ExAMPLER

An ExCALIBUR Project

Moving ABMs to exascale:
Challenges and possible solutions

Gary Polhill, with

Matt Hare, Richard Milton, Doug Salt, Ricardo Colasanti, Alison Heppenstall and Mike Batty

Urban Big Data Centre

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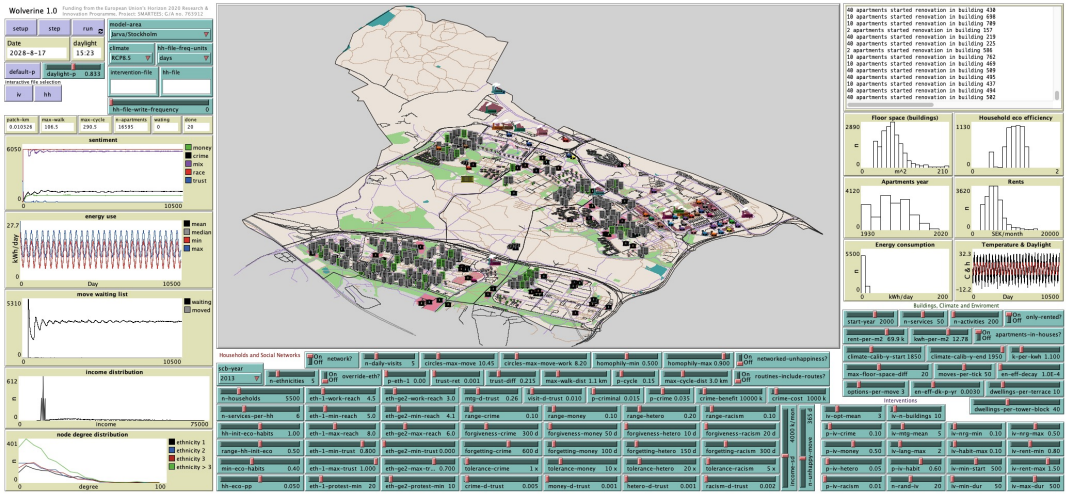
The James Hutton Institute

Outline

- What is agent-based modelling?
- Why would we want to run ABMs at exascale?
- Technical and institutional obstacles
- Possible solutions

What is agent-based modelling?

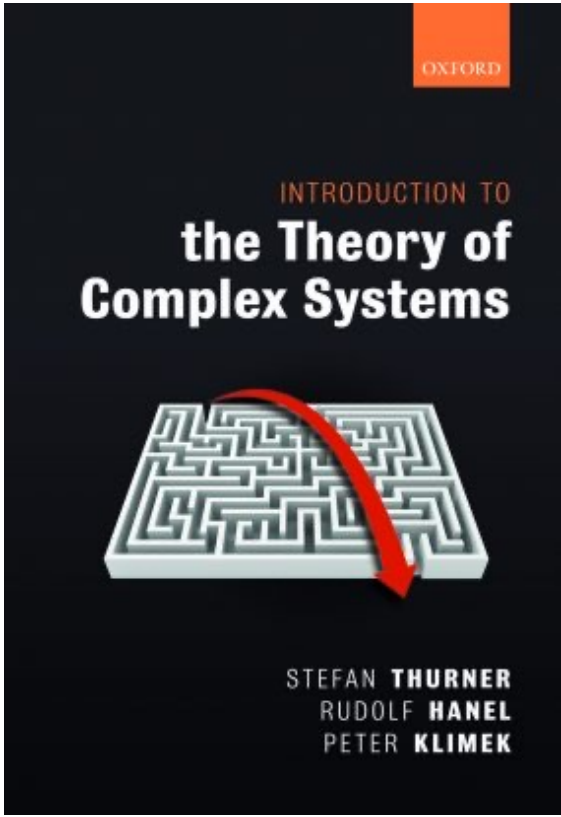
- Computer simulation
- Explicit representation of heterogeneous individuals (‘agents’)
  - Data structure and behaviour (methods)
- And their dynamic interactions
- In space
  - Usually



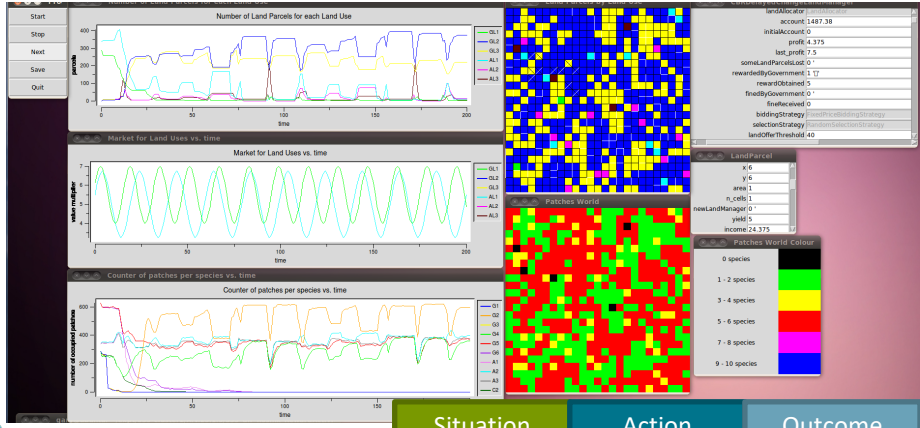
Screenshot from model of District Regeneration in Järva, Stockholm (SMARTEES project)

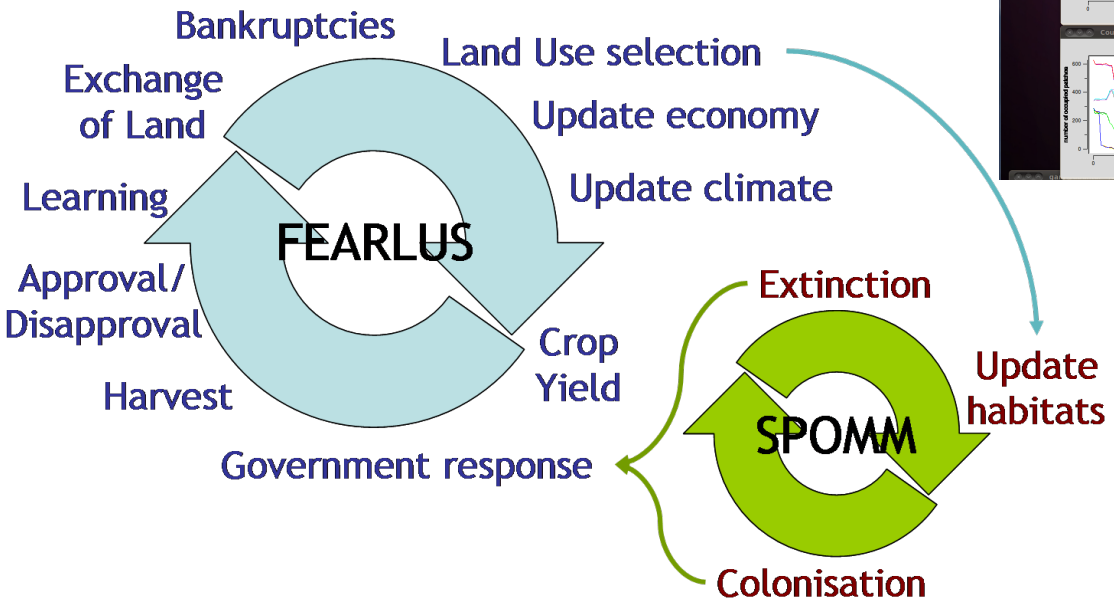
Why?

- Complexity science – the ‘maths’ stops working…
  - Path-dependent, non-Markovian and out-of-equilibrium dynamics
  - Learning, adaptation, evolution
  - Nonlinear behaviour
  - Leptokurtic distributions
    - Law of large numbers does not apply
    - Extreme events more likely than normal distributions suggest
  - Heteroskedastic time series
    - No constant variance; possibly no constant mean!
- But also:
  - Geography: Natural representation of space
  - Sociology: Explore formalizations of theory
  - Psychology: Emergent effects of dynamic, interacting individuals
  - (Heterodox) Economics: Escape ‘heroic’ assumptions



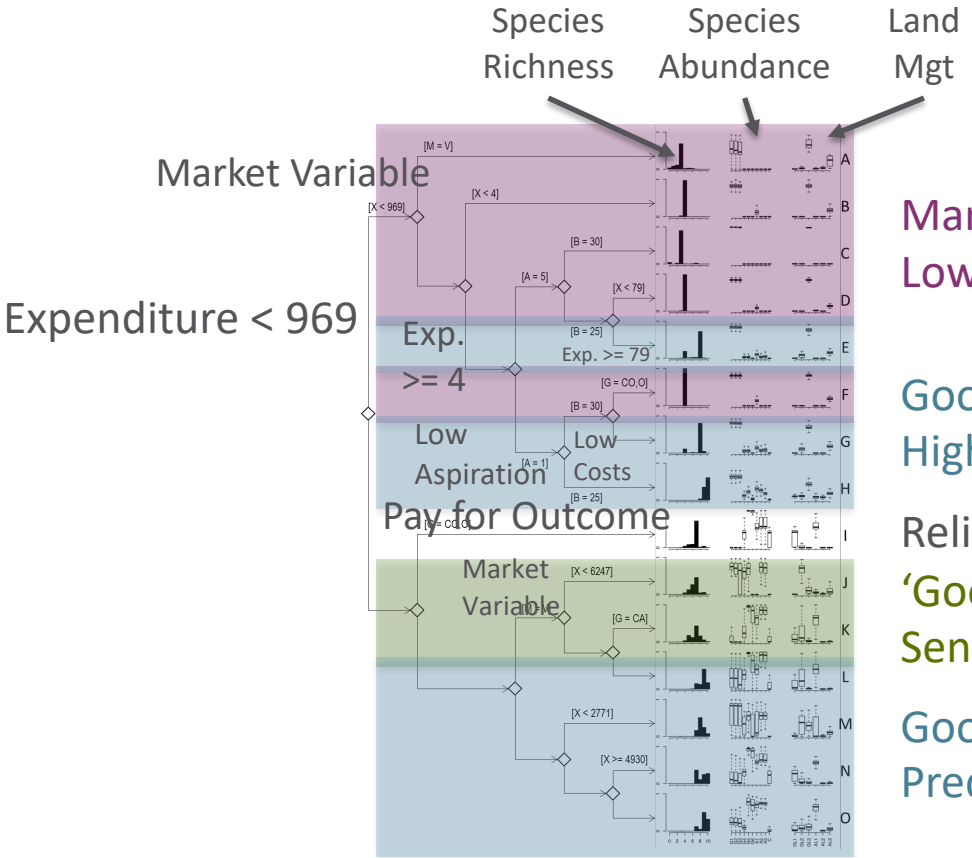
Example


Start
Stop
Next
Save
Quit
Number of Land Parcels for each Land Use
Market for Land Uses vs. time
Counter of patches per species vs. time
Patches World
LandParcel
Patches World Colour
0 species
1 - 2 species
3 - 4 species
5 - 6 species
7 - 8 species
9 - 10 species


Bankruptcies
Land Use selection
Exchange of Land
Update economy
Learning
Update climate
FEARLUS
Approval/ Disapproval
Crop Yield
Harvest
Government response
Extinction
Update habitats
SPOMM
Colonisation


Situation
Action
Outcome

Example



Market drives outcomes;
Low species richness

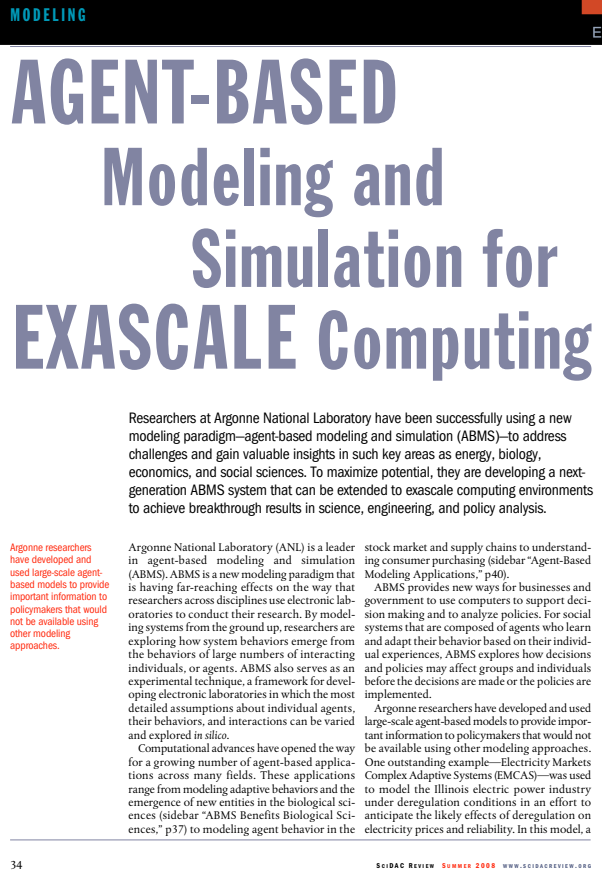
Good / best species richness (possibly);
High sensitivity / unrealistic context

Reliably ‘good enough’ richness (modally)?
‘Good enough’ richness modal;
Sensitivity to market / expenditure

Good / best species richness (possibly);
Predictable (constant) market prices needed

Exascale ABM planned as far back as 2008

- SciDAC Review, Summer 2008, pp. 34-41
  - Charles Macal & Michael North
  - Argonne
- No reply when we emailed to ask what happened…
  - …but Exascale computing relies on high levels of parallelism (e.g. on GPUs)
  - Agent interactions challenge that
  - Other sciences finding the same



MODELING

AGENT-BASED Modeling and Simulation for EXASCALE Computing

Researchers at Argonne National Laboratory have been successfully using a new modeling paradigm—agent-based modeling and simulation (ABMS)—to address challenges and gain valuable insights in such key areas as energy, biology, economics, and social sciences. To maximize potential, they are developing a next-generation ABMS system that can be extended to exascale computing environments to achieve breakthrough results in science, engineering, and policy analysis.

Argonne researchers have developed and used large-scale agent-based models to provide important information to policymakers that would not be available using other modeling approaches.

Argonne National Laboratory (ANL) is a leader in agent-based modeling and simulation (ABMS). ABMS is a new modeling paradigm that is having far-reaching effects on the way that researchers across disciplines use electronic laboratories to conduct their research. By modeling systems from the ground up, researchers are exploring how system behaviors emerge from the behaviors of large numbers of interacting individuals, or agents. ABMS also serves as an experimental technique, a framework for developing electronic laboratories in which the most detailed assumptions about individual agents, their behaviors, and interactions can be varied and explored *in silico*.

Computational advances have opened the way for a growing number of agent-based applications across many fields. These applications range from modeling adaptive behaviors and the emergence of new entities in the biological sciences (sidebar "ABMS Benefits Biological Sciences," p37) to modeling agent behavior in the stock market and supply chains to understanding consumer purchasing (sidebar "Agent-Based Modeling Applications," p40).

ABMS provides new ways for businesses and government to use computers to support decision making and to analyze policies. For social systems that are composed of agents who learn and adapt their behavior based on their individual experiences, ABMS explores how decisions and policies may affect groups and individuals before the decisions are made or the policies are implemented.

Argonne researchers have developed and used large-scale agent-based models to provide important information to policymakers that would not be available using other modeling approaches. One outstanding example—Electricity Markets Complex Adaptive Systems (EMCAS)—was used to model the Illinois electric power industry under deregulation conditions in an effort to anticipate the likely effects of deregulation on electricity prices and reliability. In this model, a

Example

- ~20,000 runs
- 76 CPU days of computing time
  - 4G MIPS CPUs
- 3×10^{16} CPU instructions
- 1.5 days on 200 CPUs
- 0.3s at exascale

ELSEVIER

Environmental Modelling & Software

Volume 45, July 2013, Pages 74-91

Nonlinearities in biodiversity incentive schemes: A study using an integrated agent-based and metacommunity model ☆

J. Gary Polhill, Alessandro Gimona, Nicholas M. Gotts

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https://doi.org/10.1016/j.envsoft.2012.11.011

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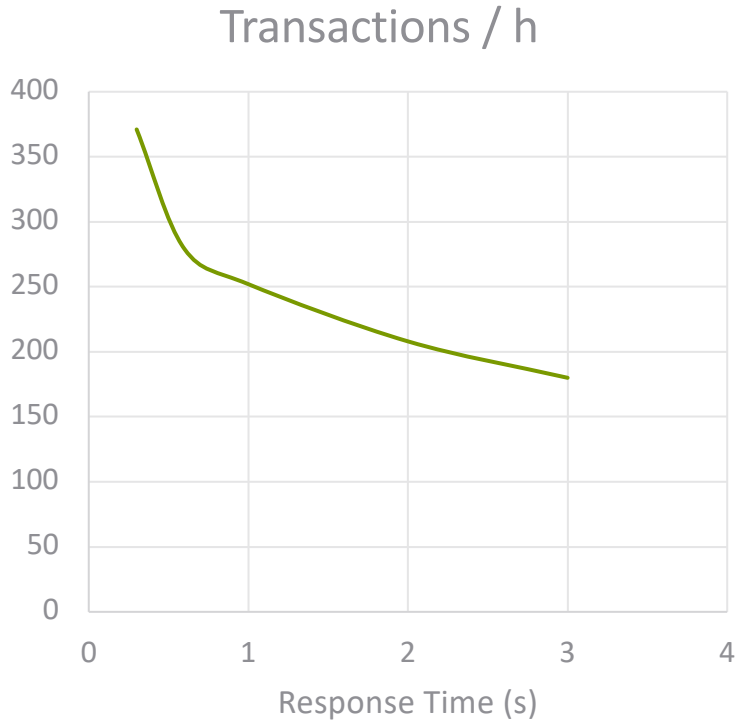
Doherty-Thadani threshold



Doherty, W. J. & Thadhani, A. J. (1982) The economic value of rapid response time. IBM Research Technical Report. https://jlelliotton.blogspot.com/p/the-economic-value-of-rapid-response.html

Thadhani, A. J. (1984) Factors affecting programmer productivity during application development. *IBM Systems Journal* **23** (1), 19-35. https://doi.org/10.1147/sj.231.0019

Search Medium

Write

The Doherty Threshold and Designing for Human-Computer Interaction

There's a split second difference between an engaged user and a frustrated one

Kubo Media Team · Follow

Published in Kubo · 6 min read · Jul 4

https://medium.com/kubo/the-doherty-threshold-and-designing-for-human-computer-interaction-f0a47c8ab583

Appeal of exascale ABM

- Sub-second response times…
  - if really possible for exascale ABSS
- …suggests experiments with simulations could be part of a creative conversation about how to handle a developing crisis
  - Next pandemic; trade crisis; financial meltdown; extreme weather event

Never mind exascale: what about HPC?

- Steep learning curve
  - Yet another bit of unstable computing science tech for social scientists to learn
  - Alessa et al. (2006)
  - An et al. (2020)
- ‘HPC snobbery’
  - ‘Embarrassingly parallel’ multiple parameter samples
  - HPC admins prefer within-run parallelization
- Resource needs are unpredictable…
  - Provably

CONTENT

ANTISOCIAL SIMULATION: USING SHARED HIGH-PERFORMANCE COMPUTING CLUSTERS TO RUN AGENT-BASED MODELS

DECEMBER 14, 2022 THESUBMISSIONAUTHOR LEAVE A COMMENT

By Gary Polhill

Information and Computational Sciences Department, The James Hutton Institute, Aberdeen AB15 8QH, UK.

‘Technical Assessment’ form for ARCHER2

Please see notes in the Service Specification document regarding the maximum amounts of time that can be applied for and technical specifications.

	Largest Job	Typical Job	Smallest Job
Number of nodes	[Please Complete Table]		
Number of cores/GPUs used per node			
Wallclock time for each job*			
Number of jobs of this type			
Memory per node required.			

*The maximum permitted wallclock time per job is a function of local Service centre policy.

Rice, H. G. (1953) Classes of recursively enumerable sets and their decision problems. *Transactions of the American Mathematical Society* **74**, 358-366. https://doi.org/10.1090/S0002-9947-1953-0053041-6

ExAMPLER: project summary

Using exascale computing, what software support do we need to co-design, build, validate, and explore policy scenarios with empirical ABM in a one-day transdisciplinary workshop?

1. Assess 'exascale readiness' using Systematic Literature Review and Benchmarking
2. Vision of exascale ABM and one-day transdisciplinary workshop scenario s/w requirements
3. Roadmap for delivering the vision founded on exascale training and learning
4. Engage with ABM community and other ExCALIBUR projects; respond to opportunities

HPC in ABM: State-of-the-art and ways forward

HPC/ABM Review

Exascale Empirical Agent-Based Modelling

Position paper

Skills
Training
Software
Barriers
Networks
Research
Funding

ExAMPLER Roadmap

W'shops
SSC/ESSA
iEMSs
GIScience
AAMAS
AAG

Community Report

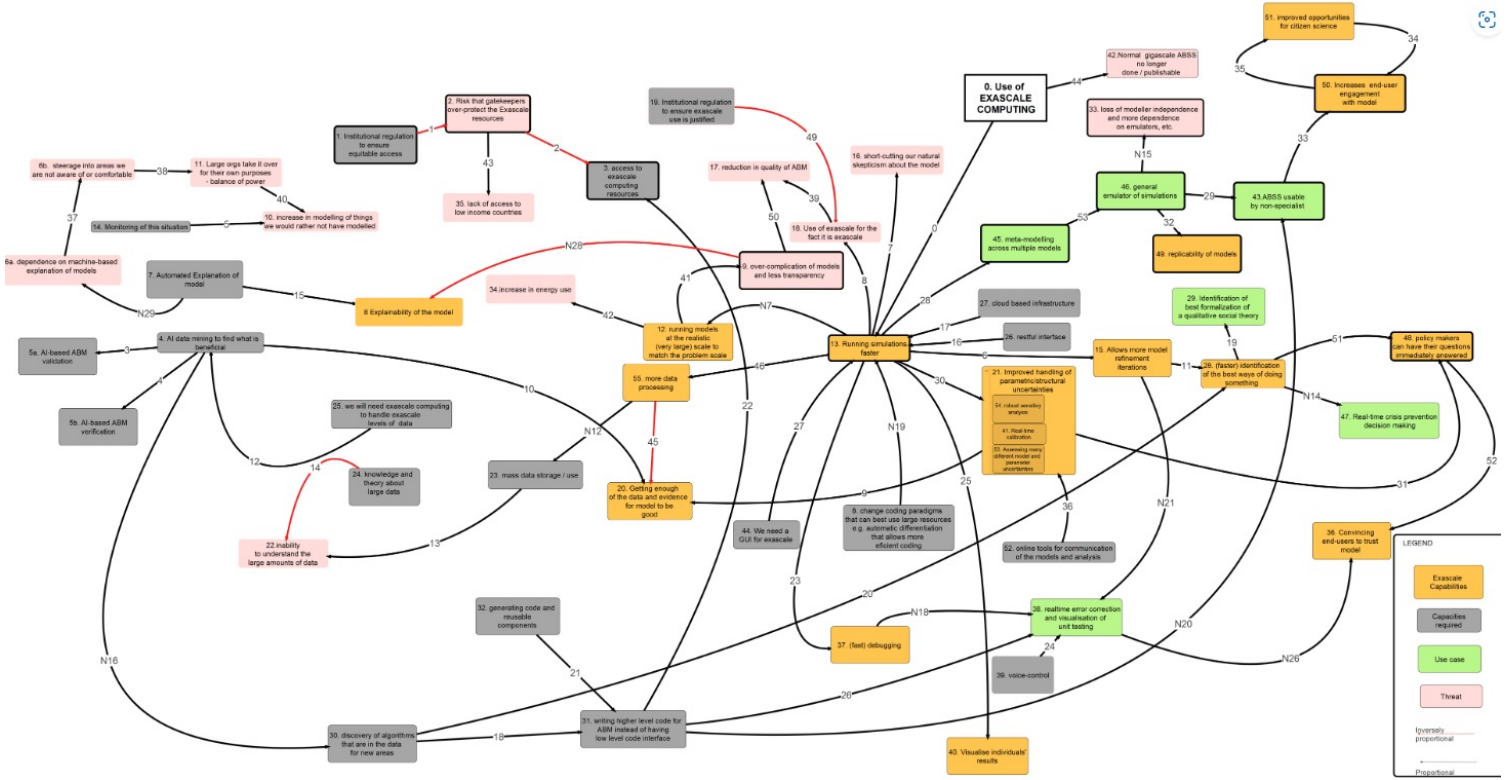
(Polhill et al. 2023)

Visions workshops; Glasgow & London ’23

- Explored potential of exascale for ABM
- Participatory approach
  - Used group model building to co-create causal loop models
- Glasgow (Social Simulation Conference)
  - 2h (1h introduction; 1h group modelling)
- London
  - 1.5 days (expert presentations; 1.5h group modelling; refinement discussions)

Combined Causal Loop Model

ExAMPLER



Exascale Capabilities

Capacities Required

Use Cases

Threats

Inversely Proportional

Proportional

Submitted to SSC 2024, Cracow

Visions model: Use Cases

- Individual-based social science as a new field
- Identifying best formalizations for social theories
- Real-time decision-making support
- Meta-modelling and general simulation emulators
- Real-time visualization and debugging tools

Use Cases

Visions model: Threats

- Increased energy consumption and cost
- Inefficient use of exascale resources
- Loss of research community control over agent-based modelling
- Overly complex models and gatekeeper control
- Over-reliance on AI for development and interpretation

Threats

Visions workshops: Challenges

- High cost of hardware might limit funding for research and development
- Parallelization of agent-based models not trivial
  - Risk that this is ignored, and we ‘oversimplify’ ABMs to enable full benefits of parallelism
    - Synchronous behaviour, matrix/network-based formalisms, simplified interactions, simplified decision-making
  - Introduce artefacts ‘for the sake of simplicity’
    - Exactly what ABM was supposed to avoid!

Roadmap workshops

- Glasgow
  - By invitation
- iEMSs 2024
  - Just held

Emerging themes

The requested HPC resource was also deemed very high and lacking evidence of demand by the panel.

- Skills, training, access to skills
- Local and exascale bureaucracy
  - IT policy/standard equipment provision
  - We cannot answer the questions for ARCHER-2!
    - And when we try to, we are not believed!
- Cost
  - Equipment for testing/development
  - Paying for skills – research opportunity cost
- Need modular, reusable software for exascale ABM
  - That's as easy to teach as NetLogo…
  - … and addresses semantic heterogeneity
- Imposter syndrome
  - Can we compete for compute with prize-winning physicists!?

					3				3
					2			1	3
			6 × T2		2	2			4
		1 × A2	1 × A2		2	1			3
		1 × A2	1 × A2	1 × A2	6 × T2	2	1			3
		2 × A2	2 × A2	4 × A2		4	4			8
		1 × A2	1 × A2	1 × A2	1 × A2	1	1	1		3
		2 × A2	3 × A2	2 × A2	2 × A2	2	2	3	2	9
					TOTAL	24	14	7	3	48

	Very La…	Large Job	Medium Job	Small Job
Number of nodes	2	1	1	1
Number of cores used per node (usually 128)	128	64	64	128
Wallclock time for each job (Max. 48h)	6	24	12	6
Number of jobs of this type	196,608	114,688	114,688	49,152
Total memory required.	512 GiB	256 GiB	256 GiB	256 GiB

	Small	Medium	Large	Very Large
RAM per run	8GiB	32GiB	64GiB	512GiB+
Cores per run	4	8	16	256
Assumed minimum garbage collection threads per run for JVM	3	7	15	N/A
Wallclock hours per run	6	12	24	6
Runs per 48h	8	4	2	8
Simultaneous runs per 256GiB RAM, 128 core node	32	8	4	0.5
Node hours for 65,536 runs	12,288	98,304	393,216	786,432
Minimum no. of jobs per expt.	256	2,048	8,192	8,192
Assumed no. of jobs per expt.	2,048	8,192	16,384	65,536
Maximum unused cores per node	0	64	64	0
Number of experiments	24	14	7	3
Computing Units	294,912	1,376,256	2,752,512	2,359,296
Total number of jobs	49,152	114,688	114,688	196,608

How could we…?

- Abstract GPU implementation away
  - e.g. Port NetLogo to GPUs; FlameGPU

Access GPU programming skills

How could we…?

- RCUK refuses funding to institutions with bureaucratic obstacles to non-standard provision!

Access GPU programming skills

Buy non-standard IT equipment

How could we…?

ExAMPLER

Your application for funding will not be progressed to assessment

This application did not pass our preliminary checks.

The reason it did not pass was:

> Your application did not conform to the requirements set out in the opportunity document.

100% Unsuccessful

Opportunity:
OPP503: EPSRC Access to High Performance Computing facilities 2024

Application reference:
APP35952

Applicant:
Gary Polhill

> Your application did not conform to the requirements set out in the opportunity document.

Access GPU
ogramming skills

Buy non-standard
IT equipment

Make a successful
HPC request

How could we…?

Access GPU
ogramming skills

Buy non-standard
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HPC request

100% Unsuccessful

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100% Unsuccessful

Opportunity:
OPP503: EPSRC Ac
facilities 2024

Application referen
APP35952

Applicant:
Gary Polhill

> Your application did not conform to the requirements set out in the opportunity document.

How could we…?

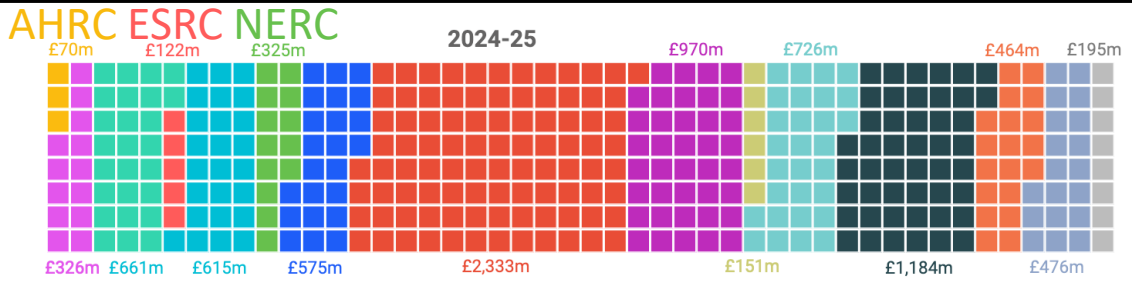
- Configure and administrate HPCs to support *all* science
  - Not just the science that's convenient/easy to support
- HPC admins apply to support scientists!

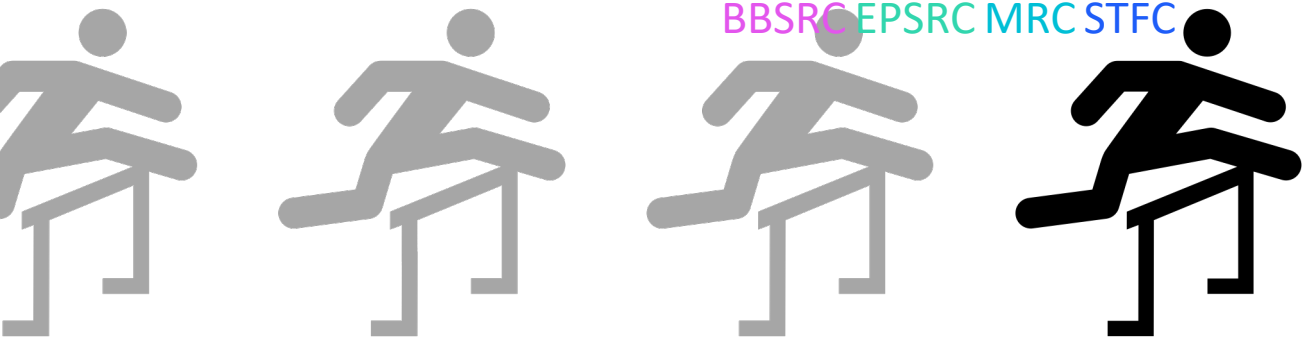
Access GPU
ogramming skills

Buy non-standard
IT equipment

Make a successful
HPC request

How could we…?





cess GPU
mming skills

Buy non-standard IT equipment

Make a successful HPC request

Justify investment and opportunity costs

Central Funding
Existing Strategic Prog.
New Strategic Prog.
Infrastructure
Collective Talent
Existing Commitments
Core IUK
Core RE

How could we…?

- Non-exascale benefits
  - Reusable model components / low-energy computing
- ‘Un-discipline’ UKRI…
  - Is ABM EPSRC, ESRC, AHRC, NERC, MRC, or even BBSRC?

cess GPU mming skills

Buy non-standard IT equipment

Make a successful HPC request

Justify investment and opportunity costs

How could we…?

- Patterns, specifications and standards
  - Can be reimplemented by anyone on their preferred platform
- Standards-driven software stacks

s GPU
ning skills

Buy non-standard IT equipment

Make a successful HPC request

Justify investment and opportunity costs

Design, build and maintain reusable software

How could we…?

Why do you want to model the whole of the UK?

The women's session is in the other room

U skills

Buy non-standard IT equipment

Make a successful Tier-2 HPC request

Justify investment and opportunity costs

Design, build and maintain reusable software

Overcome imposter syndrome & discrimination

How could we…?

- Pay more than lip-service to EDI
- Trust others' expertise – even if they aren't physicists!

…U skills

Buy non-standard IT equipment

Make a successful Tier-2 HPC request

Justify investment and opportunity costs

Design, build and maintain reusable software

Overcome imposter syndrome & discrimination

Alessa LN, Laituri M, Barton M (2006) *J. Artif. Soc. Soc. Sim.* **9**(4), 6
An L, Grimm V, Turner II BL (2020) *J. Artif. Soc. Soc. Sim.* **23**(1), 13
Doherty WJ & Thadhani AJ (1982) *IBM Research Tech. Rep.*
Macal CM, North MJ (2008) SciDAC Review, **Summer 2008**, 34-41
Polhill G (2022) *Rev. Artif. Soc. Soc. Sim.* **14 Dec 2022**
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