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Solving Large-Scale GAMS Models on HPC platforms

OR2019

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GAMS Software GmbH

H L R I S



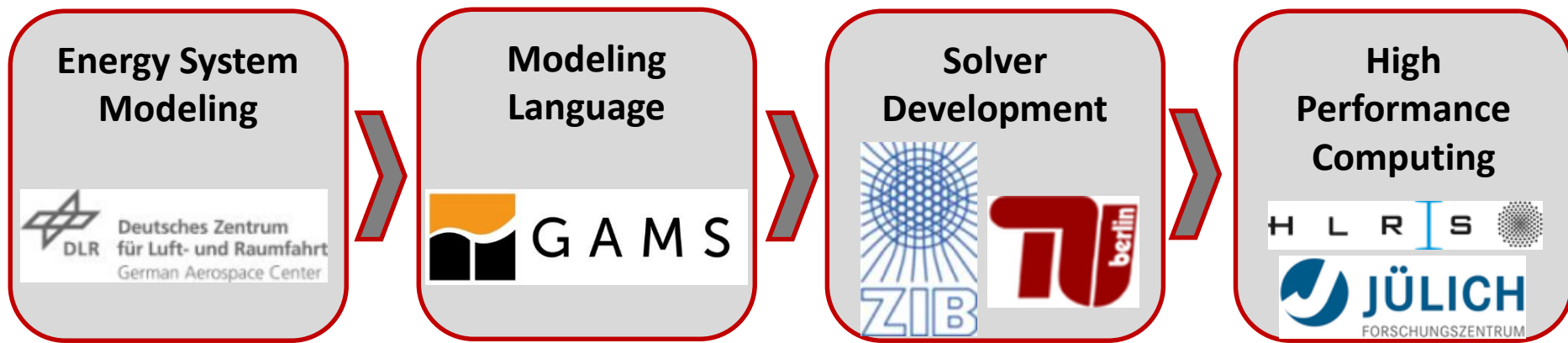
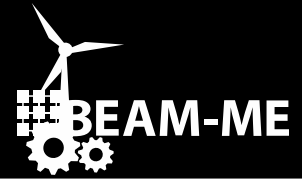
G A M S



Deutsches Zentrum
für Luft- und Raumfahrt
German Aerospace Center



BEAM-ME: An Interdisciplinary Approach



Goal: *Implementation of acceleration strategies from mathematics and computational sciences for optimizing **energy system models** (ESM)*

Model Experiment: Apply and test new solution approaches

UNIVERSITÄT
DUISBURG
ESSEN

ewi

Energiewirtschaftliches Institut an der Universität zu Köln
Energimärkte erforschen – Entscheidungen verbessern.

PAUL SCHERRER INSTITUT



Technical University
of Denmark



Karlsruher Institut für Technologie

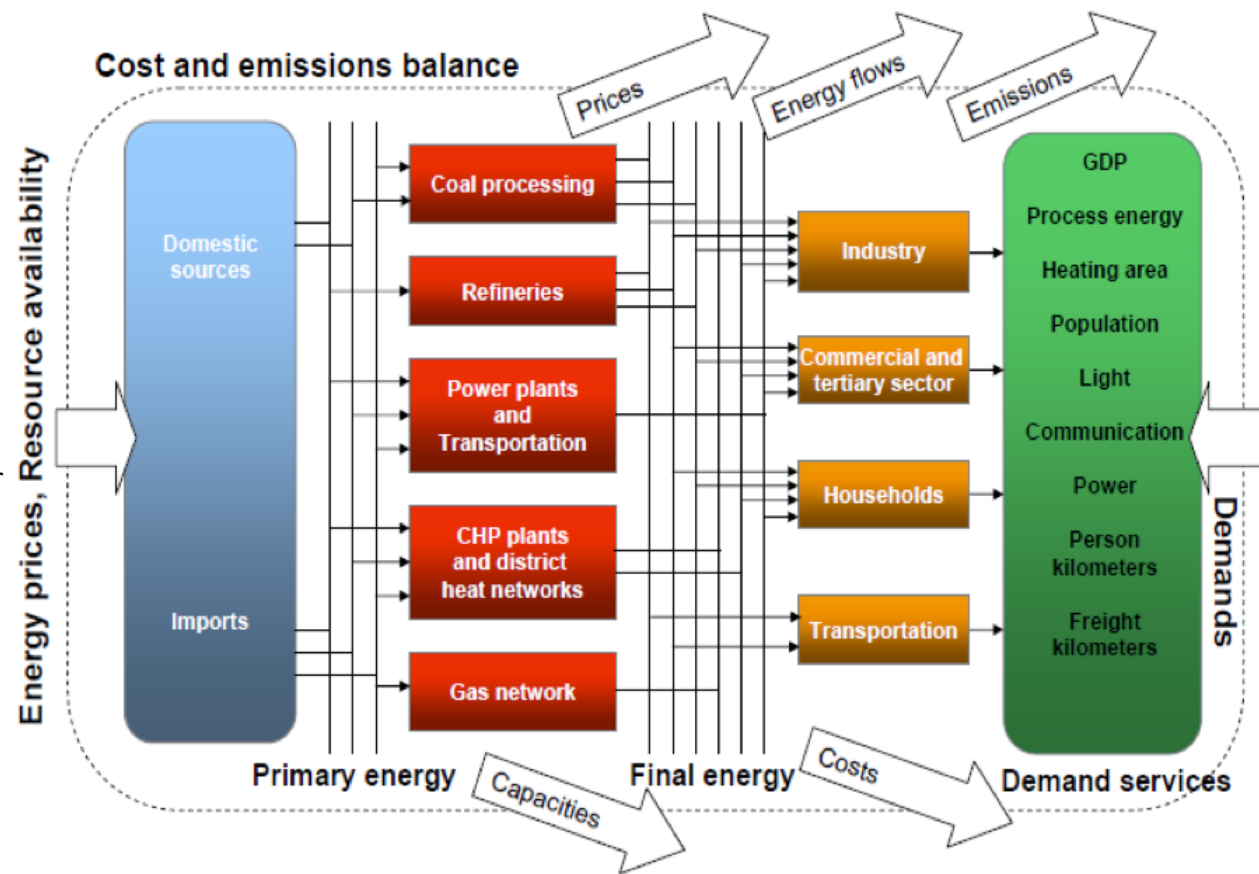


TECHNISCHE
UNIVERSITÄT
DRESDEN

ESM Principles

Model Ingredients:

- Technologies/Processes
 - Transform commodities into other commodities (e.g. fuel → electricity+emissions)
- Commodities
 - Commodity is produced or consumed by a process (e.g. fuels, electricity, emission, money)
- Time
- Region
- Policies
 - Minimum share of renewable energy
 - Maximum amount of (GHG) emissions
 - Minimum level of energy security
 - ...



→ The *mathematical, economic and engineering* relationships between these *energy producers and consumers* are basis of the ESM.

- **Significant investment!**

- E.g. MARKAL/TIMES (Energy Technology Systems Analysis Program (ETSAP) of International Energy Agency (IEA))

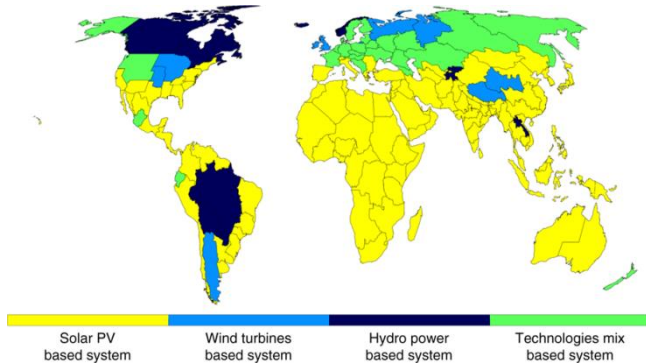
- Development & maintenance effort
 - ~10 person years
 - Lifetime of 20+ years
 - TIMES started ~1997, MARKAL ~1978)
 - Large user base
 - TIMES is used by ~200 research teams in more than 50 countries)

- E.g. REMix (German Aerospace Center (DLR))

- Start year: 2006
 - #PhD Thesis: 13 (6 in progress)
 - Person years (devel/use): 10-20
 - Maintenance: 1 PY/a
 - #Users: 11
 - #Developers: 4
 - #IT/UI Maintenance 0.25 PY/a

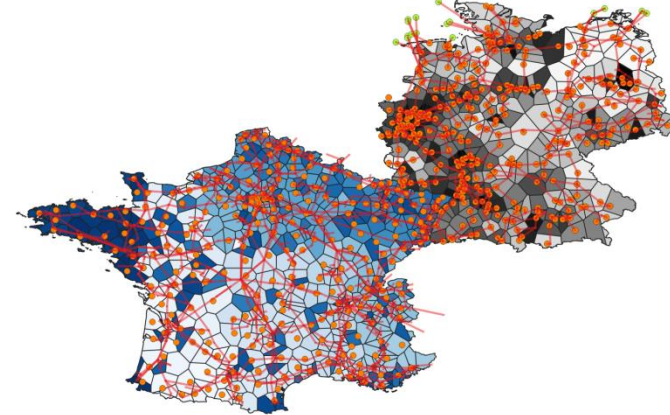
Trends in energy system models

Focus on global energy systems



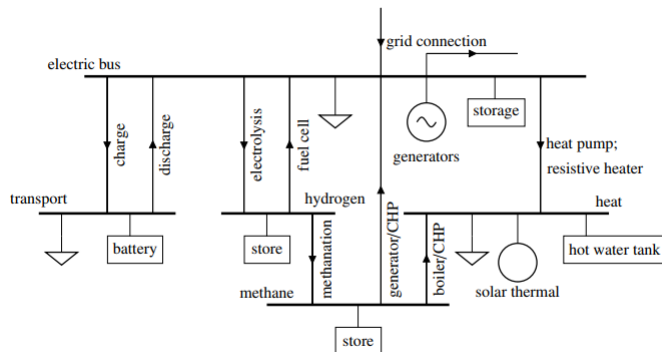
Bogdanov et al., 2019, Radical transformation pathway towards sustainable electricity via evolutionary steps

Higher granularity of regions



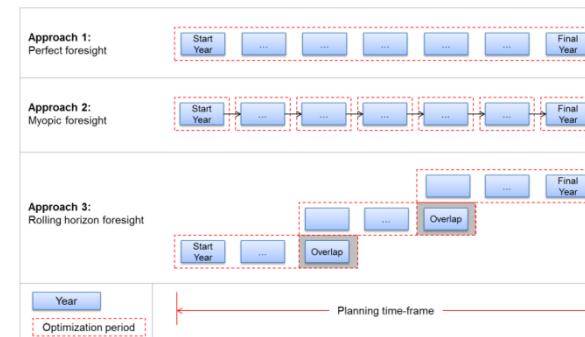
Current work-in-progress from Cao et al.

Sector integration studies



Brown et al., 2018, Synergies of sector coupling and transmission reinforcement in a cost-optimised, highly renewable European energy system

Transformation pathways



Fichter, 2018, Long-term Capacity Expansion Planning with Variable Renewable Energies

Trends in energy system models

Focus on global energy systems

Higher granularity of regions

(ES) Models challenge algorithms

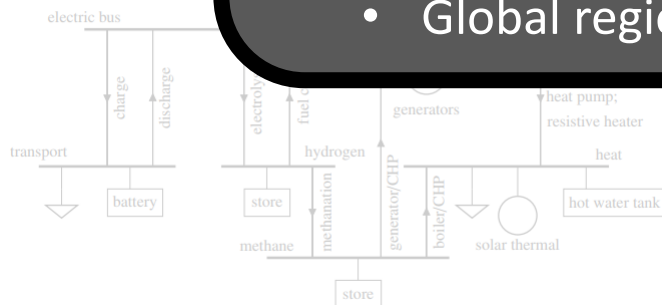
Citius, altius, fortius (faster, higher, stronger)

- Level of granularity
- Time horizon
- Global regions

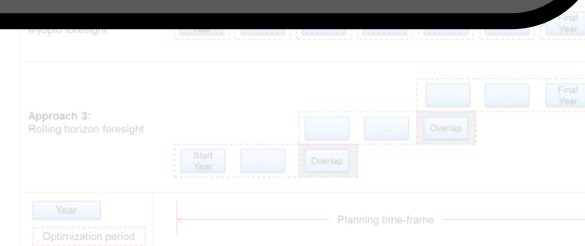
Solar PV
based system

Bogdanov et al.
towards sustain

Sector inte



Brown et al., 2018, Synergies of sector coupling and transmission reinforcement in a cost-optimised, highly renewable European energy system

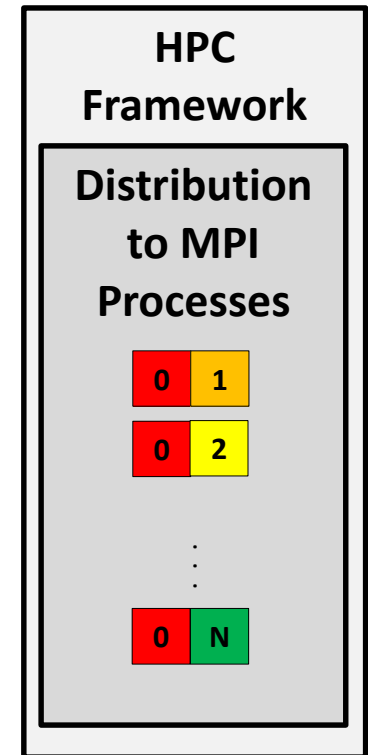


Fichter, 2018, Long-term Capacity Expansion Planning with Variable Renewable Energies

PIPS-IPM (a brief overview):

- Parallel interior-point solver for LPs (und QPs) from *stochastic* energy models
- Exploit **block structure** when solving Central Path equation system
- Main developers: Cosmin Petra
- Significant Extensions of PIPS-IPM (by ZIB, Daniel Rehfeldt, ...)
 - Linking constraints
 - (structure preserving) Presolve
 - (structure preserving) Scaling
 - ...

→ *TD-04: Nils-Christian Kempke: Optimizing Large-Scale Block Diagonal LPs by Using Parallel Interior-Point Methods*

$$\begin{array}{ll} \min & \sum_{i=0}^N c_i^T x_i \\ \text{s.t.} & \begin{array}{l} T_0 x_0 \\ T_1 x_0 + W_1 x_1 \\ T_2 x_0 + W_2 x_2 \\ \vdots \\ T_N x_0 + W_N x_N \end{array} = \begin{array}{l} b \\ h_1 \\ h_2 \\ \vdots \\ h_N \end{array} \\ & \boxed{F_0 x_0 + F_1 x_1 + F_2 x_2 + \dots + F_N x_N = g} \end{array}$$


- Block diagonal structure allows parallelization of linear algebra within PIPS-IPM
- Solve N systems of linear equations in parallel instead of one huge system

¹ Petra et al. 2014: “Real-Time Stochastic Optimization of Complex Energy Systems on High-Performance Computers”

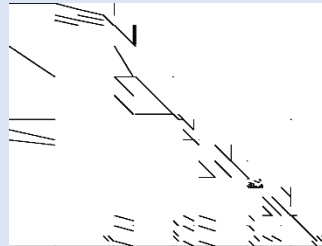
² Breuer et al. 2017: “Optimizing Large-Scale Linear Energy System Problems with Block Diagonal Structure by Using Parallel Interior-Point Methods.”

GAMS/PIPS-IPM Workflow (Comparison)

Model

$$\begin{aligned} \min c^T x \\ Ax = b \\ l \leq x \leq u \end{aligned}$$

model
generation



non-zero plot

General purpose LP solver

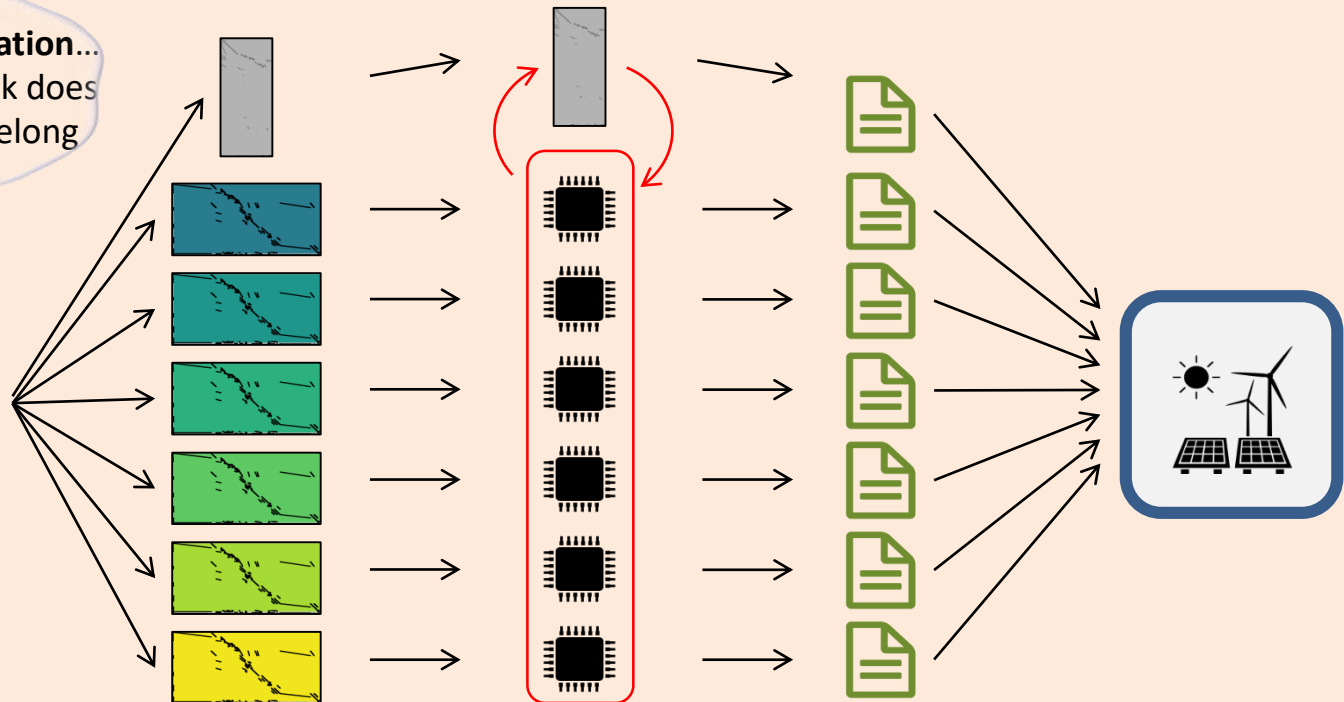


optimization results



Model annotation...
To which block does
variable x belong

model
generation



block structure

split and distribute

parallel solve

merge

optimization results

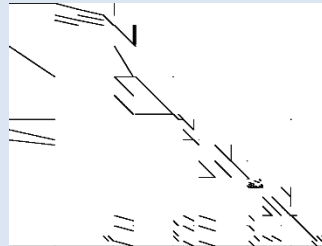
GAMS/PIPS-IPM Workflow (Comparison)

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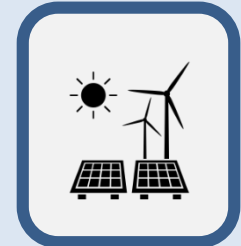
General purpose LP solver



non-zero plot

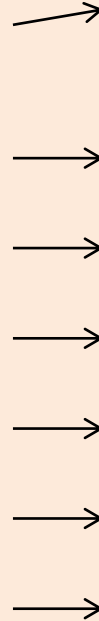
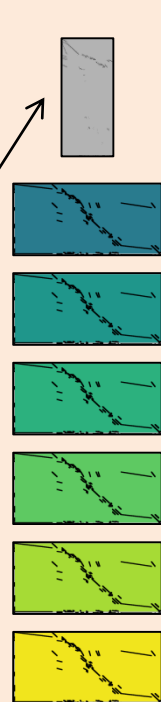


optimization results

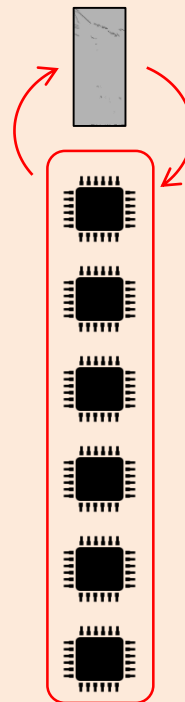


Model annotation...
To which block does
variable x belong

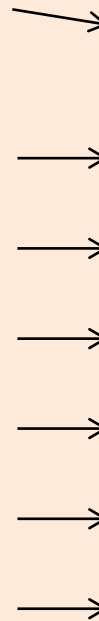
**Parallel model
generation
(work in progress)**



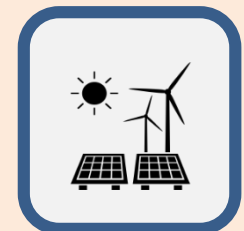
split and distribute



parallel solve

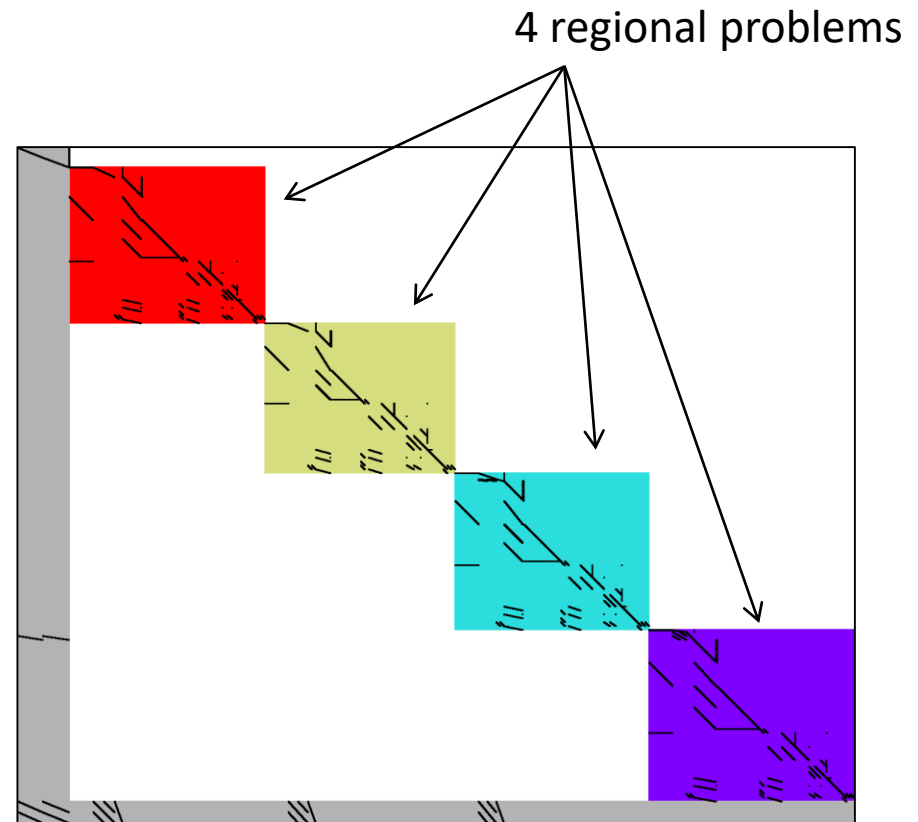
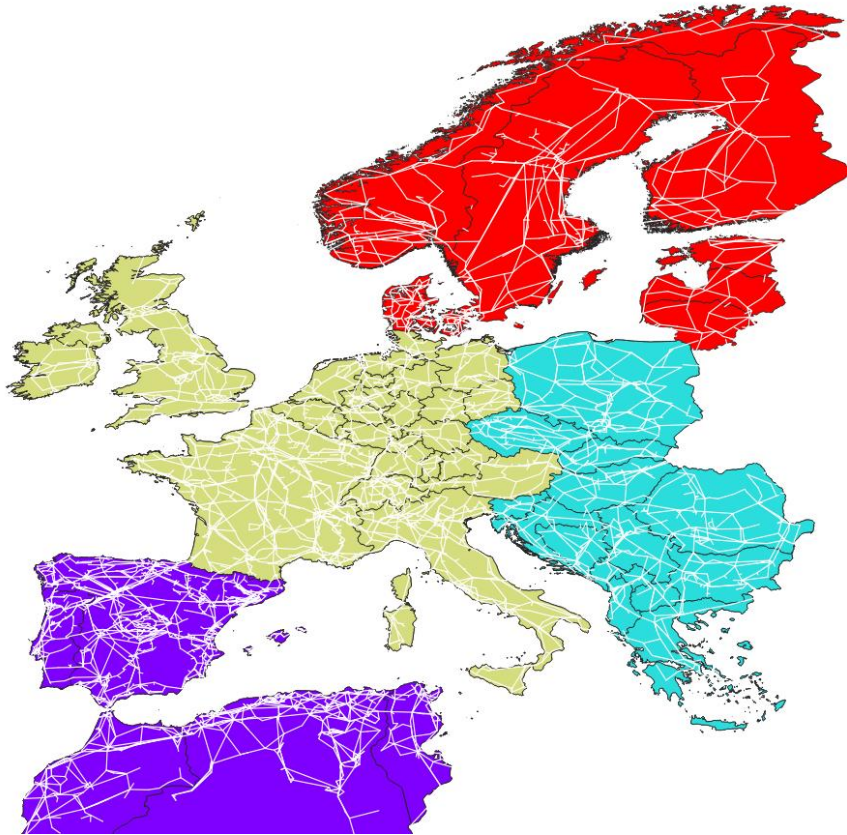


merge



optimization results

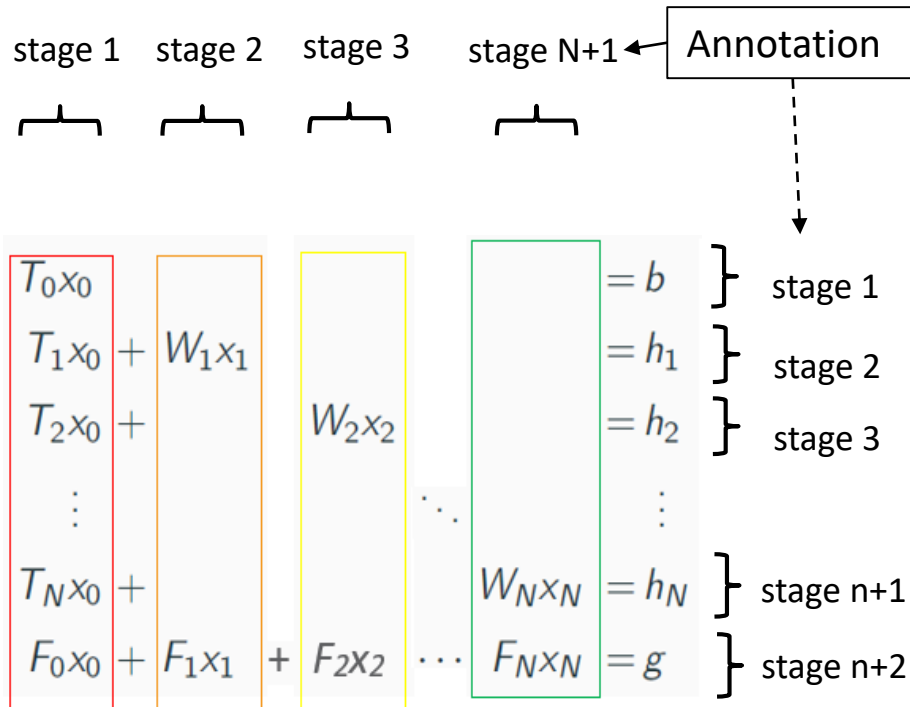
block structure



Linking elements scale with transmission lines and time steps

Model Annotation by .stage attribute

Matrix structure required by PIPS API



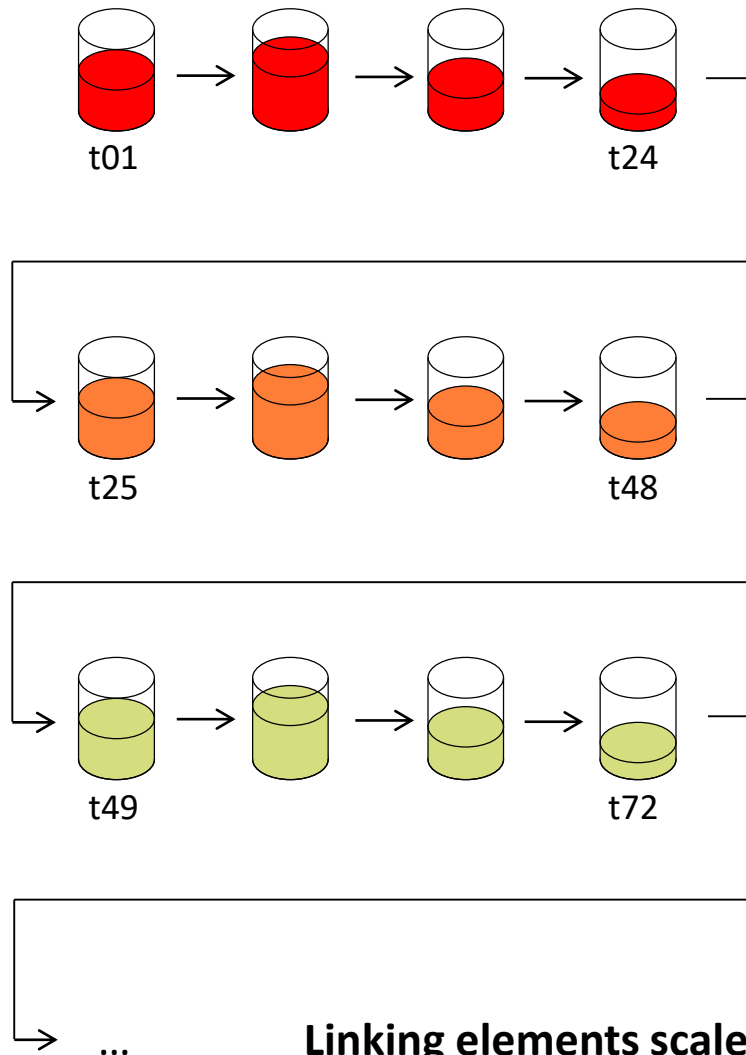
Exemplary (spatial) Annotation for SIMPLE energy system model

```

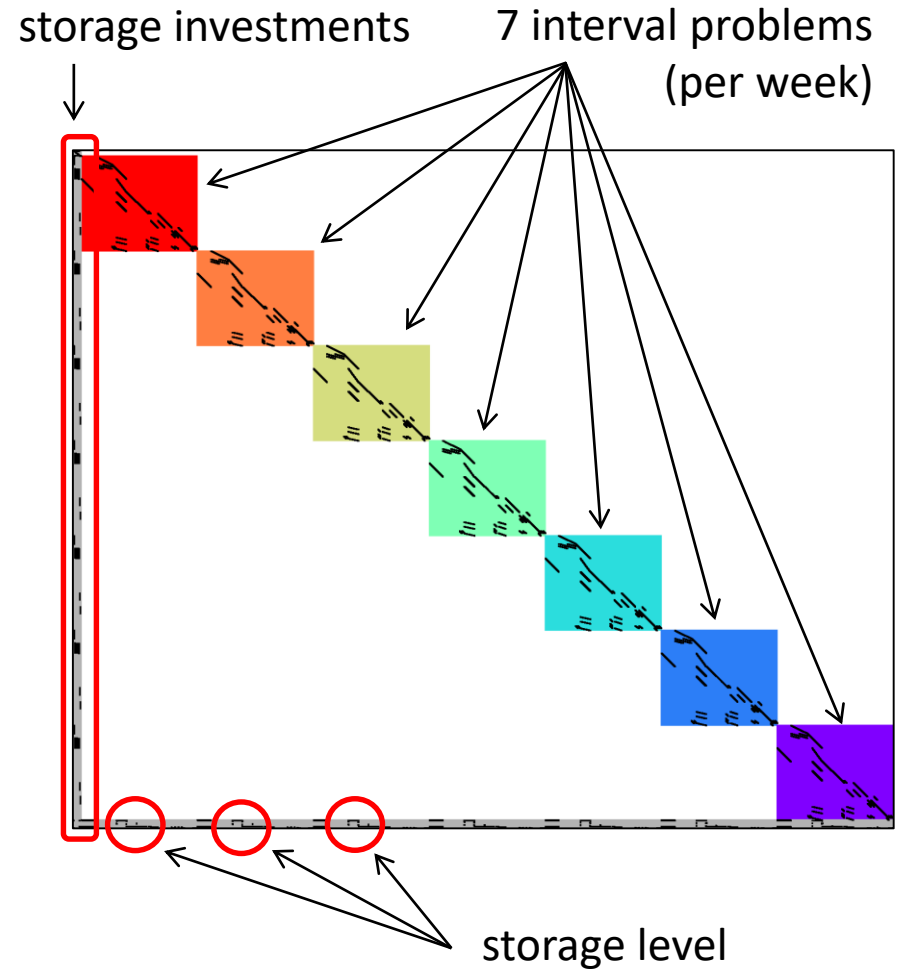
Set rr      'regions'
    p      'plants'
    s      'storages'
    tt     'time steps'
    net(rr,rr) 'transmission links'
    rp(rr,p)  'region to plant mapping'
    rs(rr,s)  'region to strg mapping'

;
[... ]
* linking variables
FLOW.stage(t,net(rr1,rr2))      = 1;
LINK_ADD_CAP.stage(net(rr1,rr2)) = 1;
[... ]
* Block variables
POWER.stage(t,rp(rr,p))         = ord(rr)+1;
STORAGE_INFLOW.stage(t,rs(rr,s)) = ord(rr)+1;
STORAGE_OUTFLOW.stage(t,rs(rr,s)) = ord(rr)+1;
STORAGE_LEVEL.stage(t,rs(rr,s))  = ord(rr)+1;
[... ]
    
```

Temporal Annotation (24h Blocks)

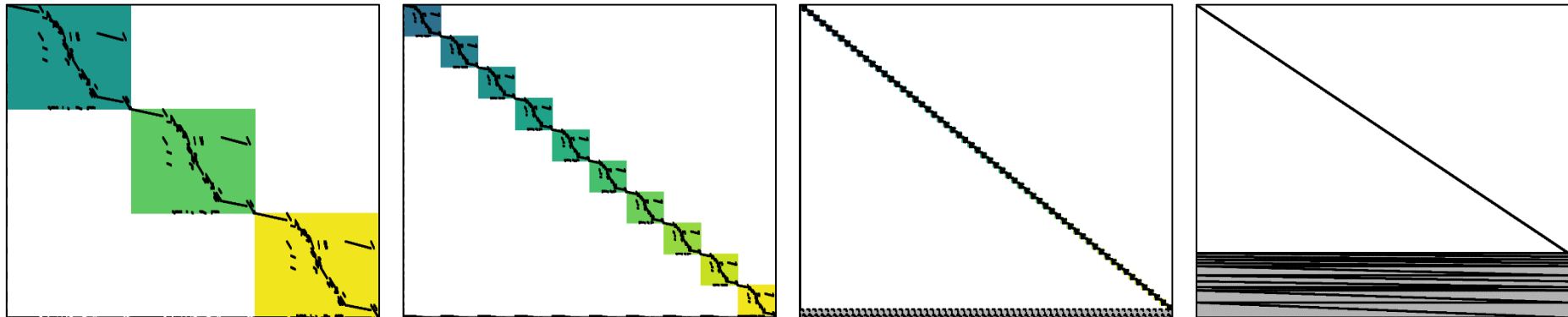


Linking elements scale with regions and technologies



Annotation – The Challenge

- How to annotate Model depends on how the model should be “decomposed” (by region, time,...)

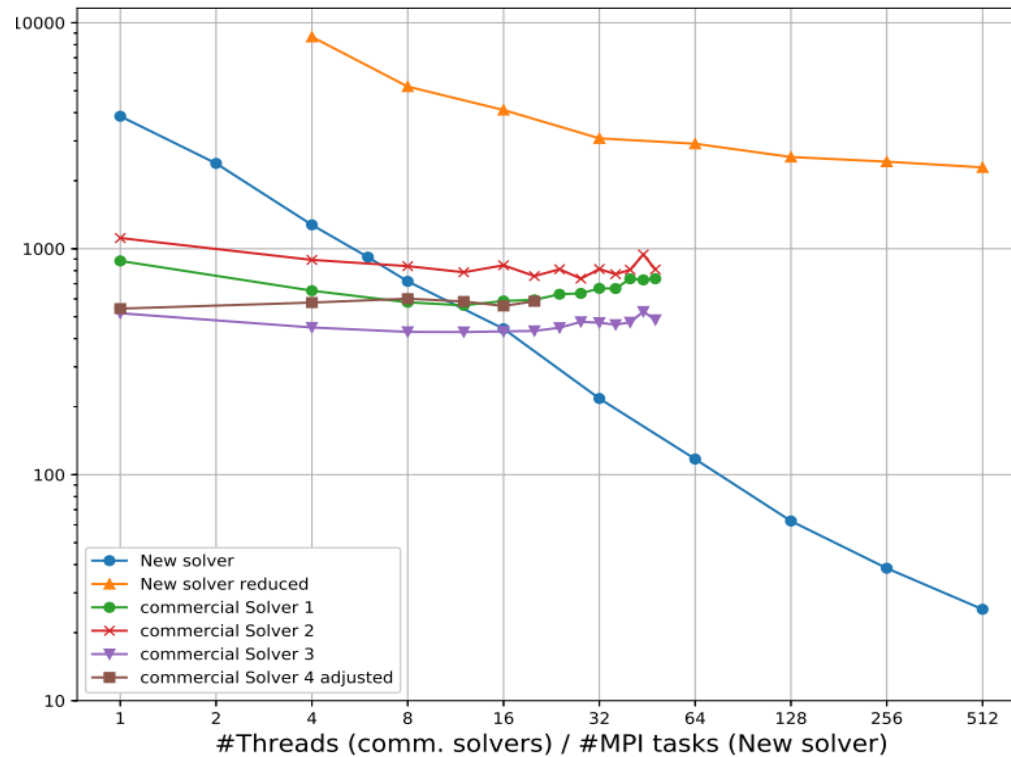


Plots show four different annotations of identical model

- Blocks of equal size are beneficial
- Few linking variables/constraints are beneficial

Computational Results

GAMS/PIPS-IPM Speedup Potential:



Scaling results of leading commercial LP solvers and the new solver on a **SIMPLE** (#rows $5.1E6$, #columns $5.6E6$, #non-zeroes $20.4E6$) model instance. The new solver was run with 2 OpenMP threads per MPI process.

Daniel Rehfeldt, Hannes Hobbie, David Schönheit, Ambros Gleixner, Thorsten Koch, Dominik Möst: A massively parallel interior-point solver for linear energy system models with block structure, ZIB-Report 19-41.

Table 1: Computational results for large-scale instances

Instance	Size				Run time (seconds)			
	Variables	Constraints	Non-zeroes	Blocks	New solver	Solver 1	Solver 2	Solver 4
SIMPLE2	95 311,531	86 551 238	344 083 267	1320	<u>244</u>	<u>25 302</u>	<u>31 101</u>	<u>23 339</u>
SIMPLE3	227 060 381	206 036 266	818 449 005	1024	<u>546</u>	<u>38 800</u>	69 377*	<u>NO</u>
ELMOD_CWE14	85 585 234	98 532 392	271 621 021	438	<u>239</u>	<u>6 181*</u>	<u>3 937</u>	<u>21 442</u>
ELMOD_CWE15	85 646 554	98 646 274	271 875 064	438	<u>181</u>	<u>6 321*</u>	<u>6 245</u>	<u>TL</u>
ELMOD_CWE16	85 883 074	98 909 074	272 602 144	438	<u>216</u>	<u>6 984*</u>	<u>5 190</u>	<u>67 941</u>
ELMOD_EU14	223 898 044	253 201 191	709 588 006	876	<u>1 220*</u>	<u>NO</u>	<u>66 105</u>	<u>NO</u>
ELMOD_EU15	224 677 686	254 304 961	712 452 541	876	<u>1 245*</u>	<u>NO</u>	<u>83 715</u>	<u>NO</u>
ELMOD_EU16	226 061 766	256 284 723	717 436 984	876	<u>1 119*</u>	<u>NO</u>	<u>79 094</u>	<u>NO</u>

* : could not be solved within the optimality tolerances, but still with a relatively small primal-dual gap (<1%).
 NO : non-optimal, specifies that the respective solver could not solve the instance within acceptable tolerances
 TL : (hard) time limit of 24 hours on JUWELS was hit

Hardware:

- **a) JUWELS**: Dual Intel Xeon Platinum 8168 CPU, 2x24 cores at 2.7 GHz, 96 GB memory
- **b) JUWELS**: Dual Intel Xeon Platinum 8168 CPU, 2x24 cores at 2.7 GHz, 192 GB memory
- **c) ZIB**: Intel Xeon CPU E7-8880 v4 2.20GHz processor, 88 cores, and **2 TB** memory

Daniel Rehfeldt, Hannes Hobbie, David Schönheit, Ambros Gleixner, Thorsten Koch, Dominik Möst: A massively parallel interior-point solver for linear energy system models with block structure, ZIB-Report 19-41.

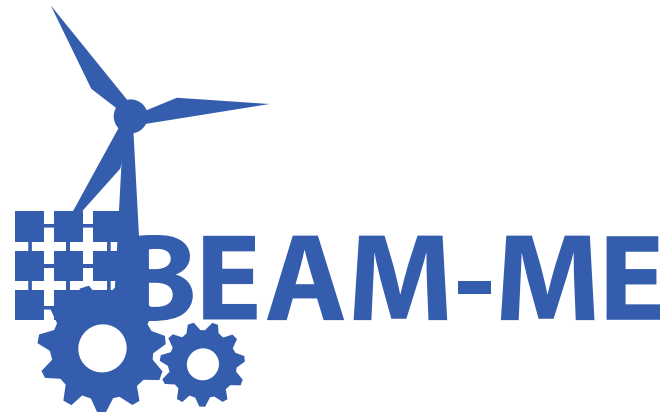
Outlook

- Parallelization can be extended to Model Generation
 - Usual Model”: model generation time \ll solver time
 - For LARGE-scale models the model generation may become significant:
 - due to time consumption
 - due to memory consumption
 - due to hard coded limitations of model size ($\#$ non-zeroes $< \sim 2.1e9$)
 - Generation of separate model blocks as required by solver
 - Fully implemented by user: possible (significant refactorization of code)
 - Annotation provided by user \rightarrow block sharp generation by GAMS: work in progress
- PIPS-IPM under constant development

Thank You!

Contact:

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