

Proceedings of the 20XX Winter Simulation Conference
M. Rabe, A.A. Juan, N. Mustafee, A. Skoogh, S. Jain, and B. Johansson, eds.

APPLYING THE STRESS GUIDELINES FOR REPRODUCIBILITY IN MODELING & SIMULATION: APPLICATION TO A DISEASE MODELING CASE STUDY

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ABSTRACT

It is arguably difficult to reproduce the results of published work in Modeling & Simulation (M&S). Authors have certainly raised concerns about this issue and attempts by journals and conferences are being made to improve the situation. As part of a movement to tackle reproducibility in M&S, the *Strengthening The Reporting of Empirical Simulation Studies* (STRESS) reporting checklists were introduced in 2018. The STRESS guidelines aimed to improve knowledge management in industry and to maximize the chance that all important M&S details are included when writing up simulation research for publication. We extend this work by providing an applied example of using the STRESS-ABS checklist for documenting an Agent Based Simulation model. It is hoped that an applied example will both encourage and guide authors and practitioners to improve their reporting.

1 INTRODUCTION

The STRESS guidelines (Strengthening the Reporting of Empirical Simulation Studies) were introduced to improve the reproducibility of computer simulation models (Monks et al. 2018). This raises the question of why we should be worried about reproducibility, a topic which has been under discussion for several years in the modeling community. In 2014, a panel discussion on the future of simulation research argued that reproducibility is key to credibility in research and went further to suggest that automated provenance tracking, discoverability across the artifacts of M&S research and the appropriate use of Creative Commons licenses was also vital (Yilmaz et al. 2014). This was followed up in a panel discussion from the Winter Simulation Conference in 2016 (Uhrmacher et al. 2016) In this it was

suggested that repeatability, replicability, and reproducibility should be at the core of reporting of applied simulation modeling studies but finds that this is not always the case.

The argument in favor of reproducibility is that it allows models to be reused, to avoid reinventing the wheel and that it is a necessity in the era of *Open Science*, which aims to make research, particularly public-funded, more widely accessible outside of academia. While applied simulation papers currently include some information about the model and the experimentation, it is rare to find one that includes sufficient information for the work to be reproduced. This is not a “simulation only” problem, and scientists across the board are concerned about the quality of the descriptions of both computer simulation and experimental studies (Baker 2016).

A wider discussion of Open Science and how its principles apply to the modeling and simulation community is given in (Taylor et al. 2017) but we further note that the benefits of good reproducibility practice might also include:

- The advancement of operational knowledge (through reusing a published model to further investigate a system);
- To enable reuse of knowledge (models are expensive to develop; reusing models (or model components) can save time and money in M&S projects that could be devoted to a wider ranging study or analysis forms);
- To further conceptual modelling knowledge (a published model will argue how a conceptualization of a system has led to a given model, simulation, results and analysis; accurately reporting this conceptualization will help other researchers tackling similar problems in deciding what to model and what not to model);
- To reuse data where none exists (in many M&S projects data cannot be collected or is limited. In this case expert opinion is captured and modelled and/or missing data is approximated; capturing these assumptions in systematic manner will help to understand the validity of the study and help others to understand and build on the techniques used); and
- Testing of novel simulation methods (the validation of new analysis methods, algorithms, experimentation techniques require careful specification so that they can be assessed and reused elsewhere).

To summarize the full discussion of the issues in (Monks et al. 2018), there have been several papers that highlight issues with reproducibility in, e.g., forecasting (Boylan et al. 2015) and agent based modeling (Janssen 2017) with corresponding efforts in system dynamics (Rahmandad and Sterman 2012) and specific areas of agent based modeling (Grimm et al. 2006) to develop guidelines for modeling studies. These are a little disjointed and STRESS is introduced to give a comprehensive view of all three modeling paradigms: discrete-event simulation (DES), agent-based modeling (ABM) and system dynamics (SD) with specific checklists for each type of modeling study (freely available online at <https://doi.org/10.1080/17477778.2018.1442155>). We also note the efforts being made by the journal ACM Transactions on Modelling and Computer Simulation, which now provides an optional reproducibility review for submitted models as does the ACM SIGSIM PADS conference. This “peer-review” of results provides a “seal of reproducibility” and more faith in the results but, arguably, it may not give researchers the necessary documentation needed to independently reproduce the contents of a paper.

This article goes beyond the initial description of STRESS to analyze how it can be used in practice, using the example of an ABM model of diseases by way of demonstration.

2 BRIEF OVERVIEW OF STRESS

The STRESS checklists attempt to provide guides for authors writing up applied simulation studies, ensuring that all of the necessary details of the study are described. While focused principally on

academic reports, it is also useful for practitioners as part of a knowledge management process. In developing the guidelines, we relied on good and bad examples of reporting within the literature as well as lessons learned from other guidelines. The authors are each experts in one or more of DES, ABM and SD, which allowed a certain amount of practical experience to be incorporated. One piece of work remaining at the end of the study was to apply the guidelines to a real problem, as is done in the following section.

There are three checklists, STRESS-ABS, STRESS-DES and STRESS-SD, and while the details differ between the three checklists, the key areas for reporting remain the same. Each is split into six sections: objectives, logic, data, experimentation, implementation and code access, covering all aspects of a modeling study that might need to be reproduced. We do not reproduce details of the checklists here and instead refer the interested reader to the full paper (Monks et al. 2018).

3 STRESS: A CASE STUDY

To illustrate how STRESS can be used to document a simulation study, we use a case study introduced in earlier work to illustrate approaches to Open Science in M&S (Fabiya et al. 2016; Taylor et al. 2017).

In what follows we describe the model and the experimentation carried out and use a STRESS record to ensure that all of the relevant characteristics of the modeling study have been described, working through the six sections in turn. The STRESS guidelines are deliberately not prescriptive as to how the checklists should be used with no requirements about the structure of a write up or the terminology that should be used. They are instead designed to be a checklist for both authors and reviewers to ensure that the work is reproducible. We break the model documentation in to 6 sections: objectives, logic, data, experimentation, implementation, and code sharing. Each section has a table that completes the checklist items. Section 3.6 is a single checklist item.

3.1 Objectives

We describe an agent-based infection model implemented in REPAST (repast.github.io). This “studies” the spread of infection in a population after an outbreak. The model is designed to be relatively straightforward, making it more obvious to see how the reporting has worked. Table 1 shows the checklist for objectives.

Table 1: STRESS Checklist of Objectives.

Section/Subsection	Item	Recommendation
1. Objectives		
Purpose of the model	1.1	Explain the background and rationale for the model. <i>The purpose of the model is to study infectious disease spread for various population dynamics.</i>
Model Outputs	1.2	State the qualitative or quantitative system level outputs that emerge from agent interactions within the ABS. <i>The outputs of the model are the sizes of the infected, susceptible and recovered population. The output is recorded every five days (simulation time unit is day).</i>
Experimentation Aims	1.3	If the model has been used for experimentation, state the research questions that it was used to answer. <i>The experimentation aim is to demonstrate the deployment of Agent-Based Simulation in Science Gateways/Open Science.</i>

3.2 Logic

Agents can be infected, susceptible or recovered. When an infected agent approaches a susceptible agent, the latter becomes infected and if there is more than one susceptible agent in the cell, only one, randomly selected agent, is infected. Infected agents recover after a period and when recovered are assumed to have some immunity to being reinfected. This immunity decreases every time they are approached by an

infected agent and, when immunity reaches zero, the recovered agent becomes susceptible and can be infected again.

The STRESS checklist follows and, as can be seen, contains a significant amount of information. We acknowledge that some of this material may be better placed in appendices in a real example of STRESS being used. Table 2 shows the logic checklist.

Table 2: STRESS Checklist of Logic.

Section/Subsection	Item	Recommendation
2. Logic		
Base model overview diagram	2.1	<p>Provide one or more of: state chart, process flow or equivalent diagrams to describe the basic logic of the base model to readers. Avoid complicated diagrams in the main text.</p> <p><i>Use case diagram of infectious disease model</i></p>
Base model logic	2.2	<p>Give details of the base model logic. This could be text to explain the overview diagram along with extra details including ABS product and process patterns. Include details of all intermediate calculations.</p> <p><i>The model starts an infection outbreak with an initial population of infected and susceptible agents. Infected agents move close to susceptible agents and infect them while susceptible agents move where the least infected agents are located. Infected and susceptible agents interact with each other every simulation time unit (day). Infected agents recover after a period of time and become recovered with a level of immunity. When an infected agent gets in touch with a susceptible agent, the susceptible agent becomes infected. When an infected agent gets in touch with a recovered agent, the recovered agent decreases its immunity. When the immunity level is 0, the recovered agent becomes susceptible and can be infected again. The outbreak occurs annually. When this happens, the population changes to reflect the initial conditions taking into account the population of the previous year.</i></p>
Scenario logic	2.3	<p>Give details of any difference in the model logic between the base case model and scenarios. This could be incorporated as text or, where differences are substantial, could be incorporated in the same manner as 2.1.</p> <p><i>N/A (only parameter sweep)</i></p>
Algorithms	2.4	<p>Provide further detail on any algorithms in the model that (for example)</p>

Section/Subsection	Item	Recommendation
		mimic complex or manual processes in the real world. <i>N/A</i>
Components	2.5	<p>2.5.1. Environment Describe the environment agents interact within, indicating its structure, and how it is generated. <i>Euclidean 2D space for free movement, Grid for neighborhood definition, Network for infection connections</i></p> <hr/> <p>2.5.2. Agents List all agents and agent groups within the simulation. Initial population: {Infected=20, Susceptible=1500, Recovered=0}</p> <p>Infected Attributes: Location, Days infected: Logic 01. Find where most susceptible are located 02. Move towards this grid location 03. If in contact with an agent { 05. If (contacted agent = susceptible){infect} 06. If (contacted agent = recovered){reduce immunity} 07. Count days infected 08. If (infected days = recovery days){change state and become recovered}</p> <p>Susceptible Attributes: Location Logic 01. Find where least infected are located 02. Move towards this grid location 03. If in contact with an infected agent {change state and become infected}</p> <p>Recovered Attributes: Location, Immunity Logic 01. Move randomly 02. If in contact with an infected agent {reduce immunity by 0.5} 05. If (immunity = 0){change state and become susceptible}</p> <p>Describe all decision-making rules that agents follow in either algorithmic or equation form.</p> <ul style="list-style-type: none"> • The data that agents access (I.e. internal attributes or external information from the environment) and how it is used. • <i>Internal distributions</i> • The objectives agents seek to achieve. • <i>Infected: move close to susceptible</i> • <i>Susceptible: move away from infected</i> • The algorithms, optimizations, heuristics and rules that agents use to achieve objectives. • <i>Infected: find where most susceptible are located</i> • <i>Susceptible: move where least infected are located</i> • How agents work together within a group along with any rules for changes in group membership. • <i>They do not work in groups</i> • Predictions of future events and adaptive action. • <i>N/A</i>

Section/Subsection	Item	Recommendation
		2.5.3. Interaction Topology Describe how agents and agent groupings are connected with each other in the model define: <ul style="list-style-type: none"> • with whom agents can interact, • <i>Interacting agents: infected with susceptible and recovered</i> • how recipients of interactions are selected • <i>Random selection</i> • what frequency interaction occurs. • <i>Every simulation time unit</i> • How agents handle and assign priorities to concurrent events • <i>No priorities (random execution of actions scheduled for the same time unit)</i>
		2.5.4 Entry / Exit Where relevant, define how agents are created and destroyed in the model. <i>All agents are created at initialization. They are not destroyed however they change state.</i>

3.3 Data

The input parameters for the model include:

- simulation period (specifies how many years the simulation will run);
- recovered count (specifies the initial recovered population);
- infected count (specifies the initial infected population); and
- susceptible count (specifies the initial susceptible population).

For this particular example, there is relatively little data but in a bigger study, this section may refer to publicly available datasets. Table 3 shows the Data checklist.

Table 3: STRESS Checklist of Data.

Section/Subsection	Item	Recommendation
3. Data		
Data sources	3.1	List and detail all data sources. Sources may include: <i>This is a demo model with no real data.</i>
Input parameters	3.2	List all input parameters in the model, providing a description of each parameter and the values used. <i>Model parameters:</i> <ul style="list-style-type: none"> • <i>Initial population: {Infected=20, Susceptible=1500, Recovered=0}</i> • <i>Recovery days: {Uniform distribution (30,50)}</i> <i>Immunity: {Uniform distribution (5,10)}</i>
Pre-processing	3.3	Provide details of any data manipulation or filtering that has taken place before its use in the simulation. <i>None.</i> <ul style="list-style-type: none"> •
Assumptions	3.4	Where data or knowledge of the real system is unavailable, state and justify the assumptions used to set input parameter values and distributions; agent interactions or behaviour; or model logic. <i>See above.</i>

3.4 Experimentation

We ran five experiments to produce five sets of results. We also created a simple visualization tool that allows easy analysis of infected/non-infected population trends. Following good Open Science practices, the model, results, visualization tool and summary pack have been deposited in an open access repository and assigned Digital Object Identifiers (DOIs) as follows:

- REPAST Infection Model Example DOI Collection (summary pack) <https://dx.doi.org/10.15169/sci-gaia:1457690398.43>
- REPAST Infection Model Virtual Appliance <https://dx.doi.org/10.15169/sci-gaia:1455182324.71>
- Graphical Visualization Tool for REPAST Infection Model <https://dx.doi.org/10.15169/sci-gaia:1457432416.29>
- REPAST Infection Model Experiment 1 Results <https://dx.doi.org/10.15169/sci-gaia:1457431676.23>
- REPAST Infection Model Experiment 2 Results <https://dx.doi.org/10.15169/sci-gaia:1457431835.0>
- REPAST Infection Model Experiment 3 Results <https://dx.doi.org/10.15169/sci-gaia:1457432005.33>
- REPAST Infection Model Experiment 4 Results <https://dx.doi.org/10.15169/sci-gaia:1457432129.78>
- REPAST Infection Model Experiment 5 Results <https://dx.doi.org/10.15169/sci-gaia:1457432242.73>

Table 4 shows the Experimentation checklist.

Table 4: STRESS Checklist of Experimentation.

Section/Subsection	Item	Recommendation
4. Experimentation		
Initialisation	4.1	State if a warm-up period has been used, its length and the analysis method used to select it. <i>No warm-up period</i> State what if any initial agent and environmental conditions have been included. <i>Initial population: {Infected=20, Susceptible=1500, Recovered=0}</i>
Run length	4.2	Detail the run length of the simulation model and time units. <i>20 years</i>
Estimation approach	4.3	State if the model is deterministic or stochastic. <i>Deterministic</i>

3.5 Implementation

The ABS model was implemented in Repast Symphony. Full details are found in Table 5.

Table 5: STRESS Checklist of Implementation.

Section/Subsection	Item	Recommendation
5. Implementation		
Software or programming language	5.1	State the operating system and version and build number. It can run in any OS, Repast Symphony 2.1, Java 7.5.1.
Random sampling	5.2	State the algorithm or package used to generate random samples within the software/programming language used. <i>Repast Random Helper.</i>
Model execution	5.3	If the ABS model has a time component, describe how time is modelled (e.g. fixed time steps or discrete-event). Fixed time steps Random execution of agent actions Last priority for recording outputs

Section/Subsection	Item	Recommendation
		First priority for annual outbreak
System Specification	5.4	State the model run time and specification of hardware used. <i>Runtime: 20 min</i> <i>VM with all dependencies (repast libraries, model source code and scenario, java runtime)</i> <i>All results and software can be found in the DOI Collection</i> https://dx.doi.org/10.15169/sci-gaia:1457690398.43

3.6 Code Access

The STRESS record for these experiments was created and assigned the following DOI: <http://dx.doi.org/10.15169/sci-gaia:1494421530.94>.

4 CONCLUSIONS

Over a series of recent publications, authors within the field of computer simulation have highlighted a problem with the reproducibility of simulation studies. The STRESS guidelines were introduced to improve the reporting of studies and minimize the chance that important details of the modelling were omitted from public records. This paper extends this work by providing an applied example of STRESS to an agent based simulation.

Reproducibility of results is one aspect of Open Science, a “movement” that encourages the digital sharing of the scientific artefacts. While reproducibility is important, we hope that our community will encourage the appropriate open sharing of models, data, results and software that will enable us all to build on each other’s work and perhaps benefit our discipline as a whole.

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