not* a division ring.

So, $\big(\Gamma(TM), \oplus, \odot\big)$ is a $C^\infty(M)$-module with addition defined as

$$\begin{aligned} \oplus : \Gamma(TM) \times \Gamma(TM) &\to \Gamma(TM) \\ \big(v_1, v_2\big) &\mapsto v_1 \oplus v_2 \end{aligned}$$

and multiplication defined as

$$\begin{aligned} \odot : C^\infty(M) \times \Gamma(TM) &\to \Gamma(TM) \\ (f, v) &\mapsto f \odot v \end{aligned}$$

where

$$\begin{aligned} \forall\, p \in M : (v_1 \oplus v_2)(p) &= v_1(p) + v_2(p) \\ \forall\, p \in M : (f \odot v)(p) &= f(p) \cdot v(p) \end{aligned}$$

with $+$ and $\cdot$ from the tangent vector spaces $\big(T_pM, +, \cdot\big)$.

**Remark.**
An $R$-module is only guaranteed to have a basis if $R$ is a division ring.
Since $C^\infty(M)$ is not a division ring, $\Gamma(TM)$ might not have a basis. This is related to the hairy ball theorem which states that there exists no nonvanishing continuous tangent vector field on even-dimensional spheres. According to Wikipedia, it is in particular not possible to comb the hair on a coconut. △

### A.5.5 Cotangent bundle and tensor fields

Similar to the construction of the tangent bundle $TM$, the cotangent bundle $T^*M$ can be constructed. Both $TM$ and $T^*M$ are smooth manifolds of dimension $2\dim(M)$.

The set of smooth sections on the cotangent bundle $\Gamma(T^*M)$ can similarly be turned into a $C^\infty(M)$-module.

This way, the concept of tensors (defined on a vector space) can be extended to the concept of tensor fields (defined on a manifold):

**Definition A.47** (tensor field)**.**
A $(p, q)$-tensor field $t$ on a smooth manifold $M$ is a $C^\infty(M)$-multilinear map

$$t : \underbrace{\Gamma(T^*M) \times \cdots \times \Gamma(T^*M)}_{p \text{ copies}} \times \underbrace{\Gamma(TM) \times \cdots \times \Gamma(TM)}_{q \text{ copies}} \xrightarrow{\sim} C^\infty(M)$$

△

## A.6 Differential forms

Differential forms are a particular class of tensor fields:

**Definition A.48** (differential $k$-form)**.**
For $0 \leq k \leq n = \dim(M)$, a (differential) $k$-form $\omega$ is a $(0, k)$-tensor field that is totally antisymmetric, i.e.

$$\forall\, X_1, \ldots, X_k \in \Gamma(TM), \forall \pi \in S_k : \omega\big(X_1, \ldots, X_k\big) = \operatorname{sgn}(\pi) \cdot \omega\big(X_{\pi(1)}, \ldots, X_{\pi(k)}\big)\,.$$

△

In particular, if two adjacent arguments (vector fields) are swapped then the $k$-form $\omega$ changes its sign. The anti-symmetric nature of a differential $k$-form encodes the orientation of a $k$-dimensional volume or density.

The set of all $k$-forms on a manifold $M$ is denoted by $\Omega^k(M)$. This set has the structure of a $C^\infty(M)$-module. Consequently, the sum of two $k$-forms is a $k$-form and the product of a smooth function and a $k$-form again is a $k$-form.

The 0-forms are by convention the smooth functions, i.e. $\Omega^0(M) = C^\infty(M)$ and the 1-forms are the covector fields, i.e. $\Omega^1(M) = \Gamma(T^*M)$.

### A.6.1 Exterior product

**Remark** (product of two tensor fields on a manifold)**.**
The tensor product can be extended in a straightforward manner: Instead of turning a $(p_1, q_1)$-tensor and a $(p_2, q_2)$-tensor into a $(p_1 + p_2, q_1 + q_2)$-tensor, it can be defined to turn a $(p_1, q_1)$-tensor field and a $(p_2, q_2)$-tensor field into a $(p_1 + p_2, q_1 + q_2)$-tensor field by applying Definition A.16 point-wise. △

Higher-dimensional forms can be built from lower-dimensional ones by means of the exterior product:

**Definition A.49** (exterior product)**.**
The exterior product is the alternating bilinear map

$$\begin{aligned} \wedge : \Omega^k(M) \times \Omega^l(M) &\xrightarrow{\sim} \Omega^{k+l}(M) \\ (\alpha, \beta) &\mapsto \alpha \wedge \beta \end{aligned}$$

defined by

$$(\alpha \wedge \beta)(X_1, \ldots, X_{k+l}) = \frac{1}{k! \cdot l!} \sum_{\pi \in S_{k+l}} \operatorname{sgn}(\pi)(\alpha \otimes \beta)(X_{\pi(1)}, \ldots, X_{\pi(k+l)})$$

△

The exterior product is the alternating version of the tensor product:
For $\alpha \in \Omega^k(M)$ and $\beta \in \Omega^l(M)$ it holds that

$$\alpha \wedge \beta = (-1)^{k \cdot l} \beta \wedge \alpha \,.$$

In particular, for $\omega \in \Omega^1(M)$ it follows that $\omega \wedge \omega = 0$. Two linearly dependent 1-forms cannot yield a nonvanishing 2-form (just like to linearly dependent vectors cannot span a nonvanishing surface (2-volume)).

Further, the exterior product is distributive with respect to addition of $k$-forms.

### A.6.2 Exterior derivative

Similarly to the tensor product, the $\mathbb{R}$-linear map $\mathrm{d}_p : C^\infty(M) \xrightarrow{\sim} T_p^* M$ can be extended: Instead of turning a $C^\infty(M)$-function $f$ into a covector $\mathrm{d}_p f \in T_p^* M$ at some

specific point $p \in M$, it can be defined to map $f$ to a covector field $\mathrm{d}f \in \Gamma(T^*M)$ by applying Definition A.43 point-wise:

$$\begin{aligned} \mathrm{d} : \Omega^0(M) &\xrightarrow{\sim} \Omega^1(M) \\ f &\mapsto \mathrm{d}f \\ \text{defined as} \qquad \big(\mathrm{d}f\big)(p) &:= \mathrm{d}_p f \end{aligned} \tag{A.1}$$

This derivative operator is just one member of a family of differential operators

$$\mathrm{d}^k : \Omega^k(M) \xrightarrow{\sim} \Omega^{k+1}(M)\,.$$

Usually, all members of this family are denoted just by $\mathrm{d}$.

**Definition A.50** (exterior derivative)**.**
The exterior derivative of a $k$-form $\omega \in \Omega^k(M)$ is defined as the unique $\mathbb{R}$-linear map

$$\mathrm{d}^k : \Omega^k(M) \xrightarrow{\sim} \Omega^{k+1}(M)$$

satisfying the following properties:

(i) $\mathrm{d}$ is an anti-derivation (of degree 1 w.r.t. $\wedge$): For $\omega_k \in \Omega^k(M)$ and $\omega_l \in \Omega^l(M)$ it holds that $\mathrm{d}^{k+l}(\omega_k \wedge \omega_l) = \mathrm{d}^k(\omega_k) \wedge \omega_l + (-1)^k\, \omega_k \wedge \mathrm{d}^l(\omega_l)$

(ii) For $f \in \Omega^0(M)$, $\mathrm{d}^0$ is defined in (A.1).

(iii) For any $\omega_k \in \Omega^k(M)$ it holds that $\mathrm{d}^{k+1}\big(\mathrm{d}^k\omega_k\big) = 0$, i.e. $\mathrm{d} \circ \mathrm{d} = 0$.

(iv) $\mathrm{d}$ is a local operator: For any open neighborhood $U \in \mathcal{O}_M$ and any $k$-form $\omega \in \Omega^k(M)$ it holds that $\mathrm{d}\big(\omega\big)\big|_U = \mathrm{d}\big(\omega\big|_U\big)$.

△

The exterior derivative is $\mathbb{R}$-linear but not $C^\infty(M)$-linear. Instead the Leibnitz rule $\mathrm{d}(f \cdot \omega) = f \cdot \mathrm{d}\omega + \mathrm{d}f \wedge g$ holds for all $f \in C^\infty(M)$ and $\omega \in \Omega^k(M)$, see property (i).

**Remark** (relationship to vector calculus)**.**
Comparing exterior calculus with vector calculus in 3 dimensions, the following relationships exists: According to property (ii), $\mathrm{d}^0$ is related to the gradient of a function. Further, $\mathrm{d}^1$ is related to the curl of a vector field and $\mathrm{d}^2$ is related to the divergence of a vector field, see A.60.

Property (iii) corresponds to the two facts that the curl of the gradient of any scalar field is zero and that the divergence of the curl of any vector field is zero. △

### A.6.3 Integration

One very important feature of differential forms is their intimate relationship with integration on oriented manifolds: A $k$-form $\alpha \in \Omega^k(M)$ can be integrated over a $k$-dimensional submanifold of $M$.

Since the exterior derivative is related to (and unifies) the gradient, curl and divergence operators from vector calculus, it is not surprising that there exists an integral theorem in exterior calculus that unifies the integral theorems of vector calculus:

**Theorem A.51** (Stokes' theorem)**.**
Let $M$ be a smooth oriented $(k+1)$-dimensional manifold with smooth ($k$-dimensional) boundary $\partial M$. Then for any $k$-form $\omega_k \in \Omega^k(M)$ it holds that

$$\int_M \mathrm{d}^k \omega_k \;=\; \int_{\partial M} \mathrm{tr}\big(\omega_k\big)\,.$$

△

This theorem clearly shows a duality between exterior differentiation and restriction to the boundary (expressed by the trace operator).

### A.6.4 Interior product and Lie derivative

The exterior derivative increases the degree of a form. In contrast, the interior product (or interior derivative or contraction) decreases the degree of a form:

**Definition A.52** (interior product)**.**
Let $M$ be a differentiable manifold and let $X \in \Gamma(TM)$ be a vector field on $M$. Then the interior product of the vector field $X$ and a $k$-form $\omega_k \in \Omega^k(M)$ is the $\mathbb{R}$-linear map

$$\imath_X : \Omega^k(M) \xrightarrow{\sim} \Omega^{k-1}(M)$$

defined by

$$\forall\, X_1, \ldots, X_{k-1} \in \Gamma(TM) : \; \big(\imath_X \omega_k\big)\big(X_1, \ldots, X_{k-1}\big) = \omega_k\big(X, X_1, \ldots, X_{k-1}\big)\,.$$

△

The interior product is an anti-derivation (of degree $-1$ w.r.t. $\wedge$):
For $\omega_k \in \Omega^k(M)$ and $\omega_l \in \Omega^l(M)$ it holds that

$$\iota_X(\omega_k \wedge \omega_l) \;=\; \big(\iota_X\omega_k\big) \wedge \omega_l \;+\; (-1)^k\, \omega_k \wedge \big(\iota_X\omega_l\big)\ .$$

The Lie derivative of a differential form can be defined with the exterior derivative and the interior product (expressing a certain duality between the two operations):

**Theorem A.53** (Cartan homotopy formula)**.**
Let $M$ be a differentiable manifold. Let $X \in \Gamma(TM)$ be a vector field on $M$ and let $\omega \in \Omega^k(M)$ be a $k$-form on $M$. Then the Lie derivative of $\omega$ w.r.t. $X$ is given as

$$\mathscr{L}_X\omega \;=\; \iota_X \mathrm{d}\omega \;+\; \mathrm{d}\big(\iota_X\omega\big)\ .$$

△

### A.6.5 Riemannian metric and related isomorphisms

The exterior product, the exterior derivative and hence also the Lie derivative are independent of a metric having merely a 'topological character'.

A Riemannian metric basically defines an inner product on every tangent space, thereby making it possible to speak for example about the length of and angles between tangent vectors.

**Definition A.54** (Riemannian metric)**.**
Let $M$ be a differentiable manifold. Further, let $g : \Gamma(TM) \times \Gamma(TM) \xrightarrow{\sim} C^\infty(M)$ be a $(0, 2)$-tensor field on $M$ that is everywhere symmetric and positive-definite. This means that the following holds:

$$\forall\, p \in M,\, \forall\, X_1,\, X_2 \in \Gamma(TM) :\ \ g(X_1,\, X_2)\Big|_p \;=\; g(X_2,\, X_1)\Big|_p \quad \text{and}$$
$$g(X_1,\, X_1)\Big|_p \geq 0 \quad \text{and} \quad g(X_1,\, X_1)\Big|_p = 0 \;\Rightarrow\; X_1\Big|_p = 0$$

Then $g$ is called a Riemannian metric on $M$ and $(M,\, g)$ is called a Riemannian manifold. △

Given a chart $(U,\ x)$ with $U \ni p$, the set $\left\{ \frac{\partial}{\partial x_1}\Big|_p, \ldots, \frac{\partial}{\partial x_n}\Big|_p \right\}$ defines a chart-induced basis of $T_pM$. The components of the metric tensor at point $p \in M$ (w.r.t. this basis) are hence given by

$$g_{ij}\Big|_p = g\left( \frac{\partial}{\partial x_i}\Big|_p, \frac{\partial}{\partial x_j}\Big|_p \right)\Big|_p$$

and the metric tensor at point $p$ is given (in terms of the basis of the cotangent space $T_p^*M$ which is the dual basis of the basis of $T_pM$) as

$$g\Big|_p = g_{ij}\Big|_p \, \mathrm{d}x^i\Big|_p \otimes \mathrm{d}x^j\Big|_p \,.$$

The canonical choice of a Riemannian metric for ($n$-dimensional submanifolds of) $\mathbb{R}^n$ is the *Euclidian metric* $g_{ij}\big|_p = \delta_{ij}$, i.e. the extension of the Euclidian inner product on every tangent space to the entire manifold.

The metric induces an isomorphism between 1-forms (covector-fields) and vector fields:

**Definition A.55** (musical isomorphism)**.**
Let $(M,\ g)$ be a Riemannian manifold and let $X, Y \in \Gamma(TM)$ be two vector fields.

The $C^\infty(M)$-linear map $\flat$ turns the vector field $X$ into a 1-form $X^\flat$:

$$\begin{aligned} \flat \ :\ \Gamma(TM) &\xrightarrow{\sim} \Omega^1(M) \\ X &\mapsto X^\flat \end{aligned}$$

defined through $X^\flat(Y) = g(X, Y)$.

In coordinates this corresponds to *lowering the index* of the components of $X$: Let $x$ be (local) coordinates and let $g_{ij}$ be the corresponding representation of the metric tensor. Then it holds that

$$X^\flat(Y) = g(X,Y) \ = \ g\Big( X^i \frac{\partial}{\partial x^i},\, Y^i \frac{\partial}{\partial x^i} \Big) \ = \ g_{ij}\, X^i\, Y^i \ = \ g_{ij}\, X^i\, \mathrm{d}x^j(Y)\,.$$

Hence, $g_{ij}\, X^i$ is the coordinate representation of $X^\flat$.

Conversely, the map $\sharp$ turns a 1-form $\omega$ into a vector field $\omega^\sharp$:

$$\begin{aligned} \sharp \;:\; \Omega^1(M) &\xrightarrow{\sim} \Gamma(TM) \\ \omega &\mapsto \omega^\sharp \end{aligned}$$

defined through $\omega = \left(\omega^\sharp\right)^\flat$.

In coordinates this corresponds to *raising the index* of the components of $\omega$:
Let $\omega^i$ be the components of $\omega^\sharp$. Then it holds that

$$\omega \;=\; \omega_j \,\mathrm{d}x^j \;=\; \left(\omega^i \frac{\partial}{\partial x^i}\right)^\flat \;=\; g_{ij}\,\omega^i \,\mathrm{d}x^j$$

Hence, $\omega^i = \left(g_{ij}\right)^{-1} \omega_j = g^{ij}\,\omega_j$ is the coordinate representation of $\omega^\sharp$. △

A *volume form* on a manifold $M$ is a nowhere vanishing top-dimensional form, i.e. a form of degree $n = \dim(M)$. A volume form exists if and only if the manifold is orientable. If $\mu_1 \in \Omega^n(M)$ is a volume form, then so is $\mu_2 = f\,\mu_1$ for any nonvanishing $f \in \Omega^0(M)$. A Riemannian metric makes one such volume form the natural choice:

**Definition A.56** (Riemannian volume form)**.**
Every oriented Riemannian manifold $(M,\, g)$ has a *natural volume form* $\mu_g \in \Omega^{\dim(M)}(M)$. Let $(U,\, x)$ with $U \ni p$ be a chart defining local coordinates around $p \in M$. Because $M$ is oriented, the chart-induced basis of $T_pM$ is positively oriented. The volume form $\mu$ at $p$ is then given as

$$\mu_g\Big|_p \;=\; \sqrt{\det\left[\,g_{ij}\Big|_p\right]}\;\mathrm{d}x^1 \wedge \ldots \wedge \mathrm{d}x^n\,.$$

△

In the Euclidian case, the determinant of the matrix of the components of the metric tensor is always 1 and the natural volume form is $\mu_g\big|_p = \mathrm{d}x^1 \wedge \ldots \wedge \mathrm{d}x^n$.

A Riemannian volume form $\mu_g$ on a Riemannian manifold $(M,\, g)$ makes it possible to determine the volume of $M$ according to the metric $g$:

$$\mathrm{Vol}(M) = \int_M \mu_g$$

If a function $f \in \Omega^0(M)$ represents a volumetric density, like for example a mass density, then it can be integrated on $M$ to yield the total mass

$$m = \int_M f \wedge \mu_g = \int_M f \, \mu_g \, .$$

The volume form $\mu_g$ serves as a measure for integrating functions (0-forms) on Riemannian manifolds.

Hence, there exists an isomorphism between 0-forms and $n$-forms. This isomporphism is expressed by the Hodge star operator:

$$\begin{aligned} \star 1 &= \mu_g \\ \star \mu_g &= 1 \end{aligned}$$

In fact, the Hodge star expresses more generally an isomorphism between $k$-forms and $n-k$-forms:

**Definition A.57** (Hodge star operator)**.**
Let $(M, g)$ be a $n$-dimensional Riemannian manifold and let $\mu_g$ be the corresponding Riemannian volume form. Then the Hodge star operator is the $C^\infty(M)$-linear map

$$\begin{aligned} \Omega^k(M) &\xrightarrow{\sim} \Omega^{n-k}(M) \\ \alpha &\mapsto \star\alpha \, . \end{aligned}$$

The *Hodge dual* of $\alpha$ is the unique $n-k$-form $\star\alpha$ which satisfies

$$\forall\, \omega \in \Omega^k(M) : \; \omega \wedge \star\alpha = \langle \omega, \, \alpha \rangle_g \, \mu_g$$

where $\langle \cdot, \, \cdot \rangle_g : \; \Omega^k(M) \times \Omega^k(M) \xrightarrow{\sim} C^\infty(M)$ is an inner product between $k$-forms induced by the Riemannian metric in the following way: For $\omega = \omega_1 \wedge \ldots \wedge \omega_k$ and $\alpha = \alpha_1 \wedge \ldots \wedge \alpha_k$

$$\langle \omega, \, \alpha \rangle_g = \det \left[ g(\omega_i^\sharp, \, \alpha_j^\sharp) \right] = \det \left[ g^{-1}(\omega_i, \, \alpha_j) \right]$$

△

The symmetry of the inner product yields the following property of the Hodge star:

$$\forall\, \alpha, \, \beta \in \Omega^k(M) : \; \alpha \wedge \star\beta = \beta \wedge \star\alpha$$

It further holds that for $\alpha \in \Omega^k(M)$

$$\star \star \alpha \;=\; (-1)^{k(n-k)}\alpha\,.$$

**Example A.58** (Hodge star and 3-dimensional Euclidian space)**.**
For the particularly simple case where $M$ is (a 3-dimensional submanifold of) 3-dimensional Euclidian space with coordinates $x$, the Hodge star operator yields the following:

$$\begin{aligned}
\star 1 \;&=\; \mathrm{d}x^1 \wedge \mathrm{d}x^2 \wedge \mathrm{d}x^3 & \qquad \star\left(\mathrm{d}x^1 \wedge \mathrm{d}x^2 \wedge \mathrm{d}x^3\right) \;&=\; 1 \\
\star \mathrm{d}x^1 \;&=\; \mathrm{d}x^2 \wedge \mathrm{d}x^3 & \qquad \star\left(\mathrm{d}x^2 \wedge \mathrm{d}x^3\right) \;&=\; \mathrm{d}x^1 \\
\star \mathrm{d}x^2 \;&=\; \mathrm{d}x^3 \wedge \mathrm{d}x^1 & \qquad \star\left(\mathrm{d}x^3 \wedge \mathrm{d}x^1\right) \;&=\; \mathrm{d}x^2 \\
\star \mathrm{d}x^3 \;&=\; \mathrm{d}x^1 \wedge \mathrm{d}x^2 & \qquad \star\left(\mathrm{d}x^1 \wedge \mathrm{d}x^2\right) \;&=\; \mathrm{d}x^3
\end{aligned}$$

◇

**Remark A.59** (distributivity and linearity)**.**
The Hodge star operator does *not* distribute with respect to the exterior product. Hence, for some $\alpha \in \Omega^k(M)$ and $\beta \in \Omega^l(M)$ in general $\star(\alpha \wedge \beta) \neq \star\alpha \wedge \star\beta$. But for $f \in \Omega^0(M)$ and $\alpha \in \Omega^k(M)$ the following holds since $\star$ is a $C^\infty(M)$-linear operator: $\star(f \wedge \alpha) = f \wedge \star\alpha$. △

**Remark A.60** (gradient, curl, divergence)**.**
Using the musical isomorphism and the Hodge star operator, the vector calculus operators gradient, curl and divergence can all be expressed with the exterior derivative: Let $\left(\mathbb{R}^3,\, g\right)$ be a Riemannian manifold with the Euclidian metric. Then for a smooth function $f \in C^\infty\left(\mathbb{R}^3\right)$ and vector fields $X,\, Y \in \Gamma(T\mathbb{R}^3)$ it holds that

$$\begin{aligned}
\nabla f \;&=\; \left(\mathrm{d}^0 f\right)^\sharp \\
\nabla \times X \;&=\; \left(\star\left(\mathrm{d}^1 X^\flat\right)\right)^\sharp \\
\nabla \cdot Y \;&=\; \star \mathrm{d}^2\left(\star Y^\flat\right)
\end{aligned}$$

The vector field $X$ corresponds to a 1-form, whereas $Y$ naturally corresponds to a 2-form, cf. Fig. A.2. △

**Theorem A.61** (interior product and Hodge star operator)**.**
Let $M$ be a $n$-dimensional smooth manifold. Further, let $X \in \Gamma(TM)$ be a smooth

$$\begin{array}{ccccccccc} 0 \to & \Omega^0(\mathbb{R}^3) & \xrightarrow{\mathrm{d}^0} & \Omega^1(\mathbb{R}^3) & \xrightarrow{\mathrm{d}^1} & \Omega^2(\mathbb{R}^3) & \xrightarrow{\mathrm{d}^2} & \Omega^3(\mathbb{R}^3) & \to 0 \\ & \cup & & \cup & & \cup & & & \\ & f & & X^\flat & & \star Y^\flat & & & \end{array}$$

Fig. A.2 De Rham complex for 3-dimensional Euclidian space

vector field on $M$ and let $\alpha \in \Omega^k(M)$ be a $k$-form on $M$. Then the interior product between $X$ and $\alpha$ can be expressed with the Hodge star operator in the following way:

$$\imath_X \alpha \;=\; (-1)^{k(n-k)} \star \left( \star\alpha \wedge X^\flat \right)$$

△

A proof is given in [20, p. 79].

# B

# Ideal gas

Equilibrium thermodynamics postulates the existence of a fundamental equation. In practice however, it may be hard to obtain an expression for a particular system. For relatively simple model such as the monatomic ideal gas, a fundamental equation can be obtained analytically on be basis of statistical mechanics.

## B.1 Sackur-Tetrode equation

The Sackur-Tetrode equation[1] is a fundamental equation in entropic representation. According to this model, the entropy $s$ of a monatomic ideal gas which has internal energy $u$, occupies a volume $v$ and comprises of $n$ particles with atomic mass $m_a$ is given as

$$s = S(u, v, n) = k_B\, n \ln\left(\left(\frac{v}{n}\right)\left(\frac{u}{n}\right)^{\frac{3}{2}}\right) + k_B\, n\, c_1 \tag{B.1a}$$

with

$$c_1 = \frac{5}{2} + \frac{3}{2}\ln\left(\frac{4\,\mathring{\pi}\, m_a}{3\,h^2}\right). \tag{B.1b}$$

Here $k_B = 1.380\,649 \times 10^{-23}\,\mathrm{J\,K^{-1}}$ is Boltzmann's constant
and $h = 6.626\,070\,15 \times 10^{-34}\,\mathrm{J\,s}$ is Planck's constant.

For sufficiently high temperatures, this model can be used in engineering applications to describe the behavior of monatomic gases. For example, noble gases such as Helium or Argon are stable as monatomic molecules.

[1] see eg. [33] which also references the original publications

## B.2 Internal energy as a thermodynamic potential

Equation (B.1a) can be solved for $u$ to obtain the fundametal equation

$$\begin{aligned} u \;=\; U(s,\, v,\, n) \;&=\; \left(\frac{n^5}{v^2}\right)^{\frac{1}{3}} \exp\!\left(\frac{2}{3}\frac{s}{n\,k_B} - \frac{2}{3}\,c_1\right) \\ &=\; \frac{3}{4\,\mathring{\pi}}\,e^{-\frac{5}{3}}\,h^2\,\frac{1}{m_a}\left(\frac{n^5}{v^2}\right)^{\frac{1}{3}} \exp\!\left(\frac{2}{3}\,\frac{1}{k_B}\,\frac{s}{n}\right) \end{aligned} \tag{B.2}$$

Sometimes it is more convenient to use the mass $m = m_a\,n$ instead of the number of particles $n$ as a state variable. Equation (B.2) can then be written as

$$u \;=\; U(s,\, v,\, m) \;=\; \frac{3}{4\,\mathring{\pi}}\,e^{-\frac{5}{3}}\,h^2\,m_a^{-\frac{8}{3}}\left(\frac{m^5}{v^2}\right)^{\frac{1}{3}} \exp\!\left(\frac{2}{3}\,\frac{m_a}{k_B}\,\frac{s}{m}\right) \tag{B.3}$$

According to Eq. (2.3), the thermodynamic equilibrium temperature is

$$\theta(s,\, v,\, m) \;=\; \frac{1}{2\,\mathring{\pi}}\,e^{-\frac{5}{3}}\,\frac{h^2}{k_B}\,m_a^{-\frac{5}{3}}\left(\frac{m}{v}\right)^{\frac{2}{3}} \exp\!\left(\frac{2}{3}\,\frac{m_a}{k_B}\,\frac{s}{m}\right), \tag{B.4a}$$

the thermodynamic equilibrium pressure is

$$\pi(s,\, v,\, m) \;=\; \frac{1}{2\,\mathring{\pi}}\,e^{-\frac{5}{3}}\,h^2\,m_a^{-\frac{8}{3}}\left(\frac{m}{v}\right)^{\frac{5}{3}} \exp\!\left(\frac{2}{3}\,\frac{m_a}{k_B}\,\frac{s}{m}\right) \tag{B.4b}$$

and the chemical potential per unit mass is

$$\mu(s,\, v,\, m) \;=\; \frac{1}{4\,\mathring{\pi}}\,e^{-\frac{5}{3}}\,\frac{h^2}{k_B}\,m_a^{-\frac{8}{3}}\,\left(5\,k_B\,m - 2\,m_a\,s\right)\left(m\,v^2\right)^{-\frac{1}{3}} \exp\!\left(\frac{2}{3}\,\frac{m_a}{k_B}\,\frac{s}{m}\right). \tag{B.4c}$$

## B.3 Internal energy density

Equation (B.3) can be turned into a local thermodynamic potential of the form $u = U(s,\, m)$ where $u$ is the internal energy density, $s$ is the entropy density and $m$ is the mass density.

According to Eq. (2.9) and Eq. (B.3) it holds that

$$u = U(s, m) = \frac{3}{4\mathring{\pi}} e^{-\frac{5}{3}} h^2 m_a^{-\frac{8}{3}} m^{\frac{5}{3}} \exp\left(\frac{2}{3}\frac{m_a}{k_B}\frac{s}{m}\right). \tag{B.5}$$

The intensive quantities are then given according to Eq. (2.10) as

$$\theta(s, m) = \frac{1}{2\mathring{\pi}} e^{-\frac{5}{3}} \frac{h^2}{k_B} m_a^{-\frac{5}{3}} m^{\frac{2}{3}} \exp\left(\frac{2}{3}\frac{m_a}{k_B}\frac{s}{m}\right) \tag{B.6a}$$

$$\mu(s, m) = \frac{1}{4\mathring{\pi}} e^{-\frac{5}{3}} \frac{h^2}{k_B} m_a^{-\frac{8}{3}} \left(5 k_B m - 2 m_a s\right) m^{-\frac{1}{3}} \exp\left(\frac{2}{3}\frac{m_a}{k_B}\frac{s}{m}\right) \tag{B.6b}$$

$$\pi(s, m) = \frac{1}{2\mathring{\pi}} e^{-\frac{5}{3}} h^2 m_a^{-\frac{8}{3}} m^{\frac{5}{3}} \exp\left(\frac{2}{3}\frac{m_a}{k_B}\frac{s}{m}\right). \tag{B.6c}$$

# References


[1] A. F. Fritzsche, H. W. Hahnemann, and Z. Rant. "Rundschau". In: *Forschung auf dem Gebiet des Ingenieurwesens A* 22.1 (1956), pp. 33–37. DOI: 10.1007/BF02592661.

[2] Henry Paynter. *Analysis and Design of Engineering Systems*. Cambridge: MIT Press, 1961.

[3] Peter H. Ceperley. "A pistonless Stirling engine—The traveling wave heat engine". In: *The Journal of the Acoustical Society of America* 66.5 (1979), pp. 1508–1513. DOI: 10.1121/1.383505.

[4] Hebert Callen. *Thermodynamics and an Introduction to Thermostatistics*. Second Edition. John Wiley & Sons Inc, 1985.

[5] Ralph Abraham, Jerrold E. Marsden, and Tudor Ratiu. *Manifolds, Tensor Analysis, and Applications*. Second Edition. Applied Mathematical Sciences. New York: Springer, 1988. DOI: 10.1007/978-1-4612-1029-0.

[6] Theodore James Courant. "Dirac manifolds". In: *Transactions of the American Mathematical Society* 319.2 (1990), pp. 631–661. DOI: 10.1090/S0002-9947-1990-0998124-1.

[7] Irene Dorfman. *Dirac Structures and Integrability of Nonlinear Evolution Equations*. Chichester: John Wiley, 1993.

[8] Arjan van der Schaft and Bernhard Maschke. "The Hamiltonian formulation of energy conserving physical systems with external ports". In: *AEU - Archiv für Elektronik und Übertragungstechnik* 49.5-6 (1995), pp. 362–371.

[9] Miroslav Grmela and Hans Christian Öttinger. "Dynamics and thermodynamics of complex fluids. I. Development of a general formalism". In: *Phys. Rev. E* 56 (6 1997), pp. 6620–6632. DOI: 10.1103/PhysRevE.56.6620.

[10] Hans Christian Öttinger and Miroslav Grmela. "Dynamics and thermodynamics of complex fluids. II. Illustrations of a general formalism". In: *Phys. Rev. E* 56 (6 1997), pp. 6633–6655. DOI: 10.1103/PhysRevE.56.6633.

[11] Morten Dalsmo and Arjan van der Schaft. "On Representations and Integrability of Mathematical Structures in Energy-Conserving Physical Systems". In: *SIAM Journal on Control and Optimization* 37.1 (1998), pp. 54–91. DOI: 10.1137/s0363012996312039.

[12] T. Yazaki et al. "Traveling Wave Thermoacoustic Engine in a Looped Tube". In: *Phys. Rev. Lett.* 81 (15 1998), pp. 3128–3131. DOI: 10.1103/PhysRevLett.81.3128.

[13] Jerrold E. Marsden and Tudor S. Ratiu. *Introduction to Mechanics and Symmetry*. Springer New York, 1999. DOI: 10.1007/978-0-387-21792-5.

[14] S. Backhaus and G. W. Swift. "A thermoacoustic-Stirling heat engine: Detailed study". In: *The Journal of the Acoustical Society of America* 107.6 (2000), pp. 3148–3166. DOI: 10.1121/1.429343.

[15] Bernhard Maschke, Romeo Ortega, and Arjan Van Der Schaft. "Energy-based Lyapunov functions for forced Hamiltonian systems with dissipation". In: *IEEE Transactions on automatic control* 45.8 (2000), pp. 1498–1502. DOI: 10.1109/9.871758.

[16] Romeo Ortega et al. "Putting energy back in control". In: *IEEE Control Systems Magazine* 21.2 (2001), pp. 18–33. DOI: 10.1109/37.915398.

[17] Romeo Ortega et al. "Interconnection and damping assignment passivity-based control of port-controlled Hamiltonian systems". In: *Automatica* 38.4 (2002), pp. 585–596. DOI: 10.1016/S0005-1098(01)00278-3.

[18] A.J. van der Schaft and B.M. Maschke. "Hamiltonian formulation of distributed-parameter systems with boundary energy flow". In: *Journal of Geometry and Physics* 42.1-2 (2002), pp. 166–194. DOI: 10.1016/S0393-0440(01)00083-3.

[19] Ernst Hairer, Christian Lubich, and Gerhard Wanner. "Geometric numerical integration illustrated by the Störmer-Verlet method". In: *Acta Numerica* 12 (2003), pp. 399–450. DOI: 10.1017/S0962492902000144.

[20] Anil N. Hirani. "Discrete Exterior Calculus". PhD thesis. California Institute of Technology, 2003. URL: https://thesis.library.caltech.edu/1885/.

[21] D. Eberard and B. Maschke. "Port hamiltonian systems extended to irreversible systems : The example of the heat conduction". In: *IFAC Proceedings Volumes* 37.13 (2004), pp. 243–248. DOI: 10.1016/S1474-6670(17)31230-2.

[22] Romeo Ortega and Eloísa García-Canseco. "Interconnection and Damping Assignment Passivity-Based Control: A Survey". In: *European Journal of Control* 10.5 (2004), pp. 432–450. DOI: 10.3166/ejc.10.432-450.

[23] Benedict Leimkuhler and Sebastian Reich. *Simulating Hamiltonian Dynamics*. Cambridge University Press, 2005. DOI: 10.1017/cbo9780511614118.

[24] Hans Christian Öttinger. *Beyond Equilibrium Thermodynamics*. John Wiley & Sons Inc, 2005.

[25] E. Hairer, G. Wanner, and C. Lubich. *Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations*. Springer, 2006.

[26] Hans Christian Öttinger. "Nonequilibrium thermodynamics for open systems". In: *Phys. Rev. E* 73 (3 Mar. 2006), p. 036126. DOI: 10.1103/PhysRevE.73.036126.

[27] R. Ortega et al. "Control by Interconnection and Standard Passivity-Based Control of Port-Hamiltonian Systems". In: *IEEE Transactions on Automatic Control* 53.11 (2008), pp. 2527–2542. DOI: 10.1109/TAC.2008.2006930.

[28] Vincent Duindam et al. *Modeling and Control of Complex Physical Systems. The Port-Hamiltonian Approach*. Springer Berlin Heidelberg, 2009. DOI: 10.1007/978-3-642-03196-0.

[29] Darryl D. Holm, Tanya Schmah, and Cristina Stoica. *Geometric Mechanics and Symmetry*. Oxford University Press, 2009.

[30] Douglas N. Arnold, Richard S. Falk, and Ragnar Winther. "Finite element exterior calculus: from Hodge theory to numerical stability". In: *Bulletin of the American Mathematical Society* 47.2 (2010), pp. 281–354. DOI: 10.1090/s0273-0979-10-01278-4.

[31] Theodore Frankel. *The Geometry of Physics: An Introduction*. Third Edition. New York: Cambridge University Press, 2011. DOI: 10.1017/CBO9781139061377.

[32] Fernando Castaños et al. "Implicit and explicit representations of continuous-time port-Hamiltonian systems". In: *Systems & Control Letters* 62.4 (2013), pp. 324–330. DOI: 10.1016/j.sysconle.2013.01.007.

[33] Walter Grimus. "100th anniversary of the Sackur–Tetrode equation". In: *Annalen der Physik* 525.3 (2013), A32–A35. DOI: 10.1002/andp.201300720.

[34] Héctor Ramirez, Bernhard Maschke, and Daniel Sbarbaro. "Irreversible port-Hamiltonian systems: a general formulation of irreversible processes with application to the CSTR". In: *Chemical Engineering Science* 89 (2013), pp. 223–234. DOI: 10.1016/j.ces.2012.12.002.

[35] Arjan van der Schaft and Dimitri Jeltsema. "Port-Hamiltonian Systems Theory: An Introductory Overview". In: *Foundations and Trends® in Systems and Control* 1.2 (2014), pp. 173–378. DOI: 10.1561/2600000002.

[36] Mitchel Craun and Bassam Bamieh. "Optimal Periodic Control of an Ideal Stirling Engine Model". In: *Journal of Dynamic Systems, Measurement, and Control* 137.7 (2015). DOI: 10.1115/1.4029682.

[37] François Gay-Balmaz and Hiroaki Yoshimura. *A Lagrangian formalism for nonequilibrium thermodynamics*. 2015. arXiv: 1510.00792 [math-ph].

[38] S. Chaturantabut, C. Beattie, and S. Gugercin. "Structure-Preserving Model Reduction for Nonlinear Port-Hamiltonian Systems". In: *SIAM Journal on Scientific Computing* 38.5 (2016), B837–B865. DOI: 10.1137/15M1055085.

[39] Kai Wang et al. "Stirling cycle engines for recovering low and moderate temperature heat: A review". In: *Renewable and Sustainable Energy Reviews* 62 (2016), pp. 89–108. DOI: 10.1016/j.rser.2016.04.031.

[40] Arjan van der Schaft. *L2-Gain and Passivity Techniques in Nonlinear Control*. 3rd ed. Springer International Publishing, 2017. DOI: 10.1007/978-3-319-49992-5.

[41] Douglas N. Arnold. *Finite Element Exterior Calculus*. Society for Industrial and Applied Mathematics, 2018. DOI: 10.1137/1.9781611975543.

[42] A. Moses Badlyan et al. *Open physical systems: from GENERIC to port-Hamiltonian systems*. 2018. arXiv: 1804.04064 [math.DS].

[43] Arbi Moses Badlyan and Christoph Zimmer. *Operator-GENERIC Formulation of Thermodynamics of Irreversible Processes*. 2018. arXiv: 1807.09822 [math-ph].

[44] Arjan van der Schaft and Bernhard Maschke. "Geometry of Thermodynamic Processes". In: *Entropy* 20.12 (Dec. 2018), p. 925. DOI: 10.3390/e20120925.

[45] Sarah-Alexa Hauschild, Nicole Marheineke, and Volker Mehrmann. *Model reduction techniques for linear constant coefficient port-Hamiltonian differential-algebraic systems*. 2019. arXiv: 1901.10242 [math.OC].

[46] Paul Kotyczka. *Numerical Methods for Distributed Parameter Port-Hamiltonian Systems. Structure-Preserving Approaches for Simulation and Control*. TUM.University Press, 2019. DOI: 10.14459/2019md1510230.

[47] Paul Kotyczka and Laurent Lefèvre. "Discrete-time port-Hamiltonian systems: A definition based on symplectic integration". In: *Systems & Control Letters* 133 (2019), p. 104530. DOI: 10.1016/j.sysconle.2019.104530.

[48] Volker Mehrmann and Riccardo Morandin. *Structure-preserving discretization for port-Hamiltonian descriptor systems*. 2019. arXiv: 1903.10451 [math.OC].