ETHOS.FINE: A Framework for Integrated Energy System Assessment

Theresa Klütz [1], **Kevin Knosala** [1,2], **Johannes Behrens** [1,2], **Rachel Maier** [1,2], **Maximilian Hoffmann** [1], **Noah Pflugradt** [1], **and Detlef Stolten** [1,2]

1 Forschungszentrum Jülich GmbH, Institute of Climate and Energy Systems – Jülich Systems Analysis, 52425 Jülich, Germany **2** RWTH Aachen University, Chair for Fuel Cells, Faculty of Mechanical Engineering, 52062 Aachen, Germany

Summary

The decarbonization of energy systems worldwide requires a transformation in their design and operation across all sectors, including the residential and commercial, industrial, and transportation sectors. Energy system models are often used to assess these changes. These models provide scenarios for potential future system designs and show how new technologies and infrastructure will meet future energy demand. Thus, they support investment decisions and policy making. The Python-based Framework for Integrated Energy System Assessment (ETHOS.FINE) is a software package that provides a toolbox for modeling, analyzing and evaluating such energy systems using mathematical optimization.

ETHOS.FINE is not limited to a single instance of energy systems. Instead, it can be freely adapted to consider multiple commodities, regions, time steps and investment periods. The optimization objective is to minimize the net present value of the system and is subject to technical and environmental constraints. If only one investment period is considered, the net present value equals the total annual costs of the system. The generic object-oriented implementation allows for arbitrary spatial scales and number of regions – from the local level, e.g., individual buildings, to the regional one, e.g., districts or industrial sites, to the national and international levels.

To reduce model size and complexity, the spatial technological resolution can be aggregated using built-in aggregation methods that are described in Patil et al. (2022). These methods include the aggregation of modeled regions and their given input parameters, and the grouping of technologies within the regions, e.g. to aggregate multiple time series for variable renewable energy sources. This also applies to the temporal resolution of the model. Apart from using the full temporal resolution defined by the input data, integrated time series aggregation methods using the built-in Python package tsam[1] allow to reduce the complexity of the model and its computation time (M. Hoffmann et al., 2022), while still allowing the flexibility of seasonal storage technologies, despite the reduced model complexity (Kotzur et al., 2018). ETHOS.FINE supports the aggregation of time steps to typical periods, the segmentation of the time series and the combination of both. The aggregation methods, spatial and temporal aggregation, can be used directly in ETHOS.FINE by calling the corresponding functions. In addition, ETHOS.FINE allows the investigation of transformation paths by considering multiple investment periods in a perfect foresight approach, as well as the stochastic optimization for a single year optimization with multiple sets of input parameters, e.g., changing energy demand forecasts or weather conditions, to find more robust energy system designs.

---

[1]tsam - Time Series Aggregation Module, https://github.com/FZJ-IEK3-VSA/tsam,

---

Methodology

ETHOS.FINE comprises seven main classes: The EnergySystemModel class can be seen as the container of the model, collecting all relevant input data for its setup. All technologies to be considered are added to this container. The Component class contains the parameters, variables, and constraints common to all system components, such as capacity limits and restrictions on the operation of technologies. The five classes - Source, Sink, Conversion, Transmission, and Storage - provide the functionality to model energy generation and consumption, conversion processes, energy storage for later use, and energy transfer between regions. Each class introduces a specific set of constraints that is added to the optimization program. The specific set of constraints is described in the additional model classes. Supplemental subclasses provide additional component features, e.g., the ability to model partial load behavior and ramping constraints for power plants. The described structure is shown in Figure 1. Objects of the Source, Sink, Conversion and Storage classes are assigned to the modeled locations, which are represented as nodes in the model. Transmission class objects are assigned to the connections between the nodes.
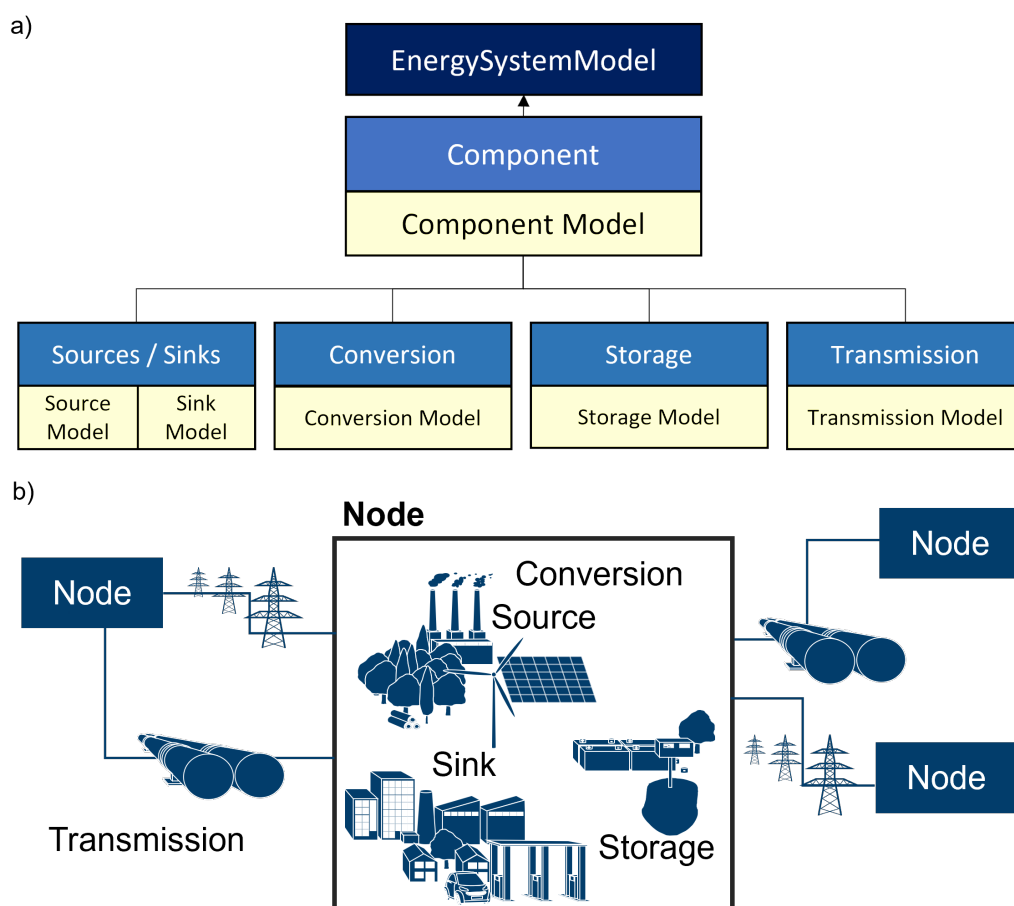
Figure 1: a) Structure of the main classes in ETHOS.FINE. Additional model classes contain the definition of the specific variables, sets and constraints for each class to build the optimization model. b) Simplified representation of the model structure in ETHOS.FINE with the corresponding component classes. Each node represents a region that can exchange goods and energy carriers via transmission components (based on Groß (2023)).

The energy system model can be set up as a linear program (LP), a quadratic program (QP), or a mixed integer linear program (MILP), depending on the chosen representation of the

added components. The optimization program is written as a Pyomo[2] instance to allow a flexible choice of solvers, i.e. `ETHOS.FINE` optimizes energy systems using both, commercial and open source solvers. In a future version, other Python libraries, e.g. linopy (Hofmann, 2023), may be integrated to improve the setup of the optimization program. Depending on the spatial and temporal resolution of the modeled system, the input parameters are primarily given as Pandas.DataFrames[3] with regions and time steps serving as indices and columns. The model output provides detailed information on the investment required in each region for the installation and operation of the selected components, as well as the temporally-resolved operation of each component. This also includes charging and discharging of storage components and commodity flows between regions via transmission components. In addition, the framework provides plotting options for spatially and temporally resolved results. Model input and output can be saved to netCDF files to support reproducibility.

Statement of need

`ETHOS.FINE` offers a unique generic model setup with a high degree of freedom for model developers. Beyond energy system models, its generic implementation allows the modeling of all kinds of optimization problems, such as material flows and resource consumption or conversion as part of life cycle analysis. `ETHOS.FINE` was developed to provide a flexible techno-economic analysis tool to analyze the energy transition on all levels of interest especially with regards to sector-coupled systems. The software exhibits many of the features described by Groissböck (2019) and is under constant development. Its code is openly accessible on GitHub which allows for contributions and feedback from a wider modeling community. The use cases described in the next section demonstrate the broad range of analyses that can be conducted with the tool.

There are several other open-source available energy system modeling frameworks that are also implemented in Python, e.g. Calliope (Pfenninger & Pickering, 2018), PyPSA (Brown et al., 2018), oemof (Hilpert et al., 2018) and CLOVER (Sandwell et al., 2023). The tools are used for similar use cases, providing different sets of functionalities and possible analysis tools. They differ mainly in the setup process of the models. `ETHOS.FINE` offers a highly flexible alternative to these tools.

`ETHOS.FINE` is designed to be used by researchers, students, and for teaching purposes in the field of energy system modeling. In particular, its exceptional capabilities with respect to complexity reduction (Kotzur et al., 2021) using spatial (Patil et al., 2022) and temporal aggregation (M. Hoffmann et al., 2020, 2021, 2022; M. A. C. Hoffmann, 2023), as well as heuristics for dealing with MILPs (Kannengießer et al., 2019; Singh et al., 2022) open a wide field of applications from small to global scale energy system models. For newcomers who are not familiar with programming, it also has the flexibility to set up models by using Excel files, the usability of which is described in one of the example Jupyter notebooks published in the GitHub repository.

Examples for previous usage

`ETHOS.FINE` has been used in various studies for energy system analyses at different scales, taking advantage of its ability to dynamically adapt to computational complexity. First applications can be found in Welder et al. (2018) and Welder et al. (2019): The authors analyzed hydrogen-to-electricity reconversion pathways in a multi-regional energy system model implemented in `ETHOS.FINE` for the northern part of Germany. Later, Welder (2022) and Groß (2023) used the framework to model the future energy system of Germany with a high spatial resolution and thereby to investigate the need for new infrastructure. D. G. Caglayan et al.

---

[2]Pyomo, Pyoton Optimization Modeling Language, https://pyomo.org/,
[3]Pandas, Python Data Analysis Library, https://pandas.pydata.org/,

(2019) built an `ETHOS.FINE` model of the European energy system, and analyzed the influence of varying weather years on the cost-optimal system design based on 100% use of renewable energy source. Their findings are also used to determine a robust system design based on variable renewable energy sources, ensuring security of supply for a wide range of weather years (D. Caglayan et al., 2021). Knosala et al. (2021) evaluated hydrogen technologies in residential buildings in a multi-commodity, single-building model. The building model from this work was also used for a sensitivity analysis of energy carrier costs for the application of hydrogen in residential buildings (Knosala et al., 2022). Spiller et al. (2022) analyzed the carbon emission reduction potentials of hotels on energy self-sufficient islands. More recently, Weinand et al. (2023) used the framework to assess the Rhine Rift Valley for its potential for lithium extraction from deep geothermal wells. Meanwhile, Jacob et al. (2023) investigated the potential of Carnot batteries in the German electricity system. Busch et al. (2023) analyzed the role of liquid hydrogen, also on a national scale, while Franzmann et al. (2023) examined the cost potential of green hydrogen for global trade. These examples illustrate the variety of applications that can be addressed by `ETHOS.FINE`.

`ETHOS.FINE` is part of the Energy Transformation paTHway Optimization Suite (`ETHOS`)[4], a collection of modeling tools developed by the Institute of Energy and Climate Research - Jülich Systems Analysis at Forschungszentrum Jülich. `ETHOS` offers a holistic view of energy systems at arbitrary scales, providing tools for geospatial analysis of renewable energy potential, time series simulation tools for residential and industrial sector, discrete choice models for the transportation sector, modeling of global energy supply routes, and local infrastructure assessments, among others. An example of the use of this model suite can be found in Stolten et al. (2022). The model framework `ETHOS.FINE` serves as a basis for several model implementations within `ETHOS`, e.g. for the optimization programs to analyse of the transformation of single buildings, the transport sector, and the local, German, European and global energy system, or to determine the cost potential of global hydrogen production.

Acknowledgements

References

Brown, T., Hörsch, J., & Schlachtberger, D. (2018). PyPSA: Python for Power System Analysis. *Journal of Open Research Software*, *6*(4, 1). https://doi.org/10.5334/jors.188

---

[4]ETHOS - Energy Transformation paTHway Optimization Suite, https://www.fz-juelich.de/en/iek/iek-3/expertise/model-services

---

Busch, T., Groß, T., Linßen, J., & Stolten, D. (2023). The role of liquid hydrogen in integrated energy systems–A case study for Germany. *International Journal of Hydrogen Energy*. https://doi.org/10.1016/j.ijhydene.2023.05.308

Caglayan, D. G., Heinrichs, H. U., Linssen, J., Robinius, M., & Stolten, D. (2019). Impact of different weather years on the design of hydrogen supply pathways for transport needs [Journal Article]. *International Journal of Hydrogen Energy*, *44*(47), 25442–25456. https://doi.org/10.1016/j.ijhydene.2019.08.032

Caglayan, D., Heinrichs, H., Robinius, M., & Stolten, D. (2021). Robust design of a future 100 [Journal Article]. *International Journal of Hydrogen Energy*, *46*. https://doi.org/10.1016/j.ijhydene.2020.12.197

Franzmann, D., Heinrichs, H., Lippkau, F., Addanki, T., Winkler, C., Buchenberg, P., Hamacher, T., Blesl, M., Linßen, J., & Stolten, D. (2023). Green hydrogen cost-potentials for global trade. *International Journal of Hydrogen Energy*. https://doi.org/10.1016/j.ijhydene.2023.05.012

Groissböck, M. (2019). Are open source energy system optimization tools mature enough for serious use? [Journal Article]. *Renewable and Sustainable Energy Reviews*, *102*, 234–248. https://doi.org/10.1016/j.rser.2018.11.020

Groß, T. M. (2023). *Multiregionales Energiesystemmodell mit Fokus auf Infrastrukturen* (Vol. 604) [Dissertation, RWTH Aachen University; Forschungszentrum Jülich GmbH, Zentralbibliothek, Verlag]. https://doi.org/10.18154/RWTH-2023-01485

Hilpert, S., Kaldemeyer, C., Krien, U., Günther, S., Wingenbach, C., & Plessmann, G. (2018). The open energy modelling framework (oemof) - a new approach to facilitate open science in energy system modelling. *Energy Strategy Reviews*, *22*, 16–25. https://doi.org/10.1016/j.esr.2018.07.001

Hoffmann, M. A. C. (2023). *Temporal aggregation methods for energy system modeling* (Vol. 605) [Dissertation, RWTH Aachen University; Forschungszentrum Jülich, Zentralbibliothek, Verlag]. https://doi.org/10.18154/RWTH-2023-01465

Hoffmann, M., Kotzur, L., & Stolten, D. (2022). The pareto-optimal temporal aggregation of energy system models. *Applied Energy*, *315*, 119029. https://doi.org/10.1016/j.apenergy.2022.119029

Hoffmann, M., Kotzur, L., Stolten, D., & Robinius, M. (2020). A Review on Time Series Aggregation Methods for Energy System Models [Journal Article]. *Energies*, *13*(3). https://doi.org/10.3390/en13030641

Hoffmann, M., Priesmann, J., Nolting, L., Praktiknjo, A., Kotzur, L., & Stolten, D. (2021). Typical periods or typical time steps? A multi-model analysis to determine the optimal temporal aggregation for energy system models [Journal Article]. *Applied Energy*, *304*. https://doi.org/10.1016/j.apenergy.2021.117825

Hofmann, F. (2023). Linopy: Linear optimization with n-dimensional labeled variables. *Journal of Open Source Software*, *8*(84), 4823. https://doi.org/10.21105/joss.04823

Jacob, R., Hoffmann, M., Weinand, J. M., Linßen, J., Stolten, D., & Müller, M. (2023). The Future Role of Thermal Energy Storage in 100% Renewable Electricity Systems. *Renewable and Sustainable Energy Transition*, 100059. https://doi.org/10.1016/j.rset.2023.100059

Kannengießer, T., Hoffmann, M., Kotzur, L., Stenzel, P., Schuetz, F., Peters, K., Nykamp, S., Stolten, D., & Robinius, M. (2019). Reducing computational load for mixed integer linear programming: An example for a district and an island energy system [Journal Article]. *Energies*, *12*(14). https://doi.org/10.3390/en12142825

Knosala, K., Kotzur, L., Röben, F. T. C., Stenzel, P., Blum, L., Robinius, M., & Stolten, D. (2021). Hybrid Hydrogen Home Storage for Decentralized Energy Autonomy. *International*

Journal of Hydrogen Energy, *46*(42), 21748–21763. https://doi.org/10.1016/j.ijhydene.2021.04.036

Knosala, K., Langenberg, L., Pflugradt, N., Stenzel, P., Kotzur, L., & Stolten, D. (2022). The role of hydrogen in German residential buildings. *Energy and Buildings*, *276*, 112480. https://doi.org/10.1016/j.enbuild.2022.112480

Kotzur, L., Markewitz, P., Robinius, M., & Stolten, D. (2018). Time series aggregation for energy system design: Modeling seasonal storage [Journal Article]. *Applied Energy*, *213*, 123. https://doi.org/10.1016/j.apenergy.2018.01.023

Kotzur, L., Nolting, L., Hoffmann, M., Groß, T., Smolenko, A., Priesmann, J., Büsing, H., Beer, R., Kullmann, F., Singh, B., Praktiknjo, A., Stolten, D., & Robinius, M. (2021). A modeler's guide to handle complexity in energy systems optimization. *Advances in Applied Energy*, *4*, 100063. https://doi.org/10.1016/j.adapen.2021.100063

Patil, S., Kotzur, L., & Stolten, D. (2022). Advanced spatial and technological aggregation scheme for energy system models. *Energies*, *15*(24). https://doi.org/10.3390/en15249517

Pfenninger, S., & Pickering, B. (2018). Calliope: A multi-scale energy systems modelling framework. *Journal of Open Source Software*, *3*(29), 825. https://doi.org/10.21105/joss.00825

Sandwell, P., Winchester, B., Beath, H., & Nelson, J. (2023). CLOVER: A modelling framework for sustainable community-scale energy systems. *Journal of Open Source Software*, *8*(82), 4799. https://doi.org/10.21105/joss.04799

Singh, B., Rehberg, O., Groß, T., Hoffmann, M., Kotzur, L., & Stolten, D. (2022). Budget-cut: Introduction to a budget based cutting-plane algorithm for capacity expansion models. *Optimization Letters*, *16*(5), 1373–1391. https://doi.org/10.1007/s11590-021-01826-w

Spiller, M., Müller, C., Mulholland, Z., Louizidou, P., Küpper, F. C., Knosala, K., & Stenzel, P. (2022). Reducing Carbon Emissions from the Tourist Accomodation Sector on Non-Interconnected Islands: A Case Study of a Medium-Sized Hotel in Rhodes, Greece [Journal Article]. *Energies*. https://doi.org/10.3390/en15103801

Stolten, D., Markewitz, P., Schöb, T., Kullmann, F., Risch, S., Groß, T., Hoffmann, M., Franzmann, D., Triesch, T., Kraus, S., Maier, R., Gillessen, B., Heinrichs, H., Pflugradt, N., Grube, T., Linssen, J., & Kotzur, L. (2022). *Neue Ziele auf alten Wegen? Strategien für eine treibhausgasneutrale Energieversorgung bis zum Jahr 2045* (Vol. 577, pp. VI, 81). Forschungszentrum Jülich GmbH Zentralbibliothek, Verlag. ISBN: 978-3-95806-627-4

Weinand, J. M., Vandenberg, G., Risch, S., Behrens, J., Pflugradt, N., Linßen, J., & Stolten, D. (2023). Low-carbon lithium extraction makes deep geothermal plants cost-competitive in future energy systems. *Advances in Applied Energy*, *11*. https://doi.org/10.1016/j.adapen.2023.100148

Welder, L. (2022). *Optimizing cross-linked infrastructure for future energy systems* (Vol. 591) [Dissertation, RWTH Aachen University; Forschungszentrum Jülich, Zentralbibliothek, Verlag]. https://doi.org/10.18154/RWTH-2022-11694

Welder, L., Ryberg, D. S., Kotzur, L., Grube, T., Robinius, M., & Stolten, D. (2018). Spatio-temporal optimization of a future energy system for power-to-hydrogen applications in germany [Journal Article]. *Energy*, *158*, 1130–1149. https://doi.org/10.1016/j.energy.2018.05.059

Welder, L., Stenzel, P., Ebersbach, N., Markewitz, P., Robinius, M., Emonts, B., & Stolten, D. (2019). Design and evaluation of hydrogen electricity reconversion pathways in national energy systems using spatially and temporally resolved energy system optimization [Journal Article]. *International Journal of Hydrogen Energy*, *44*(19), 9594–9607. https://doi.org/10.1016/j.ijhydene.2018.11.194