Introducing the Workflow and Modelling Choices Behind PyPSA-Eur-Sec

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based on many contributions from J. Hörsch, F. Neumann, F. Hofmann, M. Frysztacki, E. Zeyen, M. Victoria, K. Zhu etc.

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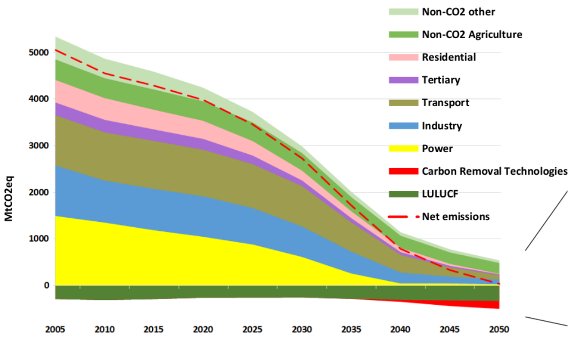
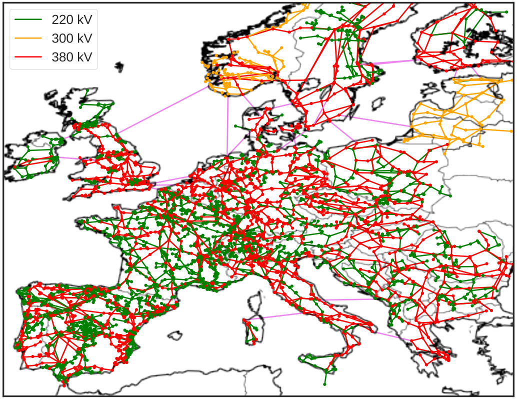
Introduction

What is PyPSA-Eur-Sec?

Need to decarbonize all sectors in Europe....



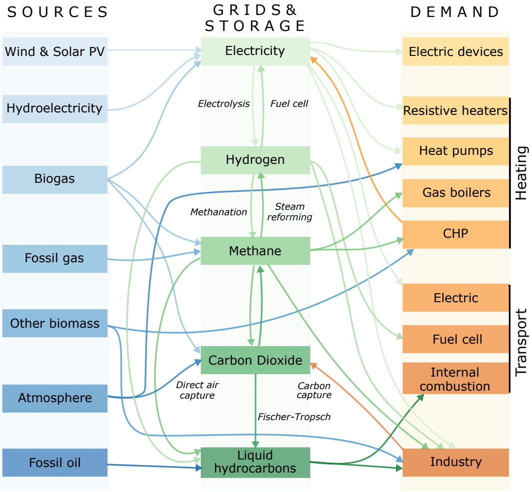
while obeying spatial and temporal constraints

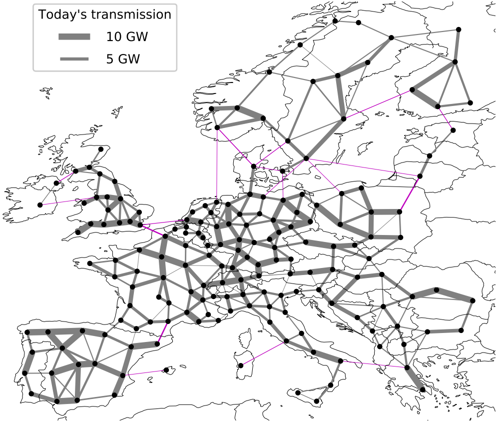


Source: European Commission 'Clean Planet for All', 2018

What is PyPSA-Eur-Sec?

Represents all energy flows... and bottlenecks in clustered network.





Goals of This Presentation

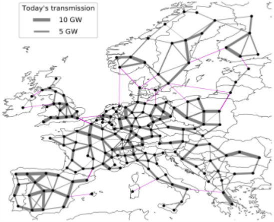
- Explain workflow management with **snakemake**
- Show concretely how this works for the open model of the European tranmission system **PyPSA-Eur**
- Explain the modelling choices behind the sector-coupled version of the model, **PyPSA-Eur-Sec** (what is exogenous and what is determined endogenously inside the model)

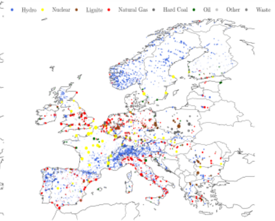
Workflow Management with Snakemake

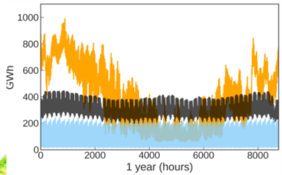
Data-Driven Modelling

Lots of different types of data come together for the modelling...

- Clustered network model
- Power plants & technology assumptions
- Renewable potentials & decades of hourly time series for each point in space
- Demand forecasts & time series







Analysis and optimisation

Problems

- Many different data sources
- Many data sources need cleaning and processing before they can be used
- Many intermediate scripts and datasets
- Many colleagues hack something together in a folder - hard to reproduce later
- Often dependencies are not clear (both data and software)
- Data and code change over time
- Want to run many parametric scenarios for same model

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What we need is a **workflow management tool**.

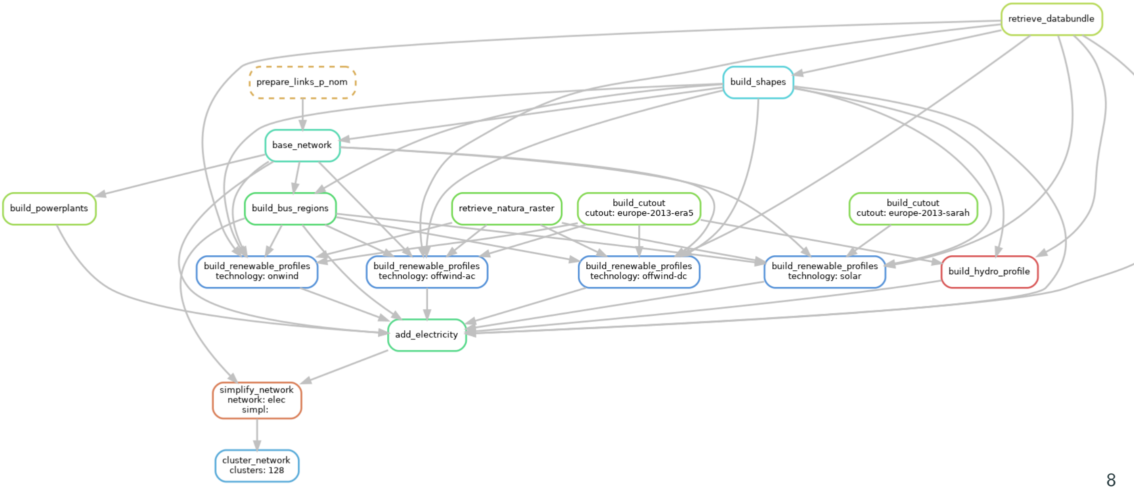
Workflow Management Tool: Snakemake

"The Snakemake workflow management system is a tool to create **reproducible and scalable data analyses**. Workflows are described via a human readable, Python based language. They can be seamlessly scaled to server, cluster, grid and cloud environments, without the need to modify the workflow definition. Finally, Snakemake workflows can entail a description of required software, which will be automatically deployed to any execution environment."

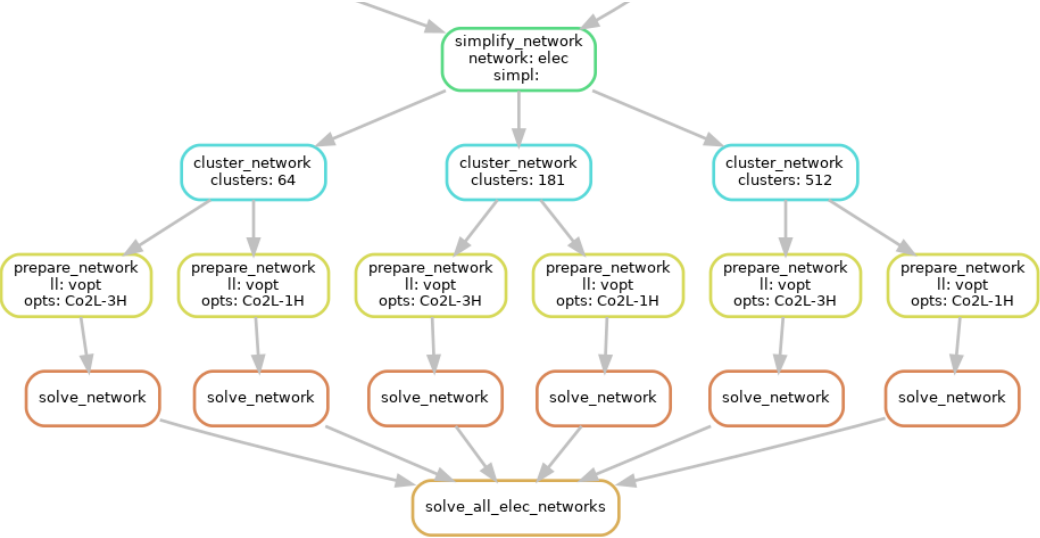
See snakemake presentation.

Snakemake for PyPSA-Eur: Building Model

A graphical unpacking of the dependencies in the PyPSA-Eur Snakemake file:



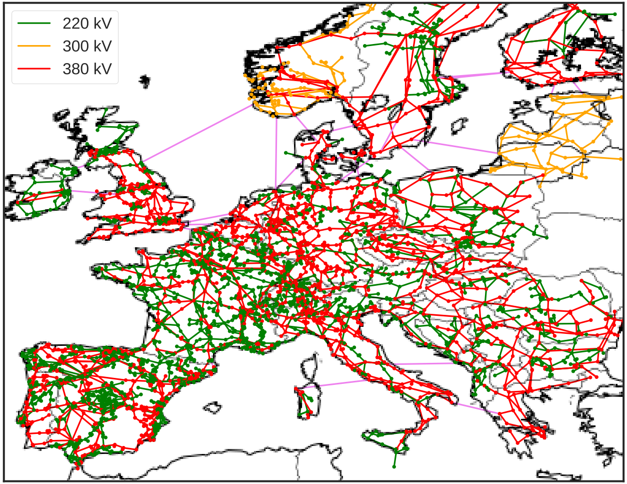
Snakemake for PyPSA-Eur: Managing Scenarios



PyPSA-Eur

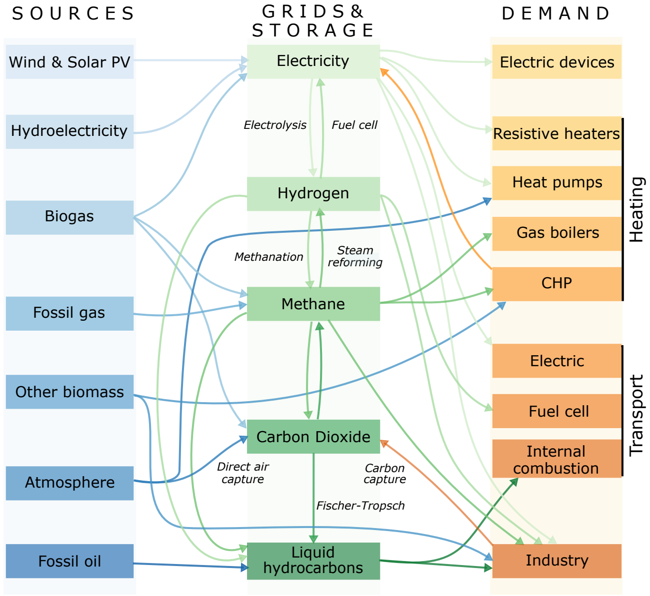
PyPSA-Eur

See other slidedeck for breakdown of PyPSA-Eur snakemake rules.



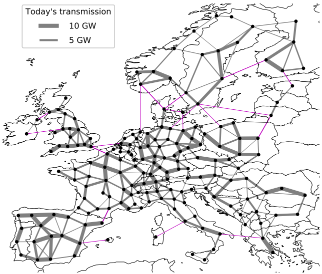
PyPSA-Eur-Sec

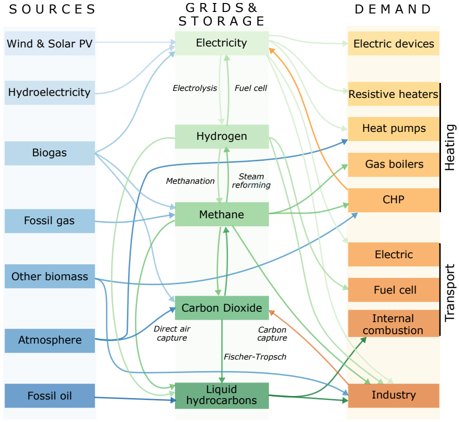
Sector coupling: A new source of flexibility



PyPSA-Eur-Sec builds on PyPSA-Eur

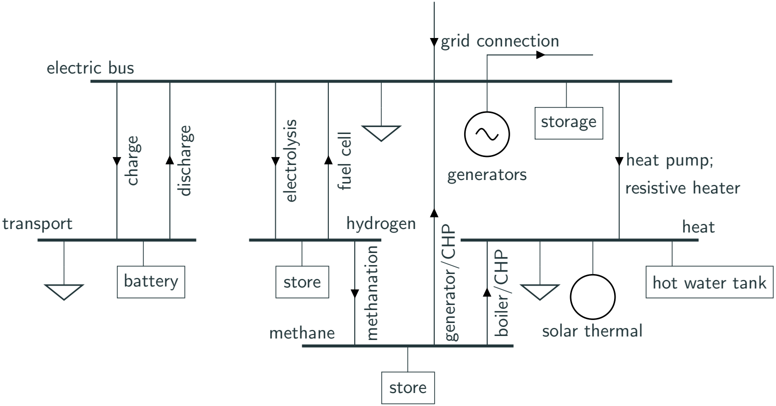
- PyPSA-Eur-Sec includes PyPSA-Eur as a **snakemake subworkflow**.
- PyPSA-Eur builds the clustered power grid and renewable generators.
- Then PyPSA-Eur-Sec adds other sectors.





Sector coupling: A new source of flexibility

In PyPSA other sectors are represented with buses for energy carriers, demand time series, (multi-)links for energy conversion and material flow, stores and generators. Partial graph:



Technology Choices: Exogenous Versus Endogenous

The model **minimises total costs given constraints** (CO_2 budgets, renewable targets, limits on wind/solar potentials, etc.). The model can choose some technologies itself, i.e. **endogenously**, while others we choose beforehand, i.e. **exogenously**.

Endogenous:

- electricity generation
- transmission reinforcement
- space and water heating technologies (including building renovations)
- supply of process heat for industry
- carbon capture

Exogenous:

- energy carrier for road transport (2050: BEV for light-duty, BEV or FCEV for heavy-duty)
- kerosene for aviation
- energy carrier for shipping (2050: LH_2)
- steel production: DRI with hydrogen, then electric arc (could make it compete with blast furnace)
- electrification in industry

Technology Choices: Exogenous Versus Endogenous

Rationale?

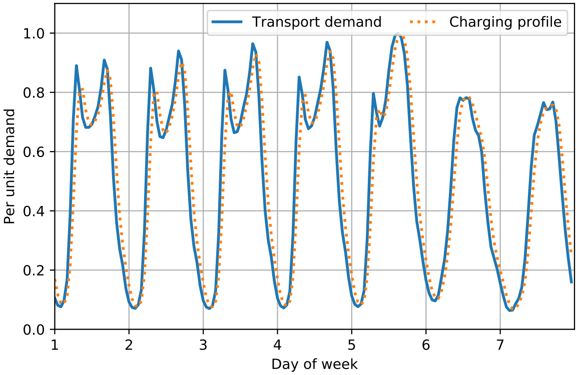
It depends where study is focused.

In some areas we know where things are going (e.g. electric vehicles for light-duty vehicles), and want to limit computation times.

Many things determined by external considerations (electric vehicles driven by air pollution, building renovations by comfort, etc.).

Choices all debatable (iron with CCS versus DRI with H_2, whether retrofitting is fixed or not, shipping fuels, etc.).

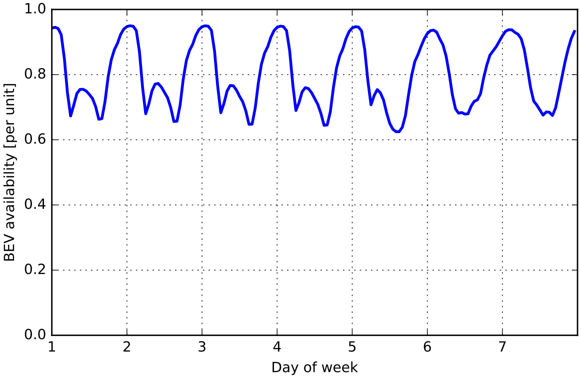
Transport sector: Electrification of Transport



Weekly profile for the transport demand based on statistics gathered by the German Federal Highway Research Institute (BASt).

- Road and rail transport is fully electrified (vehicle costs are not considered)
- Because of higher efficiency of electric motors, final energy consumption 3.5 times lower than today at 1100 TWh_{el}/a for Europe
- In model can replace Battery Electric Vehicles (BEVs) with Fuel Cell Electric Vehicles (FCEVs) consuming hydrogen. Advantage: hydrogen cheap to store. Disadvantage: efficiency of fuel cell only 60%, compared to 90% for battery discharging.

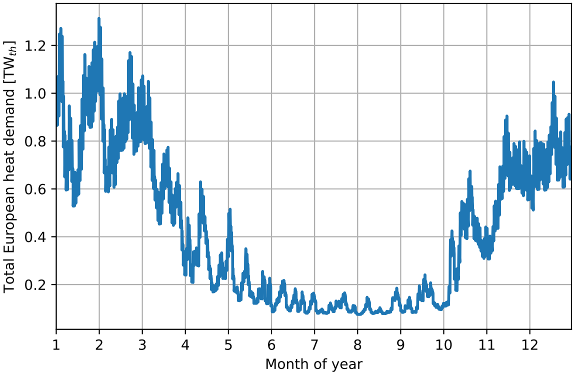
Transport sector: Battery Electric Vehicles



Availability (i.e. fraction of vehicles plugged in) of Battery Electric Vehicles (BEV).

- Passenger cars to Battery Electric Vehicles (BEVs), 50 kWh battery available and 11 kW charging power
- Can participate in DSM and V2G, depending on scenario (state of charge returns to at least 75% every morning)
- All BEVs have time-dependent availability, averaging 80%, max 95% (at night)
- No changes in consumer behaviour assumed (e.g. car-sharing/pooling)
- BEVs are treated as exogenous (capital costs NOT included in calculation)

Heating sector: Many Options with Thermal Energy Storage (TES)



Heat demand profile from 2011 in each region using population-weighted average daily T in each region, degree-day approx. and scaled to Eurostat total heating demand.

- All space and water heating in the residential and services sectors is considered, with no additional efficiency measures (conservative) - total heating demand is 3585 TWh_{th}/a.
- Heating demand can be met by heat pumps, resistive heaters, gas boilers, solar thermal, Combined-Heat-and-Power (CHP) units. No industrial waste heat.
- Thermal Energy Storage (TES) is available to the system as hot water tanks.

Centralised District Heating versus Decentralised Heating for Buildings

We model both fully decentralised heating and cases where up to 45% of heat demand is met with district heating in northern countries. Heating technology options for buildings:

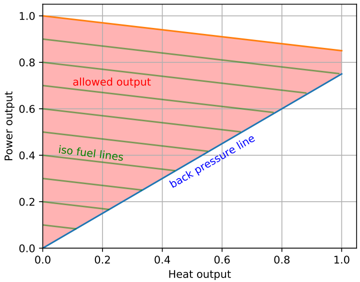
Decentral individual heating can be supplied by:

- Air- or Ground-sourced heat pumps
- Resistive heaters
- Gas boilers
- Small solar thermal
- Water tanks with short time constant $\tau = 3$ days

Central heating can be supplied via district heating networks by:

- Air-sourced heat pumps
- Resistive heaters
- Gas boilers
- Large solar thermal
- Water tanks with long time constant $\tau = 180$ days
- CHPs

CHP feasible dispatch:



Building renovations can be co-optimised to reduce space heating demand.

Remaining sectors: non-electric industry processes, aviation, shipping

For ‘hard-to-defossilise’ sectors, we assume some process- and fuel-switching (under review):

Iron & Steel	70% from scrap, rest from direct reduction with 1.7 $MWhH_2$/tSteel + electric arc (process emissions 0.03 tCO_2/tSteel)
Aluminium	80% recycling, for rest: methane for high-enthalpy heat (bauxite to alumina) followed by electrolysis (process emissions 1.5 tCO_2/tAl)
Cement	Waste and solid biomass
Ceramics & other NMM	Electrification
Chemicals	Synthetic methane, synthetic naphtha and hydrogen
Other industry	Electrification; process heat from biomass
Shipping	Liquid hydrogen (could be replaced by other liquid fuels)
Aviation	Kerosene from Fischer-Tropsch

Carbon is tracked through system: 90% of industrial emissions are captured; direct air capture (DAC); synthetic methane and liquid hydrocarbons; transport and sequestration 20 €/tCO_2

PyPSA-Eur-Sec: Preliminary Results

Electrification of other sectors is critical for decarbonisation...

Electrification is essential to decarbonise sectors such as transport, heating and industry.

Some scenarios show a **doubling or more of electricity demand**.

Source: Tesla; heat pump: Kristoferb at English Wikipedia

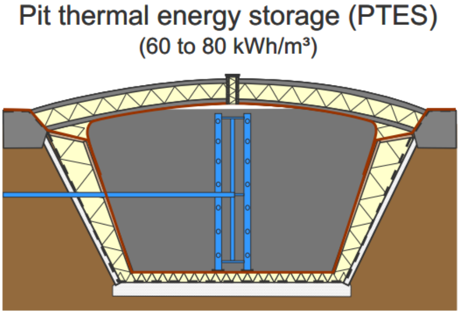
…but must take account of variabilility & social & political constraints

Sustainability doesn't just mean taking account of environmental constraints.

There are also **social and political constraints**, particularly for transmission grid and onshore wind development.

Fortunately other sectors offer flexibility back to grid

Other sectors offer **flexibility** (e.g. battery electric vehicles, power-to-gas, thermal storage), enabling energy to be **stored cheaply** and **transported easily** (e.g. using gas networks).



Sectoral coupling with spatial resolution, European scope

The Issue: Most cross-sectoral studies are at country level, but don't have the resolution to resolve transmission bottlenecks or the variability of renewables

Our Goal: Model full energy system over Europe with enough resolution to understand the effects of congestion and the cost-benefits of transmission reinforcement

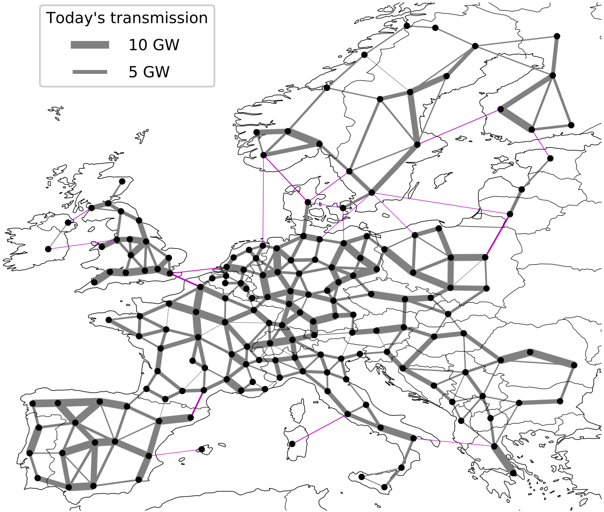
The Challenge: Enormous datasets, computability, complexity

Today: Some preliminary results from my group and our cooperation partners

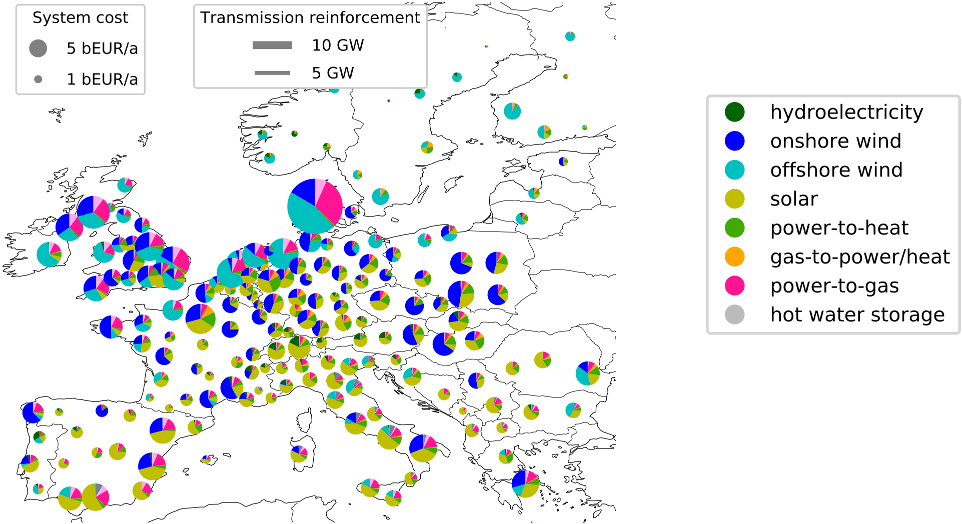
Example results: 181-node model of European energy system

Some brief, preliminary results from our sector-coupled, 181-node model of the European energy system.

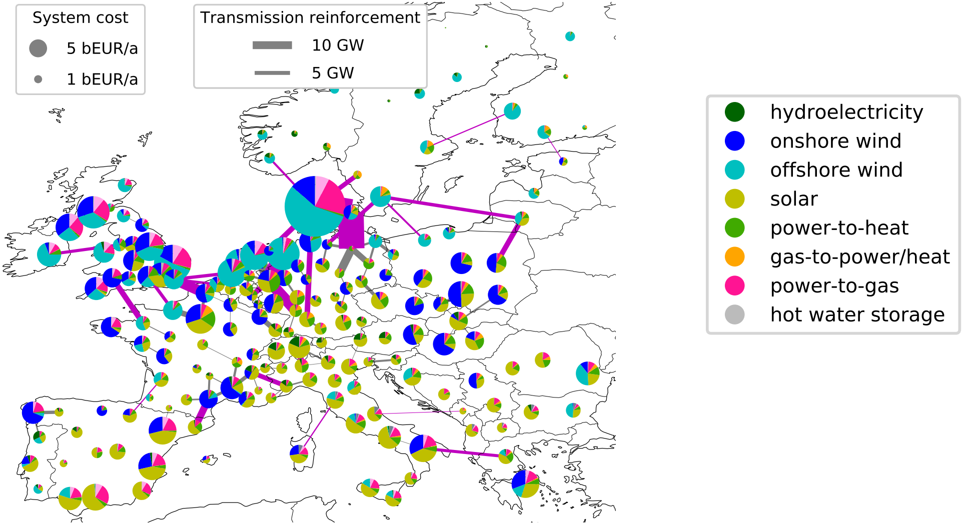
- Couple **all energy sectors** (power, heat, transport industry)
- Reduce CO_2 emissions **to zero**
- Assume **smaller bidding zones** and **widespread dynamic pricing**
- **Conservative** technology assumptions
- Examine effect of **acceptance** for **grid expansion** and **onshore wind**



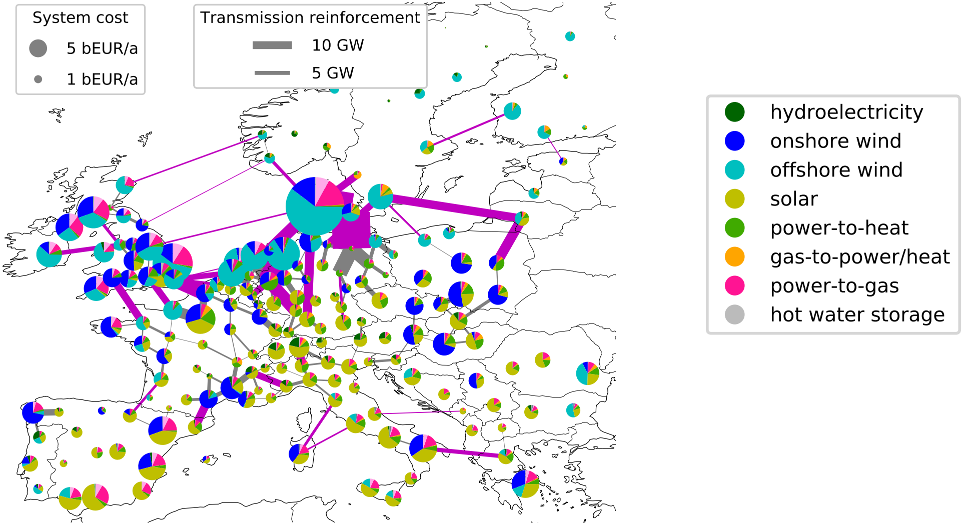
Distribution of technologies: No grid expansion



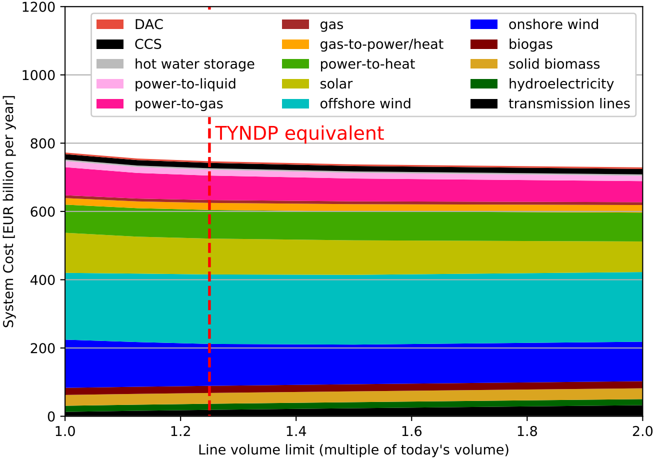
Distribution of technologies: 25% more grid volume - similar to TYNDP



Distribution of technologies: 50% more grid volume - double the TYNDP

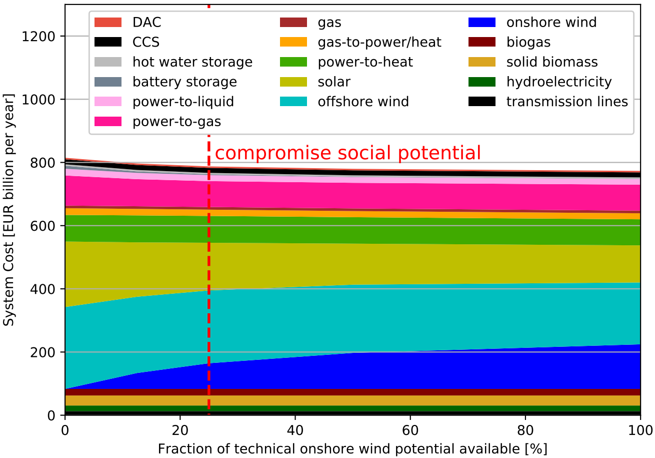


Benefit of grid expansion for sector-coupled system



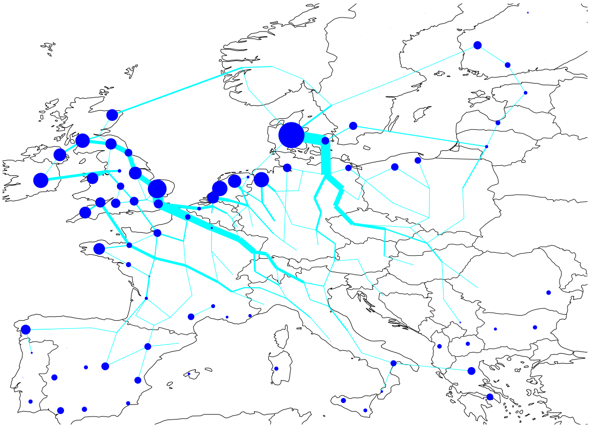
- Direct system costs **bit higher than today's system** (€ 700 billion per year with same assumptions)
- Systems **without grid expansion** are feasible, but more costly
- As grid is expanded, **costs reduce** from solar and power-to-gas; more offshore wind
- Total cost benefit of extra grid: ∼ € 47 billion per year
- **Over half of benefit available at 25% expansion** (like TYNDP)

Benefit of full onshore wind potentials



- **Technical potentials** for onshore wind respect land usage
- However, they do not represent the **socially-acceptable potentials**
- Technical potential of ∼ 400 GW in Germany is **unlikely to be built**
- Costs rise by ∼ € 42 billion per year as we **eliminate onshore wind** (with no grid expansion)
- Rise is only ∼ € 14 billion per year if we **allow a quarter of technical potential** (∼ 100 GW for Germany)

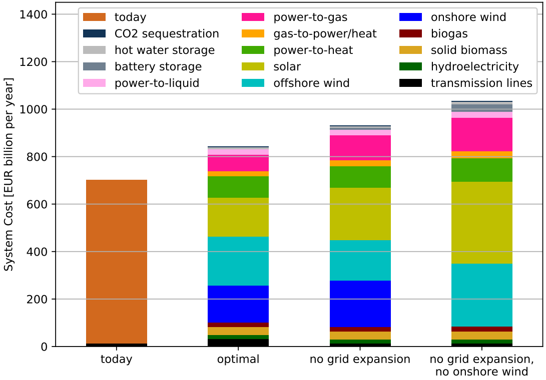
Role of hydrogen network



- New hydrogen network takes over role of transporting energy around Europe when no electricity grid expansion allowed
- Annualised cost of network: € 8 billion per year
- Largest H2 pipeline capacity: 81 GW in GB
- Largest H2 electrolyzer capacity: 178 GW in DK
- Energy moved per hour: AC is 99 TWhkm/h, DC is 3.3 TWhkm/h, H2 is 209 TWhkm/h

Should also consider indirect costs, which change the picture

Costs increase as we reduce emissions and accommodate public acceptance...



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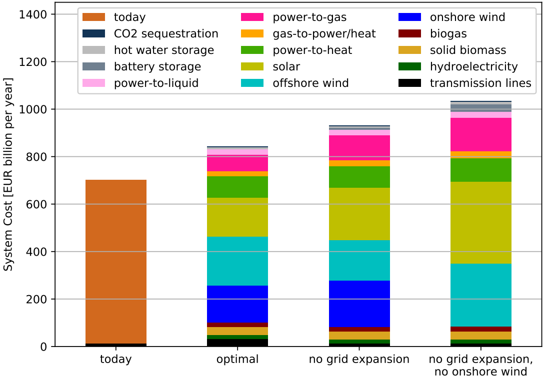
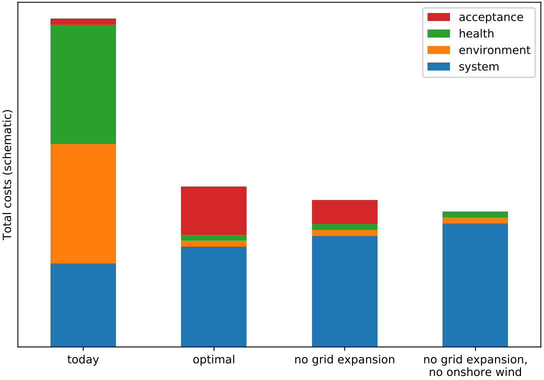
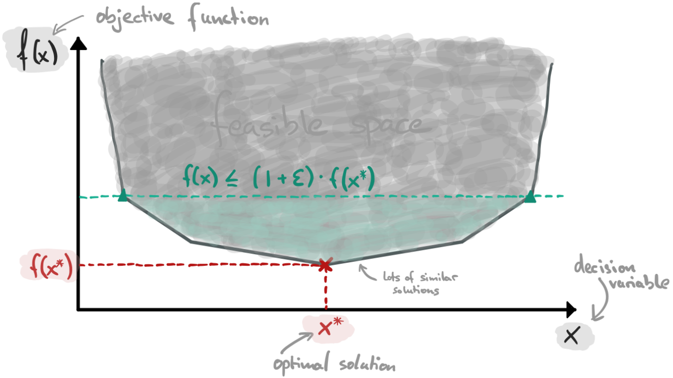
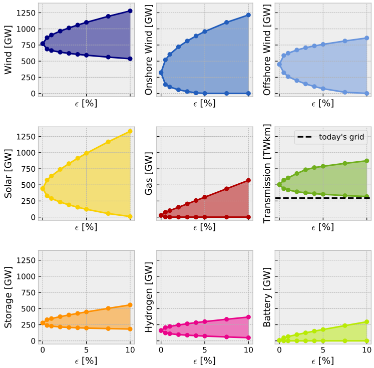


but not if we include indirect environmental, health and social costs (schematic example)



Large Space of Near-Optimal Solutions





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