

Reproducibility report for: Multi-scale modeling of macrophage – T cell interactions within the tumor microenvironment and impacts of macrophage-based immunotherapies. Submitted to: PLoS Computational Biology Manuscript number/identifier: PCOMPBIOL-D-20-01387

Curation outcome summary: Unable to determine reproducibility of the model presented.

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)
\Box 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
\Box 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
\Box The paper indicates how the algorithms yield the desired output



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^a

^aModel credibility is assessed using the Interagency Modeling and Ananlysis Group conformance rubric: https://www.imagwiki.nibib.nih.gov/content/10-simple-rules-conformance-rubric

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

Box 4: Evaluation

- \square Model and its simulations could be repeated using provided declarative or procedural code
- $\hfill\square$ Model and its simulations could be reproduced



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

Summary comments: Model source code were made available for download via a Github link provided in the manuscript (https://github.com/FinleyLabUSC/Early-TME-ABM-PLOS-Comp-Bio). These were used in our attempt to reproduce the results presented in the paper. We successfully built the executable model using the CMake file present in the Github repository, however there is no information provided describing how to use the compiled application to reproduce the results presented in the manuscript. We believe further clarity on the model execution will resolve this issue.

And Ragalanth

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

Al Ala

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

Auckland Bioengineering Institute, University of Auckland

¹Email: a.rampadarath@auckland.ac.nz