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Hybrid metapopulation-agent-based epidemiological models for efficient insight on the individual scale: a contribution to green computing

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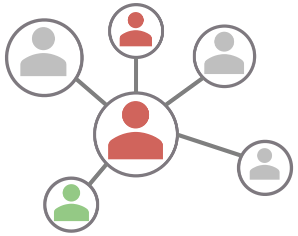
3RD (INTER-) NATIONAL CONFERENCE ON INFECTIOUS DISEASE MODELING

26 – 28 FEBRUARY 2025 IN BERLIN

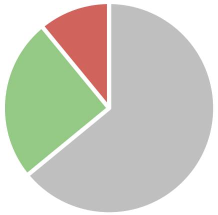
Motivation

Agent-based models (ABM)



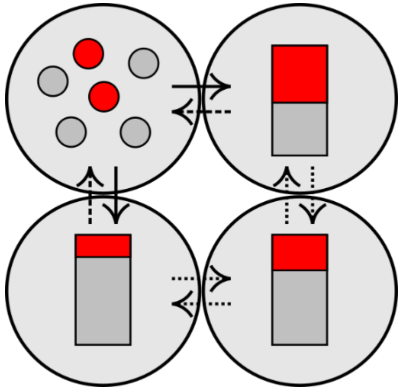
+ Resolution on individual scale
+ Capture heterogenous contact behavior and mobility patterns
- Computational complexity is dependent on number on agents
- Many parameters and lots of data needed

Population-based models (PBM)



- Aggregated results on compartment level
- Homogeneous and well-mixed population
+ Runtime independent of population size
+ Low complexity and few parameters

Hybridization framework – Spatial-hybrid model

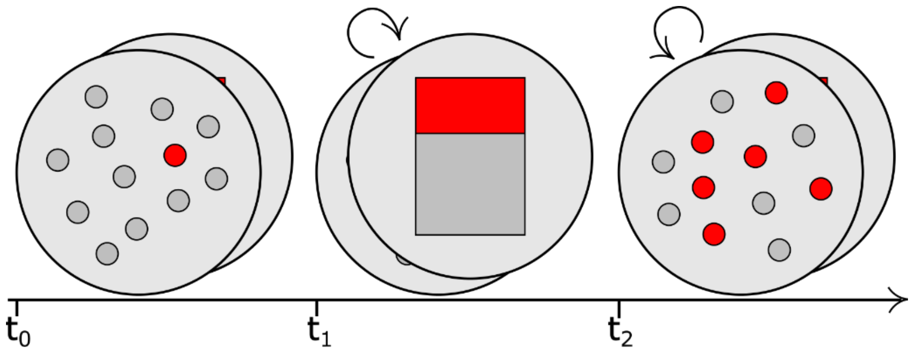


- Idea:
  - Interest in infection spread in particular region
  - Exclusive availability of data in specific region
- Concept:
  - Agent-based model in region of interest (focus region)
  - Population-based model (ODE-based in our application) for surrounding regions

→ **Detailed results** in focus region while considering **influence of connected regions** in **runtime efficient** manner

Hybridization framework – Temporal-hybrid model

- Idea:
  - Low case numbers: High stochasticity and individual behavior is important
  - High case numbers: Individual behavior is less influential and single simulation outcomes are close to averaged results



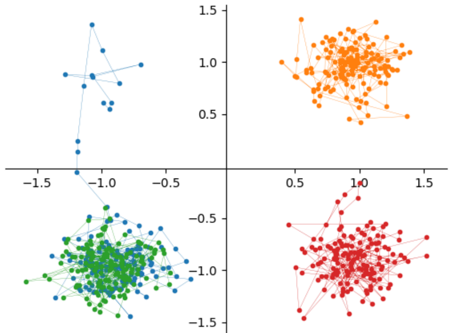
- Concept:
  - Switch between agent-based and population-based model during the simulation according to a threshold value

→ Capture stochasticity and individual behavior when necessary for **accurate outcomes** while using **runtime advantage** when possible

Proof of concept – Models[1]

Agent-based model

- Agent has position $x \in \mathbb{R}^2$ and infection state $z \in \{S, E, C, I, R, D\}$
- Infection state adoptions are modeled by stochastic jump processes
- Movement is modeled with independent diffusion processes



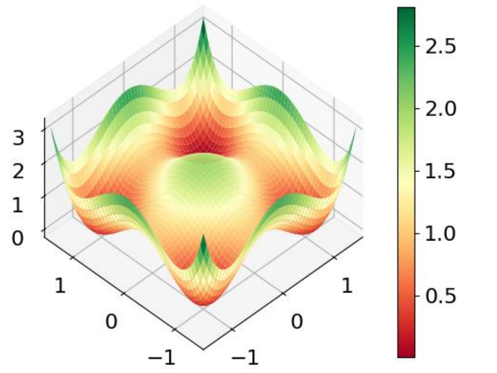
Metapopulation model

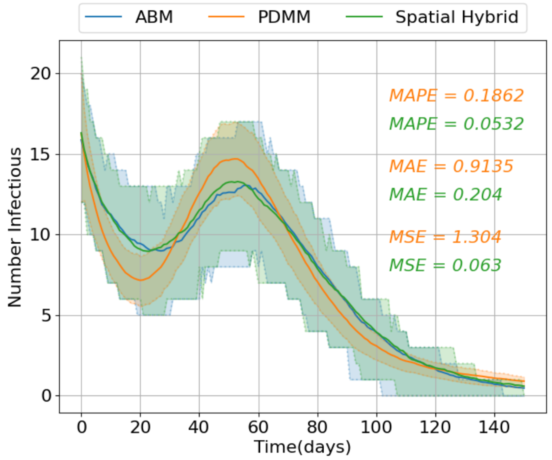
- Agents aggregated to subregions
- Infection state dynamics are given by ordinary differential equations (ODEs)
- Movement between subregions modeled with stochastic jump processes

[1]Winkelmann, Zonker, Schütte, Conrad: Mathematical modeling of spatio-temporal population dynamics and application to epidemic spreading. Mathematical Biosciences 336, 108619 (2021), https://www.sciencedirect.com/science/article/pii/S0025556421000614

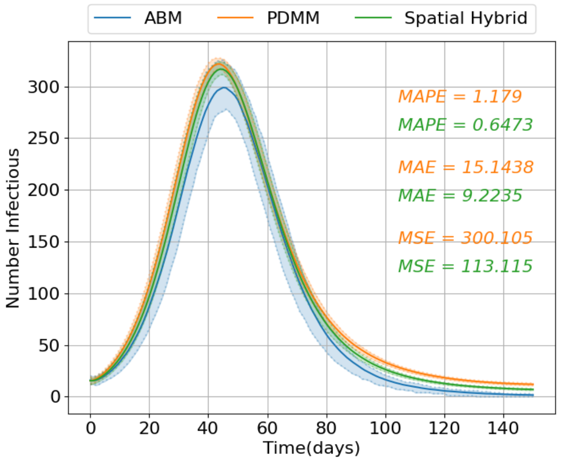
Spatial hybridization - Quadwell potential

- Setup: 8000 agents, 1% of population initially infected
- Focus region: $\Omega_1 = (-\infty, 0) \times (0, \infty)$
- Transmission rate in $\Omega_2 = (0, \infty) \times (0, \infty)$ corresponding to $R_0 = 2.4$
- Transmission rate in other regions corresponding to $R_0 = 0.8$

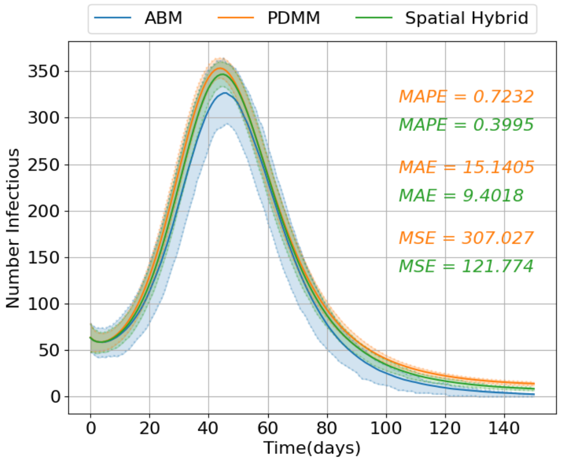




Focus region



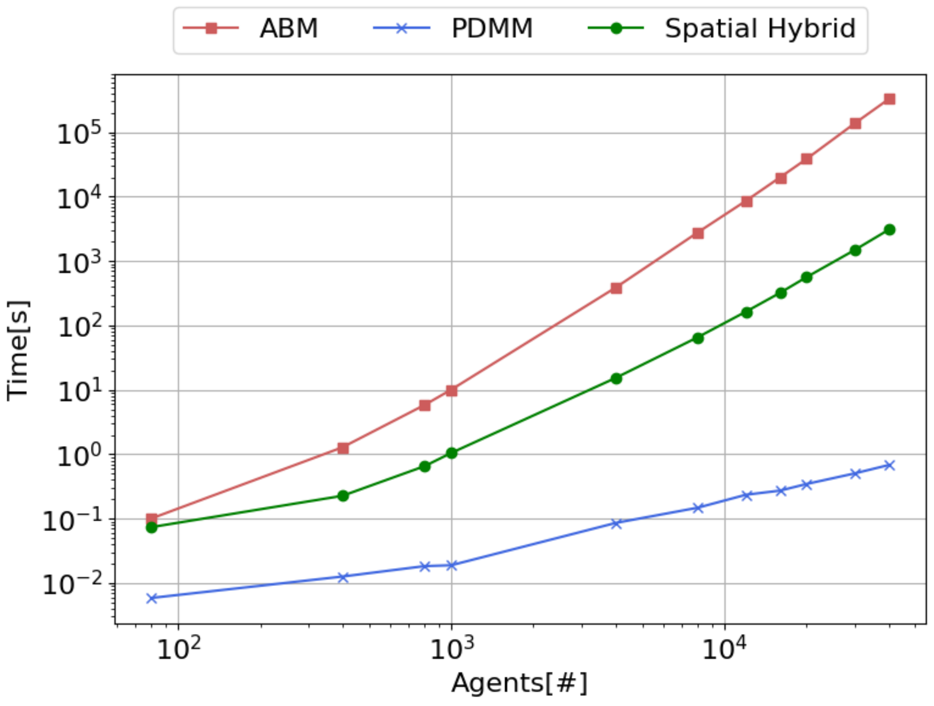
Ω_2



All regions

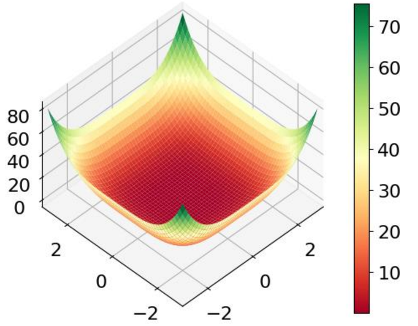
Quadwell potential – Runtime scaling

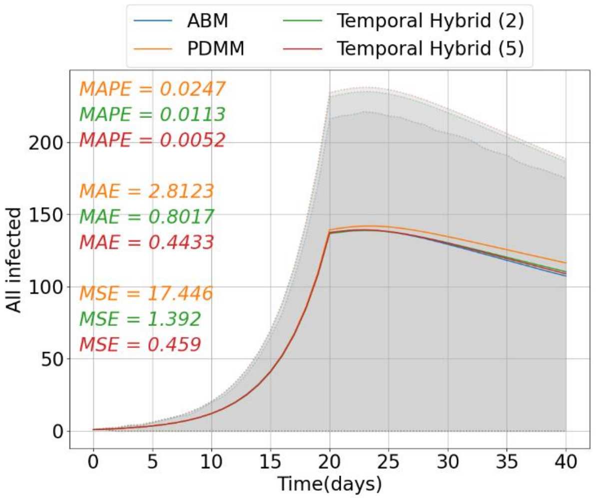
- Spatial-hybrid has same scaling behavior like ABM
- For **400 agents**: Runtime of spatial-hybrid **1 order of magnitude** lower than for ABM
- For **40,000 agents**: Spatial-hybrid reduces runtime by **98%**



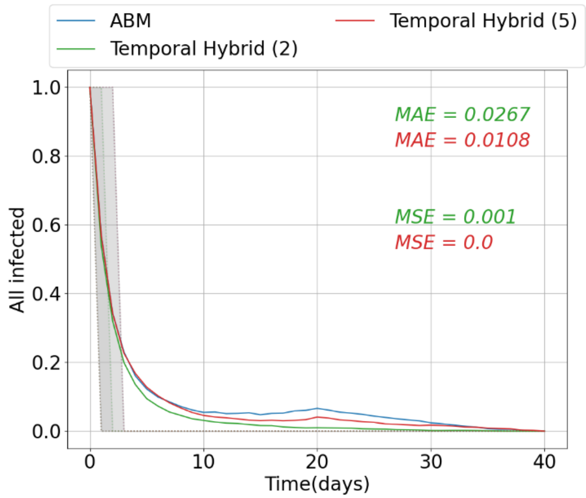
Temporal hybridization - Singlewell potential

- Setup: 10,000 agents, 1 agent initially infected, small contact radius
- Initial transmission rate corresponding to $R_0 = 4.8$
- Reduction of transmission rate by 80% after 20 days

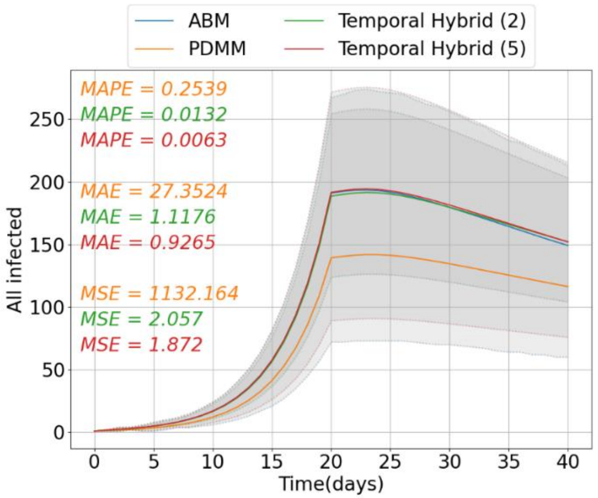




All runs



Extinction runs



Survival runs

Singlewell potential – Runtime

- Temporal-hybrid (5) is **8-times** (extinction runs) to **22-times** (survival runs) faster than ABM
- Temporal-hybrid (2) is **9-times** (extinction runs) to **49-times** (survival runs) faster than ABM

	All simulations		
Model	**min**	**mean**	**max**
ABM	41.80	331.76	1835.93
PDMM	0.00040	0.00047	0.01140
Temporal-hybrid $s=2$	0.5587	8.4082	92.6604
Temporal-hybrid $s=5$	0.5591	16.6405	104.497

	Extinction simulations			Survival simulations		
Model	**min**	**mean**	**max**	**min**	**mean**	**max**
ABM	41.80	48.77	109.147	91.07	442.20	1835.93
PDMM	-	-	-	0.00040	0.00047	0.01140
Temporal-hybrid $s=2$	0.5587	5.4414	85.2773	0.8115	9.5341	92.6604
Temporal-hybrid $s=5$	0.5591	6.2384	99.2354	2.9843	20.7604	104.497

CO_2 emissions[2]

- **Spatial-hybrid** models reduced CO_2 emissions by **70-98%** compared to ABM
- **Temporal-hybrid** models reduced CO_2 emissions by at least **94.67% up to 97.28%** compared to ABM

Model	Power[kWh]	CO_2 emissions[g]	CO_2 reduction
ABM quadwell	3.17889	1207.97915	-
Spatial-hybrid quadwell	0.07162	27.21423	97.75%
ABM Munich	4.15400	1578.51937	-
Spatial-hybrid Munich	1.20890	459.38063	70.90%
ABM single well	7.01801	2666.84380	-
Temporal-hybrid (5) single well	0.37380	142.04358	94.67%
Temporal-hybrid (2) single well	0.19095	72.56005	97.28%

[2]Icha, Lauf: Entwicklung der spezifischen Treibhausgas-Emissionen des deutschen Strommix in den Jahren 1900-2023. (2024), https://www.umweltbundesamt.de/publikationen/entwicklung-der-spezifischen-treibhausgas-10

- **PAPER:** BICKER, SCHMIEDING, MEYER-HERMANN, KÜHN, 2025, HTTPS://DOI.ORG/10.1016/J.IDM.2024.12.015.
- **SIMULATIONS:** HTTPS://GITHUB.COM/RENESCHM/MEMILIO/RELEASES/TAG/HYBRID-PAPER-V2
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