The third way of doing science in agent-based complex systems

Li An

Professor of Geography

California State University, San Diego

International Symposium on Social Simulation 2020

August 6, 2020

Wuhan, Huazhong Agricultural University, China

Photo: http://www.sdsu.edu/

Photo: Ron Niebrugge

Agent-based models in complex systems: Achievements, challenges, and future directions

Agent-based modeling as a third way of doing science in social-ecological systems

Agent-based modeling as a third way of doing science in complex systems

The third way of doing science in agent-based complex systems

A science of agent-based complex systems: more needed than ever

A new science of agent-based complex systems: merging data mining and generative modeling

Li An, Volker Grimm, Derek Robinson, Abigail Sullivan, Billie L. Turner II., Zhangyang Wang, Xinyue Ye, Emilie Lindvist, Jianguo (Jack) Liu, Nicolas Malleson, Alison Heppenstall, Christian Vincenot, Wenwu Tang, Viktoriia Radchuk.

(Temporary order; to be changed according to contribution; more invitees possible; V12.1 agent behavioral rules]

Grand challenges

- Land transformation

- Resource depletion

- Extinction of natural species

- Prevalence of invasive species

    ...

- Pandemics like Covid-19

Agents

- Individuals
  - Their behavior
  - Interactions with one another and with their environment
- Agent
  - An entity (object), notion, or software abstraction that wraps the methods (or actions) and attributes within one unit, often pursuing a certain goal

ACS Science

- Agent-based complex systems (ACS; Grimm et al. 2005)
  - Complex system
  - Complex adaptive system
- (ACS) science
  - Understand (and track) the behavior of autonomous, decision-making agents of different kinds that constitute such systems
  - Explaining and predicting the emerging patterns from the bottom up

V. Grimm, E. Revilla, U. Berger, F. Jeltsch, W. M. Mooij, S. F. Railsback, H.-H. Thulke, J. Weiner, T. Wiegand, D. L. DeAngelis, Pattern-oriented modeling of agent-based complex systems: Lessons from ecology. *Science*. **310**, 987–991 (2005).

Agent-based modeling

- A fundamental philosophy
  - Methodological individualism
  - A bottom-up style

- A major tool and paradigm
  - Computational social science
  - A "new kind of science" (Wolfram 2002)
  - The "third way of doing science" (Axelrod 1997)

- Climax of ABM
  - USA National Academy of Sciences' Sackler Colloquiu
  - Special issue in the Proceedings of the National Academy of Sciences (Bankes et al. 2002)
  - Journal of Artificial Societies and Social Simulation in 1998, etc.
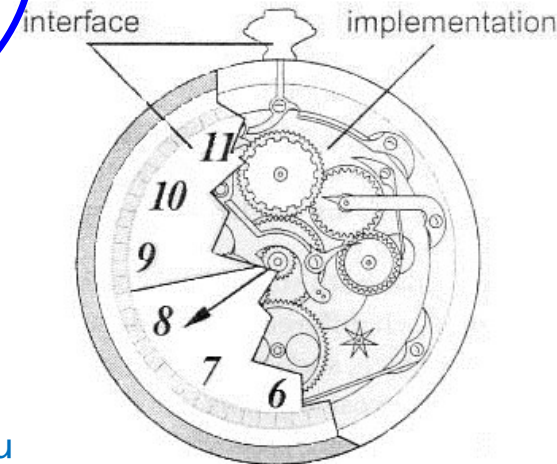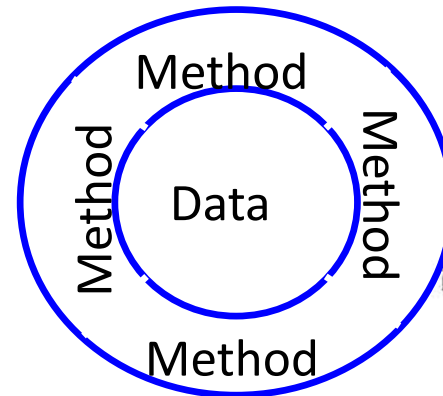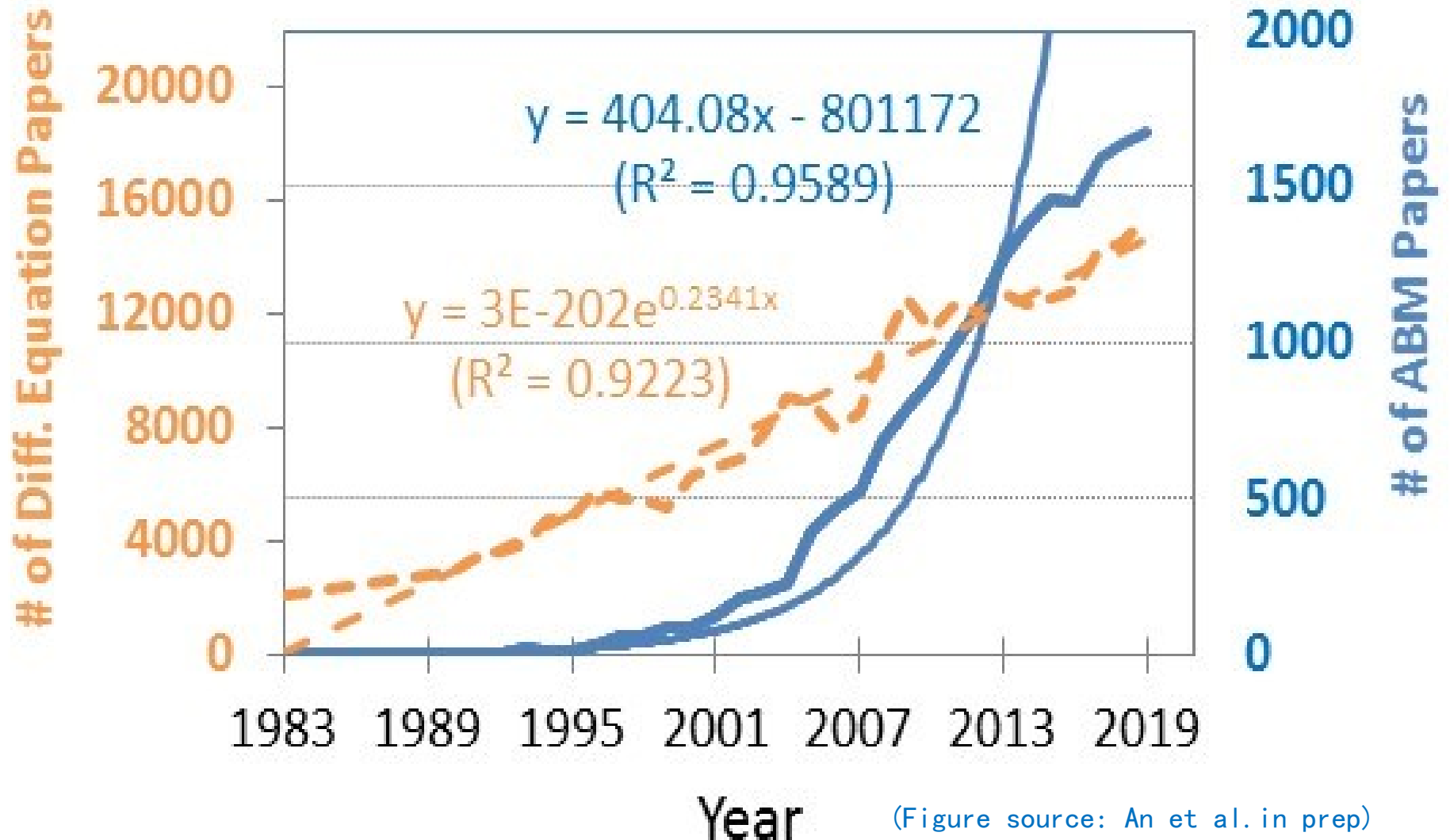
S. Wolfram, *A New Kind of Science* (Wolfram Media, Champaign, Illinois, 2002);
S. Bankes, R. Lempert, S. Popper, Making Computational Social Science Effective: Epistemology, Methodology, and Technology.
Soc. Sci. Comput. Rev. 20, 377–388 (2002).
R. Axelrod, in Simulating Social Phenomena, R. Conte, R. Hegselmann, P. Terna, Eds. (Springer Berlin Heidelberg, Berlin, Heidelberg, 1997), pp. 21–40.

Number of papers over time

$y = 404.08x - 801172$
$(R^2 = 0.9589)$

$y = 3E\text{-}202e^{0.2341x}$
$(R^2 = 0.9223)$

(Figure source: An et al. in prep)

An, L., V. Grimm, D. Robinson et al. (in preparation). The third way of doing science in agent-based complex systems

ABM challenges
(An et al.in prep)

- Integrated human-environment ABMs

- Modeling human behavior (*)

- ABM transparency and reusability

- ABM verification and validation

- Big data and AI (*)

- High-performance ABM

- Spatially explicit ABMs

- ABM education and communication

An, L., V. Grimm, D. Robinson et al. (in preparation). The third way of doing science in agent-based complex systems

Pivotal ABM levers

- Behavioral rules
  - Generative theories or models
  - Data driven "insight" (data science, artificial intelligence)
- Hybrid rules
  - Theory-informed, data-enabled machine learning

Generative theories

- The Belief-Desire-Intention (BDI) framework (Georgeff et al. 1999)

- The physical, emotional, cognitive, and social factors model (PECS) framework (Conte and Paolucci 2014)

M. Georgeff, B. Pell, M. Pollack, M. Tambe, M. Wooldridge, in *Intelligent Agents V: Agents Theories, Architectures, and Languages*, J. P. Müller, A. S. Rao, M. P. Singh, Eds. (Springer Berlin Heidelberg, Berlin, Heidelberg, 1999), pp. 1–10.
R. Conte, M. Paolucci, On agent-based modeling and computational social science. Front. Psychol. (2014), doi:https://doi.org/10.3389/fpsyg.2014.00668.

Data driven "insight"

- Big data (often new forms of data)
  - 5 Vs
  - innovative pathways
  - Facing challenges
- Data science
  - (Machine learning) From basic to advanced "training"
  - Derive some basic model structures
  - Verifying or rebutting underlying theories

Neural network

- Layers of nodes that are connected by links
  - Recurrent neural networks (RNNs)
  - Graph neural networks (GNNs)
- Nodes and links
  - Notes: agents
  - Agent-agent or agent-environment relationships
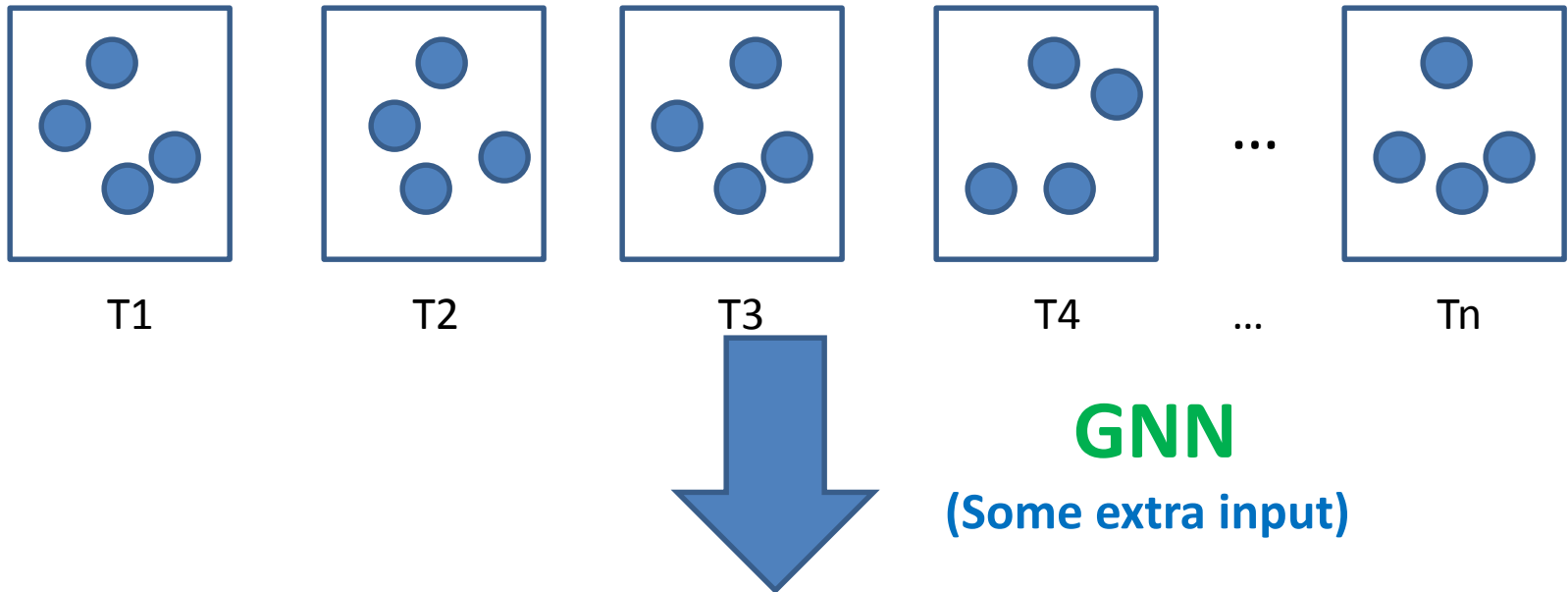
Challenges/opportunities

- Black boxes
  - Little or zero mechanism
  - Hard to interpret
- Good news
  - AI-informed, deep learning algorithms
  - Some closed-form equations can be recovered (reconstructed)
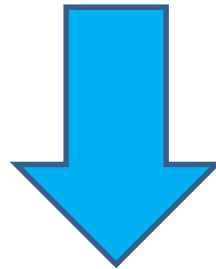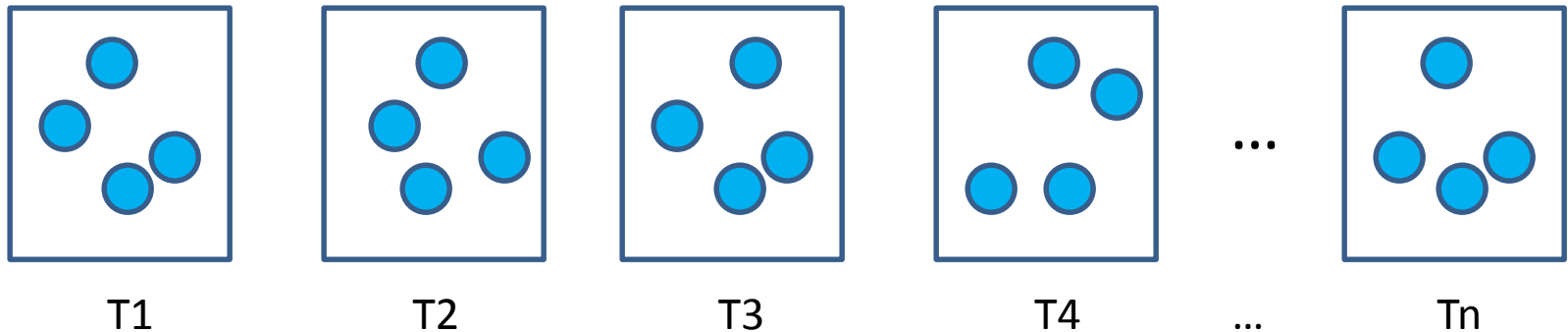
Newtonian force laws
(Cranmer et al. 2020)

- Given mass, charge, & location:

Closed-form, symbolic expressions

M. Cranmer, A. Sanchez-Gonzalez, P. Battaglia, R. Xu, K. Cranmer, D. Spergel, S. Ho, Discovering symbolic models from deep learning with inductive biases (2020), (available at https://arxiv.org/abs/2006.11287).

Decision rules

- Given a set of attributes (counterparts of mass, charge, & location)

GNN

(Domain knowledge, qualitative data, etc.)

(Closed-form) symbolic expressions

Hybrid ABM

- Generative theories

- Data-informed rules
  - Black-box ABM (predictive power)
  - AI-informed ABM (internal mechanism): 1) An edge model to represent links/edges; 2) A node model; and 3) A global model

- Hybrid ABM
  - Internal mechanism (Generative theories & AI informed)
  - Predictive power (Some nodes or edges: black boxes)

Concluding remarks

- Science
  - Multidisciplinary
  - Interdisciplinary
  - Transdisciplinary
- ABM
  - Domain knowledge-based (generative theories)
  - Data science & AI informed

Way to go

Agent-based Complex System (ACS) science, along with ABM, will provide **generative theories** and **predictive power**

- Advancing a new generic systems theory
- Facilitating an effective means to tackling the grand challenges

Acknowledgement

- All coauthors

- San Diego State University

- National Science Foundation

- Evan Casey, student assistant

Contact information

- Center for Complex Human-Environment Systems (http://complexities.org/)

- Personal website (http://complexities.org/An/)

- Email: anli@complexities.org