# Demonstrating Open Science for Modeling & Simulation Research

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***Abstract*— Most conference and journal publications present contributions based on research artefacts (data, results, software, etc.) that are difficult for researchers to access. Open science aims to promote open access to research presented in academic works. Ideally, the software, data and results presented in a scientific article should be available for other scientists to use, validate and build upon for their own research. This is particularly true in some Modeling & Simulation (M&S) research where in addition to the above access might also be required to complex models. Using a case study based on an Infection Model, this demonstration shows how Open Science approaches based on Digital Object Identifiers, Researcher Registries, Open Access Data Repositories, Scientific Gateways and e-Infrastructures project can support M&S research.**

***Keywords—Open Science; Modeling; Simulation; Research; Open Access;, Open Data; e-Infrastructure***

## I. INTRODUCTION

Encouraged by bodies such as the European Commission [1], the National Science Foundation [2] and Research Councils UK [3] there is arguably a global shift towards making research findings available free of charge via Open Access under some globally recognized sharing agreement (such as a Creative Commons license [4]). Open Science builds on this by encouraging scientific practices that all research outputs and methods are openly shared under terms that enable reuse, redistribution and reproduction [5]. Potential benefits include improved scientific efficiency, increasing transparency and quality in research validation, faster knowledge transfer, better knowledge spillovers to national and international economies, a more effective approach to address global challenges and increased citizens' engagement in science and research [6]. There are many initiatives promoting Open Science. One of these is the *Energising Scientific Endeavour through Science Gateways and e-Infrastructures in Africa* (Sci-GaIA) (www.sci-gaia.eu) project. To support Open Science, and to promote Open Science in Africa, Sci-GaIA has created the Open Science Platform [7].

What impact could Open Science approaches have on Modeling & Simulation (M&S) research? In this demonstration we attempt to show a possible future where all elements of a M&S project are openly shared and, importantly, made more visible to international communities.

## II. MODELING AND SIMULATION RESEARCH OUTPUTS

What are the outputs of M&S research? Consider the following case study. A researcher is studying the spread of disease across a population by using simulation. To do this he or she creates a simulation in some language or software package, collects data, runs simulations under different experimental conditions and collects results for analysis. The researcher then writes up their work in a scientific paper which is then published in a conference or journal. The outputs are therefore the simulation, the data, the experiments and results, the analysis and the published paper. Typically in contemporary M&S research only the final artefact of this list is normally available. The article could be made open via self-archiving under a Green Open Access agreement such as a University research archive (e.g. Brunel's BURA - bura.brunel.ac.uk) after some embargo period, or via Gold Open Access through a publisher's website (an associated publishing charge (APC) is usually incurred) – a major exception to this is in M&S is the Winter Simulation Conference archive that makes all conference papers freely available (www.wintersim.org). Importantly, a published article typically has a Digital Object Identifier (DOI) that is assigned by a publisher via agencies such as CrossRef or DataCite. A DOI is a persistent digital identifier of an object that can have associated metadata such as a URL linked to the physical location of the object (i.e. the DOI does not change but the associated metadata can). The unique DOI makes the object (in this case the published paper) both discoverable (searchable), accessible and specifically citable (rather than just "text" in a reference list). Can the other research outputs be treated in the same way?

## III. DEMONSTRATING OPEN SCIENCE FOR M&S

The outputs of simulation research can all be considered digital objects. To obtain a DOI for each of these, each output must be deposited in an Open Access Document Repository (OADR) hosted by a body that has permission to assign a DOI. As an object is deposited various metadata can be added that identify the authors, the URL, the sharing/use agreement, etc. It is also possible to create a DOI Collection that collects all the relevant DOIs together in a single reference. To demonstrate this we have created an agent-based Infection Model in the open source agent-based simulation API REPAST [8]. We ran five experiments to produce five sets of results. We also created a simple visualization tool that allows easy analysis of

TABLE 1: List of outputs and their DOIs

| Item | DOI |
|---|---|
| REPAST Infection Model Example | http://dx.doi.org/10.15169/sci-gaia:1457690398.43 |
| REPAST Infection Model Virtual Appliance | http://dx.doi.org/10.15169/sci-gaia:1455182324.71 |
| Graphical Visualisation Tool for REPAST Infection Model | http://dx.doi.org/10.15169/sci-gaia:1457432416.29 |
| REPAST Infection Model Experiment 1 Results | http://dx.doi.org/10.15169/sci-gaia:1457431676.23 |
| REPAST Infection Model Experiment 2 Results | http://dx.doi.org/10.15169/sci-gaia:1457431835.0 |
| REPAST Infection Model Experiment 3 Results | http://dx.doi.org/10.15169/sci-gaia:1457432005.33 |
| REPAST Infection Model Experiment 4 Results | http://dx.doi.org/10.15169/sci-gaia:1457432129.78 |
| REPAST Infection Model Experiment 5 Results | http://dx.doi.org/10.15169/sci-gaia:1457432242.73 |

infected/non-infected population trends (in HTML5 and Javascript). We deposited all these research outputs in the Sci-GaIA Open Access Document Repository (oar.sci-gaia.eu). The list of outputs and their DOIs is shown in Table 1.

Note that the simulation has been packaged as a virtual appliance that can be run directly on a virtual machine.

In our experience it can be difficult to download and run a simulation as researchers may not have the IT expertise to install and run the simulation software or have access to a simulation package. An alternative is to put the simulation online for people to use. Creating web-based simulations can be quite difficult to create, especially if high performance computing is required to process a simulation quickly. Science Gateways have been developed to allow easy access and deployment of web-based software. Building on e-Infrastructure research, a science gateway allows federated single-sign-on access to a range of resources (software, computers, data, sensors, etc.) To demonstrate this we have created the Africa Grid Science Gateway (http://sgw.africa-grid.org/), a Science Gateway that hosts a range of applications developed for African scientific communities of practice. We have deployed the REPAST Infection Model on the AGSG. To access this, users must first login via an Identify Federation. First time users will be asked to register (use the catch-all GrIDP Identify Federation and IDPOPEN GARR Identify Provide if your own regional provider is not listed). After registration a user can access the Infection Model via the drop down application list. In this demonstration users can select any of the five experiments with parameters to run via a form. Results can be accessed via the AGCG workspace and visualized by uploading the results file to the visualization tool (also accessible via the application list). Further details on the REPAST Infection Model deployment can be found in an accompanying paper in this conference [9]. A cloud-based high performance computing version of the Infection Model can also be found on the AGSG.

Once the outputs of research can be openly accessed and used, it is useful to uniquely identify associated researchers and link these outputs to them. Research registries can give unique identifiers to researchers. The Open Researcher and Contributor ID (ORCID – orcid.org) provides unique IDs for researchers and facilities to "claim" research outputs or "works". All the works mentioned in this paper can be found under ORCID for each of the authors. For convenience, Taylor's ORCID ID is orcid.org/0000-0001-8252-0189.

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## IV. Summary

This paper has demonstrated an Open Science approach to M&S research. Outputs can be openly shared via DOIs and OADRs. Science Gateways can also be used to make complex software easily accessible. The role of social media impact, or Altimetrics, will also be discussed with respect to more traditional Scientometrics, highlighting emerging career "narrative" tools such as Impactstory (impactstory.org).

The Sci-GaIA project is continuing to promote Open Science in Africa and beyond. For example Sci-GaIA has helped to setup a major document repository for the West and Central Research and Education Network (WACREN – wacren.net) and the Tanzanian National Research and Education Network (TERNET – www.ternet.or.tz), and a range of Scientific Applications on the AGSC. See the project website for a wealth of material on the building blocks of Open Science, for example training materials and guides on how to setup an institutional OADRs [10], Science Gateways and Science Gateway Applications [11]. Help to promote Open Science in Africa by signing the Dakar Declaration on Open Science http://www.sci-gaia.eu/dakar-declaration/ [12].

## References

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