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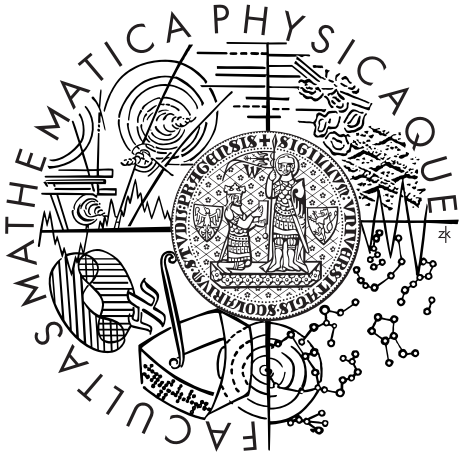

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Optimization of operation of renewable electric energy sources based on fuel cells, accumulators and FV panels for small powers

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Děkuji panu profesorovi Maršíkovi za podporu při vypracování a zkontaktování s výzkumnými kolegy a panu Douckovi za vzorová data pro testování.

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Název práce: Optimalizace funkce obnovitelných zdrojů elektrické energie na bázi palivových článků, akumulátorů a FV panelů pro malé výkony.

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Abstrakt:

První část práce je věnovaná hlubší rešerši do literatury optimálního řízení, shrnutí principů a způsobů jak je aplikovat na prezentovaný problém. Následně je sestaven a popsán model použitelný pro samostatnou energetickou jednotku s použitím vodíkových článků, akumulátoru a fotovoltaických panelů, spolu s nejčastějšími používanými rovnicemi z literatury. Také je formulován problém optimálního řízení řečeného systému pro optimální cenu v provozu při nejlepších podmínkách. Dále jsou popsány algoritmy numerického řešení systému spolu s implementací konkrétního numerického algoritmu „multiple shooting" na tento problém a numerické testy a výsledky.

Klíčová slova: řídící systémy, palivové články, stacionární zdroje energie

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Abstract:

The first part of the research is motivated to provide citations deeper to the literature of optimal control principles that could be linked to the system optimization problem, discuss these principles and various ways to apply them. Then we describe one fuel cell, accumulator and photovoltaic standalone system along with the most used equations from the literature. Next, we formulate the problem of optimal control for this system to optimize the system financial cost in the best case and we process to describe and discuss the numerical optimal control algorithm - multiple shooting - that will be used to solve the problem, that was not used in literature so far in conjunction with the problem. The codes and numerical simulations are also provided.

Keywords: control systems, fuel cells, stationary electric energy sources

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Nomenclature

η_F	Faraday efficiency
η_{ac}	battery efficiency
η_{conv}	effectivity of photovoltaic output power
λ	usual notation for costate
σ_{ac}	battery discharge rate
A_{elec}	area of electrolyzer (m^2)
$B(t)$	energy stored in the accumulator (J)
B_{max}	maximal energy in battery (J)
E_{GO}	band gap of the used PV material
G	Incident radiation (W/m^2)
i	area current (A/m^2)
I_L	light current (A)
I_0	diode reverse saturation current (A)
I_{ac}	battery current (charge or discharge) (A)
I_{bat}	battery current (A)
I_D	diode current (A)
I_d	current at inflection point in fuelcell V-I curve (A)
I_{elec}	current through electrolyzer (A)
I_{pv}	Current from photovoltaic model circuit (A)
I_{sh}	shunt current (A)
K	general notation for one parameter in empiric model for fuelcells
m_{H_2}	hydrogen production rate (kilograms instead of mols) ($\frac{kg}{hr \cdot A}$)
n_e	Electrons in H_2
N_{cell}	number of cells

n_{H_2} hydrogen production rate ($\frac{mol}{hr \cdot A}$)

$P_{batt+max}, P_{batt+max},$ Maximal/minimal power flow to the battery (W)

$P_{batt-max}, P_{batt-max},$ Maximal/minimal power flow from the battery (W)

P_{H_2+min}, P_{H_2+max} Maximal/minimal current to electrolyzer (A)

P_{H_2-min}, P_{H_2-max} Maximal/minimal current from fuelcell (A)

p_{O_2} oxygen partial pressue (Pa)

P_{pv} Power from photovoltaic model circuit (J)

P_{src} source power as energy from solar collectors minus electricity demand (W)

$Q_{bat.i}$ battery capacity (J)

R_{sh} shunt ressistor ressitance (Ω)

R_s parallel resistor ressistance (Ω)

$S(t)$ stored hydrogen ($2F \cdot mol$)

S_{max} maximum of hydrogen in tank ($2F \cdot mol$)

SOC battery state of charge

u usuall notation for control function

u_2 current flow from hydrogen (A)

V_{cell} cell voltage (V)

V_{elec} electrolyzer voltage (V)

V_{fc} fuel cell voltage (V)

V_o open circuit voltage for fuel cell (V)

$V_{pol,ch}$ charging polarization voltage (V)

$V_{pol,dch}$ discharging polarization voltage (V)

V_{pv} operation voltage (photovoltaic) (V)

$V_{rev,fc}$ fuelcell, reversible voltage (V)

x usuall notation for state

AC, DC Analog current, direct current

CFD Computational fluid dynamics

HJB Hamilton Jacobi Bellman (equations)

NLP Nonlinear programming

ODE Ordinary differential equation

PDE Partial differential equation

PEM Proton exchange membrane

PMP Pontryagin maximum principle

PV Photovoltaic, usually photovoltaic panels

SOFC Solid oxide fuelcell

SQP Sequential quadratic programming

Motivation and introduction

For better understanding of the whole problem and work, lets imagine a model situation, that we can follow. Lets say, we want to make an energy independent unit - ecologic house, for example.

Lets add renewable energy source (photovoltaic panels) and a system for storing energy. Batteries alone are not sufficient, because they would need to be changed, due to degradation. So lets add available hydrogen technologies - electrolyzer, hydrogen tank, fuel cells. And, to finish the setting, backup energy unit (or electric grid). The goal is to determine the system parameters (and develop the strategy to do so) and power management strategy in a manner to make the system independent as much as possible (minimizing the consumption of backup energy or energy from grid).

For now, lets look at the theoretical and practical tools needed to solve this problem in the following part "research and previous works". Later we will return to our model problem, and we will use the tools to analyze the setting and rewrite it into mathematical formulation.

Lastly, there will be a brief note about the developed algorithms.

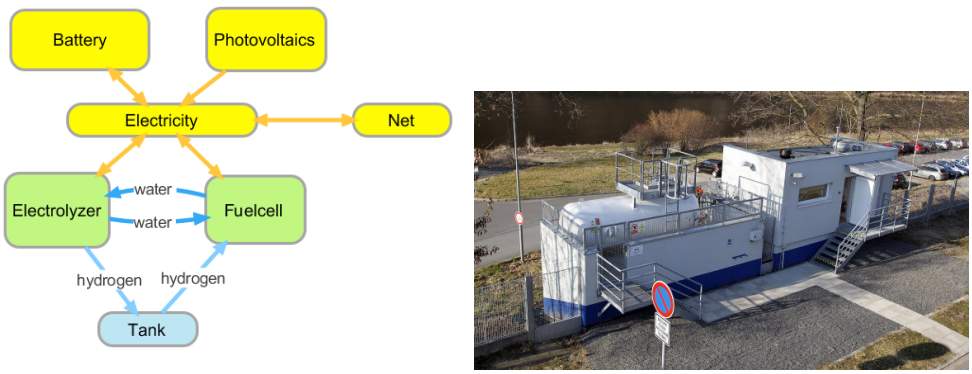

Figure 1.1: Schema of functional units (left) and a photo of existing installation in ÚJV Řež (right) [Kot15]

Basic assumptions and definitions

In this section, lets look at other works and summarize concepts from the relevant fields.

2.1 Optimization and hydrogen technology

Fuel cells and hydrogen technologies (as a part of renewable resources [MDM+11]), extend the possibilities of energy storage [eJ12] and create a need for deeper research of various systems using mathematical tools to model and optimize these systems. One example of such a system are standalone energetic units [MS04].

Some methods of optimization of these standalone systems are summarized in [EU12], optimization of standalone energetic units and power management strategies are being researched too (in, for example [IVS+09]), and some works are also focused on specific installations [AK14], [SCB+14], [TM14], [CAB14]. Also optimization problems are solved for vehicles [MKAD14]. In the article [CdAVvS06], there is proposed an optimal system even for the powerplant of SOFC (solid oxide fuel cell) type. Practical measurements of standalone systems efficiency are described together with theoretical background in [Dou14].

From the other side, practical application of optimization in the theory of optimal control is described in the books [Eva], [Lew12], [War72]. An example of a method used for global optimization is an application of metropolis algorithm, so called Simulated annealing [BM95] (that was originally used for the design of electric circuits or in chemistry [CD97]). There is even a method taking in account the uncertainty of data, called Stochastic annealing [PD95]. This method is used in [GPSV10] for optimization of the parameters of a control strategy.

Another interesting optimization principle, the Pontryagin principle, is used to prolong the lifetime of such systems [XOL+13, ZXZ13, ZXP+14].

Needed to say, that new algorithms of global optimization are often being used (ex. particle swarm, or genetic algorithms). For these algorithms, the question of convergence is still an open problem (about this and another possibilities of such algorithms see the text [Alv06]).

2.2 Models for batteries, fuel cells, electrolyzer, photovoltaics...

There are rich available model descriptions (for example also in [Vep13]), complex models (with PDEs) are used for complicated problems and for detailed desription of inside processes (for example in a battery), but these models aren't meant and suited for simulations taking longer time or scale. More simple models with less variables (for example like curve fitting) are better in case in which we do need to evaluate the model more times per run (as in our case).

2.2.1 Photovoltaics

When looking at photovoltaic (PV) panels, if we want a better model than just saying "general power source", we need to consider that the photoelectric effect (the power source) happens at the P-N junction, which is, of course, a diode, and that there is also some resistance present. That is the reason, why the following (2.1) equivalent circuit - "5 parameter circuit" - is used (there exists even the so called "7 parameter circuit" which has another diode in parallel to the first diode).

Construction details, like material used (single crystalline silicon, polycrystalline and semicrystalline, thin films, amorphous silicon, spheral...) or additional tricks (concentrated cells, lens, antireflexive and other coating) affect the parameters and the efficiency.

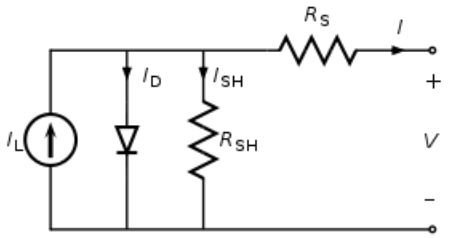

Figure 2.1: 5 parameter equivalent circuit for photovoltaic panel

The circuit supplies current $I = I_{pv}$ at voltage $V = V_{pv}$, I_L is generated current by photovoltaic effect and from that we subtract diode current and shunt current. This way we can derive the model:

$$I_{pv} = I_L - I_D - I_{sh} = I_L - I_0(\exp(\frac{V_{pv} + I_{pv}R_s}{\alpha})) - \frac{V_{pv} + I_{pv}R_s}{R_{sh}} \tag{2.1}$$

$$I_L = C_1 G,\ I_0 = C_2 T^3 \exp(\frac{-E_{GO}}{kT}) \tag{2.2}$$

$$P_{pv} = V_{pv} I_{pv} \eta_{conv} \tag{2.3}$$

- α curve fitting parameter (model requires test runs and measurements)
- G incident radiation $[W/m^2]$
- T surface temperature (K)
- E_{GO} band gap of the used PV material
- C_i constants

- I_L light current $[A]$
- I_D diode current $[A]$
- I_{sh} shunt current $[A]$
- I_0 diode reverse saturation current (comes from the Shockley's diode equation) $[A]$
- V_{pv}, I_{pv}, operational voltage and current $[V]$, $[A]$
- R_s, R_{sh}, parallel and shunt ressistors $[\Omega]$
- P_{pv}, η_{conv} output power and effectivity $[W]$, [dimensionless]

Parameters commonly used to characterize the output of the unit are: short circuit current, open circuit voltage and maximum power point. Nice derivation is in the work [A.98] together with a method on how to compute the parameters from manufacturer supplied information from datasheet, notes on behavior with changing temperature, and finally even a fortran code for PV panels.

In a work focused on solar panels and water electrolysis [Olu11], there is deeper description and analysis and measurement of output power dependency on illumination and even thermal effects. The efficiency of PV energy generation is said to be from 5 to 20 %.

Needed to say, that detailed analysis of output power includes an observation [Vou11], that there is a maximal power point in the voltage current characteristic; this is ideally exploited by a microcontroller, traking this point. (In addition this book covers many interesting details, even about AC/DC converters.) Algorithms for tracking maximal power point are also being developed in [BHB04, SOBL06], also using neural networks is considered [CNCP11].

2.2.2 Battery

Why to use both batteries and hydrogen (tanks) to store energy? Batteries have higher efficiency, but can not store as much energy as we can with hydrogen. Moreover, the state of charge of batteries tends to decrease and batteries tends to lose quality over time. But using them as quick source, or buffer of energy, is generally a good idea. Moreover, in a case, where electrolyzer works more efficiently at lower loads, battery can lower the load by taking it on itself.

The main variables for a common battery model are the voltage and state of charge (SOC). Lets speak about a model of lead acid accumulator from [Vou11] - the model is generally valid for batteries charged more than 20 %, has relations for charging and discharging and is parametrized by parameters that need to be computed experimentally. (Needed to say, that there exist models even for overcharged batteries and other specific cases.)

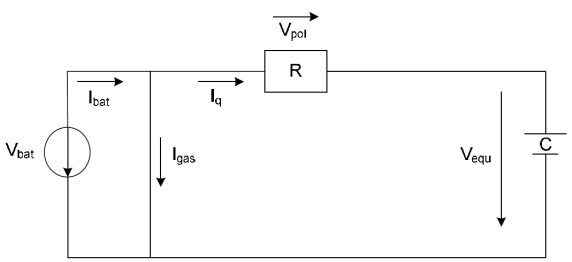

Figure 2.2: Equivalent circuit for lead acid accumulator.

$$I_{bat} = I_q - \frac{Q_{bat,nom}}{10} g_0 \exp(\frac{V_{cell}}{g_1} - \frac{g_2}{T_{bat}}) \tag{2.4}$$

The battery current is the reaction current (I_q) minus the gas current losses, that are modelled using nominal capacity of accumulator ($Q_{bat,nom}$ in Ah), cell voltage, temperature and gassing current parameters. The cell voltage is the equillibrium voltage plus polarization voltage:

$$V_{cell} = V_{equ,0} + \frac{V_{equ,l} SOC}{100} + V_{pol} \tag{2.5}$$

The equillibrium voltage is approximated linearily by its value at $SOC = 0$ and slope $V_{equ,l}$, the polarization voltage is different for charging and discharging (with coefficients dependent on the battery):

$$V_{pol,ch} = U_{ch} a_{ch} (1 - \exp(-\frac{I_{q,norm}}{b_{ch}}) + c_{ch} I_{q,norm}) \tag{2.6}$$

$$V_{pol,dch} = U_{dch} (1 - \exp(-\frac{I_{q,norm}}{b_{dch}}) + c_{dch} I_{q,norm})(1 + (g_{100} - 1) \exp(\frac{SOC - 100}{k_{100}})) \tag{2.7}$$

The indexes "ch" stand for charging and "dch" for discharging. The parameters g_{100}, k_{100} are height and slope parametes for fully charged battery ($SOC = 100\%$).

A discrete model for a capacity of the battery is

$$Q_{bat,i} = Q_{bat,i-1} + I_q(t_i - t_{i-1}) = Q_{bat,nom} SOC_{i-1}/100 + I_q(t_i - t_{i-1}) \tag{2.8}$$

The state of charge of the accumulator is a fraction of the current capacity at each time instant divided by its nominal capacity. So for SOC we have a model with efficiency (η_{ac}), discharge rate (σ_{ac}) and charge or discharge current I_{ac}.

$$SOC(t+1) = SOC(t)(1 - \sigma_{ac}) + I_{ac} \eta_{ac} (\Delta t) \tag{2.9}$$

SOC cannot be directly measured, it needs to be derived from the model or indirectly from experiements.

2.2.3 Electrolyzer and Fuel cell

Electrolyzer and fuel cell both basically operate from a simple chemical reaction ([RS03]) :

$$H_2O \longleftrightarrow H_2 + \frac{1}{2} O_2 \tag{2.10}$$

By adding (electric) power, the reaction occurs from left side to the right, producing hydrogen and oxygen, whereas combining hydrogen and oxygen allows us to get the energy back. The first way is the basic function of electrolyzer and the latter is of the fuel cell. By Faradays law, the (molar) quantity of produced/consumed hydrogen is proportional to transfered charge.

Interesting details arise from the exact engeneering of both processes (parameters like temperature, material of electrolyte or membrane, catalyzators etc...), anyway the basic common variables are voltage, current and temperature.

It is good to note, that hydrogen has the best heating value (energy to fuel ratio). The higher heating value is $142.12\,MJ\,kg^{-1}$, the pure standard heat formation of the product water. The lower heating value is $120.21\,MJ\,kg^{-1}$, calculated from the fact, that the product oxygen goes out unused as a steam (at said 150 °C). Electrolysis is not the only way to get hydrogen, other ways are being considered too, for example by reforming natural gases.

2.2.3.1 Electrolyzer

Common types of electrolyzers are alkaline based (operates using an alkaline solution) and proton exchange membrane electrolyzer (PEM).

As presented in [Vou11], there are many ways that lead to the voltage-current model of the electrolyzer: regression, models based on analysis of processes on anothe, cathode and membrane (and calculating then V-I relationship by subtracting from the open circuit voltage the voltages of activation polarization and ohmic polarization), and even rigorous CFD models.

2.2.3.2 Butler Volmer equation

In the work [A.98], it is noted, that at low voltages, the electrolyzer is more efficient, but generates small amounts of hydrogen. The Butler-Volmer equation is used to model the system:

$$I = I_{0e}(\exp(\frac{(1-\alpha_e)n_eF}{RT}(U-U_{eq})) - \exp(-\frac{\alpha_e n_e F}{RT}(U-U_{eq}))) \tag{2.11}$$

With unknown parameters I_{0e}, α_e (symmetry factor) and U_{eq}. Hydrogen production rate is computed as follows:

$$n_{H_2} = \frac{N_{cell} I_{elec}}{n_e F}\eta_F \tag{2.12}$$

where F is Faraday constant and η_F is Faraday efficiency (relation between theoretical and actual electron transfer, often to be determined by experimental measure), $n_e = 2$.

One empirical model

$$V_{elec} = V_{rev,elec} + \frac{r_1 + r_2 T}{A_{elec}} I_{elec} + (s_1 + s_2 T + s_3 T^2)\log(\frac{t_1 + t_2/T + t_3/T^2}{A_{elec}} I_{elec} + 1) \tag{2.13}$$

This model primary expresses dependency on temperature ([Vou11]). There exists even empirical model for the faraday's efficiency, that also accounts for the fact, that with decreasing current and/or higher temperatures, the parasitic currents increase (because of the electrolyte).

$$\eta_F = B_1 + B_2 \exp(\frac{B_3 + B_4 T_{el} + B_5 T_{el}^2}{i}) \tag{2.14}$$

2.2.3.3 Fuel cell

The exact process in fuel cell happens in this way:

$$\begin{aligned} H_2 &\rightarrow 2H^+ + 2e^- \\ \frac{1}{2}O_2 + 2e^- &\rightarrow O^{2-} \\ 2H^+ + O^{2-} &\rightarrow H_2O \end{aligned}$$

And the calculation (from [Olu11]) for the amount of hydrogen produced is:

$$n_{H_2} = \epsilon \cdot 0,01866 \frac{mol}{hr \cdot A},\ m_{H_2} = \epsilon \cdot 3,77 \cdot 10^{-5} \frac{kg}{hr \cdot A} \tag{2.15}$$

... where ϵ is the fuel cell efficiency:

The simplest way to model fuel cell V-I relationship is to look at it as a reverse electrolyzer, this way is followed by the following model from [Vou11].

First empiric model Takes into account the overvoltages (ohmic and activation), but not effects of mass. The model computes the cell voltage V_{fc} using open circuit voltage V_o, current density i (in A/m^2), model parameter b, current at the inflection point of the V-I curve I_d and slope Δ at the linear stage of ohmic overvoltage:

$$V_{fc} = E + \frac{b}{\ln(1/I_d\, i)} - (\Delta - \frac{b}{4I_d})\, i \tag{2.16}$$

The parameters ($K \in \{E,\ I_d,\ b,\ \Delta\}$) vary with fuel cell temperature T and oxygen partial pressure p_{O_2}:

$$K = K_1 + K_2 T + K_3 T \ln(p_{O_2}) \tag{2.17}$$

It is said, that this model is suitable more for low voltages and powers. But it can be used even for electrolyzer (p_{O_2} is then the operating pressue for the electrolyzer at which the oxygen is produced).

Second empiric model This model takes into effect even the mass transport limitation. For computation of a cell voltage V_{fc} and open circuit voltage V_o, the following applies:

$$\begin{aligned} V_{fc} &= V_o - a_T \log(i) - ir + m \exp(il) \\ V_o &= V_{rev,FC} + B \log(i_o) \end{aligned} \tag{2.18}$$

Where $V_{rev,FC}$ is the reversible voltage, i the current density (fuel cell current per unit area of the electrode, in units of milliampers per square centimeter),i_0

and B the Tafel parameter (i_0 is the value on the Tafel plot when the current begins to move away from zero), a_T the Tafel slope, r the resistance (in $\Omega \cdot cm^2$), and finally the model parameters m, l representing the overvoltage due to mass transport limits. All these parameters can depend on temperature.

Hydrogen and oxygen then flows according to this equations (by Faradays law, already substitued $n_{e,H_2} = 2$, $n_{e,O_2} = 4$):

$$H_{2,g} = \frac{N_{cell} I}{2F\eta_F}\, mol/s,\; O_{2,g} = \frac{N_{cell} I}{4F\eta_F}\, mol/s \tag{2.19}$$

All these models are empirical and are important because of their low computational complexity. For greater complexity, there are, of course, more sophisticated models using partial differential equations. For more in depth description, there is also a book about fuel cells, that examines every aspect of fuel cell design and explains the details of how fuel cells work [LDM03].

Lets add a word about the storage of hydrogen. The possibilities for storage are to store it at the output pressue of the electrolyzer, or at higher pressue or liquidified. These possibilities are covered in most of presented resources and citations. If we wanted to store the hydrogen in any other way, than at the output pressue, we would need to add the compressor into the equation (like it is done in [VSS$^+$]).

2.3 Optimization and optimal control - general theory

Optimization is a rich field with many subproblems arising from the specific problem settings. Optimal control is actually applied optimization together with variational calculus [Mil99] and has similar subproblems (or subclasses).

As (global) optimization is concerned about finding the minimum of a function with number of parameters, optimal control theory takes this idea to the next step and solves minimum of a functional ("objective function" or "cost function" J that consists of final time objective and integrated Lagrangian) of a dynamic system, evolving in time, controlled by a function (system dynamics).

$$\begin{aligned} \text{minimize } J &= \phi(x(T), T) + \int_0^T L(x, u(x,t), t)\, dt && \text{...cost function / objective function} \\ \dot{x} &= f(x, u(x,t), t) && \text{...system dynamics} \\ x(0) &= x_0 && (2.20) \\ g(x, u(x,t), t) &\leq 0 && \text{...constraints} \end{aligned}$$

In free final time case, the function ϕ is not present.

Problems from calculus of variations can be formulated as an optimal control problem, so the ideas from this field apply in optimal control too. Moreover, optimal control theory has methods for solving the problem of controllability and observability and the presence of noise.

2.3.1.1 Basic terms

Optimization problems have many subclasses (2.3) and optimal control is not an exception.

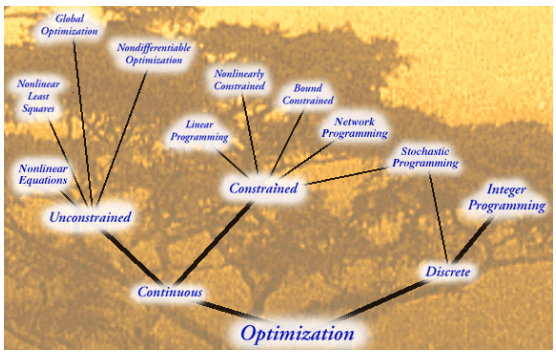

Figure 2.3: Optimization Tree, neos.mcs.anl.gov

So, in formulating the problem, there are many decisions that need to be made, or many features, that can be adressed. To get a grasp of the field, lest summarize the most common features. (More details can be found in the book [BBBB95], the developement of this field over time is summarized in the article [Sar00]).

First, the problem can be formulated in **finite time** or **infinite time**, or the **time can be varied** too ("free time, fixed endpoint" problem vs "fixed time free endpoint"). The model can be **continuous** or **discrete**, not only in **time, but also in states**. Lastly, we can account for **statistical uncertainities**. When we add probability to the problem, we will be dealing with markov chains theory.

The goal, control policy, can be made **open loop** or **closed loop** formulation. Closed loop does care for values and decisions in intermediate states, whereas open loop control has the control function predetermined in advance and does not rely on intermedate states and values. Methods for solving optimal control problems are: **dynamic programming**, **Hamilton Jacobi Bellman (HJB) equations** and **Pontryagin maximum principle** (or minimum principle ... it is called by both names in literature). Only some of the problems can be solved analytically, for example the class of **linear quadratic control** problems, that can be solved through Riccati equations.

Long story short, there are two main approaches - direct methods and indirect methods. Indirect methods take the optimal control problem and reformulate it as differential equation problem with possible boundary conditions - this approach is best used for continuous functions, of course. Direct methods, on the other hand, would see the problem as a problem of nonlinear programming

Both approaches are supported by the strength of calculus of variations [GF64] and both approaches are actually used in numerical solutions.

2.3.1.2 Hamiltonian of the system

Many problem formulations could be efficiently written using Hamiltonian of the system. We will use it too, so lets state the Hamiltonian as a Lagrangian (from cost function) plus adjoint variable times system dynamics, how the Hamiltonian is usually defined:

$$H(x, u, \lambda, t) \quad = \quad L(x, u, t) + \lambda^T f(x, u, t) \tag{2.21}$$

Said efficiency comes from the fact, that the system dynamics is a sort of a constraint and we translate constrained optimization problem to unconstrained - the adjoint variable comes from this idea to introduce lagrangian multipliers (as in [Eva, Lew12, Bry75]) or from HJB equations. There are two ways to get the equations presented later, one gives the name "adjoint variable" to one of the derivatives, so it is conveniet to use the name. It is essential for formulations, that will come later. Lets just note here, that Hamiltonian is constant for systems with parameters independent on time.

To summarize, the problem is then to optimize the value of Hamiltonian - finding such optimal control function u, state function x and costate function λ.

Dynamic programming

Dynamic Programming is a principle well known for problems, that can be decomposed into smaller subproblems. The principle is easy - if the optimal solution of a problem can be composed from optimal solutions of subproblems, we can use this information to build the solution. Whenever this is true (needs, for example, additive cost function), we just do not need to search the whole state space, but we can construct the solution by constructing subsolutions one from another in a clever order. Like, for example, the problem of finding the shortest path in a graph.

Dynamic programming needs discretized problem formulation. Ultimately, going to the limit with discretization points gives rise to the HJB equations.

2.3.1.3 Hamilton-Jakobi-Bellman equations

HJB eqs. are partial differential equations of the problem (here we need the Hamiltonian), the last equation is just system dynamic written using Hamiltonian:

$$J^\star(x(T),T) = \phi(x(T),T) \tag{2.22}$$
$$-\frac{\partial J^\star}{\partial t} = \min_u H(x,u,J^\star_x,t) = L(x,u,t) + J^\star_x f(x,u,t)$$
$$\dot{x} = \frac{\partial H}{\partial \lambda} = f \quad \text{...state equation}$$

When using this apporach, the first step to solve is to get the optimal value function first and from that the other values.

Hamilton-Jakobi-Bellman equations from optimal control gave life to the theory of viscosity solutions (more can be found in the articles [BCD08, Dra, LZ13].) These equations can be solved using finite element methods, but their numerical stability is said to not be good in practise.

2.3.1.4 Pontryagin principle of maximality, PMP

The last step - or method - is principle of maximality (Pontryagin principle of maximality, PMP) and can be - for continuous control functions - derived using the HJB equations (as in [BBBB95]). Using that, we get to formulate equations for adjoint variable - the first equation is pontryagin maximum principle and the second we get by differentiating HJB equation, as in [Die11]. The last condition is the transversality condition for fixed time free endpoint problem.

$$u^\star(t,x,\lambda) = \arg\min_u (H(x,u,\lambda,t))\phi(x(T),T) \tag{2.23}$$
$$-\dot{\lambda} = \frac{\partial H}{\partial x} = \frac{\partial f^T}{\partial x}\lambda + \frac{\partial L}{\partial x} \tag{2.24}$$
$$\lambda(T) = \nabla\phi(x(T),T) \tag{2.25}$$

As was said, we get the same results even from the perspective of taking the system dynamic as constraint for lagrange multipliers.

In the presence of state constraints $x \in R = \{x \in \mathbb{R}^n,\, g(x) \leq 0\}$, PMP is formulated a bit differently [Eva] - we need to define a function

$$c(x,u) = \nabla g(x) \cdot f(x,u) \tag{2.26}$$

and the costate equation becomes:

$$-\dot{\lambda} = \frac{\partial H}{\partial x}(x,u,t) + \mu\frac{\partial c}{\partial x}(x,u) \tag{2.27}$$

While the PMP now states the existence of the function $\mu : [0,T] \to \mathbb{R}$.

Needed to say, that PMP equations are only necessary condition for optimality, so analytical proof of existence and uniqueness is needed.

All these analytic methods will give us equations, to solve the equations is a concern of numerical optimal control.

- HJB Equations - tabulation in state space
- Indirect methods, Pontryagin - solve boundary value problem
- Direct Methods - change to nonlinear programming
  - Single shooting - discretized controls to NLP
  - Multiple shooting - controls and node start values discretized
  - Collocation - disretized controls and states

Figure 2.4: Numerical optimal control cases

2.4 Numerical optimal control

Numerical optimal control can be, again, used to solve either continuous or discretized problems. Heavily relies on the problem analysis and follows the said methods. It would seem, that it is sufficient to just solve HJB PDE's, but it is not used everytime. For example, the problem is, so called, curse of dimensionality - when state and/or control, has many components, the problem becomes exponentially hard to solve. Suggested remedy, in the article [Die11], is, for example, to approximate cost function by another means, for example using neural network methods. Second clue, to know when to use state and costate equations, is, that when we want to have continuous control function, we can just solve the boundary value problem (as in, for example, [Wan09]). When we want to allow discontinuities, we need to rewrite the problem to nonlinear optimization problem (an excellent book about this topic is [Cha07]).

As said above, the main classes are **indirect methods** (first optimize then discretize) and **direct methods** (first discretize, then optimize). Indirect methods result in algorithms similar to ODE solvers, but the resulting system can be badly conditioned or unstable in some cases. Direct methods just rewrite the problem to the area of nonlinear programming problem and then apply convenient solver.

There are three main cases of direct methods - **single shooting**, **multiple shooting** and **collocation**.

Single shooting discretizes the control to piecewise constant function and uses numerical integrator for the evaluation of the cost function (ODE). This way we get a finite dimensional optimization problem, which can be solved by any nonlinear programming algorithm [Bec04], more in section below.

Single shooting algorithm is useful, but the stability can sometimes depend heavily on starting value.

Collocation discretizes both the control function and state function and approximates the integral. We get larger system for nonlinear programming, but the good news is that the system is sparse (in the meaning, that the Jacobian has many zero elements). Collocation can treat better even unstable systems, but refining the grid results in new problem with higher dimensions.

Multiple shooting discretizes the control, as single shooting, and additionally the time scale. So it is called "multiple" shooting, because it works like running single shooting algorithm repeatedly again from the starting times t_i. Of course we need to add constraints for continuity (the end values from the previous interval to be the same as the starting values on the next interval). Multiple shooting algorithm results in only a block sparse problem, but is easy to parallelize and can treat even unstable systems well.

Numerous implementations of numerical optimal control are available, not only in MATLAB, but for example also in C++ in [HFD11].

Nonlinear programming (NLP) Is an area of algorithms for optimizing nonlinear cost functions (on constrained and unconstrained sets). Methods include derived algorithms from ideas of gradient descend or newton method (applied on finding a point where the gradient is zero), for example. Usually these methods can also make use of derivatives (with said newton method on first derivative we, for example, need also second derivatives) and that, in case of optimal control and optimizing differential equations, leads to the need of computing sensitivity equations. That means how the functional depends on the choice of (discretized) control function $\frac{\partial J}{\partial u_i}$. When not supplied, methods usually compute these just by approximating. Algoritmical approaches for getting the results for sensitivity are, for example External Numerical Differentiation, Variational Differential Equations, Automatic Differentiation, Internal Numerical Differentiation (that makes use of the equations written directly in source code for numerical computation).

More details about computing sensitivity equations are for example in [PLCS06]. A suggested technique for solving optimal control problems is, for example, Sequential quadratic programming, SQP , [BT95], [Ott]. It is a method for solving nonlinear problems with second derivatives; uses repeated subsolutions of quadratic programming problems.

Optimal problem algorithm for actual energy source configuration

In this section we will apply the theory and methods to our setting and problem (trying to focus on issues, that were not answered elsewhere).

Contribution of this work Now, lets emphasize, that other existing works tried to model the problem using discontinuous functions and optimized only the system parameters (for minimial cost) for given power management strategy or optimized only the power management strategy (or decision constants of the said strategy).

So our aim will be to optimize the global parameters against the cost (using global optimization algorithms), but for each test case (values of variables) to use the methods of optimal control theory to find the best control strategy. That can be useful in cases, where we wonder about the following:

- How will the perception of the problem change for continuous formulation of equations?
- Will there be a case, when it is not valid to suppose, that for all system parameters the optimal control strategy are still the same through time?

At the end, we will discuss how can we use ideas from other works or how to use the designed method in practical setting.

In the scope of this work, there will be developed an implementation computing the values for an exact desired setting.

3.1 Mathematical formulation

This section will advance from writing the problem in terms of equations to actually applying knowledge and methods for rewritting for numerical solving

3.1.1 Formulation of the optimal control strategy

Since we are using continuous formulation of equations, we are able to follow the optimal control theory for continuous cases (thats one difference from other works).

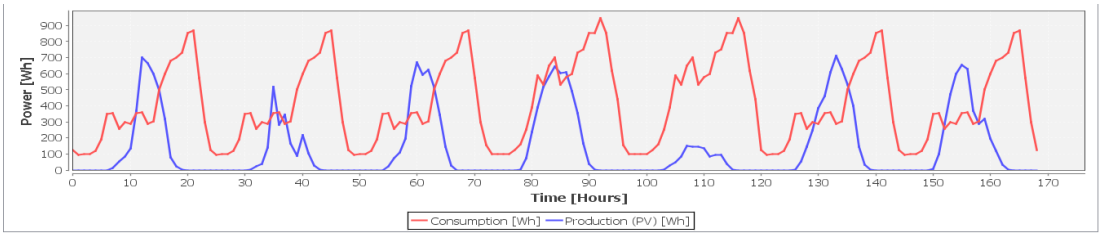

Figure 3.1: First seven days of available data (power production from PV panels from UJV Řež). As the data start with wednesday, notice bigger consumption over weekends (in the middle).

Model using power We need to rewrite the setting using mathematical formulation - to express the boundary conditions, the state variables $x(t)$, the performance index $J()$, the control function $u(t)$ and the dynamics of the system $\dot{x} = f(x, u, t)$ (using notation consistent with the optimal control theory, see eqs. 2.20).

Lets express every state variable in energy, Joules, and control variables in Watts, with exception for u_2, that will be in ampers (see next).

Because we have two state variables - the state of charge of the accumulator $B(t)$ and the stored hydrogen $S(t)$(in the scripts the units are multiplied by Faradays constant times n_e times number of moles - to not do conversion again for electrolyzer and fuelcell), our state is two dimensional real valued function $x(t) = (x_1(t), x_2(t)) = (B(t), S(t))$. These quantities are bounded by $B(t) \leq B_{max}$ and $S(t) \leq S_{max}$, bounds to maximal battery charge and maximal hydrogen stored (in means of power we used to create the hydrogen).

The boundary condition is the source power from solar collectors and power demand, defined as $P_{src}(t) = P_{in}(t) - P_{demand}(t)$, difference between input power and power demand (in Watts). Usually the data would look like in figure 3.1. The control function u is also a two dimensional function of time and will define the power flow:

- the first component tells us about charging/discharging the battery:

$$(\dot{B})(t) = P_{batt}(u_1) - \sigma B(t) \tag{3.1}$$

  Using this equation we can model the efficiency by setting $P_{batt}(u_1) = u_1 \eta_{batt}$ and also the result of auto discharge σ.

  - $u_1 > 0$ ... We are charging the battery, using the power u_1. There is a bound, how much power can we give to the battery $u_1 \in [P_{batt+min}, P_{batt+max}]$
  - $u_1 = 0$ ... Battery disconnected
  - $u_1 < 0$ ... We are discharging the battery, getting the power $-u_1$. There is a bound, how much power we can get from battery $-u_1 \in [P_{batt-min}, P_{batt-max}]$

- The second component tells us about the current flowing from the hydrogen source:

$$(\dot{S})(t) = P_{H_2}(u_2) \tag{3.2}$$

Definitely the term will be different for u_2 positive and negative, because this equation models two different devices:

- $u_2 > 0$ ... The electrolyzer is turned on, using the power$P_{H_2}(u_2)$. There is a bound, how much current can flow $u_2 \in [P_{H_2+min}, P_{H_2+max}]$
- $u_2 = 0$ ... No change in hydrogen supply
- $u_2 < 0$ ... The fuel cell is turned on, giving us the power $P_{H_2}(u_2)$. There is a bound, how much current we can get $-u_2 \in [P_{H_2-min}, P_{H_2-max}]$

Again, here we can model the efficiency (for example $P_{H_2}(u_2) = \frac{N_{cell}u_2}{2F\eta_F}\eta_{H_2}$ for $u_2 < 0$ - the current would flow to the fuelcell, so we use the equation for fuelcell 2.18 multiplied by efficiency) and even nonlinear characteristics of the efficiency. This design follows the wise rule, that the electrolyzer and fuel cell should not operate simultaneously (because that would be a waste of power). The bounds are, for example, the technical specifications set by the manufacturer. Why do we use current for u_2 as a variable and not power? Because the model equations 2.18 give us how the voltage depends on current (and from that we can get the power dependency on current and thats the function $P_{H_2}(u_2)$).

Also in many cases in literature, the result of the analysis of the optimal control problem is, that the actual control function is so called bang-bang control or bang-off-bang control. These controls are called this way, because they only use maximal allowed values and zero (turned off). In our case it would not be wise to follow this path, because the efficiency, in the means of power, varies.

So, once again and nicely written, the dynamics of our system is:

$$\begin{aligned} \dot{x} &= f(x,u,t) \\ \begin{bmatrix} \dot{B(t)} \\ S(t) \end{bmatrix} &= \begin{bmatrix} P_{batt}(u_1) \\ P_{H_2}(u_2) \end{bmatrix} + \begin{bmatrix} -\sigma \cdot B(t) \\ 0 \end{bmatrix} \end{aligned} \tag{3.3}$$

To finish our formulation, we want to find the minimizing control function $u^\star$ (and the corresponding minimizing trajectory $x^\star$ and costate $\lambda^\star$ - will be introduced later) to minimize the performance index

$$\begin{aligned} J &= \phi(x(T),T) + \int_0^T L(x,u,t)\,dt \\ &= hcost(S(T)) + bcost(B(T)) + \int_0^T pcost(P_{src} - P_{batt} - P_{H_2})\,dt \end{aligned} \tag{3.4}$$

where $hcost(x)$ is a function that gives a price for hydrogen, $bcost(x)$, price for power in the battery and $pcost(x)$ is a function that translates power exchange with the grid to its money cost. Generally $pcost(0) = 0$, $pcost(x) \cdot x \geq 0$, $|pcost(x)| \leq |pcost(-x)|$ and all the functions are bounded on bounded intervals.

That simply says, that for not using the grid we pay nothing, selling gives us money, by buying we lose money and that selling the power to grid would not give us such an amount of money as we would lose by buying the power.

Generally we can think of any *pcost* function, in the solution and scripts below we will simply use $pcost(x) = c_1 x$ if $x \geq 0$, otherwise $= c_2 x$, for $c_1, c_2 \geq 0$.

As we will see later, the most important thing is, that the function $J[x(u)]$ would be continuous.

Note If we wanted to not optimize the cost, but the effectivity (in means of power), we would simply use $L(x, u, t) = |P_{src} - P_{batt} - P_{H_2}|$, $\phi = 0$.

Thats exactly the power, we are outputting to the net (or withdrawing from) over selected time interval $[0, T]$. We are not interested in the final value (even not in minimizing any function of the final state) so it is classified as final state free problem.

Models for business problems As a note, every optimal control problem, whose aim is to find the optimal strategy and the minimum of the functional, can be upgraded so it can compute parameters for the most economic installation. The adjustment is just adding parameters to the equation, that will allow us to use components with different efficiency and tie these to a cost. The cost, in turn, can then be added to the cost functional (with keeping an eye on the fact that then the physical units will become a currency and making any necessary adjustments) and the parameters can be also passed to the numerical optimalizator.

For the test run in the scripts attached, very simple models are used, that bind the efficiency quadraticaly to cost (bounded on an interval).

3.1.2 Construction of solutions and rewriting the problem

Now we will look at different formulations and used methods from the literature, that will give us necessary conditions for minimality, even from different views.

Hamiltonian The Hamiltonian of our system, using $\lambda \in \mathbb{R}^2$ as lagrange multipliers is

$$\begin{aligned} H(x, u, \lambda, t) &= L(x, u, t) + \lambda^T f(x, u, t) \\ &= |P_{src} - P_{batt} - P_{H_2}| + \lambda_1(P_{batt}(u_1) - \sigma \cdot B(t)) + \lambda_2 P_{H_2}(u_2) \end{aligned} \tag{3.5}$$

By the way, because our state equations do not depend on time, our Hamiltonian is constant. If we would include the fact that, for example, the battery gets old and less efficient in time, the hamiltonian will suddenly become non constant.

Additionally, in the presence of state constraints (for example $x \in [0, B_{max}] \times [0, S_{max}] \iff \{x \in \mathbb{R}^2,\, g(x) \leq 0,\, g(x) = -((x_1 - 1/2 B_{max})^2 + 1/4 B_{max}^2)((x_2 - 1/2 S_{max})^2 + 1/4 S_{max}^2)\}$), the definition of Hamiltonian alone is not sufficient and the theory usually also defines the function

$$c(x, u) = \nabla g(x) \cdot f(x, u) \tag{3.6}$$

(that will be used later).

Conditions for minimum Other (necessary) conditions for minimum are: (state equation, costate equation, boundary conditions)

$$\begin{aligned}
\dot{x} &= \frac{\partial H}{\partial \lambda} = f && \text{...state equation}\\
-\dot{\lambda} &= \frac{\partial H}{\partial x} = \frac{\partial f^{\mathsf{T}}}{\partial x}\lambda + \frac{\partial L}{\partial x} && \text{...costate equation}\\
x(t_0) &= (0,0) && \text{...boundary condition}\\
0 &= (\phi_x + \psi_x^{\mathsf{T}}\nu - \lambda)^{\mathsf{T}}|_T dx + (\phi_t + \psi_t^{\mathsf{T}}\nu + H)^{\mathsf{T}}|_T dT && \\
& && \text{...boundary condition prototype}\\
0 &= \psi(x(T),T) && \text{...final state constraint (if present)}\\
0 &= \lambda^{\mathsf{T}}|_T dx + H^{\mathsf{T}}|_T dT && \text{...boundary condition in our case } (dT = 0)\\
\lambda_i(T) &= \frac{\partial \phi}{\partial x_i}(x(T),T) && \text{...boundary condition for costate (for free final state)}\\
\lambda_i(T) &= 0 && \text{...boundary condition for costate in our case}
\end{aligned} \tag{3.7}$$

Pontryagin minimum principle Because values of control function are bounded (maybe even discrete for degenerated intervals), we need to use Pontryagin maximum principle (we are dealing with constrained input problem) "the Hamiltonian must be minimized over all admissible u for optimal values of the state and costate." If we had continuous control function, the problem could be tackled by more traditional approach using derivative of Hamiltonian with respect to u.

In other words $H(x^\star, u^\star, \lambda^\star, t) \geq H(x^\star, u, \lambda^\star, t)$ for all admissible u. (We have this instead of the stationary condition $0 = \frac{\partial H}{\partial u} = \frac{\partial L}{\partial u} + \frac{\partial f^T}{\partial u}\lambda$)

In the presence of state constraints ("maximum principle for state constraints"), we have the existency of a costate function $p^\star$ and a function $\lambda^\star$, such that:

$$\begin{aligned}
\dot{p^\star}(t) &= -\nabla_x H(x^\star(t), p^\star(t), u^\star(t)) + \lambda^\star(t)\nabla_x c(x^\star(t), u^\star(t)) && (3.8)\\
H(x^\star, p^\star, u^\star) &= \max_u \{H(x^\star, p^\star, u) \,|\, c(x^\star, u) = 0\} && (3.9)
\end{aligned}$$

... for $u^\star$, $x^\star$ solving the control problem (eqs. 2.20) and function c defined above 3.6. (Instead of simple $-\dot{\lambda} = \frac{\partial H}{\partial x} = \frac{\partial f^T}{\partial x}\lambda + \frac{\partial L}{\partial x}$ ...costate equation.)

Hamilton Jacobi Bellman The equation for developement of the optimal cost (computed backwards) is

$$\begin{aligned}
J^\star(x(T),T) &= \phi(x(T),T) && (3.10)\\
-\frac{\partial J^\star}{\partial t} &= \min_u H(x,u,J_x^\star,t) = L(x,u,t) + J_x^\star f(x,u,t) &&
\end{aligned}$$

And to get $u^\star$ using HJB and Minimum principle:

$$u^\star(t,x,\lambda) = \arg\min_u (H(x,u,\lambda,t))\phi(x(T),T) \tag{3.11}$$

3.1.3 Approach using direct methods

Above methods and conditions for minimum come from the indirect approach. Allowing countable number of discontinuities would rise the need to rewrite the problem, as in [GF64]. If we would like to use direct methods with functions with discontinuities, the thoughts will go in different way (eg. not using the notation of Hamiltonian).

3.1.3.1 Ritz method, finite differences and existence

As an important known result about direct methods, the direct way to get to the minimum is the following (using [GF64] as a reference, where also proofs can be found):

In a general situation (application to our specific case will come later), where we want to evaluate a functional $J[y]$ depending on a function y from an general function space $\mathcal{M}$ ($y \in \mathcal{M}$), we first construct an approximating sequence of spaces $\mathcal{M}_i$. Each space $\mathcal{M}_i$ is defined by the basis functions $\{\varphi_i\}_{i=1}^n$, such that their every linear combination $\sum^n \alpha_i \varphi_i$ together make the whole particular space $\mathcal{M}_i$. The sequence of spaces will need to approximate (in subset sense $\mathcal{M}_1 \subseteq ... \subseteq \mathcal{M}_i \subseteq ... \subseteq \mathcal{M}$) the space $\mathcal{M}$ in which we would like the solution to lie. This approach is called Ritz method.

Note, that the space $\mathcal{M}$ is likely to be infinite dimensional, because the solution is, of course, a control function.

Definition of complete sequence Approximating sequence of spaces is called complete, if, for any given $y \in \mathcal{M}$ and $\epsilon > 0$, we can have a function y_n (of the form of linear combination) that differs less than epsilon from the given function - $\|y_n - y\| < \epsilon$.

The convergence results then continue in this way:

Theorem If a functional $J[y]$, $y \in \mathcal{M}$ is continuous (in the norm of the space $\mathcal{M}$) and if a sequence $\mathcal{M}_i$ is complete, then $\lim_{n\to\infty} \mu_n = \inf_y J[y]$ (μ_n's are realized by functions $y_n \in \mathcal{M}_n$, that is then, in fact, a minimizing sequence of functions for the functional $J[y]$).

The finite differences idea then adds, that the approximation in each particular space is done by piecewise linear function.

Together then, if we have a sequence (y_n), of optimal solutions of our problem constrained to space $\mathcal{M}_n$, we are approaching the limit if the given functional is continuous.

3.1.3.2 The application of Ritz method

Does our problem, from the point of view of direct methods from calculus of variations, have this property?

The space $\mathcal{M}$ is, in our case, defined as the space of real valued functions $y(t) = (x(t), u(t)) : \mathbb{R}^4 \to \mathbb{R}$, that are bounded on a bounded interval, $x(t)$ is continuous, and do satisfy the state equation $\dot{x} = f(x, u, t)$ and J is the cost function of our problem, that was given by (in 3.4):

$$
\begin{aligned}
J[x,u] &= \phi(x(T),T) + \int_0^T L(x,u,t)\,dt \\
&= hcost(S(u(T),x(T))) + bcost(B(u(T),x(T))) + \\
&\quad + \int_0^T pcost(P_{src}(x(t)) - P_{batt}(u(t),x(t)) - P_{H_2}(u(t),x(t)))\,dt
\end{aligned}
$$

And because everything comes down to functions P_{batt} and P_{H_2}...

$$
\begin{bmatrix} \dot{B(t)} \\ S(t) \end{bmatrix} = \begin{bmatrix} P_{batt}(u_1) \\ P_{H_2}(u_2) \end{bmatrix} + \begin{bmatrix} -\sigma \cdot B(t) \\ 0 \end{bmatrix} \tag{3.12}
$$

... that are selected to be continuous (see models presented before - 2.18, 2.13, 2.9 - it is not only physically-wise selection that makes approximating easier, computation faster, but it also gives us the needed results here), we just need to clarify our demands on functions *hcost*, *bcost* and *pcost* - to be continuous. Because these functions just translate amouts of physical variable to cost in money, we can assume continuity without causing any harm.

In this analysis we omitted any constraints, but given the fact that the constraints are, in the basic sense, constant, not dependent on anything (because they just limit the maximal allowed powers of components), they are not going to affect continuity in the presence of multipliers, or any clever tricks meant to incorporate the multipliers (and they also dont affect the existence of minima, because they constrain the spaces on which we are searching for the minima).

Our functional is, in the end, easier to work with, than normally presented problems from the calculus of variations, because we do not have derivatives of the control function in our functional.

3.2 Applied numerical procedures and results

Using all previously mentioned, we developed a program capable of answering the following questions:

- "What is the most economic setting for photovoltaic and hydrogen system and what is the specific power management strategy (the optimal control function) of such system?".
- "What is the most economic control function for a specified time scale, given a prediction of consumption and energy generation"

From now on, we will look on the second, easier question, with the goal to verify the effectivity of numerous NLP solvers. So, lets suppose, that we already have measured yearly power consumption and have already installed photovoltaic panels and measured power output. If it is not this case, we can, of course, use the model and approach from [A.98] to get the estimated power output from manufacturer's datasheets. If we would like to answer the first question, the only remaining work would be to add the equation tying together the cost of a PV panels and other equipment and their effectivity.

Lets now have a look at all the implementation details and all the used tools (because this way it would make the actual usage of the scripts less time consuming work) and the accompanynig numerical experiments.

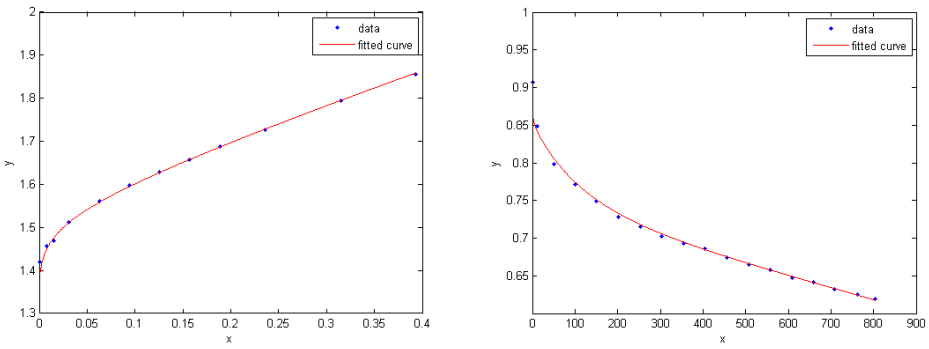

Figure 3.2: Results of the fitting for electrolyzer (left) and fuelcell (right), x axis is current density ($mA \cdot m^{-2}$), y axis is voltage (V). Actual values of parameters are kept in the file `consts.m` together with all the other model constants and numerical settings.

3.2.1 Setting up the constants

Two datasets standing for the boundary conditions of power consumption and demand are supplied. The first data of generated solar energy and house consumption were taken from this dataset `http://www.networkrevolution.co.uk/project-library/dataset-tc5-enhanced-profiling-solar-photovoltaic-pv-users/` (using the monthly average averaged with weekday average for weekdays and monthly average averaged with weekends average for weekends) and through the scripts, the results are in a file `data.txt`. The second dataset is a dataset that was also used in planning of a real standalone system in the work [Dou14], `data2.txt`. (The first dataset was used in first experiments, in this text there will be presented the data from the second dataset to allow comparsion.)

For setting the constants for electrolyzer and fuelcell empiric models, we used the dataset [Bau] and a plot digitizer software from `http://plotdigitizer.sourceforge.net/`. The model parameters were fitted using MATLAB fitting toolbox (and from the results below we can see, that the empiric models are indeed useful and sufficient). The source codes are in the directory "fit".

3.2.2 The scripts and usage

First attempt was to use the ACADO optimization toolkit. Even though the scripts (and tests) were not able to run completely, the source codes using this library are also attached, in the directory AcadoLinearVersion (waiting for the next release of the toolkit).

The next step was to use MATLAB and to write multiple shooting algorithm (as was said, in a way to reformulate the optimal control problem as NLP problem), the formulation is independent on actual solver used and so it is able to run with MATLABs original fmincon function and with any algorithm from OPTI toolbox (`http://www.i2c2.aut.ac.nz/Wiki/OPTI/`). In the case of algorithm breakdown on a specific problem setting, we can just easily switch to a different algorithm.

All used approaches to the problem are reported with respective sources in these directories:

- Directory `MatlabSinglShooting1` contains implementation using single shooting technique. This implementation was not effective for this problem.
- In the main directory, there is an implementation of multiple shooting using MATLAB function fmincon.
- Directory `TrySensitivity` contains the same problem implementation with multiple shooting, but with employed sensitivity equations for computing the derivatives. This approach has not proved to be working effectively (probably because the precise computation of the derivatives results in breakdown of the algorithm more often, than it did when approximating them).
- Directory `4dformulation` contains the code of a slightly differently formulated problem, with 4 control functions (one for electrolyzer, one for battery input, one for battery output and one for fuelcell) in an attempt to try to cure said problem with derivatives, using more dimensional problem, with only positive valued control functions and more constraints. Unfortunately this approach failed, because the resulting matrices in the computation were detected to be badly conditioned by the algorithms.
- Directory `Opti` contains the code for multiple shooting using Opti toolbox solver.
- Directory `AsBusiness` has sample scripts for optimization of the cost - variables that influence the efficiency of the fuelcell are added to the formulation, optimizer and final cost.
- Directory `Test` contains all the code for the numerical test cases presented below.

All the matlab scripts in each directory follow this structure:

- `main.m` - main file, executing in matlab will execute the whole computation
- `ctr.m` - function for computing the constraints (physical and the ones resulting from multiple shooting approach)
- `obj.m` - computing the objective function for optimization
- `fun.m` - computing the whole equation, integration over the time
- `state.m` - evaluation of state equation
- `statesens.m` - script for computing sensitivity equations
- `consts.m` - file for storing the constants and options defining the problem
- `dispopt.m` - script for displaying graphs
- `nlpoutfun.m` - script for displaying the approximations after each iteration
- `interpt1qr.m` - script for fast linear interpolation of the source data

- `controldata` - points on piecewise lienar function defining the power demands
- `dispsaved.m` - the script that would print, after the solver finishes, the graphs like in this work and compute the constraint violation and final cost for comparing.

Every variation of the scripts can be run in the same manner - executing `main.m`. The solved problem is set to examine the effectivity over one year period (or one week in the main folder). You can also notice rescaling constants in `consts.m` - because letting the integrators integrate functions depending on very high time ranges in basic physical units (seconds) would take unreasonable amount of time (also because the boundary conditions are set to change on hour by hour basis and that means that nothing interesting happens for the numerical integrator that tries to watch for sudden changes and keep the precision).

For more discretization points the program becomes, of course, slower. If we want to see some results earlier, we can set the constants "Data.cLogBegin" and "Data.cLogEnd" in `consts.m` to specify at which power of two discretization points to begin and at which to end. This also affects the selection of the initial values - on the first run they are set randomly and on each consecutive run they are copied from previous run (this is because the selection of initial point in the search space can affect the outcome of certain solvers and also their running time).

3.2.3 The numerical experiments

The scripts will start solving the problem on discretized control function to number of discretization points beginning at 2^{cLogBeg} and ending at 2^{cLogEnd} (constants from `consts.m`), using the results from previous run as a starting point for the next run. Some iterations can fail to satisfy the bounds, thinking that the problem is infeasible, because at a lower number of discretization points, achieving the result might be difficult or impossible. This flaw is fortunately automatically fixed when the number of discretization points grows bigger, because higher number of available decision points can steer the system to allowed set of states.

For correct one-year long prediction, the optimization process would take long time (2^{14} discretization points would require more than 4 days of processor time per iteration), so we would chose smaller time scale for testing purposes - one day and 2^5 discretization points (also called number of stages, or "ns=32" in the graphs). The main goal is to explore, which NLP solvers would perform reasonably well on this type of problem.

This test case was set up to control a production of one day, where the photovoltaic power income was less than it would be needed and the test case starts with empty batteries and fuel tank. The goal is to observe lesser cost of electricity over the day.

The currency is set to a virtual one, where to buy an unit of power costs 200 units, to sell it costs 100 units and the energy remaining in batteries and fuel at the end of the run can be sold for 150 units. The efficiency of the battery is set to 70% and the fuelcell is considered ideal in this test case (to see if the algorithm would use the fuelcell even though it's nonlinear characteristic).

The initial point is chosen to be random, because some solvers would consider zero to be a local optimum.

3.2.3.1 Understanding the results

After each iteration, the environment will show the state of the optimization in 4 graphs, like in Figure 3.4 on page 29.

Left top graph shows the state of energy in battery and hydrogen in tank, right top graph shows the evolution of the cost function in time (this curve is an integral of our virtual currency flow, which is just weighted power flow to the system), left bottom graph shows the control function (2 dimension - power to battery and current to hydrogen - so two lines) and right bottom graph shows the state trajectory. The axes in each subfigure are scaled for better run of the algorithm.

At the beginning, the algorithm starts from a point far from optimum. As for multiple shooting, the graph for states is not even continuous during the computation, because the solvers need more iterations to guess correctly the beginnings of the states.

3.2.3.2 Results of test runs

Usually, the results verify, that with lower number of discretization points, the algorithms tend to fail, because they are not able to even meet the provided conditions on such small scale level - the power input and demand oscillates faster, than the number of control points allows for compensation.

From MATLAB and OPTI toolbox, we have applied the algorithms listed in the table 3.3, together with the evaluation of the success of every solver.

Solver	Figure	Note	Optimal cost found	Max constraint violation
FILTERSD	3.4	$\otimes$	-2.429403e+08	7.920000e+06
NLOPT	3.5	$\otimes$	-1.062047e+09	7.919988e+06
SQP	3.6	$\heartsuit$	-2.072860e+08	2.851336e-05
LBFGSB	3.7	T	-3.524222e+08	7.919967e+06
interior-point	3.8	T	8.456483e+13	5.526876e+06
IPOPT	3.9	T	-2.768536e+08	7.919997e+06

Figure 3.3: Results of test runs. All the solvers performed on 32 discretization points, some did time out (T), some broke down and indicated infeasibility ($\otimes$), some finished and satisfied the constraints ($\heartsuit$).

All the solvers managed to find a better strategy than to just buy the power from the grid (which can be seen from the top right graph that would go steeply linearly down), unfortunately some of them did 'cheat' in a sense, that the constraints were not satisfied or were terminated by the time condition (those that did time out were roughly three times slower, than SQP solver). The best performance can be observed for SQP (Sequential quadratic programming) solver, which is in line with the suggested approach from various sources.

The solver converged to make decisions (as seen in figure 3.6) copying the peaks from boundary conditions and mostly using the ideal fuelcell over the bat-

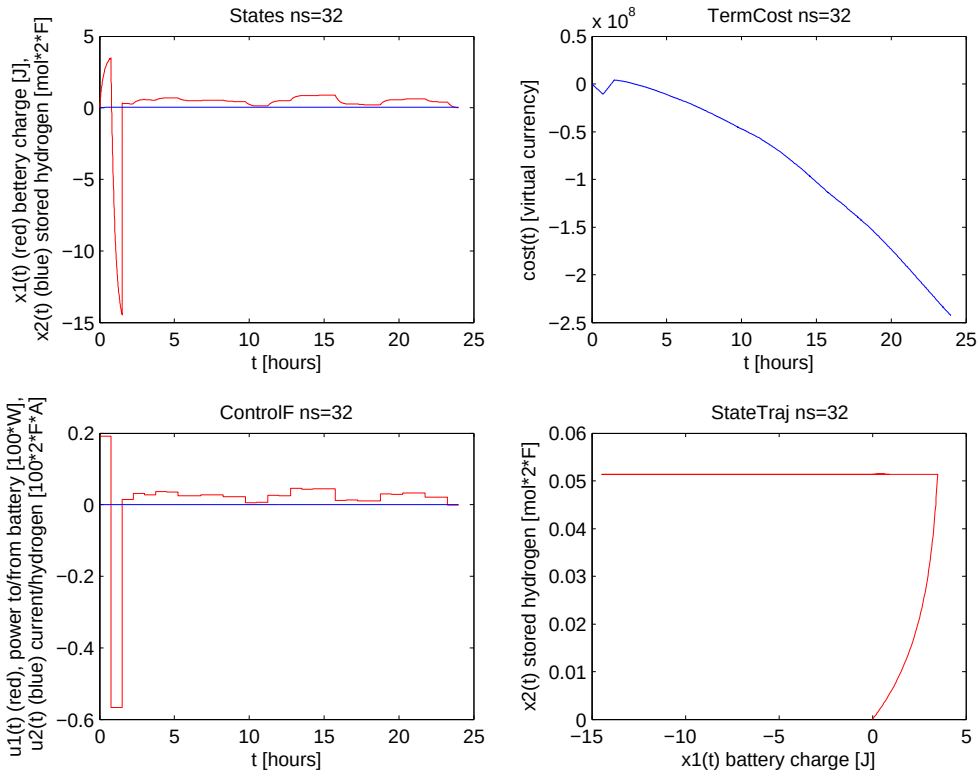

Figure 3.4: FilterSD solver results (failed to satisfy the constraints).

tery - even in spite of accompanying nonlinearities - and used the battery as a backup for one moment of need. In reality, the roles would be reversed and fuelcell used more as long term storage, but that might not be the same challenge for the numerical test of the solver.

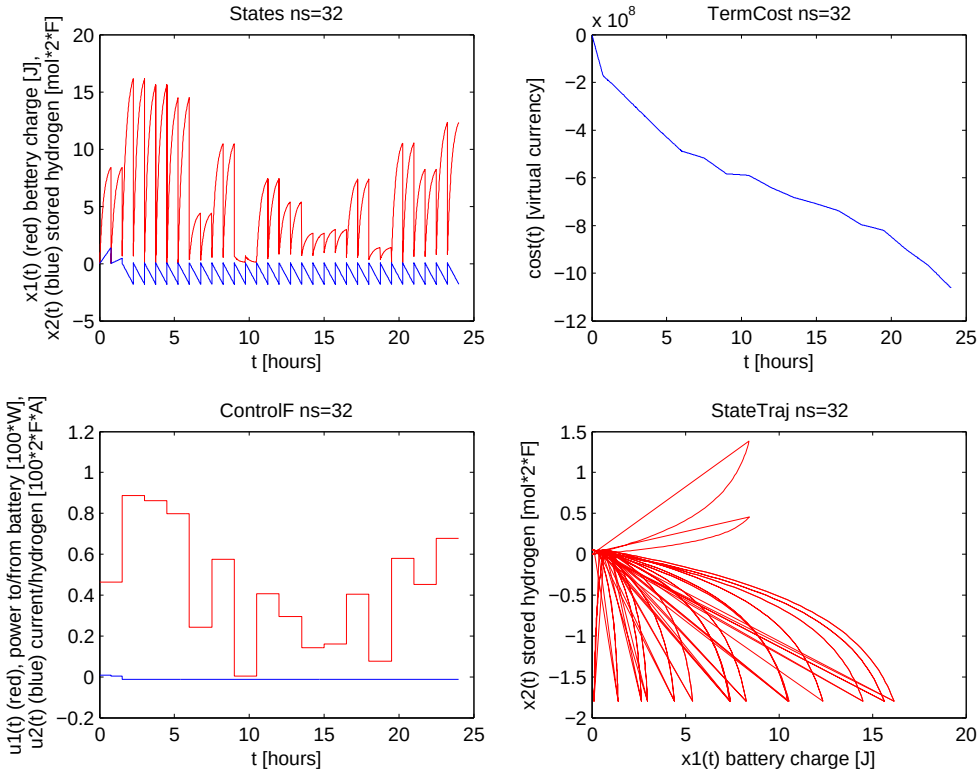

Figure 3.5: NLOPT solver results. Note that it did not manage to satisfy the constraints.

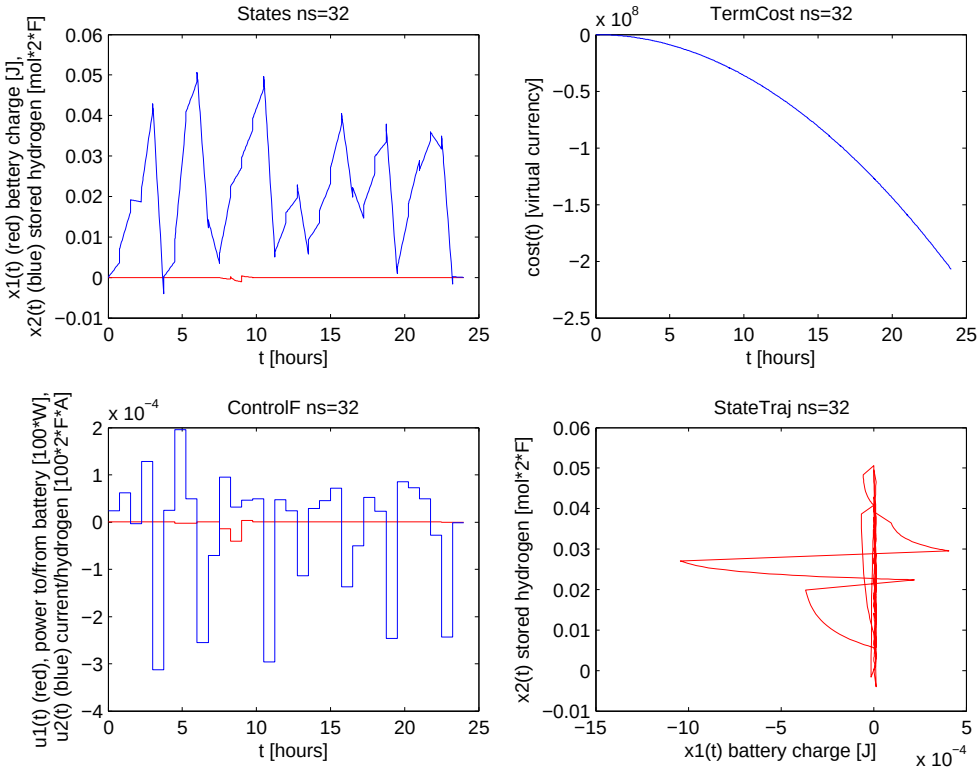

Figure 3.6: SQP solver results (so far the most suited one).

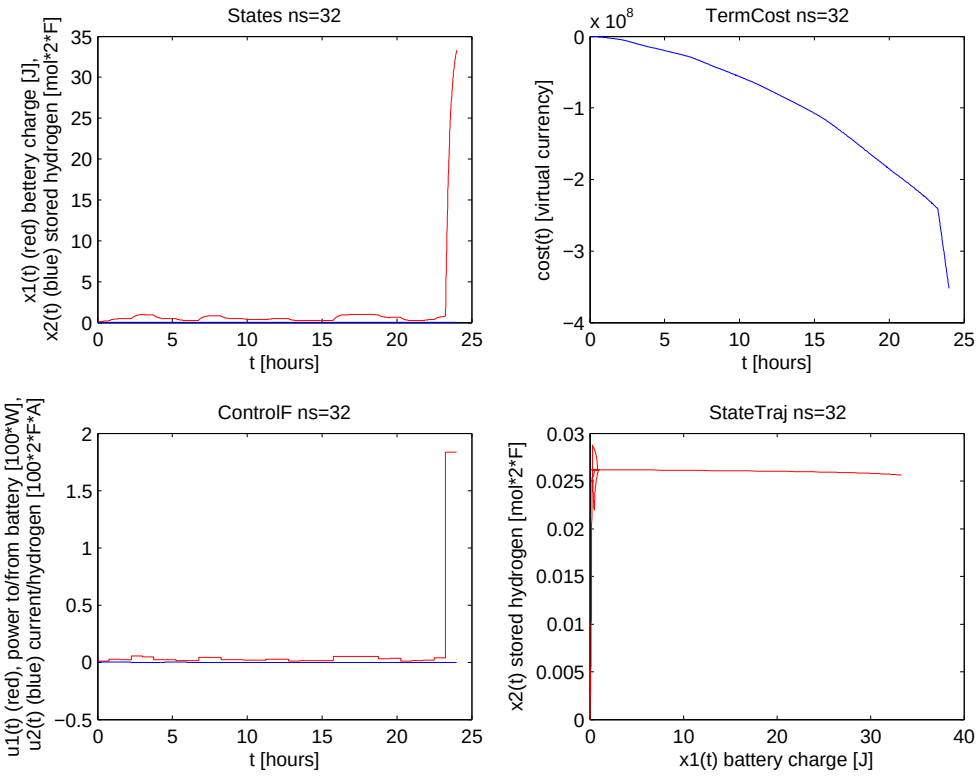

Figure 3.7: LBFGSB solver results (timed out).

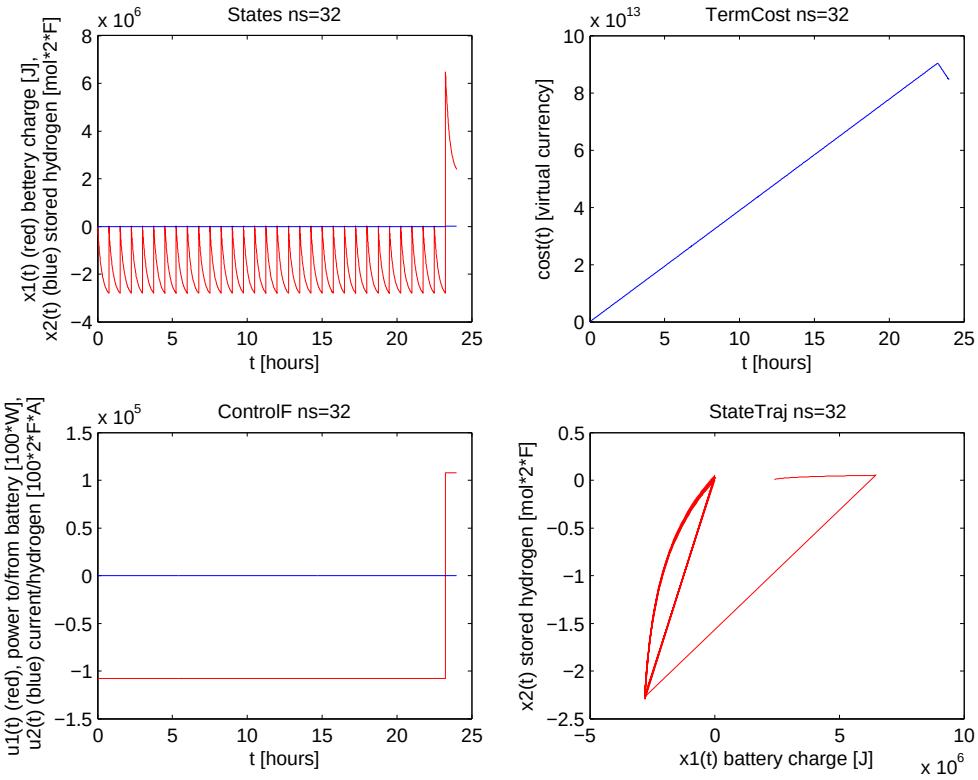

Figure 3.8: Interior-point solver results (timed out).

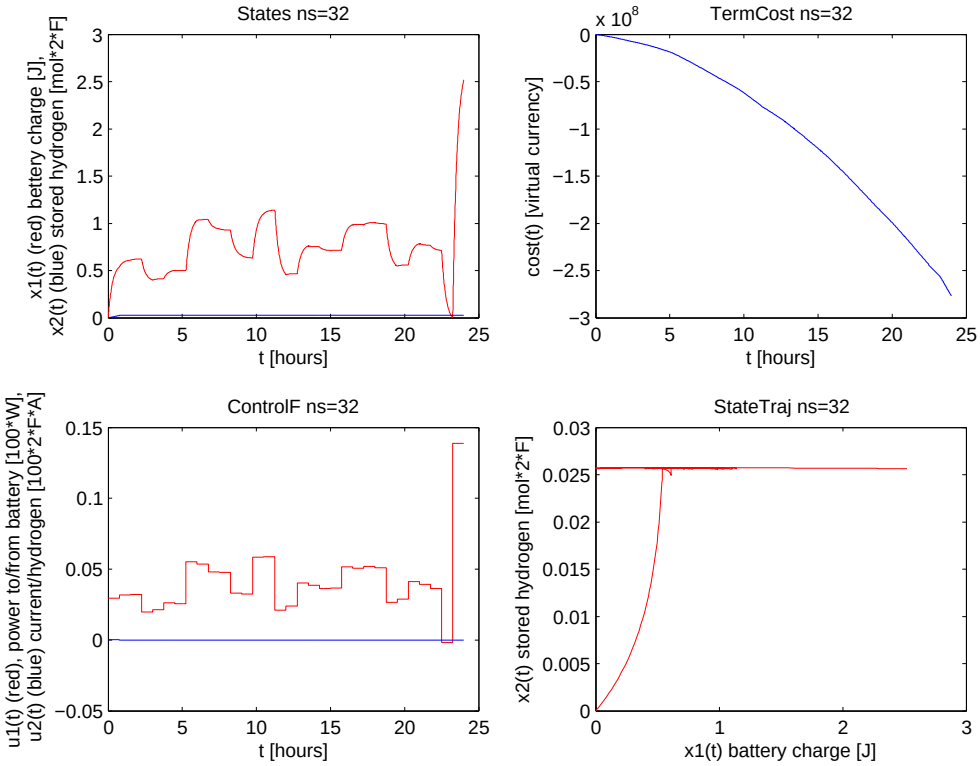

Figure 3.9: IPOPT solver results (timed out).

Conclusion

We have looked up optimal control and fuel cells works and articles, including deeper links to existence results and have applied a numerical optimal control method on a physical problem in a specific way, so that we got:

- method for optimizing system (and system's cost) not against a certain strategy, but against ideal maximum instead (which would work even better in the need of additional control strategy change in runtime).
- method for comparing strategies against ideal maximum - to allow to answer a question whether we can get better, that could not be otherwise answered.
- matlab implementation allowing for solver changes for testing different minimum finding algorithms (in case of breakdowns)

The implemented numerical optimal control method shows, that it is possible to find effective algorithms for controlling small photovoltaic powerplants. It is also shown, that not every numerical solver is able to converge on this specific problem setting.

From the numerical experiments, the solver SQP was verified to be well suited for the problem, which is in line with the literature on the topic of multiple shooting method. Other solvers were compared and found to be unbearably slower (in the case of interior point, IPOPT and LBFGSB) or prone to breakdown (FILTERSD and NLOPT).

Future work could include tuning the method for real applications - the process would need to be implemented, for example, on a graphic card or a computer cluster to be faster. The strength of multiple shooting approach is, that it is already prepared for parallelization.

The implementation can aid in the design of specific photovoltaic powerplant to optimize the initial cost, the implementation can aid in fulfilling this need.

Also given a reasonable forecast of sunshine and power consumption, it can control the system (by precalculating the control for the next week each specified step in time), though this would need to be tested against other (currently considered) best power management strategies.

So we have successfully reached the initial goals:

- Preparing a computer program for modeling of stationary energetic source with commercially available fuelcells and accumulators in combination with available PV installations.
- To propose a control program for storing and using electrical energy in a stationary installation.

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