Powering a Sustainable Future: The Importance of Open-Source Energy Modelling & Energy Data

Sylvain Quoilin

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Integrated and Sustainable Energy Systems (ISES)

- The ISES research group at the University of Liège/KU Leuven
- Part of the Mechanical Engineering department
- Main focus on the modeling of energy systems
- Young research group

Marco Navia

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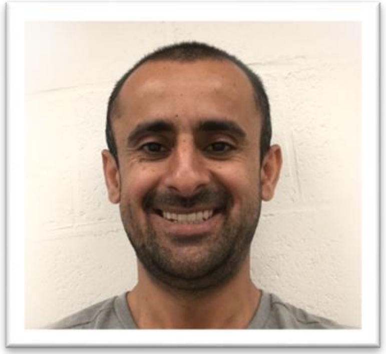
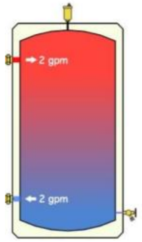


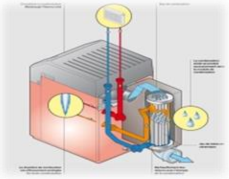
Umair Tareen

What we do at the thermodynamics laboratory

Component Level:

- Monitoring, Dynamic Modeling, Optimal control



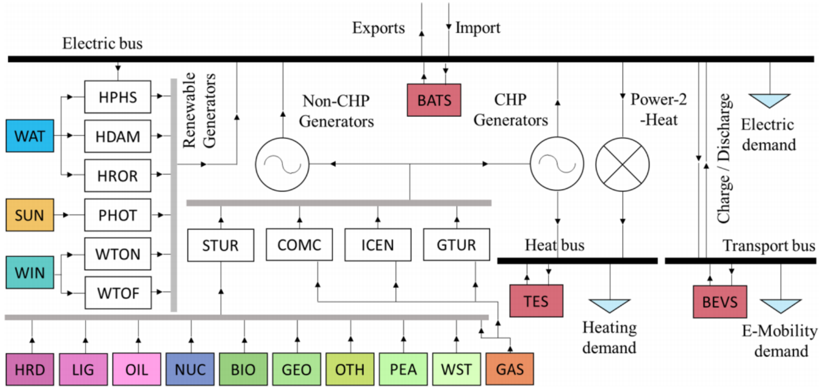



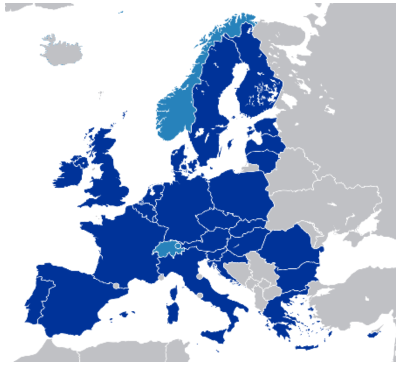




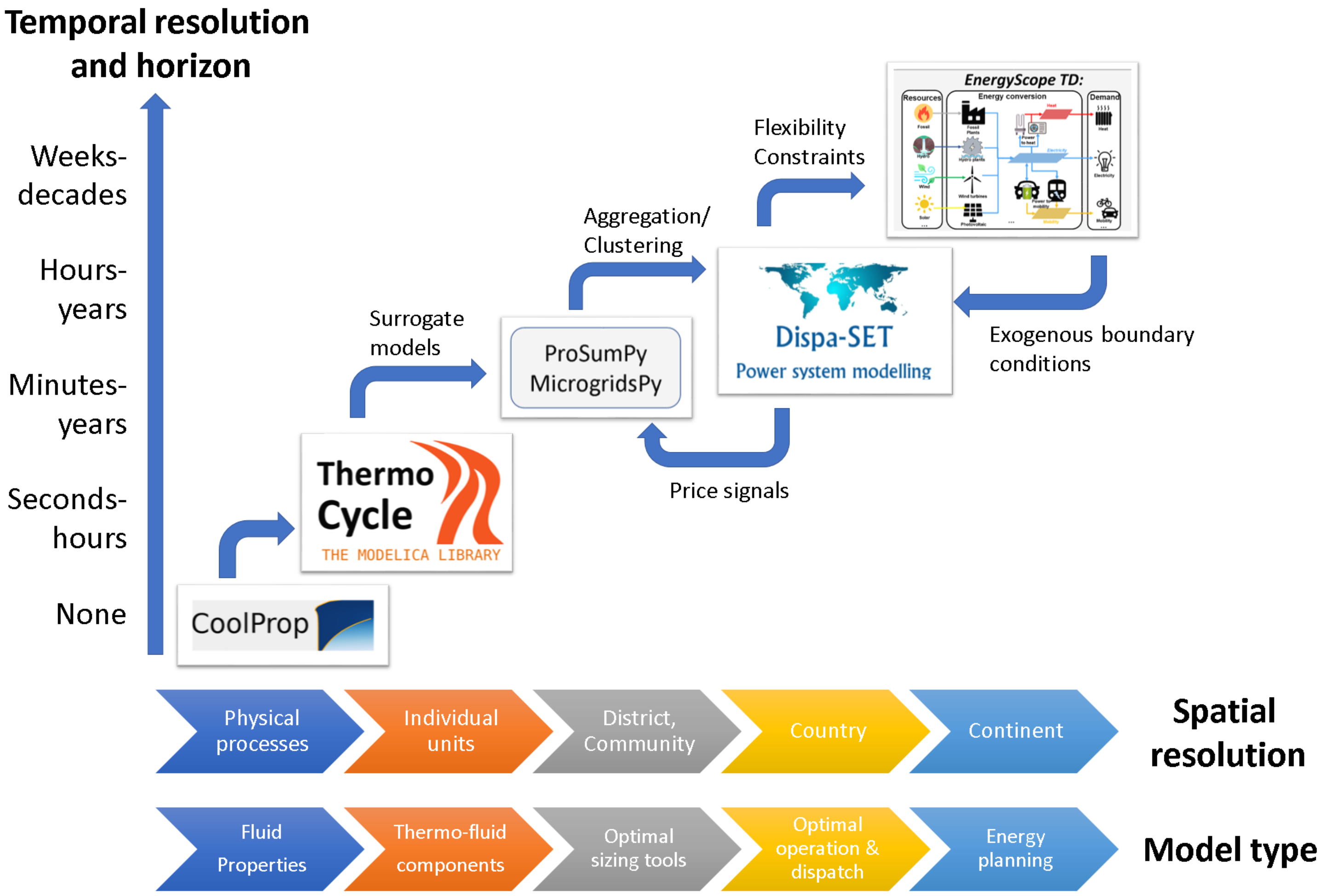

System level:

- Optimal integration, multi-scale simulations, flexibility provision by thermal systems
- Development and use of open-source models:



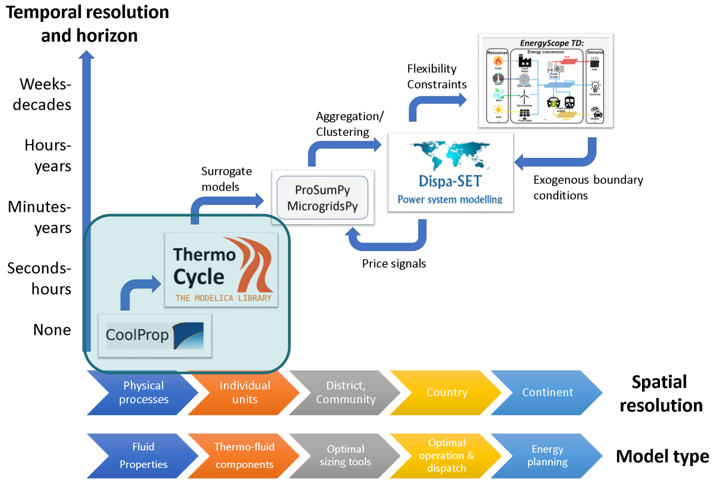


Models to support the energy transition



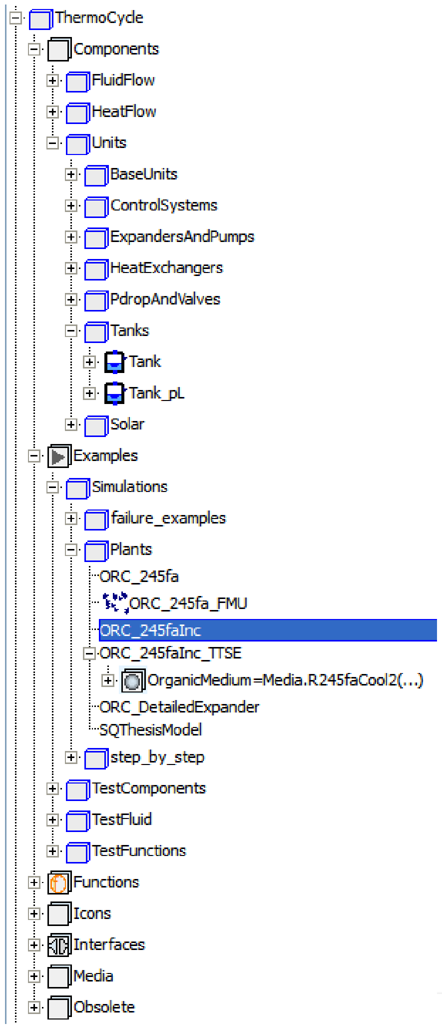
- Multi-scale portfolio of models:
  - **From** the accurate characterization of thermal processes
  - **To** their widespread deployment at country/continental level

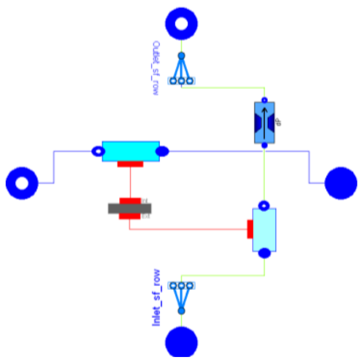
ThermoCycle – CoolProp: dynamic modelling and fluid properties

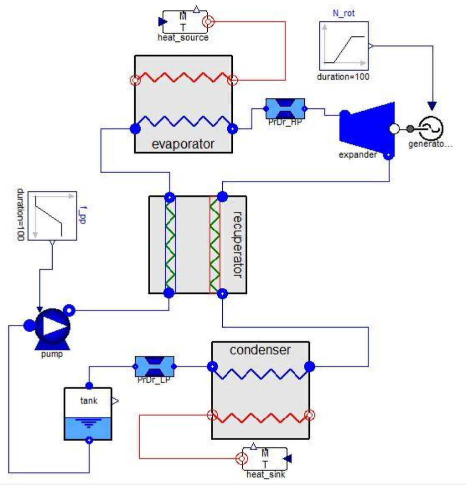


The ThermoCycle Library

- Modelica: Open-source language for the modeling of complex multiphysics systems.
- Acausal language
- ThermoCycle => Open-source Library for the modeling of thermal systems
- Cross-Platform
- Special focus on thermodynamic cycles
- Computational efficiency and robustness are key aspects of the library







Thermo-physical fluid properties: *CoolProp*

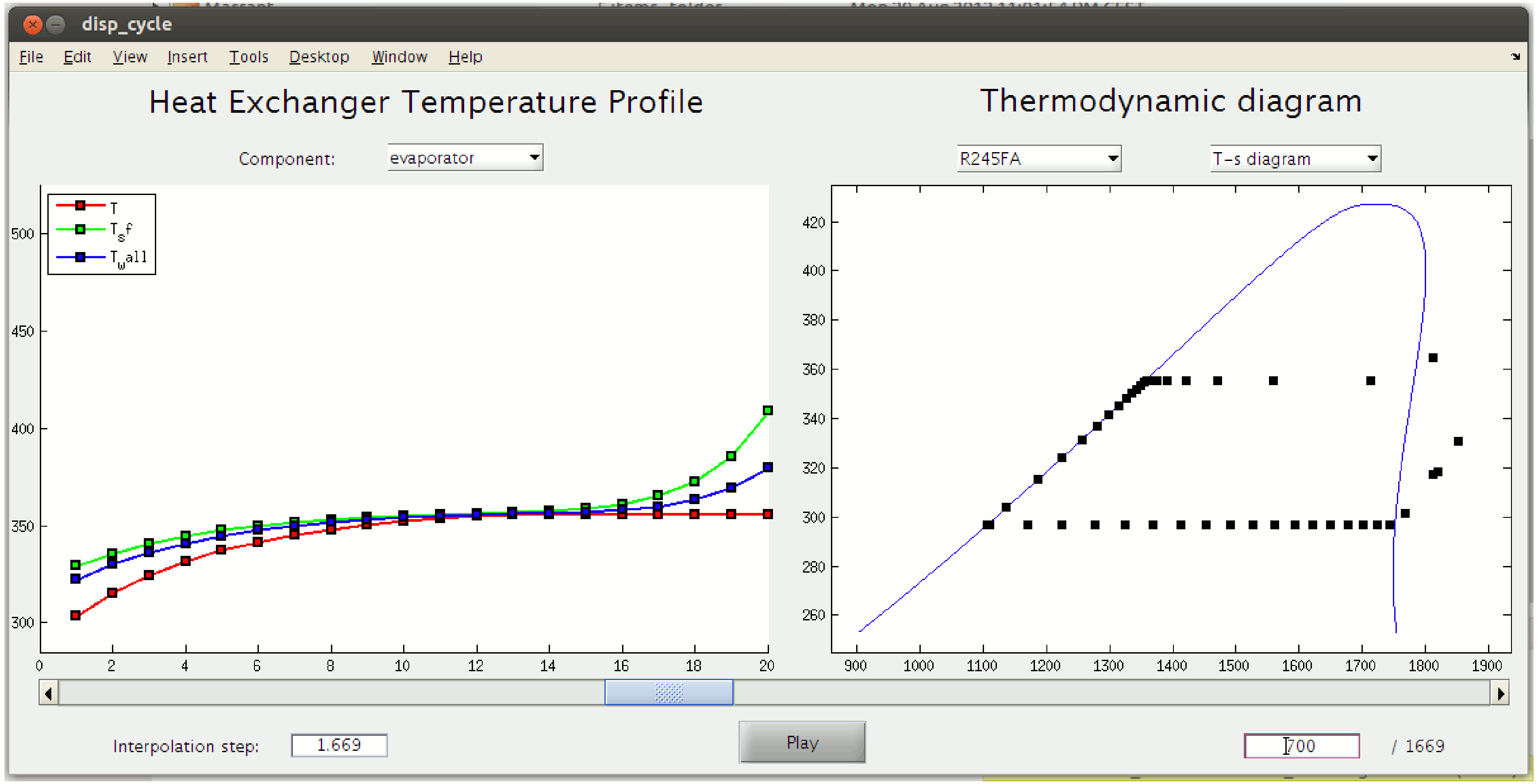
REFPROP:

- Historical, reference software for thermophysical properties for:
  - 151 pure and pseudo-pure fluids
  - Unlimited mixtures
- Written in Fortran
- Non-free

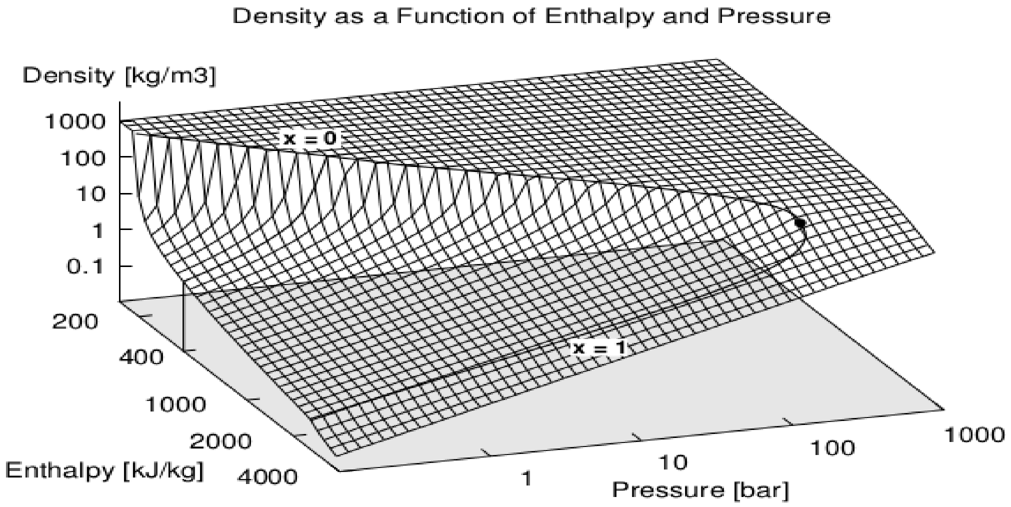
CoolProp:

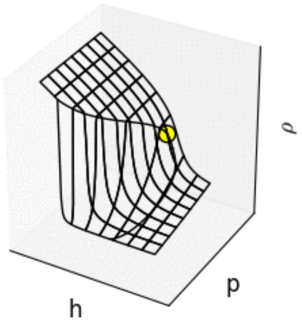
- Open-source thermophysical properties for:
  - 125 pure and pseudo-pure fluids
  - 35 mixtures
  - 57 incompressible pure fluids
  - 47 incompressible mixtures
- Written in C++
- MIT license

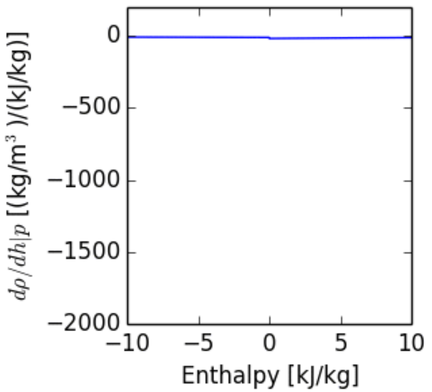
Simulation display



Robustness of dynamic two-phase flows: *Chattering*

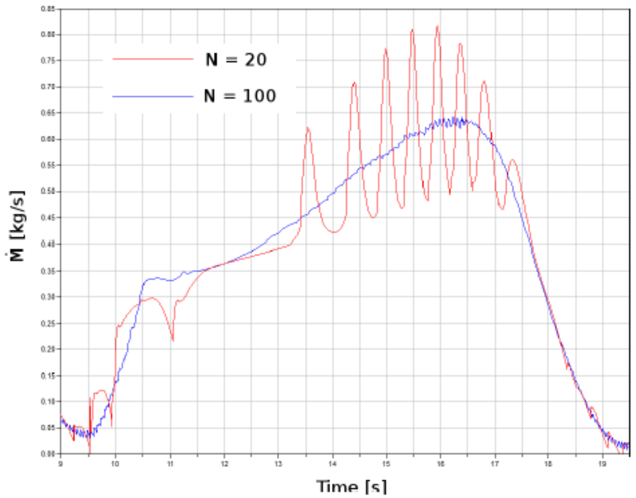




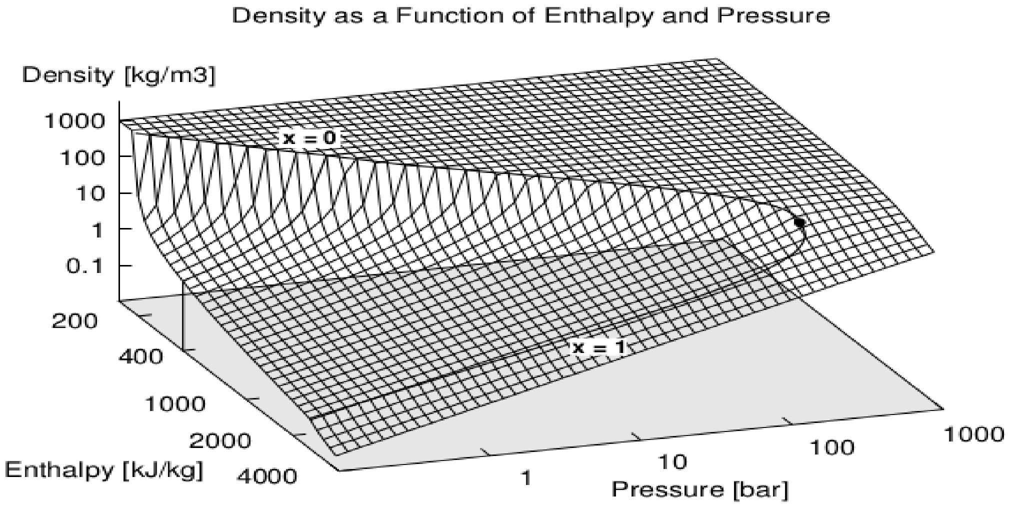


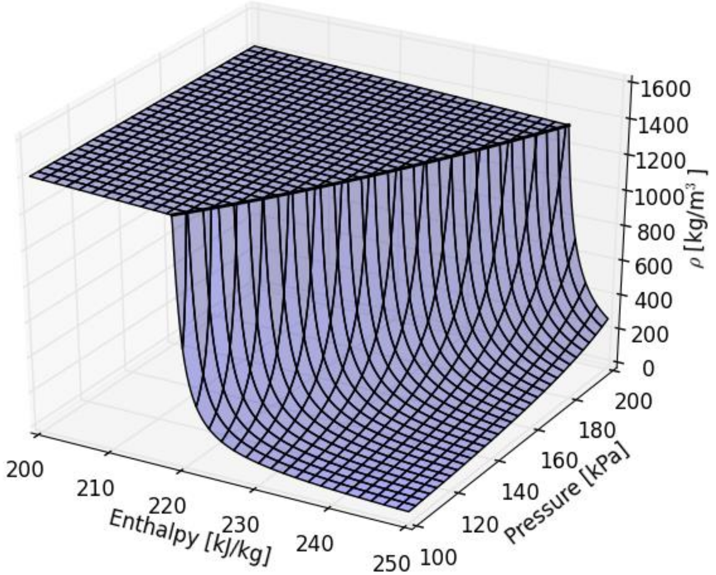
Non-physical flow reversals and simulation failures can occur if:

$$V_i \cdot \frac{d\rho_i}{dt} \approx \dot{M}_{su}$$



Benefits: *Hacking into the code*





- Discontinuities in thermodynamic properties:
  - Multiple numerical issues
  - Simulation failures
- Solution:
  - Smoothing of the thermodynamic properties
  - Implemented directly into Coolprop

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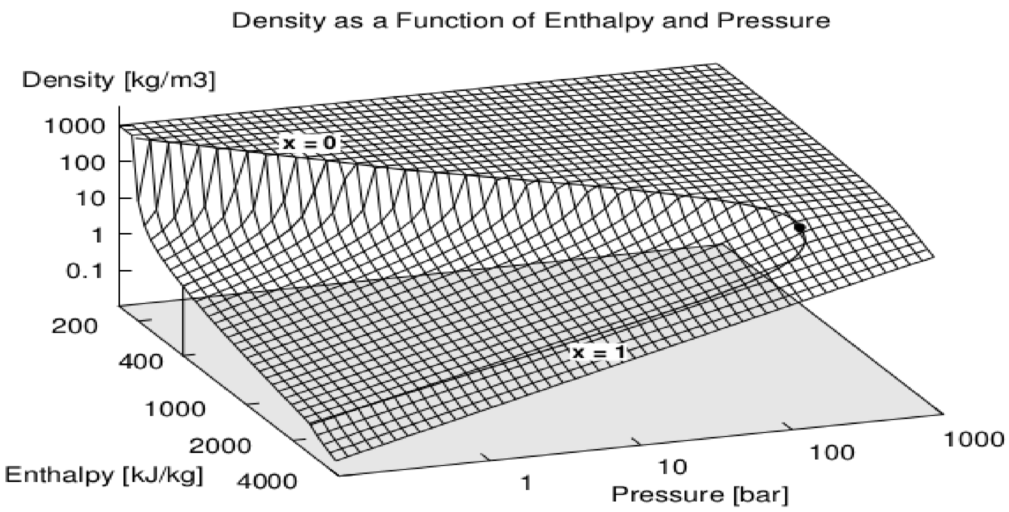

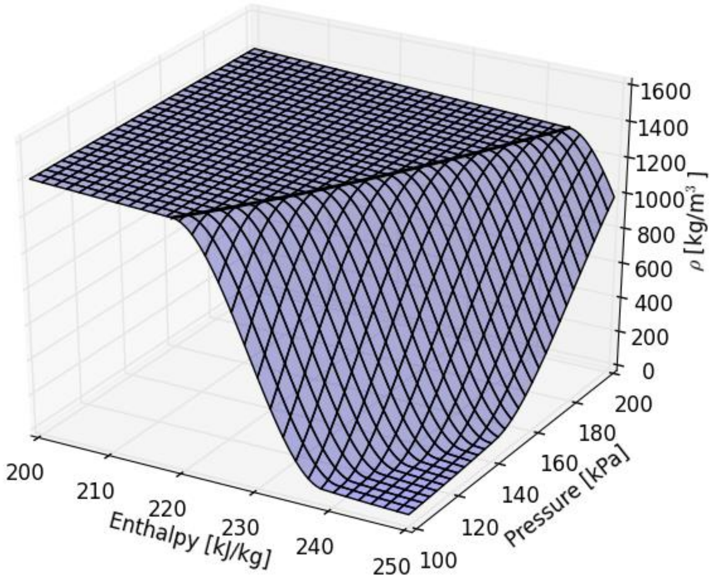

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  - Simulation failures
- Solution:
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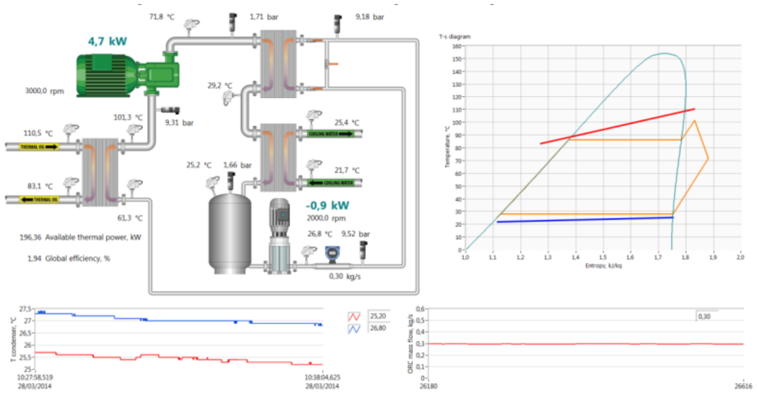
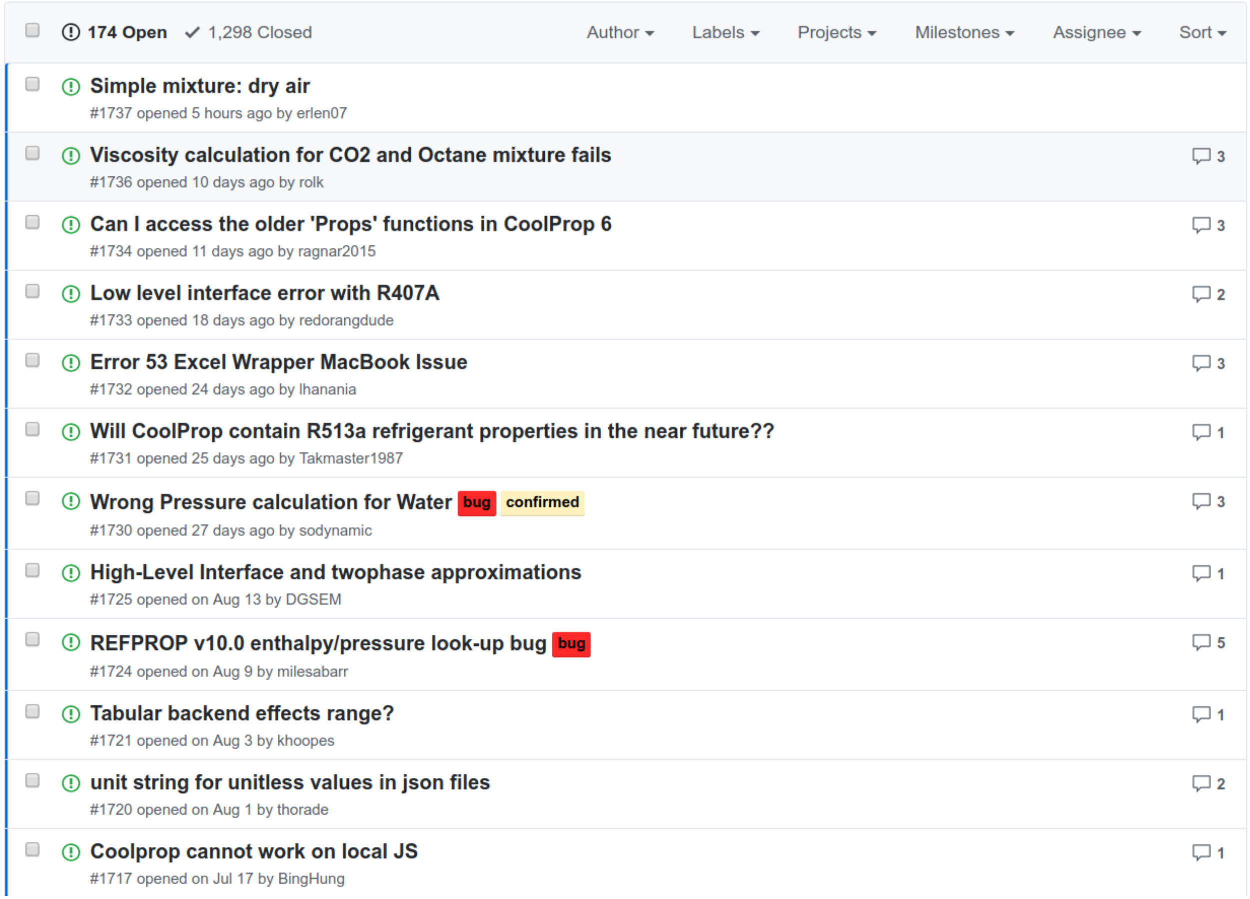
Benefits: *Software compatibility and portability*

- Interface to multiple engineering softwares
  - Fully-featured wrappers: Python (2.x, 3.x) , Modelica, Octave, C#, VB.net, MathCAD, Java, Android, MATLAB
  - High-level interface only: Labview, EES, Microsoft Excel, LibreOffice, Javascript, PHP, FORTRAN, Maple, Mathematica, Scilab, Delphi & Lazarus, Julia
- Runs in Windows, OSX, Linux, IOS, Android



Benefits: *Collaborative work*

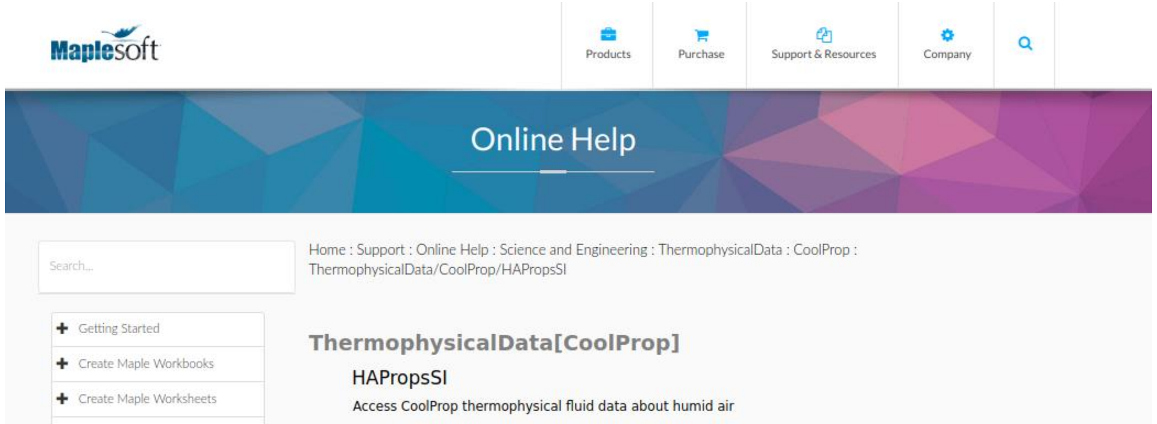
- More than 40 contributors
- However: one main developer
- Github / Sphinx / ReadTheDocs / Travis ecosystem

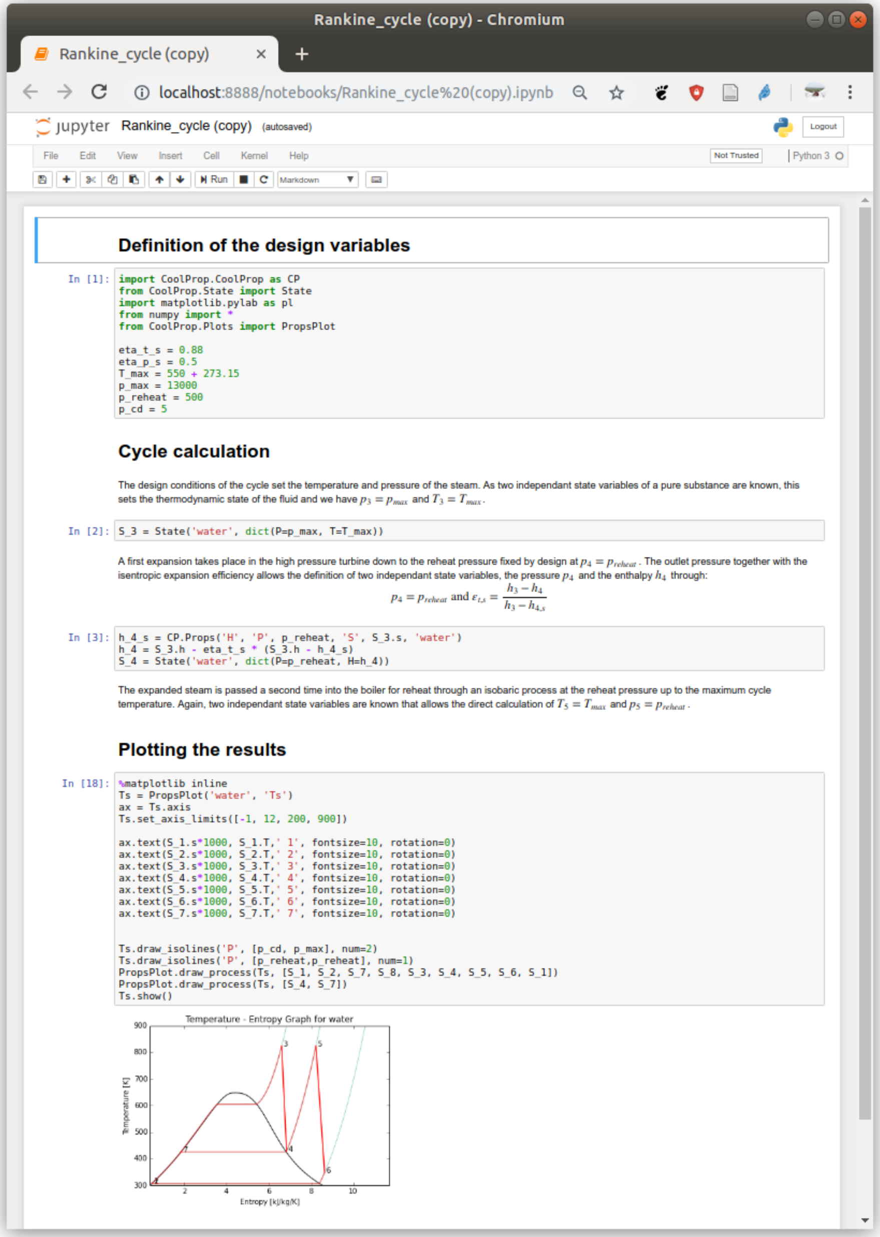


Benefits: *Free access for everyone*

Examples:

- Teaching thermodynamics in developing countries
- Private companies





Benefits: *Scientific recognition*

I&EC research
Industrial & Engineering Chemistry Research

ACS AuthorChoice

Article

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Terms of Use

Pure and Pseudo-pure Fluid Thermophysical Property Evaluation and the Open-Source Thermophysical Property Library CoolProp

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†Energy Systems Research Unit, University of Liège, Liège, Belgium

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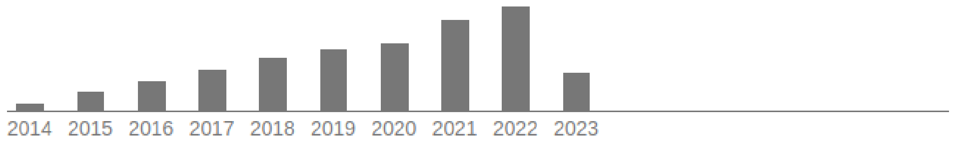
Supporting Information

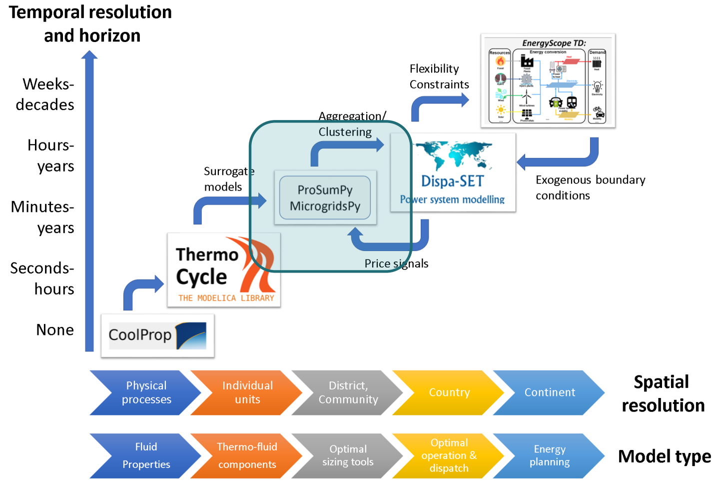
ABSTRACT: Over the last few decades, researchers have developed a number of empirical and theoretical models for the correlation and prediction of the thermophysical properties of pure fluids and mixtures treated as pseudo-pure fluids. In this paper, a survey of all the state-of-the-art formulations of thermophysical properties is presented. The most-accurate thermodynamic properties are obtained from multiparameter Helmholtz-energy-explicit-type formulations. For the transport properties, a wider range of methods has been employed, including the extended corresponding states method. All of the thermophysical property correlations described here have been implemented into CoolProp, an open-source thermophysical property library. This library is written in C++, with wrappers available for the majority of programming languages and platforms of technical interest. As of publication, 110 pure and pseudo-pure fluids are included in the library, as well as properties of 40 incompressible fluids and humid air. The source code for the CoolProp library is included as an electronic annex.

Total citations Cited by 2005



Scholar articles Pure and pseudo-pure fluid thermophysical property evaluation and the open-source thermophysical property library CoolProp
IH Bell, J Wronski, S Quoilin, V Lemort - Industrial & engineering chemistry research, 2014
Cited by 2005 Related articles All 17 versions

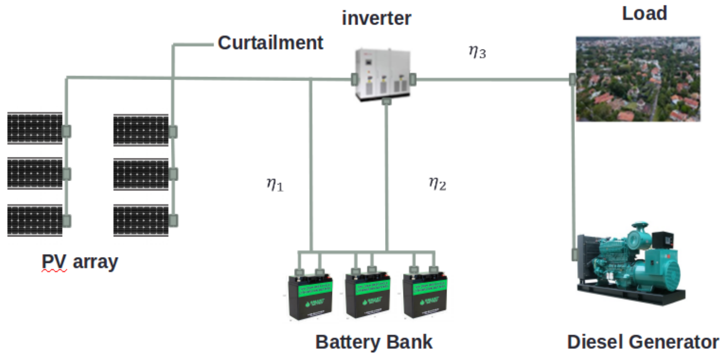
Modeling rural electrification in developing countries



Available Solutions for rural electrification

Grid extension

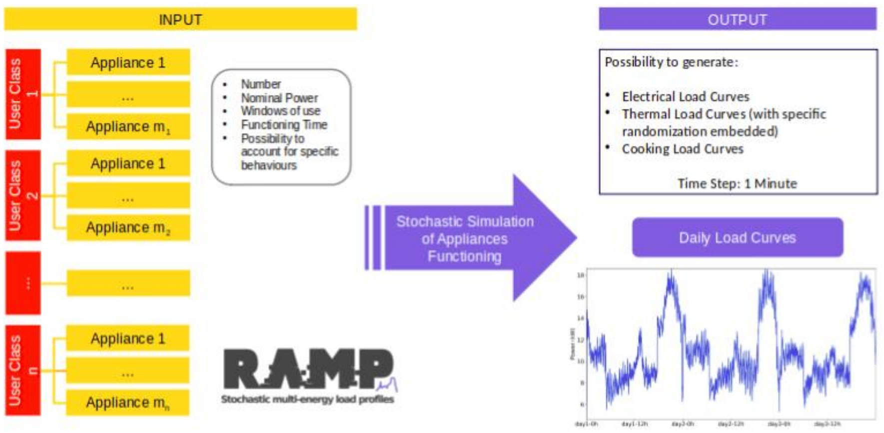
Hybrid Microgrids



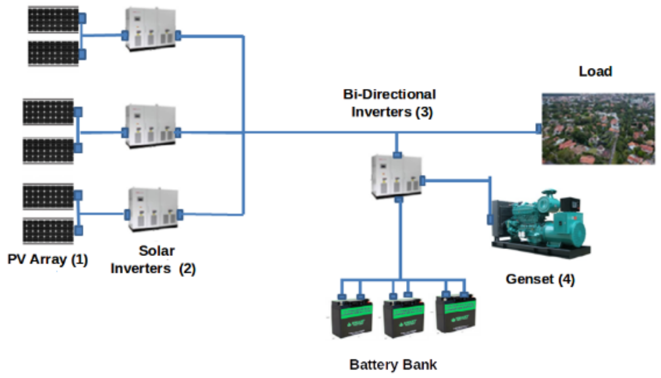
Solar home systems

Integrate detailed community-level data into GIS

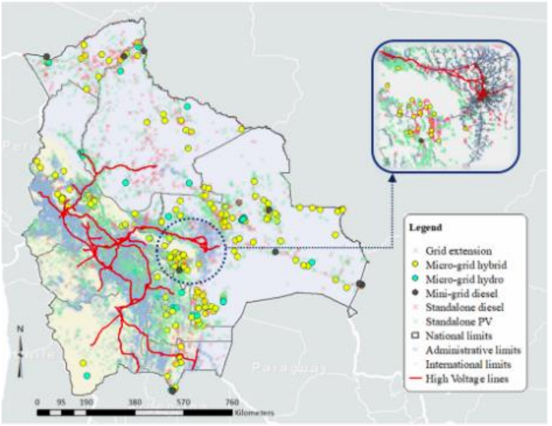
Bottom-up load curves generation



Optimal design of microgrids and solar home systems



GIS-based optimal electrification

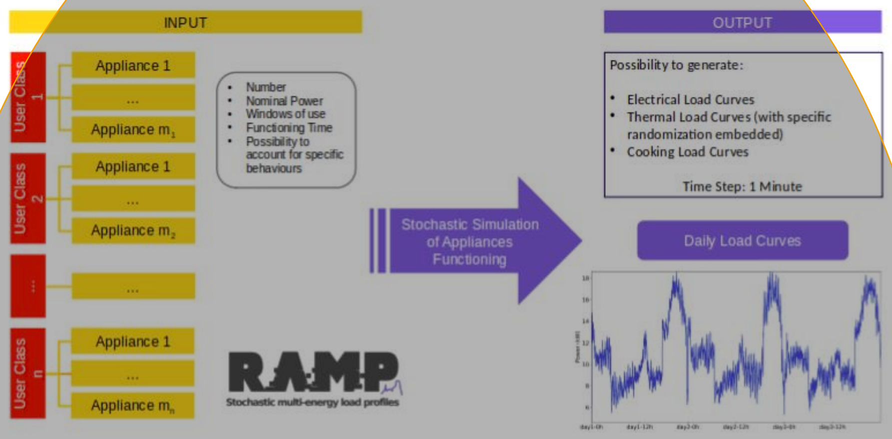


- Surveys among Bolivian communities (Both electrified and non-electrified)
- Allows predicting consumption patterns

Surrogate models

Integrate detailed community-level data into GIS

Bottom-up load curves generation



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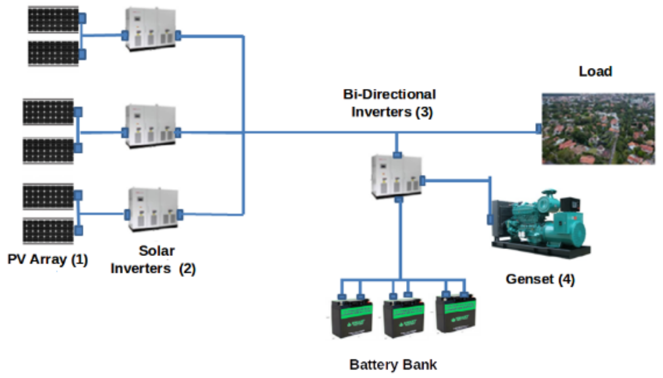
RAMP

Optimal design of microgrids and solar home systems



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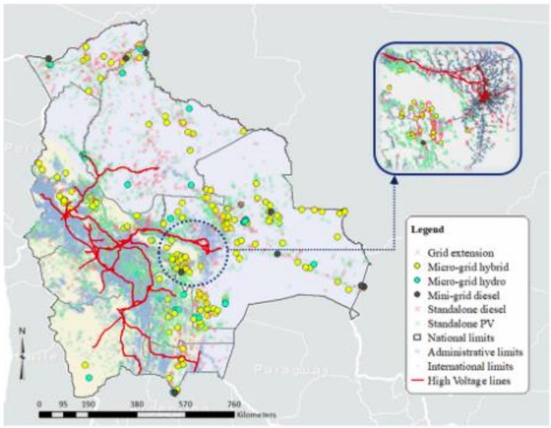

Surrogate models

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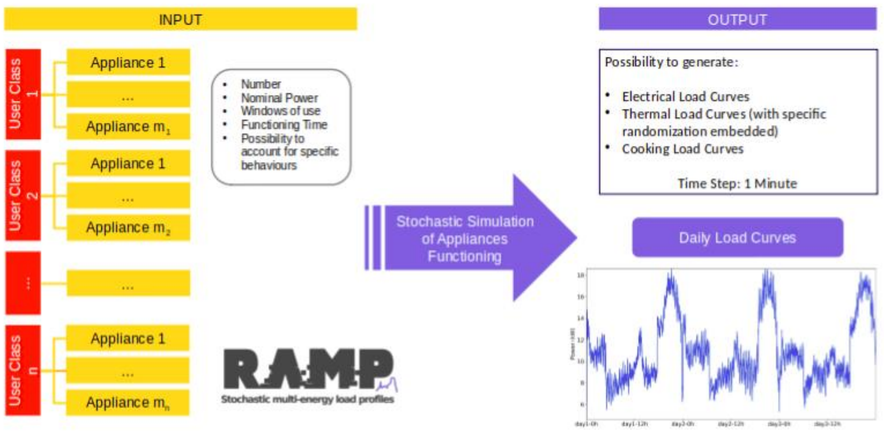
Integrate detailed community-level data into GIS

Bottom-up load
curves generation



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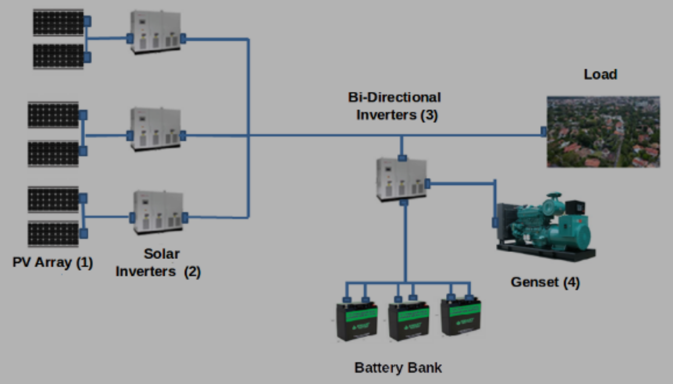
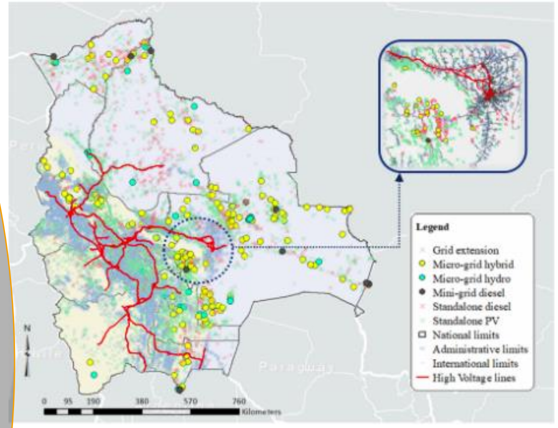
Optimal design of microgrids
and solar home systems



MicroGridsPy

GIS-based
optimal electrification



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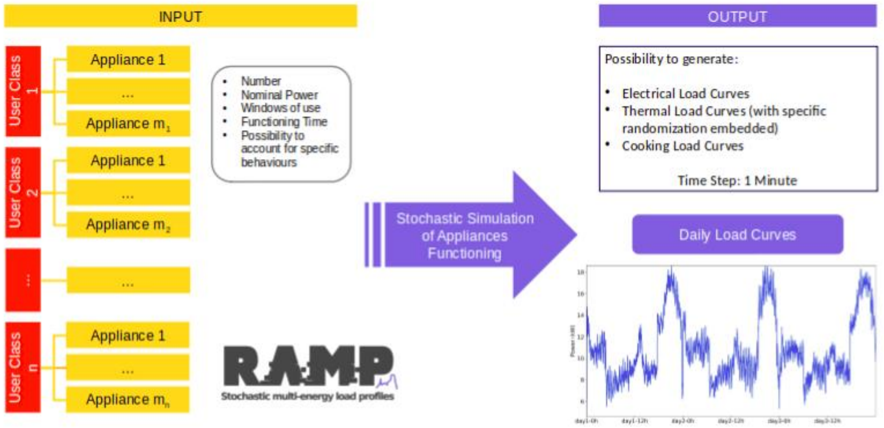

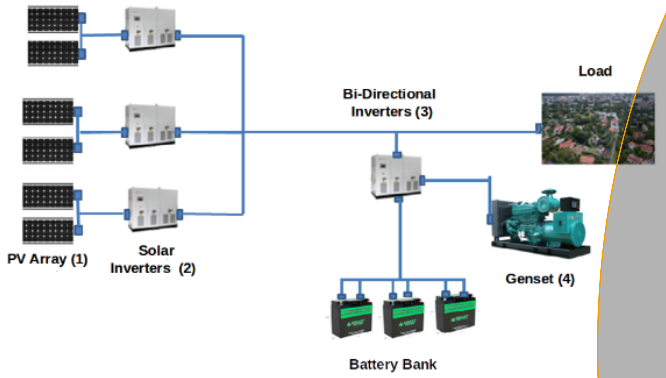

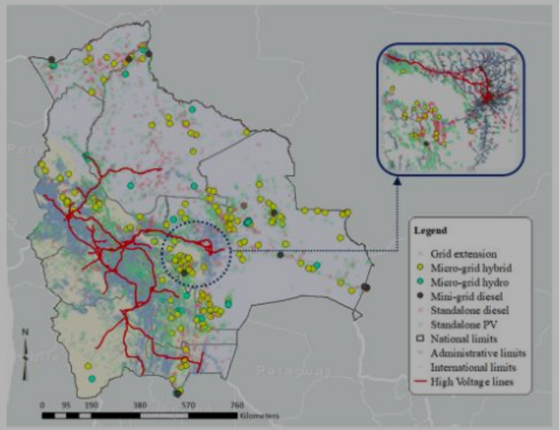

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Surrogate models

OnSSET

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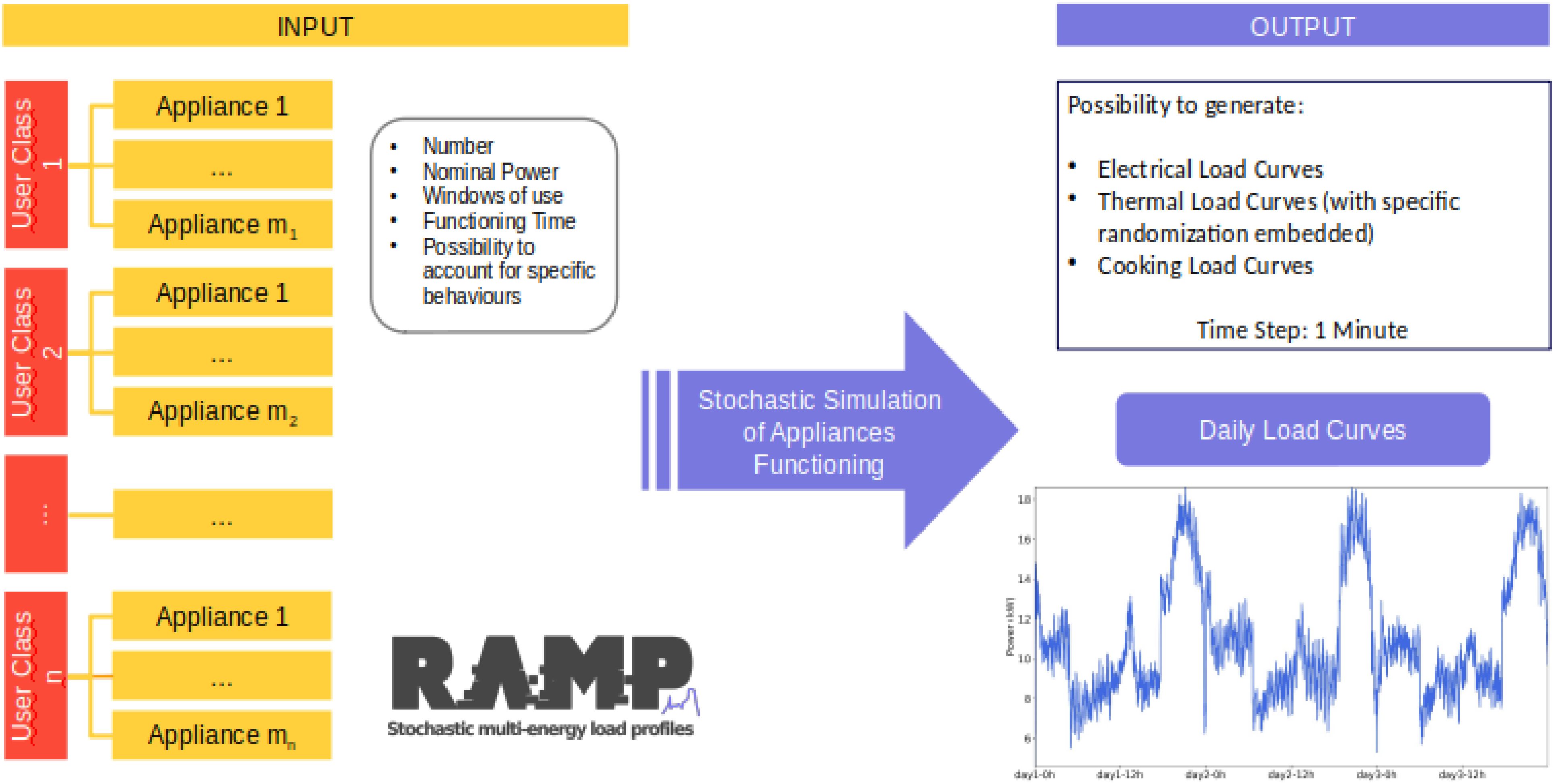
RAMP stochastic bottom-up demand model



MicroGridsPy: Optimal sizing of isolated energy systems

- Objective function:
  - Minimize investment and operational costs

$$Inv + \sum_{s=1}^{S}\left(\sum_{y=1}^{Y}\frac{YC_s}{(1+e)^y}\cdot I_s^{occurrence}\right)$$

- Optimization variables:
  - Nominal capacity of generators, battery and renewable sources.
  - Dispatch of generators, battery and renewable sources.

- Optimization characteristics
  - Deterministic or two-stage stochastic
  - LP or MILP.
  - Time period is one year.
  - Time step is one hour.

python

PYOMO

GUROBI OPTIMIZATION

MicroGridsPy: Example results

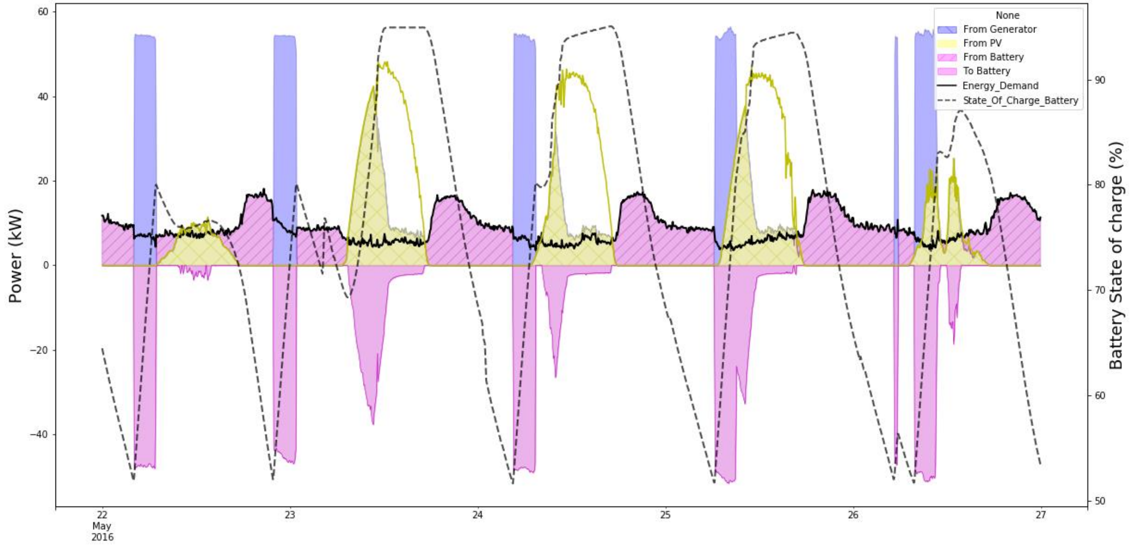
Monitoring of the “El Espino” microgrid:

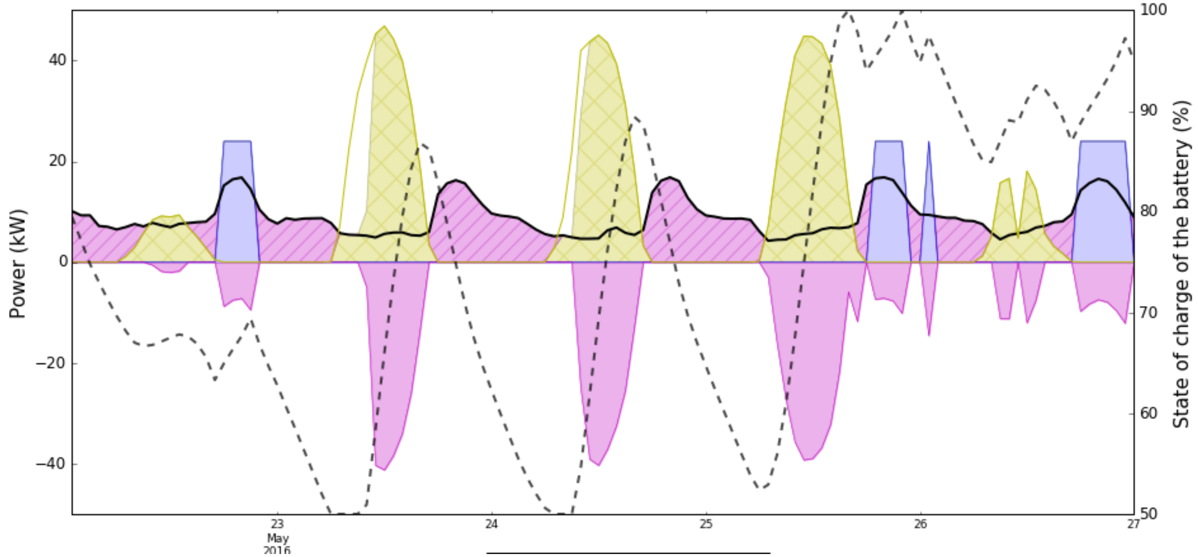


Re-optimization of the system:

- Smaller diesel generator
- Better battery charging strategy

→ - 34% diesel consumption

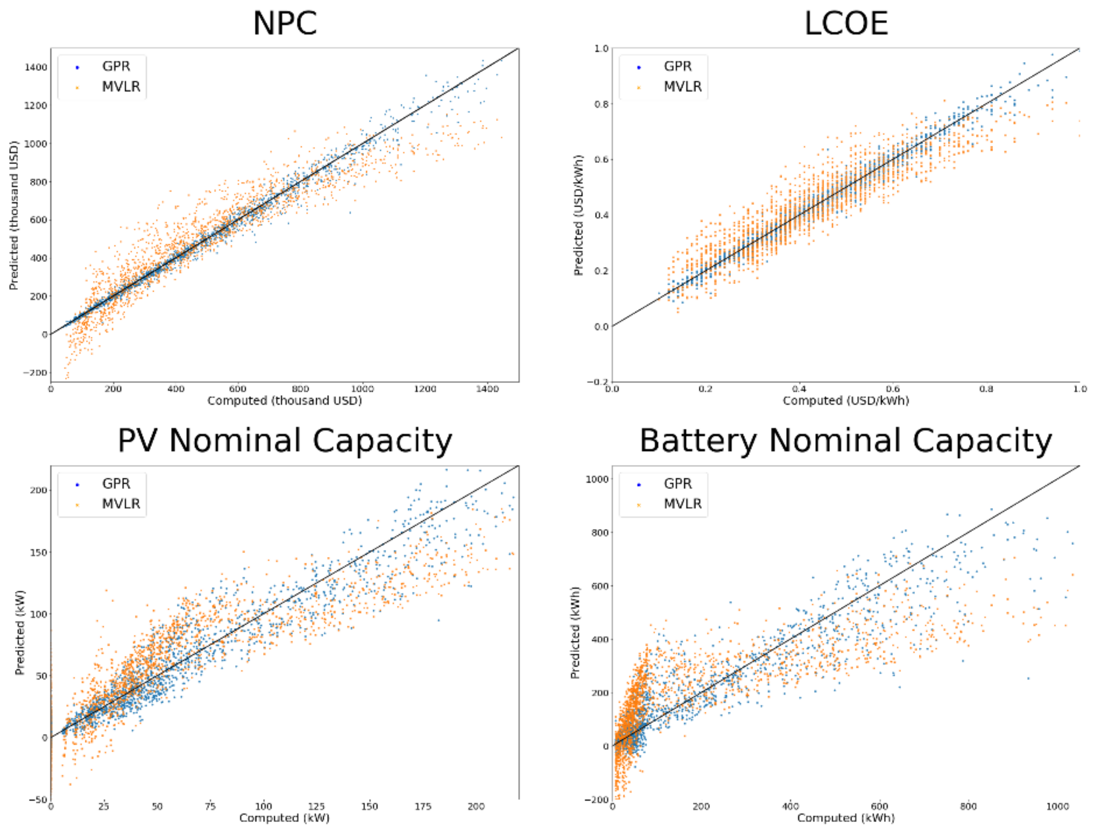




Surrogate model creation

Input output parameters

Input parameters	Output parameters
PV invesment cost	NPC
Battery invesment cost	LCOE
Depth of discharge	PV installed capacity
Battery Cycles	Battery installed capacity
Generator investment cost	
Generator efficiency	
Low heating valuer	
Fuel cost	
Toto demand in the year	
Total PV production from one unit	



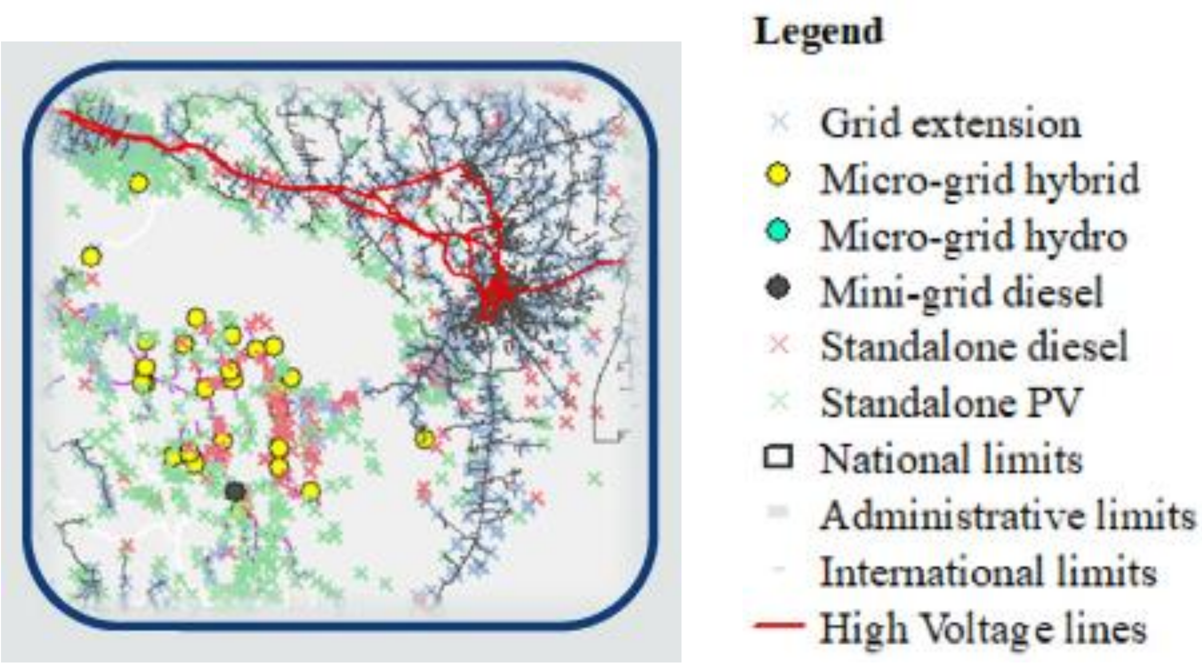
Selected machine learning methods:

- Multi-linear regression.
- Gaussian process regression.

OnSSET open-source spatial electrification tool

Electrification algorithm:

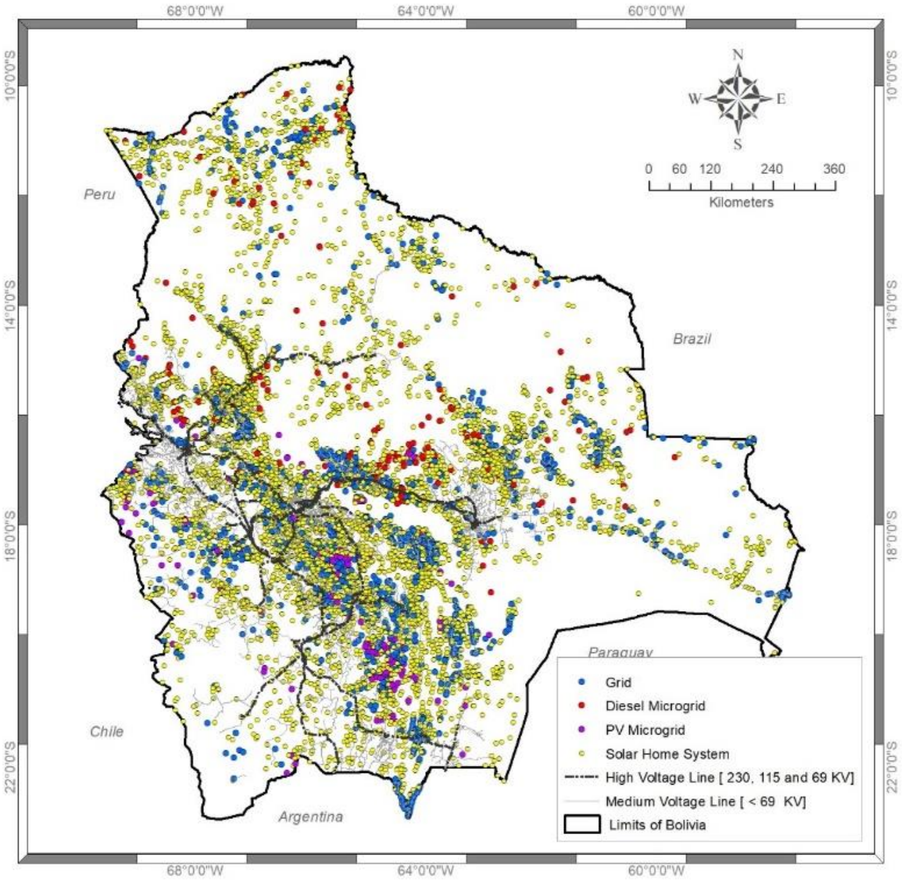
1. Calculates LCOE for each each isolated system technology.
2. Calculates the LCOE cost of extending the grid.
3. Compares LCOE grid with isolated systems in each community.
4. If at least 1 community has been electrified with grid, come back to step 2.
5. Calculates all relevant indicators.



Results: Universal access in Bolivia

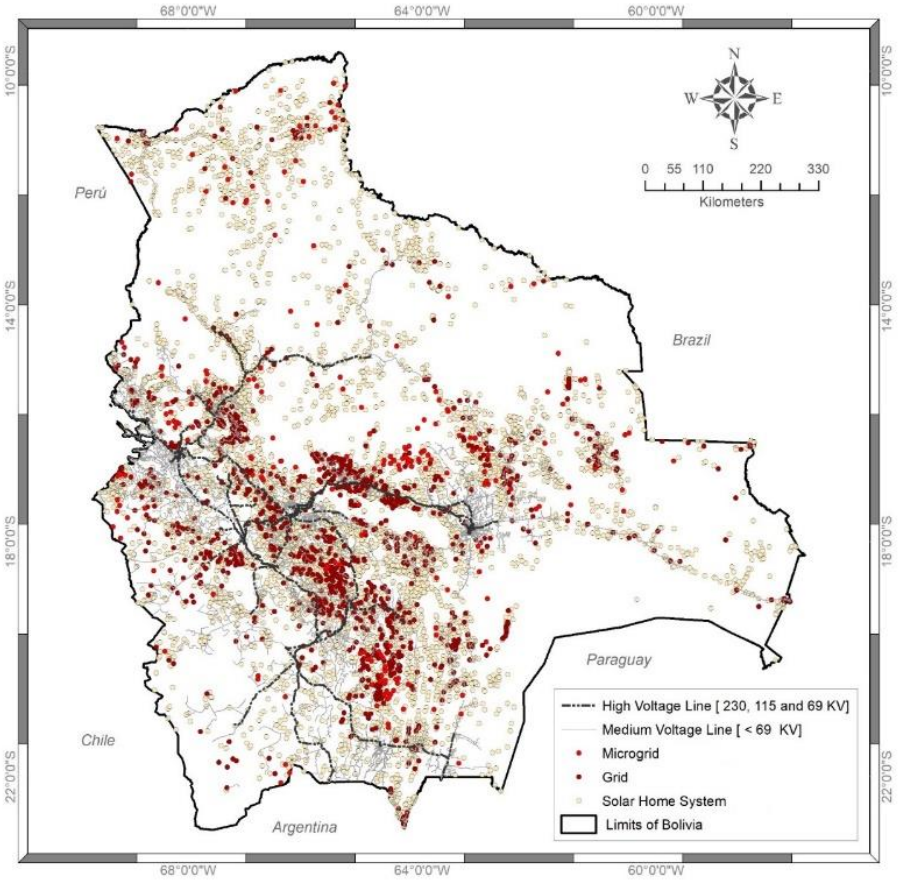
Naïve formulation

OnSSET only

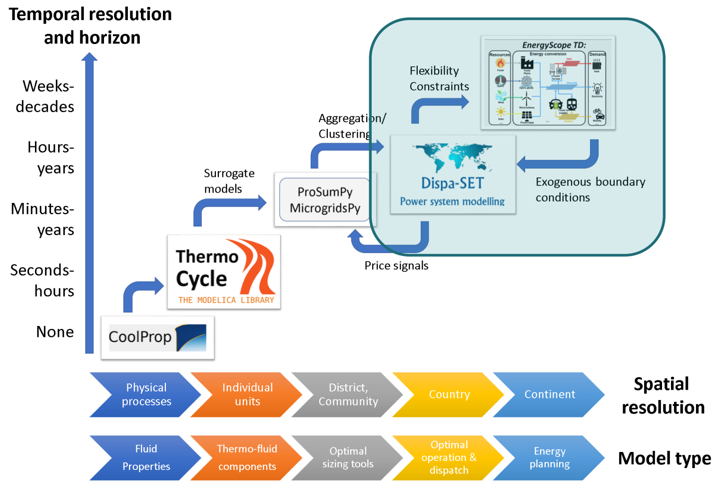


Interlinked framework

RAMP + MicroGridsPy + OnSSET



EnergyScope and Dispa-SET: A bi-directional soft-linking



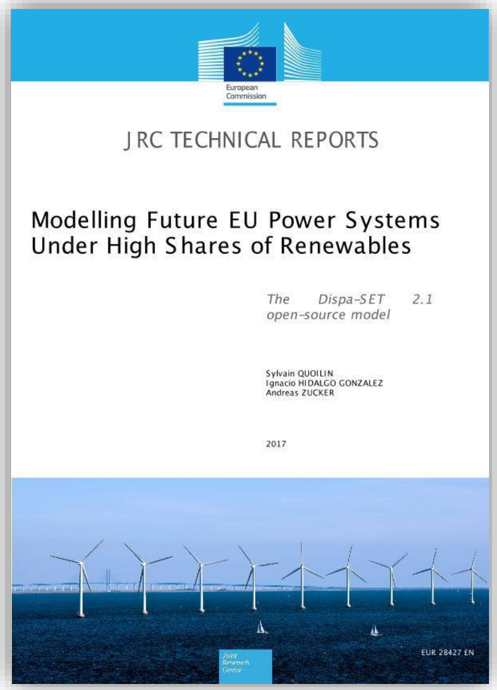
Dispa-SET in a nutshell

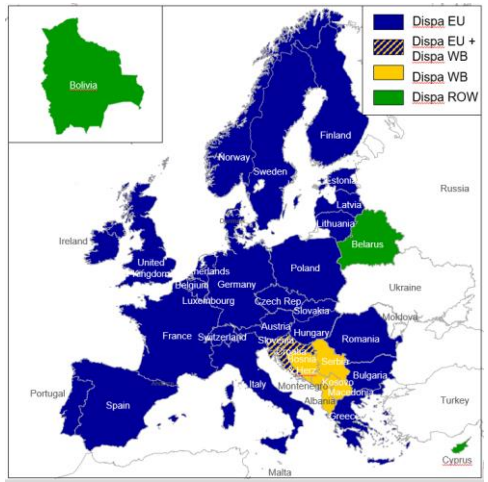
What Dispa-SET is:

- A unit commitment and dispatch model of the European power system
- Two successive optimizations:
  - Mid-term scheduling of power stations
  - Short-term unit commitment (rolling horizon)
- Probabilistic assessment of system adequacy and flexibility needs of power systems, with growing share of renewable energy generation
- Easily "pluggable" to the outputs of long-term planning models

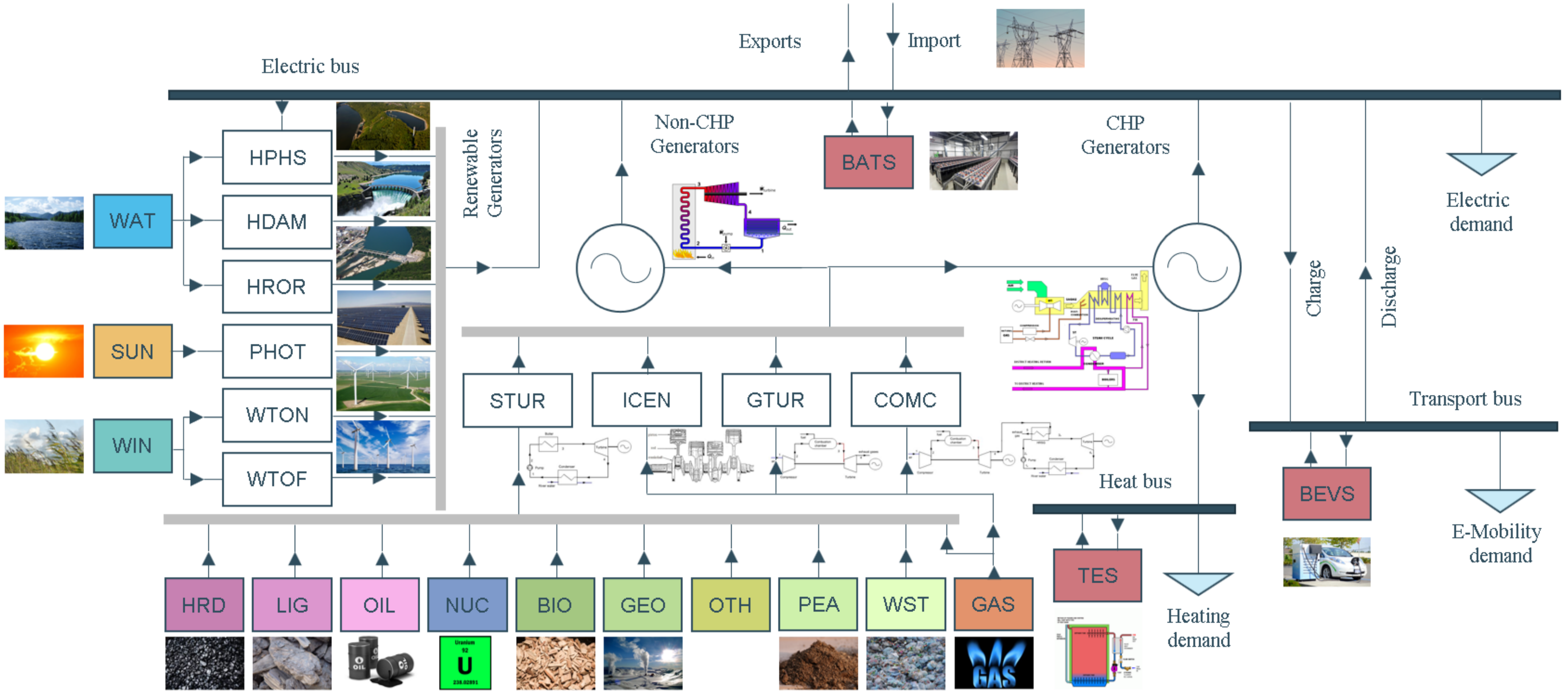
What Dispa-SET is <u>not</u>:

- An expansion planning model
  - Only operational costs are optimized
  - No investments





Dispa-SET 2.3: System structure & technology overview in a single node

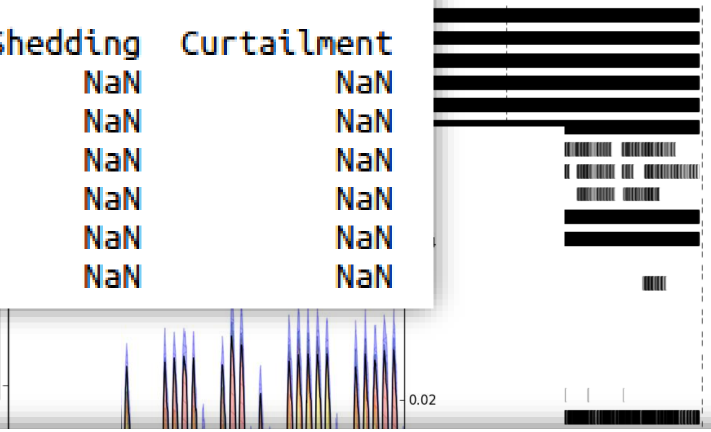


- Sector coupling options: P2H, P2V, P2P…

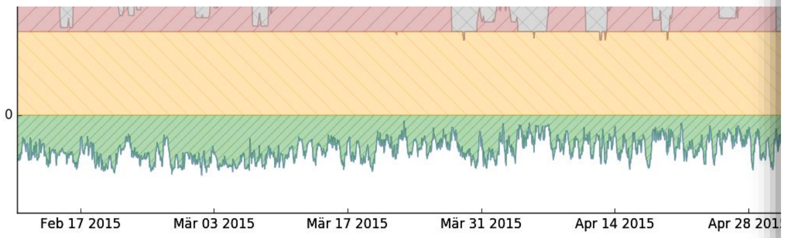
Dispa-SET 2.1: typical outputs

Country-Specific values (in TWh or in MW):

	Demand	PeakLoad	NetImports	LoadShedding	Curtailment
AT	59.375448	10144.000000	5.144132	NaN	NaN
BE	86.971154	13632.250000	8.911190	NaN	NaN
CH	44.694098	7794.262468	7.199527	NaN	NaN
DE	478.030824	76212.250000	-17.260122	NaN	NaN
FR	470.075612	90588.000000	-51.878128	NaN	NaN
NL	87.925973	16285.500000	5.682672	NaN	NaN



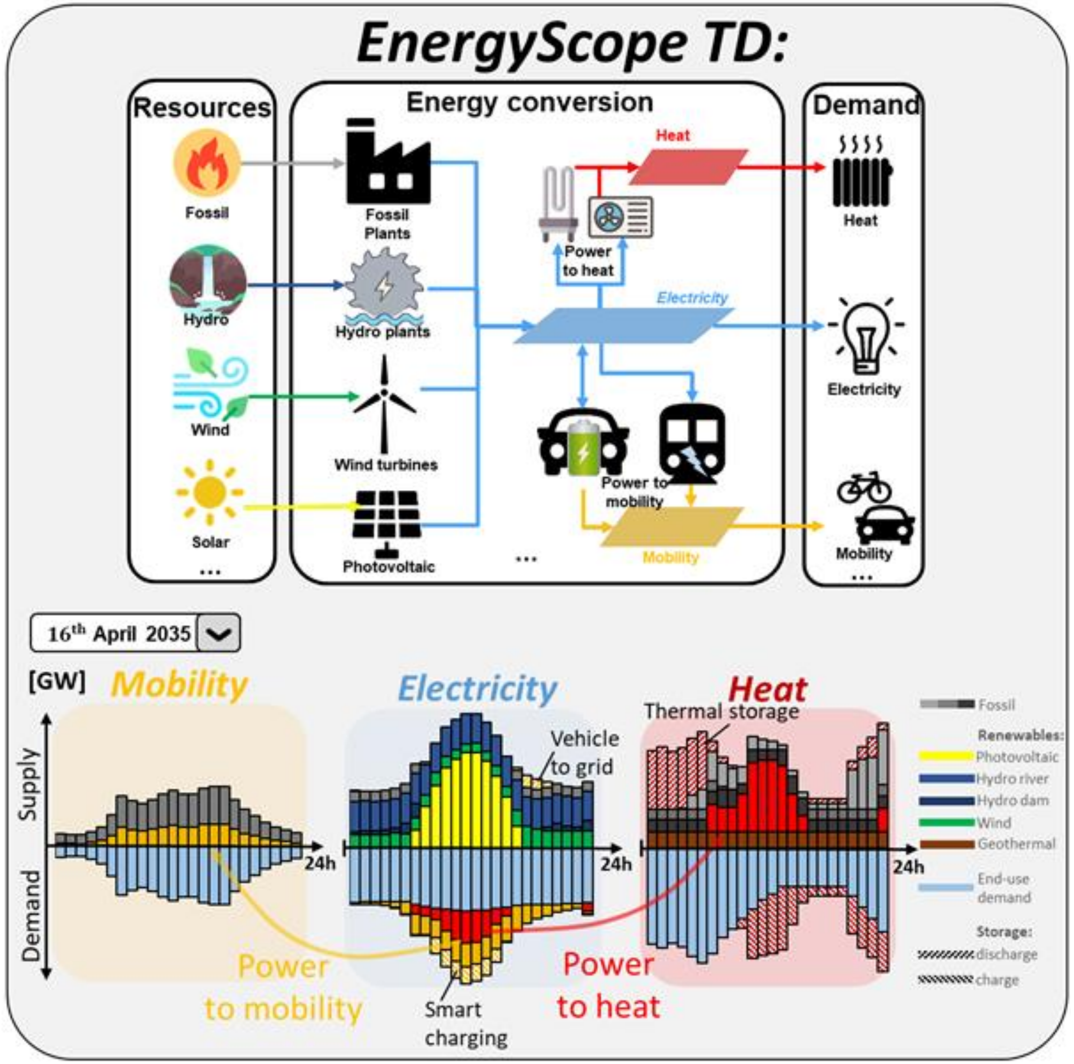

```
Aggregated statistics for the considered area:
Total consumption:1227.07310992 TWh
Peak load:203182.461067 MW
Net importations:-42.20072928 TWh
```



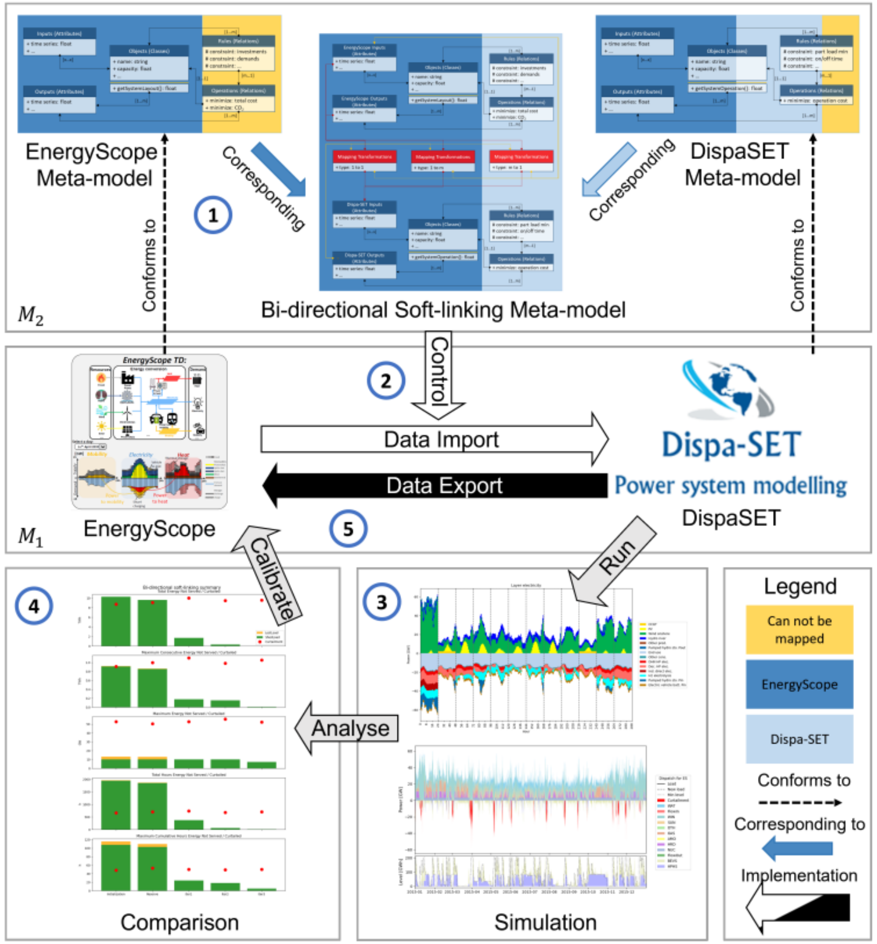

```
Number of hours of congestion on each line:
{'AT -> CH': 5917,
 'AT -> DE': 430,
 'BE -> FR': 62,
 'BE -> NL': 344,
 'CH -> AT': 720,
 'CH -> DE': 15,
 'CH -> FR': 56,
 'DE -> AT': 1522,
 'DE -> CH': 4378,
 'DE -> NL': 2803,
 'FR -> BE': 2689,
 'FR -> CH': 7665,
 'NL -> BE': 1403,
 'NL -> DE': 60}
```

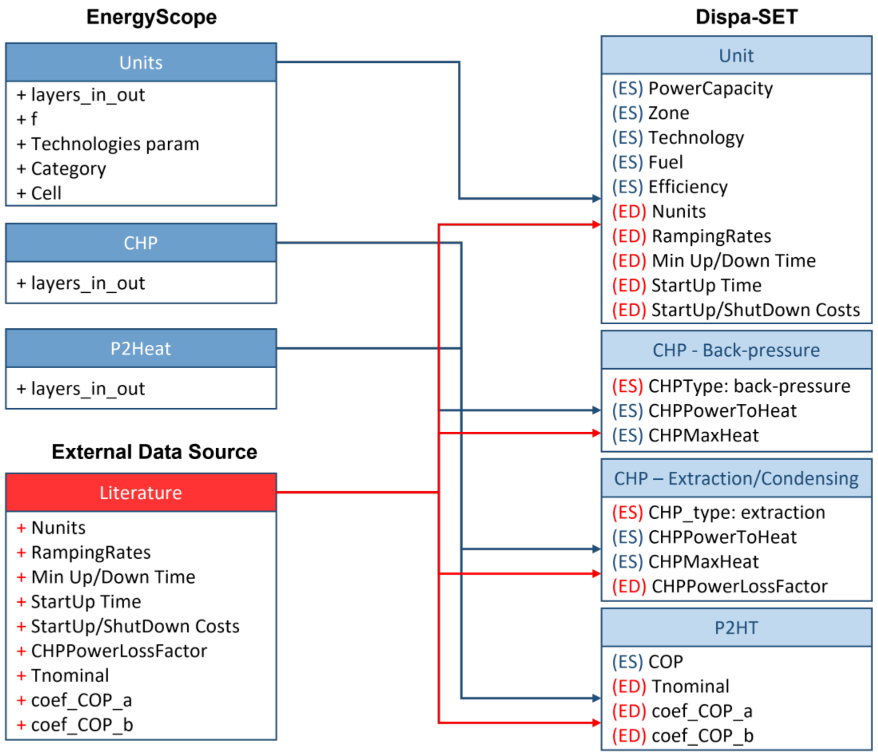
The EnergyScope model:

- EnergyScope TD:
  - *Advantages:*
    - Hourly resolution over a year
    - Whole-energy system: heat, elec. mob…
    - Optimisation of design & operation
    - Open source & documented[1-2]
  - *Disadvantages:*
    - Space resolution: 1 cell
    - Technico-economic: simplified representation of technologies
    - No market equilibrium



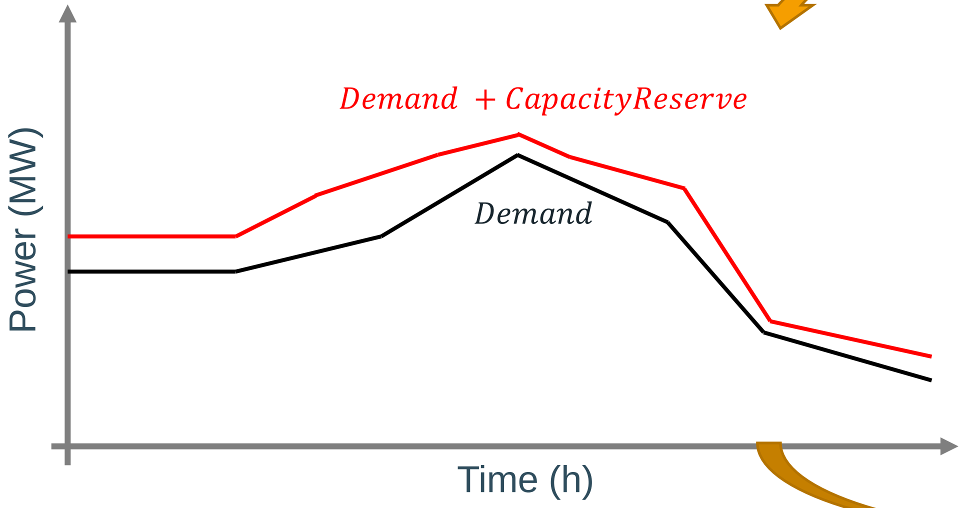
Mapping variables between both models

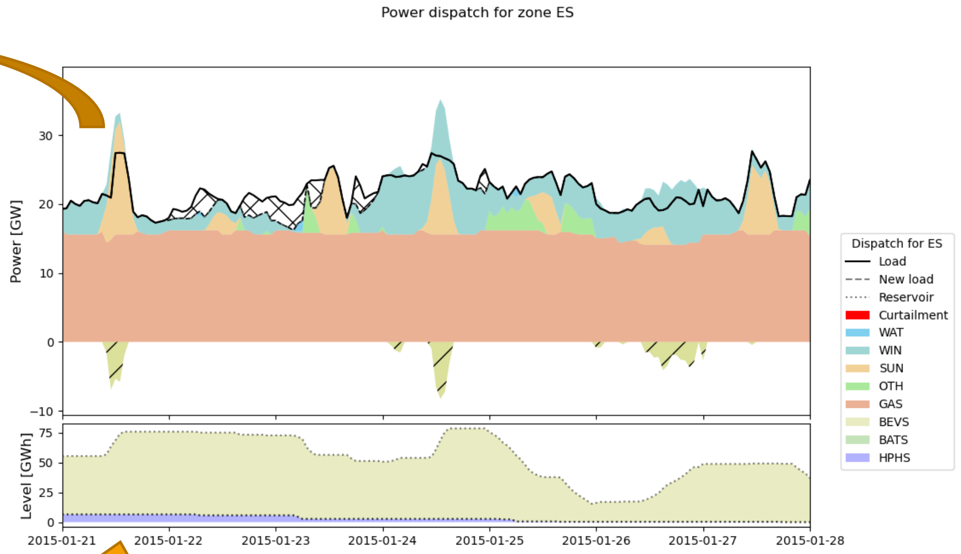




The output of Dispa-SET is fed to EnergyScope as a reserve demand

$$\boldsymbol{CapacityReserve} \mathrel{+}= \boldsymbol{Max}(\boldsymbol{ShedLoad})$$





- The installed capacity should allow to run with this additional demand
- Operational cost is computed on « actual » operation

33

Stop condition

- MILP issue with the solvers optimality gap
- Optimization accuracy:

j – soft-linking iteration
z – UCED rolling horizon loop
i – UCED time interval

$$Accuracy_z = OptimalityGap \cdot ObjectiveFunction_z$$

- UCED error:

$$Error_z = \sum_i ShedLoad_i \cdot CostLoadShedding + \sum_i LostLoad_i \cdot CostLostLoad + \sum_i SlackLoad_i \cdot CostSlack$$

- Stop condition:

$$StopCondition = \begin{cases} j+1: \ Error_z \geq Accuracy_z \\ stop: \ otherwise \end{cases}$$

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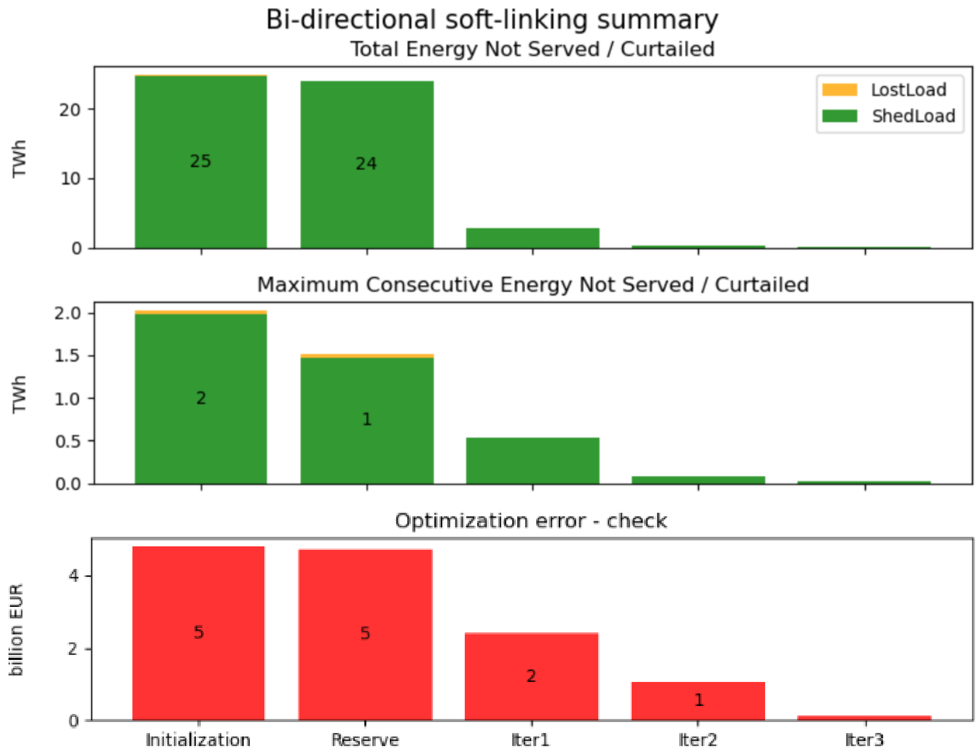
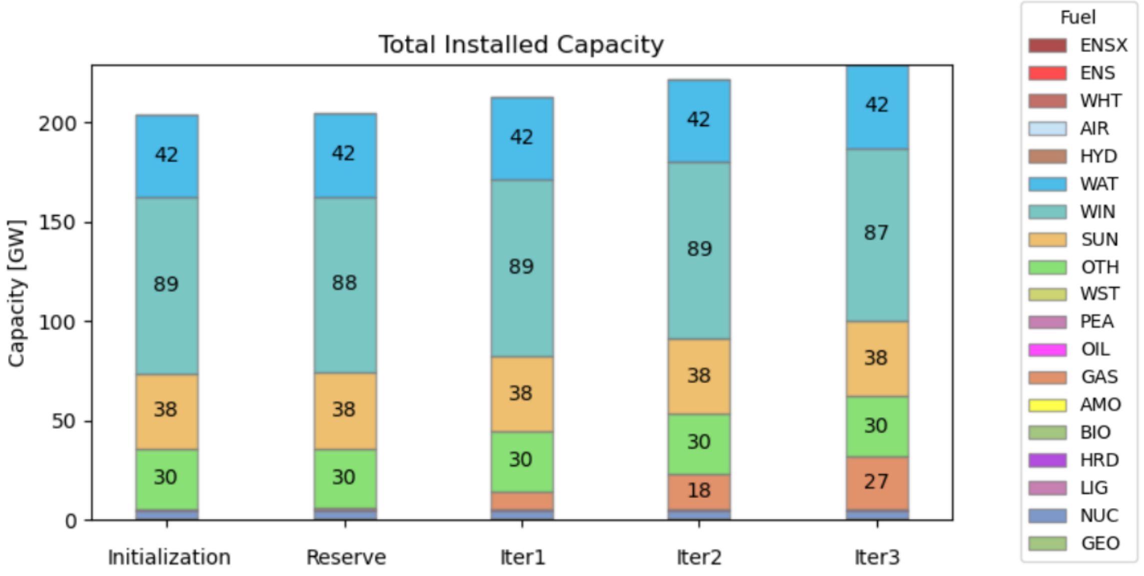
Over the iterations, the installed flexible capacity increases





Convergence between both models is attained after 3 iterations!

Final remarks

Why transparency and reproducibility matter

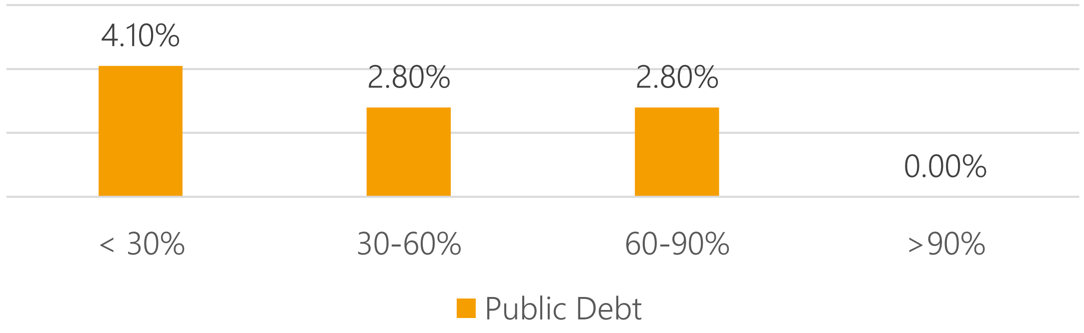
Calculation spreadsheet for:

Growth in a Time of Debt by Carmen M. Reinhart and Kenneth S. Rogoff. Published in volume 100, issue 2, pages 573-78 of American Economic Review, May 2010

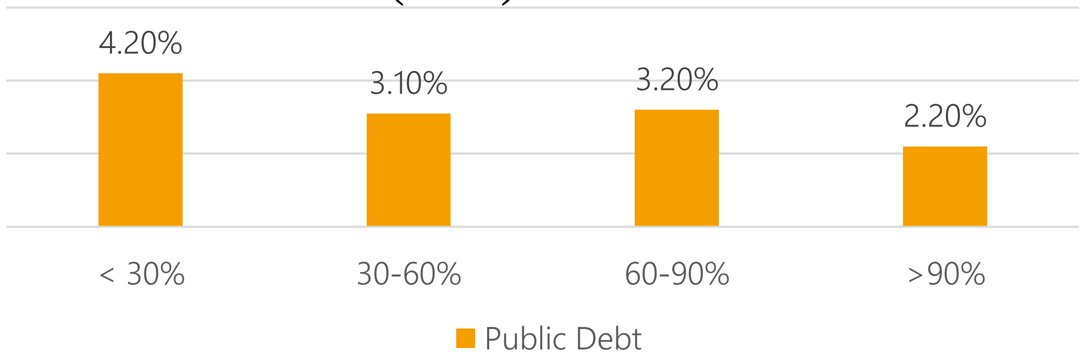
	B	C	I	J	K	L	M
2			Real GDP growth				
3			Debt/GDP				
4	Country	Coverage	30 or less	30 to 60	60 to 90	90 or above	30 or less
26			3.7	3.0	3.5	1.7	5.5
27	Minimum		1.6	0.3	1.3	-1.8	0.8
28	Maximum		5.4	4.9	10.2	3.6	13.3
29							
30	US	1946-2009	n.a.	3.4	3.3	-2.0	n.a.
31	UK	1946-2009	n.a.	2.4	2.5	2.4	n.a.
32	Sweden	1946-2009	3.6	2.9	2.7	n.a.	6.3
33	Spain	1946-2009	1.5	3.4	4.2	n.a.	9.9
34	Portugal	1952-2009	4.8	2.5	0.3	n.a.	7.9
35	New Zealand	1948-2009	2.5	2.9	3.9	-7.9	2.6
36	Netherlands	1956-2009	4.1	2.7	1.1	n.a.	6.4
37	Norway	1947-2009	3.4	5.1	n.a.	n.a.	5.4
38	Japan	1946-2009	7.0	4.0	1.0	0.7	7.0
39	Italy	1951-2009	5.4	2.1	1.8	1.0	5.6
40	Ireland	1948-2009	4.4	4.5	4.0	2.4	2.9
41	Greece	1970-2009	4.0	0.3	2.7	2.9	13.3
42	Germany	1946-2009	3.9	0.9	n.a.	n.a.	3.2
43	France	1949-2009	4.9	2.7	3.0	n.a.	5.2
44	Finland	1946-2009	3.8	2.4	5.5	n.a.	7.0
45	Denmark	1950-2009	3.5	1.7	2.4	n.a.	5.6
46	Canada	1951-2009	1.9	3.6	4.1	n.a.	2.2
47	Belgium	1947-2009	n.a.	4.2	3.1	2.6	n.a.
48	Austria	1948-2009	5.2	3.3	-3.8	n.a.	5.7
49	Australia	1951-2009	3.2	4.9	4.0	n.a.	5.9
50							
51			4.1	2.8	2.8	=AVERAGE(L30:L44)	

The Reinhart-Rogoff spreadsheet error arguably skewed the international debate on austerity

Calculated economic growth (Published version, 2010)



Corrected calculations (2013):



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Open-science

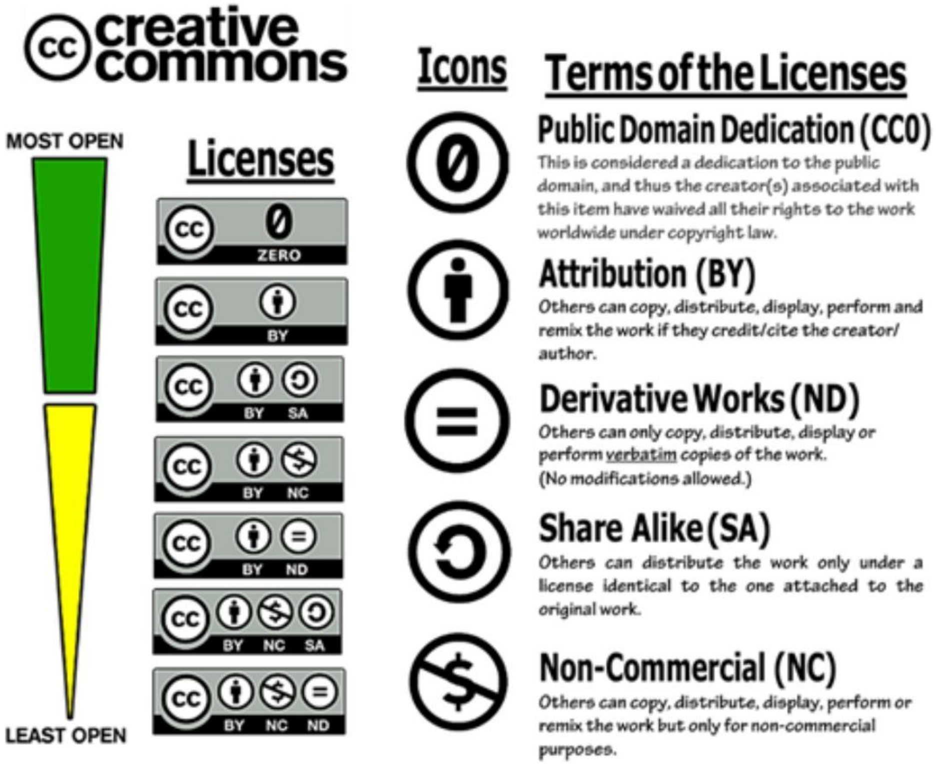
What does Open Science involve?

- **Open Access**: freely accessible publications for everybody via: gold and green Open Access
- **Open Data** is the practice of opening your data (e.g. measurement data) as unlimited as possible to as many people as possible. The best practice is to commit to the FAIR – principles when it comes to sharing data. Your data should be Findable, Accessible, Interoperable and Reusable.
- **Open Source** (Software) is the practice of sharing the source code of your software freely with everybody. The open-source practice is about releasing your source code under a free license that allows others to use, adapt and redistribute your software freely.
- **Open Methodology**: transparency regarding the uniform laboratory processes e.g., lab work.

Other concepts: FOSS, FAIR principles

Selecting a license for data

- Creative commons (CC) is well-known
  - Only use version 4.0
- Example: CC BY-NC
  - Others can remix, adapt, and build upon your work
  - their new works must acknowledge you
  - non-commercial use only
- Alternatives include ODbL, ODC-By, PDDL



Selecting a license for code

- Are you okay with your code becoming part of a closed-source commercial software product?
  - No: GPL
  - Yes: permissive licenses (MIT/BSD/Apache)
- Do you want to force users to publish their improvements to your software, or to software they develop based on your software, under the same license?
  - No: permissive licenses (MIT/BSD/Apache). This makes the code more broadly usable, but also allows people to take the code without sharing their improvements.
  - Yes: GPL. This ensures that any future changes and improvements to the code remain free and open

	Code	Data	Documentation
Copyleft	GPL, (AGPL)	ODbL	CC BY SA
Permissive	ISC, MIT, BSD, Apache [1]	CC BY, ODC-By	CC BY
Public domain	not recommended	PDDL, CC0	CC0

Source: https://wiki.openmod-initiative.org/

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Why energy models and data should be open

- Quality of science: peer review, reproducibility, traceability
- More effective collaboration between science and policy
    - Transparent social debate
- Collaborative burden sharing (=> increased productivity)
- Research funded by public money should be public

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ENERGY POLICY

The importance of open data and software: Is energy research lagging behind?

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ARTICLE INFO

ABSTRACT

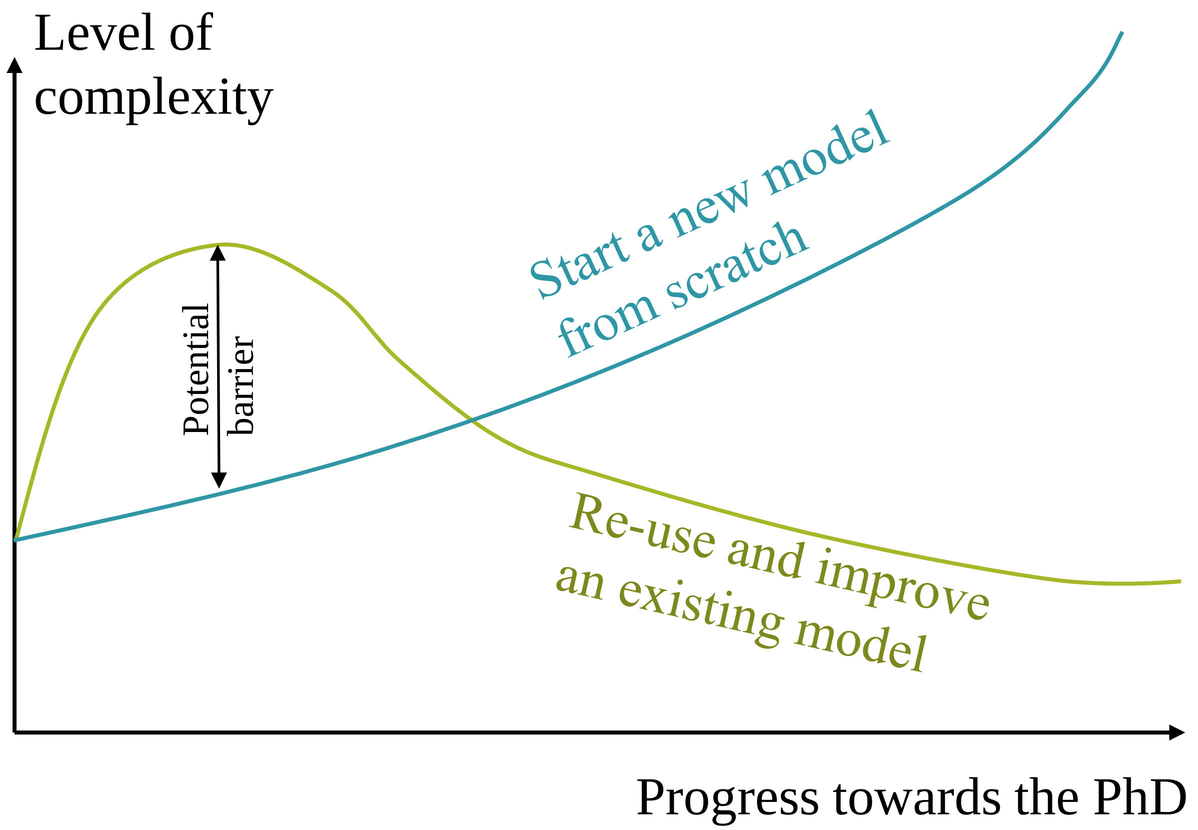
From the H2020 website: "*the European Commission is now moving decisively from Open Access into the broader picture of Open Science*"

Why energy models and data are not open

- Ethical and security concerns (particularly for data)
  - E.g. Information in household consumption data
- Unwanted exposure and scrutiny
  - *"My code is not good enough to be published"*
  - Reluctance to share data was shown to be associated with weaker evidence
- Fear of the code being stolen
  - *"The code is valuable intellectual property that belongs to my institution"*
- Time-consuming: documenting the code, providing a documentation
  - *"It is too much work to polish the code"*
- Institutional and personal inertia
  - *"It is not common practice to publish code in my institution"*
- License is omitted
  - ➢ *"The inputs are proposed as open data and are available upon request"*
  - ➢ standard copyright rules apply
  - ➢ no re-use or distribution of the code/data is permitted

Why energy models are proliferating

- Recent years have seen a proliferation of energy system models, open or not
- Reasons include:
  - Limited knowledge of the modeling landscape by young researchers
  - Lack of guidance and inertia of the promotors
  - Willingness to make "something new"
  - The initial potential barrier to get into someone else's model



Thank you very much for you attention!

For more information on the topic:

openmod open energy modelling initiative

https://openmod-initiative.org/