Scaling Complexity: High-Performance Computing at the Intersection of Agent-Based Modeling and Complex Networks

2 December: Workshop

09:00 – 09:30	*Registration*
09:30 – 10:00	Introduction
10:00 – 10:45	*Talk:* The dynamics of social systems with higher-order interactions – **Vito Latora** (*Queen Mary University of London*)
10:45 – 11:15	*Coffee break*
11:15 – 12:00	*Talk:* Complex Symptoms at Scale: Best practices surrounding epidemic modelling across time and space – **Sarah Wise** (*University College London*)
12:00 – 12:45	*Talk:* From social science theory to formalized agent behaviour: challenges and ways ahead – **Geeske Scholz** (*TU Delft*)
12:45 – 14:00	*Lunch*
14:00 – 14:45	*Talk:* Agent-Based Modelling to Support Decision-Making in Crises: Opportunities and Barriers – **Gary Polhill** (*The James Hutton Insitute*)
14:45 – 15:30	*Talk:* Challenges in Accelerating and Scaling Agent-Based Model Simulations (ABMS) with High-Performance Computing (HPC) – **Eduardo Cesar Galobardes** (*Universitat Autònoma de Barcelona*)
15:30 – 16:00	*Coffee break*
16:00 – 16:15	*Short Talk:* Utopia: a comprehensive modelling framework for complex and adaptive systems – **Yunus Sevinchan** (*Humboldt-Universität zu Berlin*)
16:15 – 17:30	Panel discussion
17:30 – 19:00	Poster session (and soup)

Talk Details and Abstracts

10:00 – 10:45 **Vito Latora** (*Queen Mary University of London*)

The dynamics of social systems with higher-order interactions

Networks are made of nodes and links. Hence, they model well dynamical processes, such as the spreading of a disease in a population, where transmission occurs through pairwise contacts. Conversely, networks are not best suited to describe the spreading of innovation, the formation of opinions or the emergence of cooperation in social systems, all processes in which more complex mechanisms of interactions,

involving groups of three or more units, are at work. In this talk, I will discuss how to use higher-order networks to better model the presence and role of groups in different types of social dynamics. With the analysis of a series of study cases, I will show that higher-order interactions produce novel collective phenomena. They lead to explosive transitions to the adoption of novelties in models of social contagion, stabilize otherwise unstable synchronized states in systems of many-body dynamical units, and even help providing a novel explanation for the survival of cooperation in social dilemmas.

11:15 – 12:00 **Sarah Wise** (*University College London*)

Complex Symptoms at Scale: Best practices surrounding epidemic modelling across time and space

After a virtual Cambrian explosion of epidemiological model development in response to the Covid-19 crisis, both the limits of and the need for agent-based modelling (ABM) are more apparent than ever. Agent-based modellers made extensive use of abstractions and simplifications of simulated populations to make their models more computationally tractable on actionable timescales. Using an epidemiological model, this talk will discuss the impact of the relative scale of the population being simulated and how this intersects with geographical and spatial dynamics.

12:00 – 12:45 **Geeske Scholz** (*TU Delft*)

From social science theory to formalized agent behaviour: challenges and ways ahead

Deciding upon a decision model and how to operationalize it into the rules or internal structure needed for every agent-based model is a critical yet challenging step. However, standards available to guide this step are yet to be established. In my talk, I share insights from several collaborative projects trying to develop such guidance, from deciding upon agents' decision rules to their formalization in computer code.

14:00 – 14:45 **Gary Polhill** (*The James Hutton Insitute*)

Agent-Based Modelling to Support Decision-Making in Crises: Opportunities and Barriers

The ExAMPLER project has been funded by the UK's Engineering and Physical Sciences Research Council to investigate the requirements for running agent-based models on the latest high-performance computers (exascale). Through a systematic literature review, a series of workshops, and engagement with various communities, we have identified a number of important institutional as well as technical barriers that need to be overcome before we have the capability needed. This talk will identify those barriers, and outline the advantages of overcoming them whether or not an agent-based model is ever executed on an exascale computer.
Authors: Gary Polhill, with Alison Heppenstall, Ricardo Colasanti, Matt Hare, Doug Salt, Richard Milton, and Michael Batty

14:45 – 15:30 **Eduardo Cesar Galobardes** (*Universitat Autònoma de Barcelona*)

Challenges in Accelerating and Scaling Agent-Based Model Simulations (ABMS) with High-Performance Computing (HPC)

As agent-based models (ABM) grow increasingly complex, their simulations demand greater computational resources, often needing the use of parallel high-performance computing (HPC) platforms. Despite the inherently parallel nature of ABMS, several challenges arise in efficiently utilizing these resources. This talk will explore key obstacles in scaling ABMS on HPC systems, present contributions from our group that address these issues, and discuss our ongoing efforts to optimize the execution of non-spatial ABMS.

16:00 – 16:15 **Yunus Sevinchan** (*Humboldt-Universität zu Berlin*)

Utopia: a comprehensive modelling framework for complex and adaptive systems

Utopia is a modelling framework strongly motivated by bringing together researchers of complex and adaptive systems, fostering collaboration and a shared language in how systems are abstracted into models. To that end, Utopia aims to make the everyday workflow of implementing models, performing simulations and evaluating the resulting data more convenient, efficient, and reproducible. It offers a powerful simulation manager, C++ and Python model backends, as well as a C++ library with tried-and-tested implementations of cellular automata, graphs and ABMs. At the same time, the framework retains flexibility for researchers in how exactly they implement their model in order to apply to a wide array of use cases.

Panel Discussion

16:15 – 17:30 **Participants:** Speakers & Organisers

This session brings together the speakers and workshop organisers to explore critical challenges and opportunities at the intersection of Agent-Based Modeling and Network Science. Key topics include methodological synergies between different modeling approaches, practical challenges in implementing large-scale simulations, and future directions for computational social science. The discussion will address both theoretical and practical aspects of complex systems modeling, examining how different computational approaches can complement each other. Audience participation is encouraged to foster dialogue between different research perspectives.

3 December: Vahana.jl Hands-On

09:30 – 10:30	Julia Essentials (for Vahana.jl)
10:30 – 11:00	*Coffee break*
11:00 – 12:30	Vahana.jl Basics & First Model Implementation
12:30 – 13:45	*Lunch*
13:45 – 15:15	Handling Simulation Data
15:15 – 15:45	*Coffee break*
15:45 – 17:15	Adding a Spatial Component & Parallal Simulations

After introducing Julia and Vahana basics, we will extend the Hegselmann-Krause model in two steps. First, we'll develop a variant where agents interact at different locations represented as vertices in a bipartite graph. Then, we'll enhance this model by introducing a spatial neighborhood structure among these locations.

For analyzing the simulations, methods for data analysis and visualization will be demonstrated and tested on our model implementations. Additionally, we will explore how to parallelize individual simulation runs and discuss the key considerations for parallel computation.

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Organizers:
Steffen Fürst (Freie Universität Berlin), Nataša Djurdjevac Conrad (Zuse Institute Berlin), Sarah Wolf (Freie Universität Berlin)