Enabling energy systems research on HPC

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Energy Systems Analysis Needs HPC

Background: The status quo

Studying the future is inherently subject to large uncertainties. The state of the art in energy system research is to tackle these uncertainties with ensemble modeling of a **small subset of all possible scenarios**. This has proven to be inadequate as the models are highly sensitive to certain input data. Additionally, the widely-used commercial solvers show poor scalability and are **limited to single shared-memory compute nodes**. Thus, models are defined with a lower temporal and spatial resolution and a lower technological diversity than necessary to ensure applicability for real world policy support.

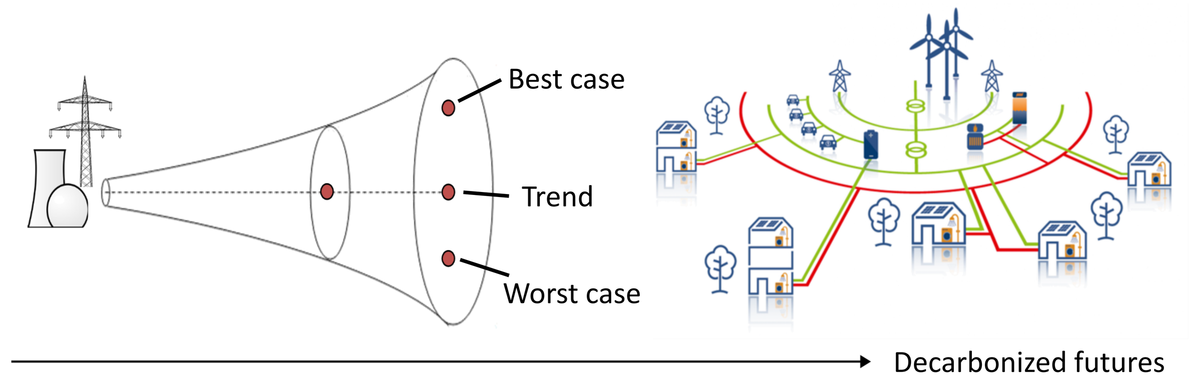

Fig. 1: The established scenario funnel for decarbonization pathways of energy systems

Objective: The theoretical best practice

We have opted to fully inspect the conceivable parameter space for the first time by using a hitherto unattained number of model-based energy scenarios. To overcome the above-mentioned limitation we use **automated parameter sampling**, **model coupling**, a self-developed **distributed memory solver**, and a **workflow environment for HPC**. Efficiently leveraging the capability of HPC could be a game changer for the energy-system analysis community.

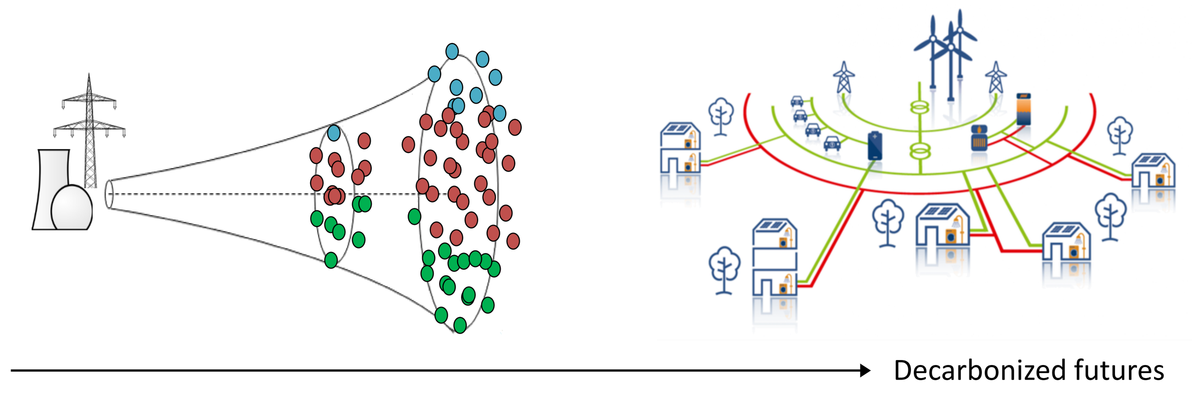

Fig. 2: The scenario funnel for decarbonization pathways of energy systems in UNSEEN

Methodological Approach

New HPC solver - PIPS-IPM++[6]

- We have designed custom algorithms for **distributed High Performance Computing (HPC)** to keep computing times manageable and to circumvent memory limitations
- PIPS-IPM++ implements a **parallel interior-point method** (IPM) for solving large-scale linear programs (LPs). It exploits the doubly bordered block diagonal matrix structure to parallelize the optimization process via **MPI** and **OpenMP**
  - The hourly optimization model is decomposed into time slices
- LP standard form:

$$\min \; c^T x \quad \text{s.t.} \; Ax = b, \; x \geq 0$$

where $c \in \mathbb{R}^n$, $b \in \mathbb{R}^m$, $A \in \mathbb{R}^{m \times n}$.

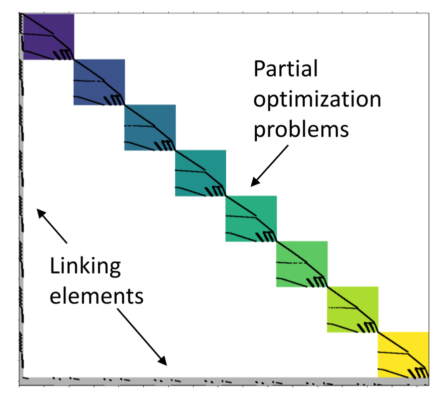

Fig. 3: Example of a typical energy system block-structured matrix

Model coupling

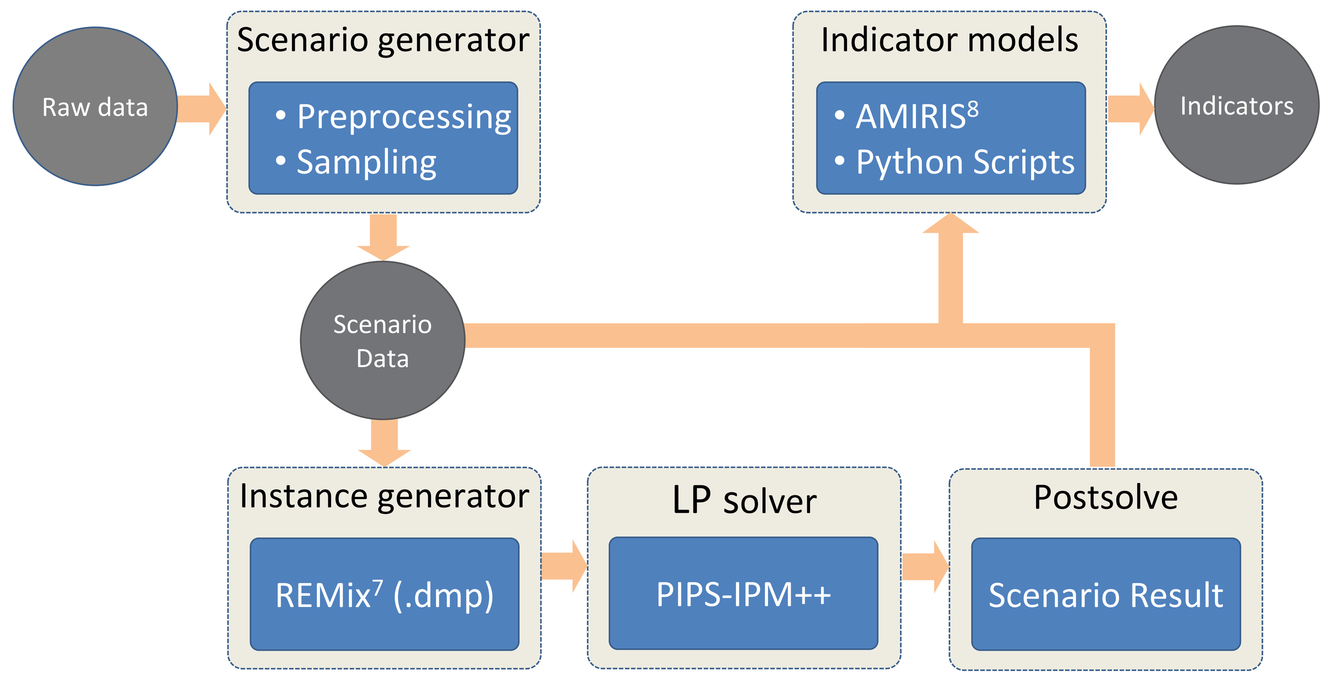

Fig. 4: High-level representation of the pipeline flow for each scenario as part of our HPC workflow

JUBE[9] – workflow environment

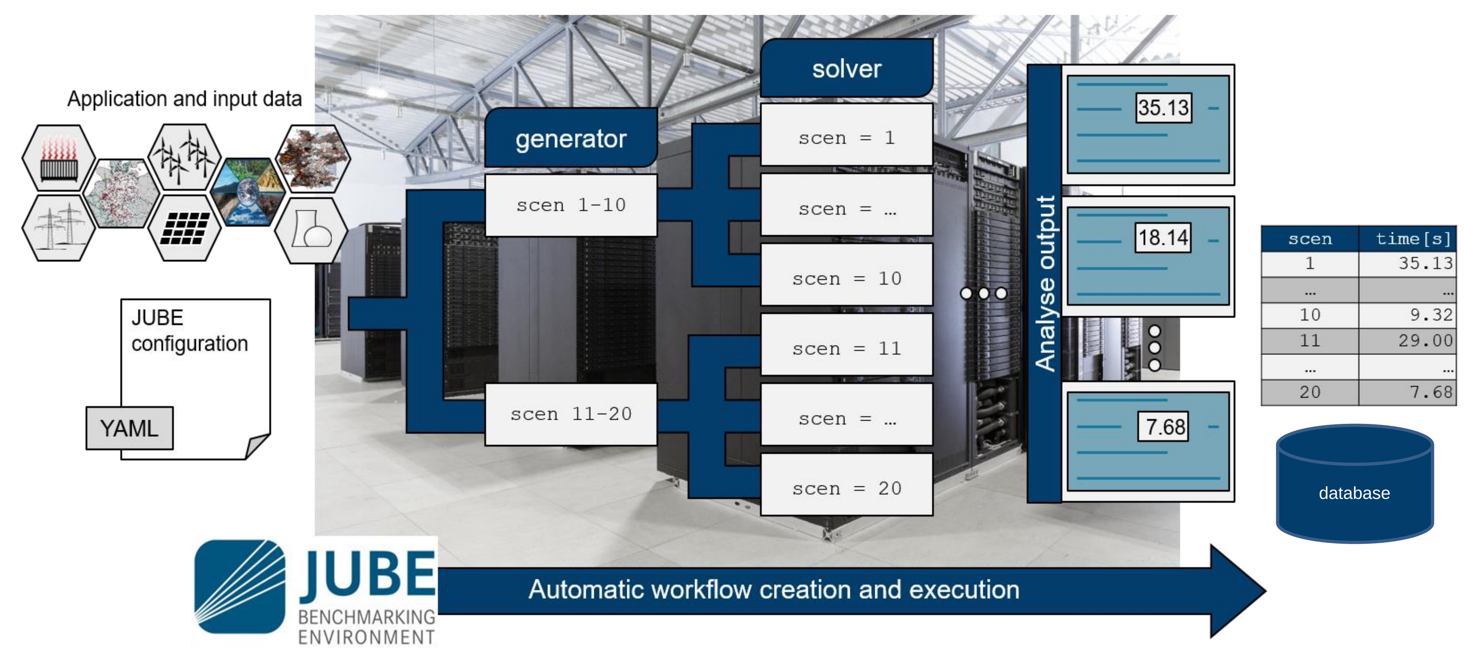

Fig. 5: Schematic representation of the HPC workflow implementation by JUBE (manages parallel pipeline flow (Fig. 4))

Preliminary Results

PIPS-IPM++ scaling

Our open-source solver PIPS-IPM++[6] **outperforms state-of-the-art commercial solvers** on massively parallel architectures. A comparison on JUWELS[10]:

SIMPLE-PIPS[11] benchmark instance:
- 5.1M rows; 5.6M columns
- Up to 32 nodes; 2 threads per MPI process

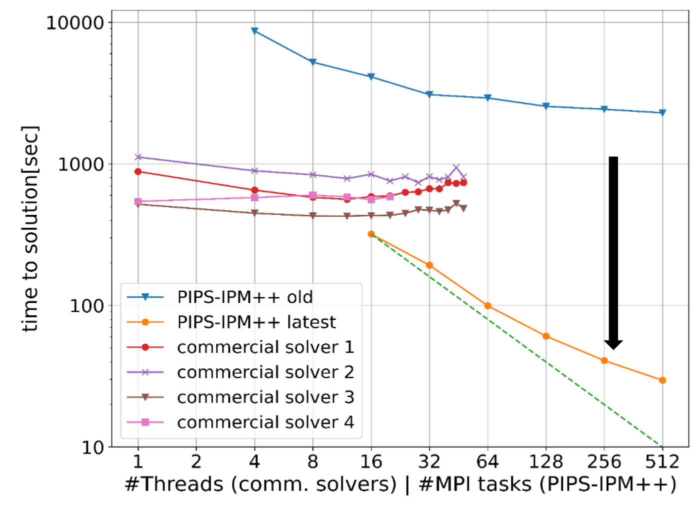

Fig. 6: Benchmark instance of the simple-pips model

PyPSA-eur[12] converted to REMix:
- 234M rows; 213M columns
- 16 nodes; 96 MPI tasks; 8 threads per task

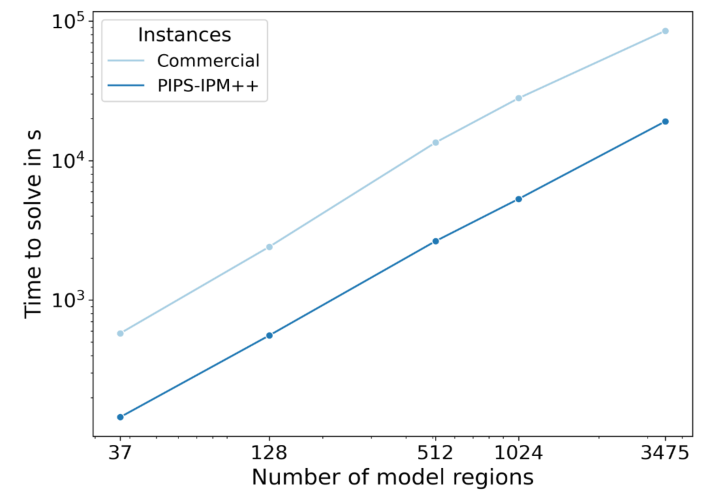

Fig. 7: REMix instance based on the PyPSA-eur dataset

Scenario analysis

1. **Proof-of-concept:** 1000 small instances of German power system scenarios
2. **Real-world models:** > 40 large instances of a highly resolved German power system scenarios
3. **Indicator evaluation:** >30 indicators build 3 clusters
   - Red (1): High gas consumption (higher CO_2 emissions and flexibility)
   - Blue (3): High share of renewables (fewer CO_2 emissions and flexibility)
   - Green (2): In between cluster 1 and 3

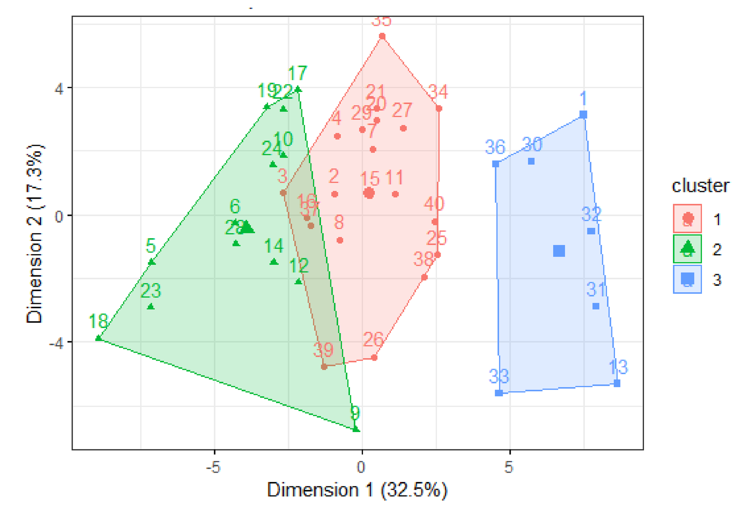

Fig. 8: Scenario cluster plot for 2 main dimensions

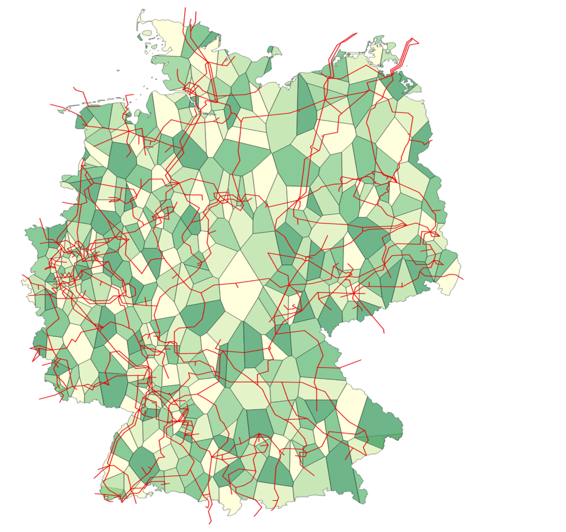

Fig. 9: Highly resolved German power system model

Outlook

Our next step is to cover the uncertainties in energy scenario modeling by performing **more comprehensive parameters variations**, e.g. on weather and demand time series. Furthermore, an increase in model resolution calls for technologically more representative modeling approaches and thus, **solving mixed-integer linear programs on HPC** becomes the next challenge. We have prepared our workflow and solver software to solve such problems. Thus, we can build upon our solver PIPS-IPM++ and integrate **methods for heuristics** such as those **based on neural networks** we are currently developing.

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1 JÜLICH Forschungszentrum
2 DLR Deutsches Zentrum für Luft- und Raumfahrt German Aerospace Center
3 GAMS
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[6] https://github.com/NCKempke/PIPS-IPMpp
[7] https://www.dlr.de/ve/remix
[8] https://www.dlr.de/ve/amiris
[9] https://go.fzj.de/jsc-jube
[10] https://go.fzj.de/juwels
[11] https://gitlab.com/beam-me/simple-pips
[12] https://github.com/PyPSA/pypsa-eur
[13] https://go.fzj.de/jsc-unseen