# IACAP25 - Reproducing Simulations


**Short abstract**

Sometimes simulationists notice that successive runs of the same simulation yield different results. There is no consensus if such variance is cause for concern or can safely be ignored. The central epistemological principle of computational modeling, namely that the computational error must be of the same magnitude as the modeling error, can be used to decide if we should be worried. If the variance of the simulation is within the bounds prescribed by the modeling error we have no reason to doubt the results. Waters get murkier once we cannot establish modeling error independently of the simulation, a case that is more common in science and engineering than often thought. I will discuss several examples from the field of dynamical systems where access to models is often mediated through computer simulations alone and therefore establishing an acceptable level of variance seems impossible. I evaluate the possibility to get at the modeling error through extrapolation from well understood toy-models and from experimentally observing analogue models.

**Long abstract**

The discovery that computer simulations do not reproduce across successive runs is made with beautiful regularity (e.g. in (Diethelm 2012) or in (Antunes and Hill 2024)). The problem seems especially pressing in HPC simulations, which - for economical reasons - cannot be repeated easily. Ludwig (Ludwig 2019) noted that failing to exactly reproduce results might be especially troublesome in climate simulations where we expect the climate system to be sensitively dependent on initial conditions. It is thus feared that a small variance might blow up to a large error and invalidate any prediction. Unfortunately there is no consensus in the field of computer simulations under which conditions reproduction failures are threatening and under which conditions they are acceptable. Diethelm (Diethelm 2012) and Fox (Fox 1971) for example argue that reproduction failures are inherent in simulations because of certain features of the numerics employed. They are thus unavoidable and should be accepted on the condition that an error analysis shows that one cannot do better. The possibility of such an error analysis relies on the central epistemological principle of computational modeling (Fillion and Corless 2014). Modeling error and computational error must be shown to be of the same magnitude. But as Fillion and Corless themselves note (Fillion and Corless 2021) often simulations seem to work without formally establishing the principle. This is surprising because many simulations, especially the ones implementing models of dynamical systems, are sensibly dependent on initial conditions. We expect the modeling error to overwhelm any numerical errors introduced during the run of a simulation and make results diverge. Thus we expect the failure to reproduce to be the norm rather than the exception in such simulations. But again simulations of dynamical systems often do work - we trust the weather forecast for about a week. But can we make the conditions when they work more explicit? Perhaps our initial distinction between modeling and computational error is too coarse. Following Corless we should actually distinguish between four levels of abstractions in which errors can propagate: "the physical reality of the problem under study, the continuous mathematical model of that physical reality, the numerical discretization of that mathematical model, and the floating-point

simulation of that discretization." (Corless 1994, p.109). Engineers are often only concerned with the first and the last level (e.g. Eck et al. 2013), but reproductions are dependent on the interplay of all levels. If the physical level already doesn't allow for them, there is no chance that a computer simulation will yield them. Numerical mathematicians on the other hand are often focused on the last two levels and are happy if their numerical methods are well behaved. And lastly physicists often study only the continuous model of physical reality and not physical reality itself. I will discuss the interplay of the four levels of abstraction for reproducing simulation results using Lorenz' famous 1963 model. For this model we can build physical analogues (e.g. as electrical circuits) giving access to physical reality, we can analyse the solutions of the differential equations defining the model and we can estimate the error for the discretization of the differential equations. I argue that all these properties together allow us to state the variance of reproductions that we can expect from simulations. I also discuss Lorenz' 1969 model, where arguably the access to physical reality is meditated by its simulations, which makes establishing the expected level of variance much harder. Thus there are cases where the expected level of variance cannot be determined exactly and these are exactly the cases where experimental realizations are lacking.


Antunes, Benjamin, and David R. C. Hill. 2024. ‘Reproducibility, Replicability and Repeatability: A Survey of Reproducible Research with a Focus on High Performance Computing’. Computer Science Review 53 (August):100655. https://doi.org/10.1016/j.cosrev.2024.100655.

Corless, R. M. 1994. ‘What Good Are Numerical Simulations of Chaotic Dynamical Systems?’ Computers & Mathematics with Applications 28 (10): 107–21. https://doi.org/10.1016/0898-1221(94)00188-X.

Diethelm, Kai. 2012. ‘The Limits of Reproducibility in Numerical Simulation’. Computing in Science & Engineering 14 (1): 64–72. https://doi.org/10.1109/MCSE.2011.21.

Eck, C., Kovalenko, Y., Mangold, O., Prohl, R., Tkachuk, A., & Trickov, V. (2013). Reduction of numerical sensitivities in crash simulations on HPC-computers (HPC-10). In High Performance Computing in Science and Engineering ‘13: Transactions of the High Performance Computing Center, Stuttgart (HLRS) 2013 (pp. 679-697). Springer International Publishing.

Fillion, Nicolas, and Robert M. Corless. 2014. ‘On the Epistemological Analysis of Modeling and Computational Error in the Mathematical Sciences’. Synthese 191 (7): 1451–67. https://doi.org/10.1007/s11229-013-0339-4.

Fillion, Nicolas, and Robert M. Corless. 2021. ‘Concepts of Solution and the Finite Element Method: A Philosophical Take on Variational Crimes’. Philosophy & Technology 34 (1): 129–48. https://doi.org/10.1007/s13347-019-00371-w.

Fox, Leslie. 1971. ‘How to Get Meaningless Answers in Scientific Computation’. IMA Bulletin 7 (10): 296–302.

Ludwig, Thomas. 2019. ‘Bitwise Reproducibility (with Exascale Machines)’. https://www.cs.fsu.edu/~nre/nre-2019/presentations/03-Ludwig.2019-06-20-ISC-Reproducibility.pdf.