

# HYBRID METAPOPOPULATION AGENT-BASED EPIDEMIOLOGICAL MODELS

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Predictive Simulation Software

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Joint work with René Schmieding, Martin Kühn and Michael Meyer-Hermann

# Motivation

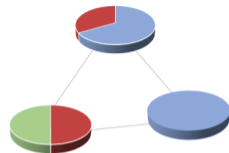


## Agent-based models



- Arbitrary level of detail
- Capture heterogenous contact behavior and mobility patterns
- Computational complexity is dependent on the number of agents

## Equation-based models



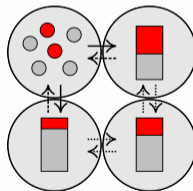
- Aggregated results (on compartmental level)
- Homogenous and well-mixed population
- Runtime independent on population size

## Motivation

- Interest in infection spread in a focus region
- Considering influence of connected regions on infection dynamics in focus region dynamically
- Exclusive availability of data in a focus region
- Reduction in computing time and energy demands

## Concept

- Agent-based model in focus region
- Equation-based model for surrounding regions

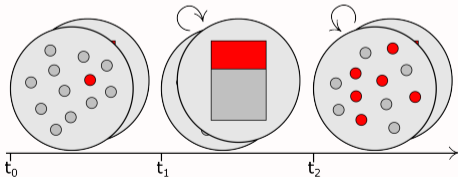


## Motivation

- Low case numbers: High stochasticity and individual behavior is important
- High case numbers: Individual behavior is less influential and simulation results are close to average
- Reduction in computing time and energy demands

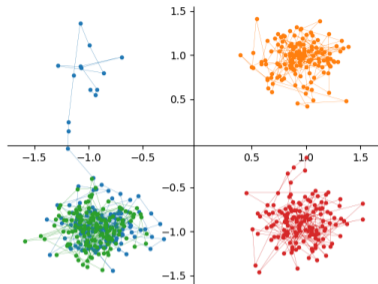
## Concept

- Agent-based model when case numbers are below a threshold
- Equation-based model when case numbers exceed threshold



# Models - Agent-based model (ABM\*)

- Agent  $(x, z) \in \Omega \times \mathcal{Z}$ 
  - $\Omega \subset \mathbb{R}^2$  compact domain
  - $\mathcal{Z} = (z_1, z_2, \dots, z_{n_I})$  set of infection states
- System state  $Y := (X, Z) \in \Omega^{n_a} \times \mathcal{Z}^{n_a}$
- Infection state dynamics: Stochastic jump processes  $\mathcal{P}_{ij}(t) := \mathcal{P}_{f_{ij}^{(\alpha)}}(Y(t))$
- Movement: Diffusion process  $\frac{dX(t)}{dt} = -\nabla F(t, X(t)) + \sigma(t, X(t))\xi(t)$ 
  - $F : \Omega \rightarrow \mathbb{R}$  a potential
  - $\sigma : [0, T] \times \mathbb{R}^2 \rightarrow \mathbb{R}^{2 \times m}$  a noise term
  - $\xi = \frac{dW}{dt}$  the derivative of the Brownian motion in  $\mathbb{R}^m$



\*Winkelmann, S., Zonker, J., Schütte, C., Conrad, N.D.: 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>

Julia Bicker, Institute for Software Technology, Department of High-Performance Computing: Hybrid metapopulation agent-based epidemiological models, 2023/06/03

- Domain  $\Omega = \bigcup_{k=1}^{n_R} \Omega_k$  split into  $n_R$  subregion  $\Omega_1, \dots, \Omega_{n_R}$
- System state  $N = (N_i^{(k)})_{i \in \mathcal{Z}, k=1, \dots, n_R} \in \mathbb{R}_{\geq 0}^{n_I \times m}$ , with  $N_i^{(k)}$  the number of agents in region  $\Omega_k$  and compartment  $i$
- Infection state dynamics: Ordinary differential equations
$$\frac{d}{dt} N_i^{(k)}(t) = \sum_{j \neq i} (f_{ji}^{(k)}(N) - f_{ij}^{(k)}(N))$$
- Movement: Stochastic jump processes  $\mathcal{L}_i^{(kl)}$  with rates  $\lambda_i^{(kl)} N_i^{(k)}$

\*Winkelmann, S., Zonker, J., Schütte, C., Conrad, N.D.: Mathematical modeling of spatio-temporal population dynamics and application to epidemic spreading.

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Julia Bicker, Institute for Software Technology, Department of High-Performance Computing: Hybrid metapopulation agent-based epidemiological models, 2023/06/03

## ABM

- **Movement:** Evaluation of diffusion process (per agent)
- **Infection state adoptions:** Calculation of adoption rate functions (per agent) + pairwise comparison of agents for adoptions that require contact

## PDMM

- **Movement:** Evaluation of spatial transitions (frequency dependent on rates  $\lambda_i^{(kl)} N_i^{(k)}$ )
- **Infection state adoptions:** Evaluation of ordinary differential equations

	ABM	PDMM
Complexity	superlinear, up to $\mathcal{O}(n_a^2)$	$\mathcal{O}(n_a)^*$
Spatial domain	continuous	discrete
Infection state dynamics	stochastic	deterministic

$\mathcal{O}(n_a)^*$  can be replaced by  $\mathcal{O}(1)$  under the assumption that spatial transitions are rare.

## *ABM* $\rightarrow$ *PDMM*

- Trivial projection from agent to subpopulation  $N_i^{(k)}$  according to infection state  $i$  and position  $x \in \Omega_k$

## *PDMM* $\rightarrow$ *ABM*

- Infection state given by subpopulation index  $i$
- Position in focus region has to be sampled from appropriate distribution

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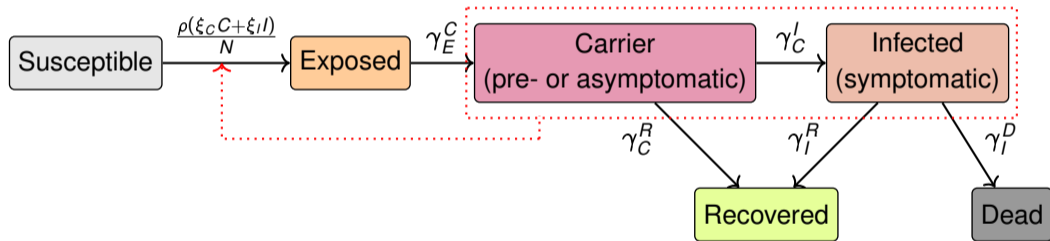
**Algorithm 1:** Spatial hybridization

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- 1 Create ABM and PDMM for  $\Omega = \bigcup_{k=1}^{n_R} \Omega_k$  and  $t = t_0$ ;
  - 2 Set and restrict rates and populations;
  - 3 ABM for  $\Omega_1$ ;
  - 4 PDMM for  $\Omega_2, \dots, \Omega_{n_R}$ ;
  - 5 **While**  $t \in [t_0, t_{max}]$  **do**;
  - 6 Define next synchronization point  $\hat{t}$ ;
  - 7 Advance ABM and PDMM from  $t$  to  $\hat{t}$ ;
  - 8 Exchange populations;
  - 9 Set  $t = \hat{t}$ ;
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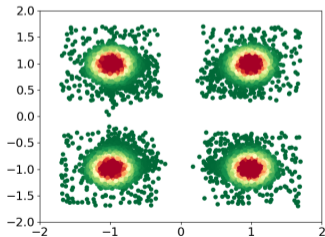
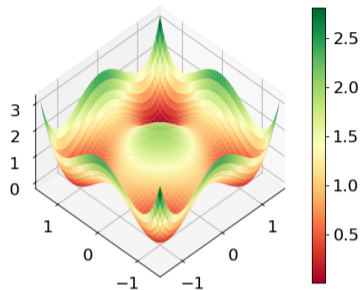


# Application: Transmission model

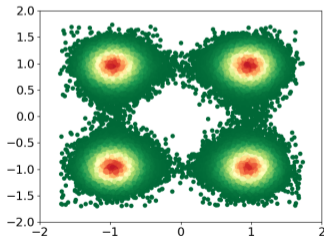


# Application 1 - Quadwell potential

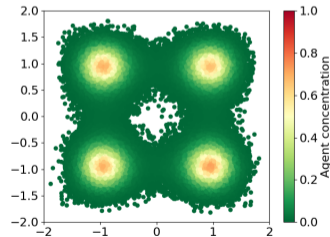
- Potential  $F(x, y) = (x^2 - 1)^2 + (y^2 - 1)^2$
- Focus region  $\Omega_1 = (-\infty, 0) \times (0, \infty)$
- Constant noise term  $\sigma \in \mathbb{R}$



$\sigma = 0.3$



$\sigma = 0.5$

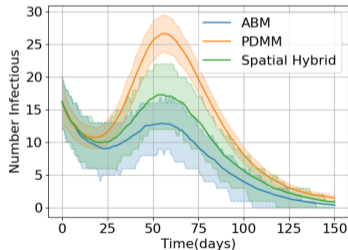


$\sigma = 0.6$

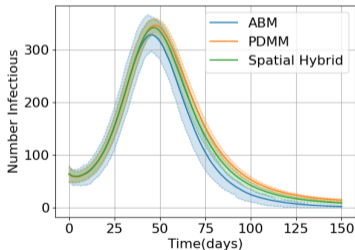
# Quadwell potential - Simulation results



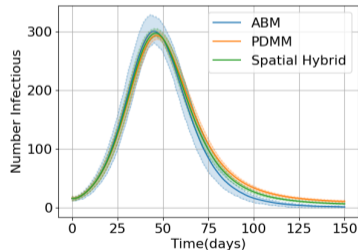
- 1% of population initially infected
- Transmission probability in  $\Omega_2$  is three times higher than in other regions



Focus region



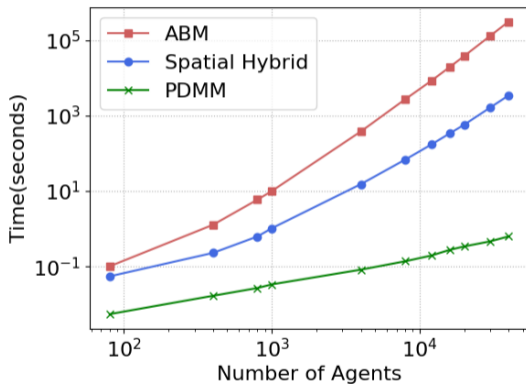
All regions



Region 2

## Quadwell potential - Runtime results

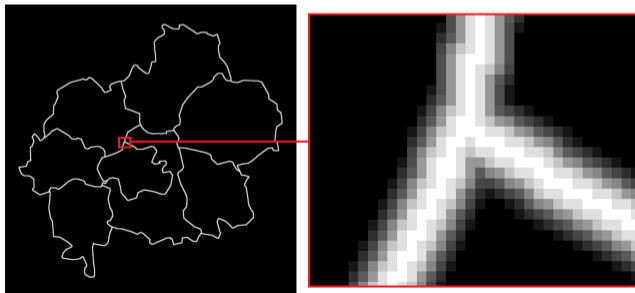
- Spatial-hybrid has same scaling behavior like ABM
- Spatial-hybrid reduces runtime by 98% for 40,000 agents compared to ABM



## Application 2 - Munich and surrounding counties

- Potential  $F$  given by map of city of Munich and its surrounding counties with Gaussian curve on borders

$$F(x) = \begin{cases} 0, & x \text{ is inside a county} \\ h, & x \text{ is on a border} \\ c \in (0, h), & x \text{ is on gradient area next to the borders} \end{cases} \quad (1)$$



- Adding commuting term to diffusion process:

$$\frac{dX(t)}{dt} = -\nabla F(t, X(t)) + \sigma(t, X(t))\xi(t) + K(t, X(t))$$

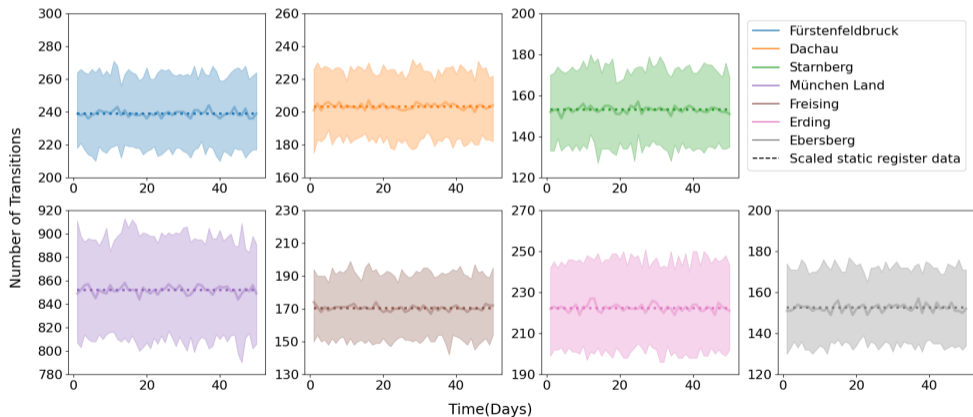
- For agent  $\alpha$  a commuter,  $\alpha$ -th element of  $K$  is

$$K_{\alpha}(t) = \begin{cases} \pi(x_{\alpha}) - x_{\alpha}, & \text{if } t_d^{\alpha} \in (t, t + \delta t] \vee t_r^{\alpha} \in (t, t + \delta t] \\ 0, & \text{else} \end{cases}$$

- $t_d^{\alpha}$  is time point agent  $\alpha$  commutes
- $t_r^{\alpha}$  is time point agent  $\alpha$  returns
- $\pi(x_{\alpha})$  is agent's new position in commuting destination region

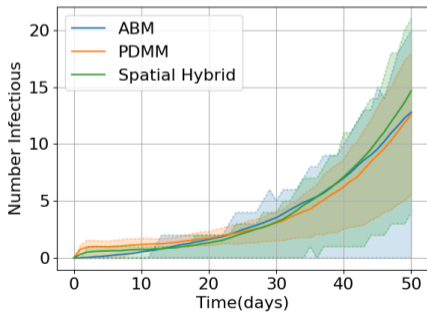


# Transitions to and from Munich City

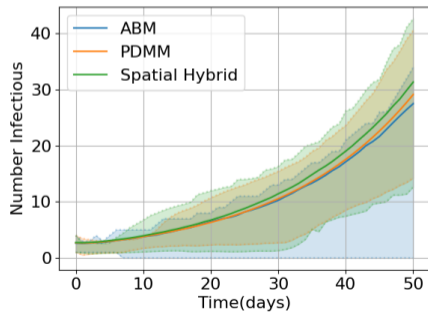


# Munich potential - Simulation results

- Transmission probability same in all regions
- Only in region next to Munich City initially infected (0.2%)



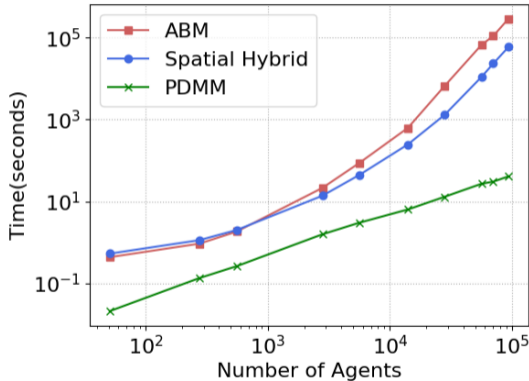
Focus region (Munich City)



All regions



- Runtime gain less than for quadwell due to percentage of agents modeled with ABM ( $\approx 75\%$  of agents located in focus region)
- ABM runtime comparably low for chosen setting, due to low number of infected agents
- Still 80% runtime gain for 90,000 agents



- In our simulations, hybridization saved up to 98% runtime
- Definition of exchange rules have essential impact on accuracy and performance of hybridization
- For spatial hybridization runtime gain depends on number of agents in focus region, relative to regions modeled with equations
- For temporal hybridization runtime gain depends on proportion of simulation time that ABM is used
- Next step: Using more advanced models for hybridization

- Github repository: <https://github.com/SciCompMod/memilio.git>, code for hybrid model on fork <https://github.com/reneSchm/memilio>

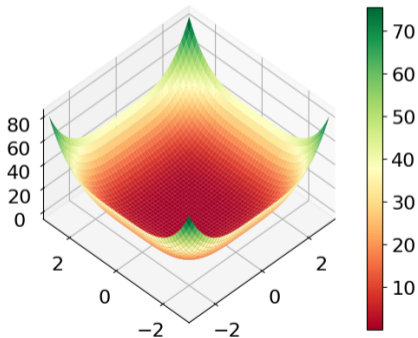


**Thank you for your attention!**

- Preprint: Bicker, Schmieding, Kühn, Submitted, 2024, <https://arxiv.org/abs/2406.04386>

# Appendix

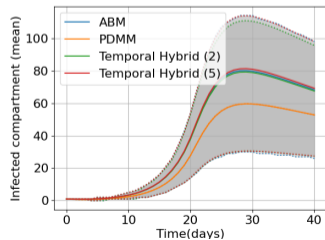
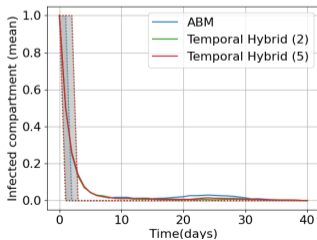
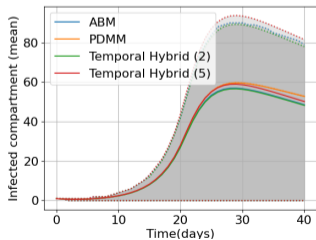
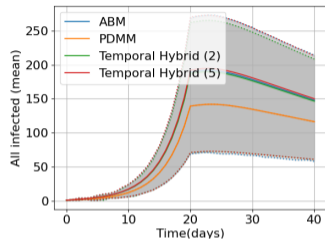
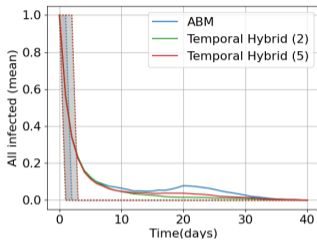
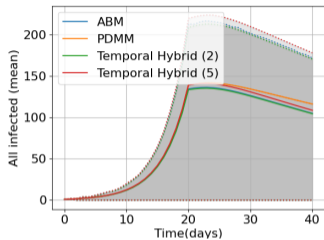
- Potential  $F(x, y) = \frac{(x^4 + y^4)}{2}$



Setup:

- Only one initially infected
- Parameters chosen such that in 30% of all ABM simulations the virus dies out
- In non-extinction scenarios, NPI (reduction of transmission probability) after 20 days

# Single well potential - Simulation results



Combined

Extinction

Survival

# Single well potential - Runtime results



Model	Extinction (seconds)			Survival (seconds)		
	min	mean	max	min	mean	max
ABM	80.9407	93.0124	112.658	93.1817	446.238	2091.56
PDMM	-	-	-	00040	0.00046	0.01000
Temporal-hybrid 2	42.33	48.79	99.75	45.09	143.97	634.26
Temporal-hybrid 5	42.31	49.37	102.76	46.02	147.47	655.27

Model	Combined (seconds)		
	min	mean	max
ABM	80.9407	344.297	2091.56
PDMM	0.00040	0.00046	0.01000
Temporal-hybrid 2	42.33	116.26	634.26
Temporal-hybrid 5	42.31	120.05	655.27