



**CENTER FOR REPRODUCIBLE
BIOMEDICAL MODELING**

Curation of computational biology models

Anand Rampadarath & David Nickerson
Auckland Bioengineering Institute, University of Auckland

<https://reproduciblebiomodels.org/>

a.rampadarath@auckland.ac.nz
d.nickerson@auckland.ac.nz



Acknowledgements

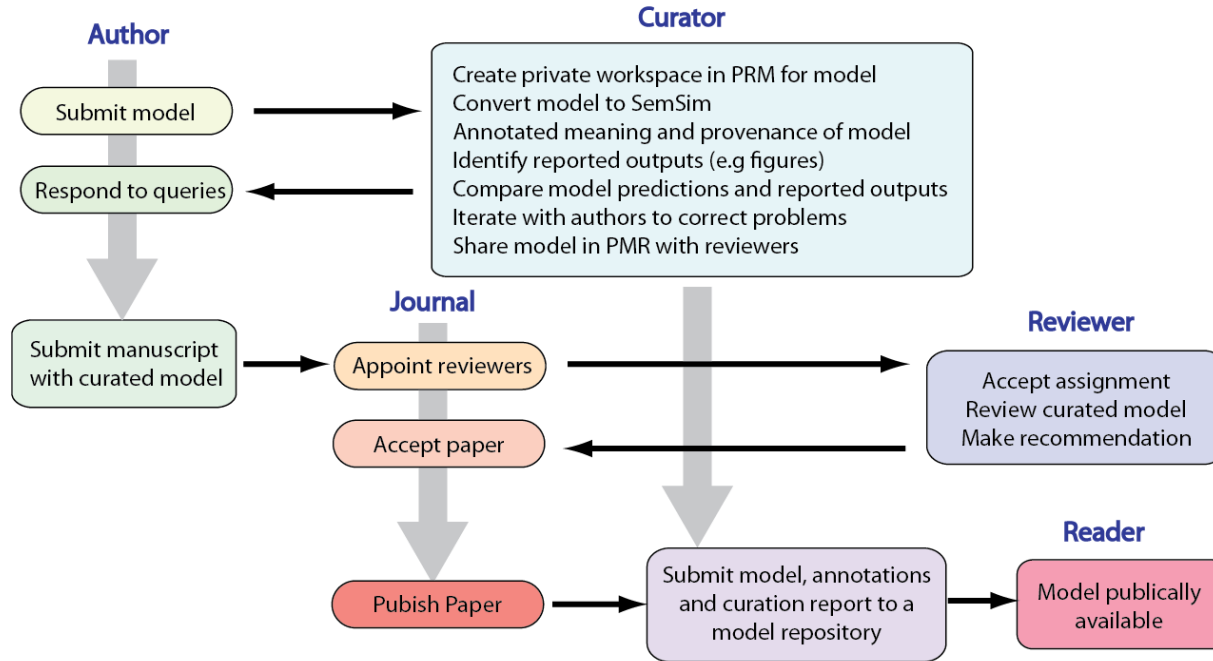
- Centre director: Herbert Sauro, University of Washington
- Co-directors:
 - Jonathan Karr, Icahn School of Medicine at Mount Sinai
 - John Gennari, University of Washington
 - Ion Moraru, University of Connecticut Health
- NIH/NIBIB Biomedical Technology Resource Center grant P41 EB023912

Model curation service for journals

- Work with journals to improve reproducibility
- Help develop common curation practices
 - Domain specific vs general curation
 - Curation != validation
- Measuring reproducibility
 - FAIRmetrics and associated pitfalls
- Annotation
 - Non-standard model formats
 - Simulation results

Initial vision

Manuscripts received by journals will be curated to make sure that any author supplied code will faithfully reproduce the results presented in the manuscript.



PLoS Comp Biol - Pilot

Author(s) submit
manuscript

Existing submission pipeline

Selected associate editors

Suitable manuscripts
sent to curation service
(as a reviewer)

Curation service checks reproducibility
and produces reproducibility report

Reproducibility report
submitted as the “review”

Editorial describing pilot:

<https://doi.org/10.1371/journal.pcbi.1007881>

Reproducibility report



Director: Professor Herbert M. Sauro
University of Washington, Seattle, WA
<https://reproduciblebiomodels.org>

Reproducibility report for: Title of the submission being evaluated.

Submitted to: Name of Journal

Manuscript identifier: Journal-identifier

Curation outcome summary: One or two sentences summarizing the outcome of the curation report.

Box 1: Criteria for repeatability and reproducibility

Model source code provided:

- Source code: a standard procedural language is used (e.g. MATLAB, Python, C)
 - There are details/documentation on how the source code was compiled
 - There are details on how to run the code in the provided documentation
 - The initial conditions are provided for each of the simulations
 - Details for creating reported graphical results from the simulation results
- Source code: a declarative language is used (e.g. SBML, CellML, NeuroML)
 - The algorithms used are defined or cited in previous articles
 - The algorithm parameters are defined
 - Post-processing of the results are described in sufficient detail

Executable model provided:

- The model is executable without source (e.g. desktop application, compiled code, online service)
 - There are sufficient details to repeat the required simulation experiments

The model is described mathematically in the article(s):

- Equations representing the biological system
- There are tables or lists of parameter values
- There are tables or lists of initial conditions
- Machine-readable tables of parameter values
- Machine-readable tables of initial conditions

The simulation experiments using the model are described mathematically in the article:

- Integration algorithms used are defined
- Stochastic algorithms used are defined
- Random number generator algorithms used are defined
- Parameter fitting algorithms are defined
- The paper indicates how the algorithms yield the desired output



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Box 2: Criteria for accessibility

- Model/source code is available at a public repository or researcher's web site
 - Prohibitive license provided
 - Permissive license provided
 - Open-source license provided
- All initial conditions and parameters are provided
- All simulation experiments are fully defined (events listed, collection times and measurements specified, algorithms provided, simulator specified, etc.)

Box 3: Rules for Credible practice of Modeling and Simulation*

*Model credibility is assessed using the Interagency Modeling and Analysis Group conformance rubric:
<https://www.imag.ki.nibb.nih.gov/content/15-simple-rules-conformance-rubric>

- Define context clearly: Extensive
- Use appropriate data: Extensive
- Evaluate within context: Adequate
- List limitations explicitly: Insufficient
- Use version control: Adequate
- Document adequately: Partial
- Conform to standards: Insufficient

Box 4: Evaluation

- Model and its simulations could be repeated using provided declarative or procedural code
- Model and its simulations could be reproduced



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Summary comments: This would be a longer bit of text, giving details about what was tested and what worked. Lorem ipsum dolor sit amet, consectetur adipiscing elit, sed do eiusmod tempor incididunt ut labore et dolore magna aliqua. Ut enim ad minim veniam, quis nostrud exercitation ullamco laboris nisi ut aliquip ex ea commodo consequat. Duis aute irure dolor in reprehenderit in voluptate velit esse cillum dolore eu fugiat nulla pariatur. Excepteur sint occaecat cupidatat non proident, sunt in culpa qui officia deserunt mollit anim id est laborum. Lorem ipsum dolor sit amet, consectetur adipiscing elit, sed do eiusmod tempor incididunt ut labore et dolore magna aliqua. Ut enim ad minim veniam, quis nostrud exercitation ullamco laboris nisi ut aliquip ex ea commodo consequat. Duis aute irure dolor in reprehenderit in voluptate velit esse cillum dolore eu fugiat nulla pariatur. Excepteur sint occaecat cupidatat non proident, sunt in culpa qui officia deserunt mollit anim id est laborum. Lorem ipsum dolor sit amet, consectetur adipiscing elit, sed do eiusmod tempor incididunt ut labore et dolore magna aliqua. Ut enim ad minim veniam, quis nostrud exercitation ullamco laboris nisi ut aliquip ex ea commodo consequat. Duis aute irure dolor in reprehenderit in voluptate velit esse cillum dolore eu fugiat nulla pariatur. Excepteur sint occaecat cupidatat non proident, sunt in culpa qui officia deserunt mollit anim id est laborum.

Anand K. Rampadarath¹, PhD
Curator
Center for Reproducible Biomedical Modeling

David P. Nickerson, PhD
Curator Service Director
Center for Reproducible Biomedical Modeling

Auckland Bioengineering Institute,
University of Auckland

¹Email: a.rampadarath@auckland.ac.nz

PLoS Comp Biol - Pilot

- ~70 submissions opt -in to pilot
- ~40 reports submitted
- 30% of submissions “reproducible”
 - At least one reported result could be reproduced
- Common reasons we are unable to determine reproducibility
 - No code submitted or will be made available after acceptance
 - Missing data files
 - Software successfully installed and runs on test data, but no mention of data used in paper
 - Insufficient descriptions of how to use outputs to obtain results
 - Code provided without comments or documentation

Physiome

- <https://journal.physiomeproject.org>
- New journal with a focus on reproducibility
- Reproducibility report included in publication

- <https://vph2020.sciencesconf.org/315725>

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Reproducibility report

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Reproducibility report

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