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Unlocking the potential of past research: using generative AI to reconstruct healthcare simulation models

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ABSTRACT

Discrete-event simulation (DES) is widely used in healthcare Operations Research, but the models themselves are rarely shared. This limits their potential for reuse and long-term impact in the modelling and healthcare communities. This study explores the feasibility of using generative artificial intelligence (AI) to recreate published models using Free and Open Source Software (FOSS), based on the descriptions provided in an academic journal. Using a structured methodology, we successfully generated, tested and internally reproduced two DES models, including user interfaces. The reported results were replicated for one model, but not the other, likely due to missing information on distributions. These models are substantially more complex than AI-generated DES models published to date. Given the challenges we faced in prompt engineering, code generation, and model testing, we conclude that our iterative approach to model development, systematic comparison and testing, and the expertise of our team were necessary to the success of our recreated simulation models.

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healthcare; model
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1. Introduction


Operational Research (OR) has a long history of working alongside health services to use models to support decisions aiming to improve patient health outcomes and reduce service costs. Discrete-Event Simulation (DES) is the most widely applied simulation method. Given its maturity, there are now multiple reviews of DES in health (Forbus & Berleant, 2022; Liu et al., 2020; Soorapanth et al., 2023; Vázquez-Serrano et al., 2021; Zhang, 2018) that highlight the breadth of DES application in areas that include chronic lung disease, COVID-19 planning, cancer services, neonatal pathways, emergency care, and stroke treatment services (Campos et al., 2023; Gjerloev et al., 2024; Harper & Mustafee, 2023; Koca et al., 2024; Ouda et al., 2023; Penn & Viana, 2025; Salmon et al., 2018; Yakutcan et al., 2022).

At the time of writing, around 100 DES articles applied to health and medical problems are published in scholarly journals, conferences and books each year (Monks et al., 2024). Many of the articles reporting applied research studies directly worked with a health service to support real decisions. In each case, key outputs of the research are the conceptual and coded DES models. The conceptual model might take many forms in the report: from an unstructured narrative description to a more

formal description, such as following a conceptual modelling framework (Robinson, 2008) or as prescribed by a reporting guideline (Grimm et al., 2020; Monks et al., 2019). Whatever the approach used by the study authors, the conceptual models are published – they are *available* to interested parties to reuse if they choose. On the other hand, the coded model – the digital artefact that generates the results reported in the paper – is rarely made available in any form – as low as 8% (Monks et al., 2024). The coded model remains with the original authors, but over time, as authors move on, or retire, it is effectively lost to the modelling and simulation community. We note that the development of the coded model is expensive. Not only did it require modeller time to code and analyse, but it also required time from medical professionals, healthcare managers, informatics specialists, and service users (patients and their families) to provide domain expertise, support validation, and challenge assumptions or results. This cost could be voluntary or could have been supported by public funding.

The publication of coded models alongside a conceptual model falls under the field of Open Science. The Facilitating Open Science in European Research (FOSTER) project¹ (Bezjak et al., 2018) defines Open Science as “the practice of science in such a

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way that others can collaborate and contribute, where research data, lab notes and other research processes are freely available, under terms that enable reuse, redistribution and reproduction of the research and its underlying data and methods.” In this article we focus on the reuse potential of DES models of health services that can be realised through Open Science. While the availability of conceptual models supports reuse, the cost of re-coding a DES model from scratch is likely prohibitive. This is particularly true from the perspective of a health service reuser. While an academic DES study will typically run over months or years, a health service may need a model to use within weeks or potentially days. We argue that the lack of availability of coded DES models reduces the potential long-term impact of DES research in health services.

Since the release of ChatGPT² there has been excitement about the potential of Artificial Intelligence (AI) to increase productivity. Pioneering simulation research proposes a “Natural Language Processing (NLP) Shortcut” framework (Jackson et al., 2024) for generating DES models. This framework combines the general coding abilities of generative AI and Large Language Models (LLMs) with prompt engineering to create a coded *and reusable* simulation model.

To date, generative AI has only been used to code simple simulation models; for example consisting of 20–30 lines of Python code (Frydenlund et al., 2024; Jackson et al., 2024) or to support a reflective modelling process (Giabbanelli, 2024). The level of detail and scope of these models are not reflective of DES models used in practice within health services. Such a model would, for example, require hundreds of lines of code, include more sophisticated process logic (e.g., balking, probabilistic routing, and multiple entity classes), make use of coding best practices, control pseudorandom number streams, and include a user interface. Our aim in this study is to build on the pioneering NLP Shortcut framework to investigate the potential of generative AI to recreate coded models from the conceptual model of a healthcare DES model reported in academic publications. We note that many DES studies make use of Commercial Off-the Shelf (COTS) packages for their simulation modelling. We take an Open Science approach to recreating these models and generate Python code. This code is then licensed and preserved using Open Science archives and a research compendium (Gentleman & Lang, 2007; Ayllón et al., 2021).

1.1. Aims

Our study investigates the feasibility of using generative AI to recreate DES models in healthcare based on textual descriptions from the academic literature. We focus on generating models in the

Python simulation package *SimPy* (Team SimPy, 2024), selected for its (i) compatibility with language models’ code-generating capabilities, (ii) growing adoption in health service Operational Research (Monks & Harper, 2023a), and (iii) our expertise in developing *SimPy* models for healthcare applications (Allen et al., 2020; Harper et al., 2023). A key advantage of *SimPy* is its seamless integration with the broader Python ecosystem, enabling researchers to construct, analyse, and share fully reproducible simulation workflows by combining *SimPy* models with open-source tools for data analysis and visualisation (Zinoviev, 2024). In contrast, models built in commercial simulation environments such as Simul8 or AnyLogic are typically stored in proprietary formats that are not accessible as plain code or text. As a result, these models cannot be directly included in the training data for LLMs, which rely on open, text-based code repositories and public datasets for training material.

To assess feasibility, we engineer prompts for Perplexity.AI to generate complete Python and *SimPy* code that captures model logic (e.g., arrival processes, queuing, activities, sampling, and balking). Additionally, we explore generating browser-based user interfaces using *Streamlit* (Streamlit, 2025) to enhance accessibility for non-programmers. Our research objectives are to:

- Determine if generative AI can produce functional, verifiable *SimPy* models from engineered prompts describing DES models
- Assess the feasibility of generating usable *Streamlit* web interfaces for these models
- Pilot this approach by recreating two published healthcare DES models
- Evaluate the reproducibility of our methodology when conducted by different modellers

This work contributes to the growing interest in generative AI applications for modeling (Frydenlund et al., 2024; Giabbanelli, 2024; Giabbanelli et al., 2024; Tolk, 2024). Our long-term goal is to develop guidance on prompt engineering and to document the opportunities, challenges, and limitations of using AI to recreate DES models—ultimately supporting result reproduction, model reuse, and educational applications.

The remainder of this paper first defines key concepts in generative AI, LLMs, and chatbots, followed by a review of generative AI applications in simulation modelling. We then detail our methodology and apply it to two case studies: a 2010 critical care model and a 2016 stroke pathway model. Finally, we present our results and discuss implications for Operational Research in this emerging field.

2. Theoretical framework and literature review

Before reviewing relevant generative AI research for simulation, we briefly define generative AI and describe popular LLMs and human interaction with them *via* Chatbot AI tools. We summarise the key concepts in Table 1.

2.1. Generating novel content using LLMs

Traditional Machine Learning (ML) paradigms, such as classification, train a model to learn patterns within historical labelled data in order to classify new unseen instances. For example, classifying if a brain scan indicates Parkinson's Disease or is healthy. Generative AI models are trained on unlabelled data and, rather than predict or classify, they aim to create novel digital content such as text, images, music, or code. One example is generating a simple simulation model in Python code (Frydenlund et al., 2024; Jackson et al., 2024). LLMs are a subset of generative AI that specialise in natural language communication between humans and computers. The Generative Pre-trained Transformer (GPT) architecture, that underpins AI Chatbot tools like ChatGPT, is perhaps the most well-known example of an LLM. GPT models are built on transformer-based neural network architectures, which use self-attention mechanisms to process and generate text (Brown et al., 2020; Vaswani et al., 2023). In simple terms, GPT models are sequence predictors, trained to predict the next token (e.g., a word) in a sequence based on the context of previous tokens.

2.2. Zero-shot learning and model scaling

A key advancement that distinguishes LLMs from traditional ML approaches is their capacity for zero-shot

learning – the ability to perform tasks on previously unseen categories without explicit training (Brown et al., 2020). This capability enables LLMs to adapt to novel contexts and tasks, such as generating code based on user specifications, without additional training. The evolution of zero-shot learning has been closely tied to the increasing scale of language models. When GPT-1 was introduced in 2018, it contained 117 million parameters (Radford & Narasimhan, 2018). Subsequent iterations have seen substantial growth in model size, with GPT-3 including 175 billion parameters (Brown et al., 2020). The exact specifications of GPT-4 and GPT-4.5 have not been officially confirmed by OpenAI, but GPT-4 is speculated to contain up to a trillion parameters (Giabbanelli, 2024).

2.3. Challenges and limitations: Data contamination and hallucination

Evaluating the zero-shot capabilities of LLMs is challenging due to the potential contamination of test data (Xu et al., 2024a). The concept of contamination is analogous to leakage in traditional supervised machine learning (Kaufman et al., 2012), i.e., the training data overlaps with test data, accuracy measures are overstated, and the model is simply outputting data it has memorised in training. In the case of LLMs, it is difficult to determine if the training data overlaps with test data and careful evaluations must be designed.

A key challenge in the use of LLMs is mitigating the risk of *hallucination*. LLMs are sequence prediction models that prioritise generating the most probable next word in a sequence, even if it is inaccurate. Simply put, given an input, a model will always produce an output, whether or not it is correct. As a result, an LLM may “hallucinate”:

Table 1. Key concepts in generative AI.

Topic	Summary
Generative AI	AI models designed to create novel digital content such as text, images, music, or code.
Large Language Models (LLMs)	A subset of generative AI specialising in processing and generating human-like text.
Transformer Architecture	Neural network design using self-attention mechanisms to process and generate text.
Zero-Shot Learning	The ability of a model to perform tasks or make predictions on categories it hasn't explicitly seen during training.
Model Scaling	The process of increasing model size (number of parameters) to improve performance and capabilities.
Hallucination	The tendency of LLMs to generate plausible-sounding but factually incorrect or logically flawed content.
Data Contamination	The overlap of training data with test data, potentially leading to overestimated model performance.
Temperature	A parameter controlling the randomness and creativity in LLM outputs.
Prompt Engineering	The process of crafting effective inputs to elicit desired outputs from LLMs.
Chatbot AI	AI-powered conversational interfaces that use LLMs to understand and generate human-like responses in real-time interactions.
Context Window	The amount of previous conversation an LLM can consider when generating responses.
RLHF (Reinforcement Learning from Human Feedback)	A technique used to fine-tune LLMs based on human ratings of model outputs.
Alignment Problem	The challenge of ensuring AI outputs align with human values and intentions.
Retrieval Augmented Generation	A technique that enhances LLMs by integrating an external information retrieval system.

confidently present content that is factually incorrect, logically flawed, or at odds with the training data provided (Dou et al., 2024; Huang et al., 2023; Ji et al., 2023).

For example, an LLM might generate plausible but fabricated references in an academic essay or produce code that appears functional but contains logical errors. These errors may go unnoticed by users, and have consequences that vary from minor (e.g., wasted time from debugging nonsensical code) to severe (e.g., incorrect decisions based on the results of a flawed simulation model). The causes of hallucination are complex and varied. In coding, for instance, it might stem from pre-training the LLM on code that contains both obvious and subtle bugs.

Hallucination is a major limitation of generative AI and hence is an active area of research (Ji et al., 2023). Promising approaches include variations on the theme of iterative retrieval of information (Khot et al., 2023; Yao et al., 2023) that can involve refining outputs through multiple iterations each providing more context or fact-checking. Another approach is to estimate model uncertainty statistics that can highlight LLM knowledge deficiencies (Farquhar et al., 2024). For the immediate future, it seems likely that hallucination will continue to be a major challenge for the safe and productive use of generative AI, with some arguing it cannot be fully eliminated (Xu et al., 2024b). As such, it is crucial to incorporate some form of fact-checking or testing mechanisms in any work that relies on content generated by an LLM.

2.4. Randomness and prompt engineering

LLMs include an element of randomness in the generation of responses. This randomness is typically controlled by a “temperature” parameter, where higher values increase variability in outputs (and increase hallucinations), while lower values produce more deterministic results. The use of randomness allows LLMs to generate diverse and creative solutions but it also means that, given the same prompt, an LLM may produce different code outputs across multiple runs. This variability poses challenges for reproducibility in contexts such as code generation for simulation models, where consistent and replicable results are important. By default, Chatbot AI tools may not offer direct user control over temperature.

Given the randomness used in generative AI, and as LLMs tend to hallucinate, another important concept to define is the formation of prompts. This has given rise to the discipline of prompt engineering: the process of writing a prompt that results in the most effective LLM performance (Liu et al., 2021; Pornprasit & Tantithamthavorn, 2024). This is a

very recent area of research and there is not yet a consensus on the most effective approaches although various patterns are available (Wang et al., 2024; White et al., 2023). For example, in *one-shot* or *few-shot* learning, the prompt includes one or more simple examples of the task to clarify the context for the LLM.

2.5. Retrieval Augmented Generation

Retrieval Augmented Generation (RAG) is a promising research area that can reduce the occurrence of hallucinations in language models (Shuster et al., 2021). In the RAG process, a knowledge base is queried, and relevant information is incorporated into the prompt’s context before it is processed by the language model (Lewis et al., 2021). In simple terms, this can be thought of as providing the language model with more factual information within the prompt. A knowledge base could be the internet; for example, Perplexity.AI retrieves web pages, and online documents prior to generating an answer. Hallucinations can be reduced as RAG provides trained LLMs access to knowledge it has not seen before; for example, up to date information not used in training, or advancements in scientific fields that came post training. Hallucinations are not completely mitigated by RAG, for example, if a user’s question cannot be answered from the knowledge base then the language model may still generate an incorrect answer (Barnett et al., 2024).

2.6. AI chatbots and alignment

Since 2022, and at the time of writing, wide-scale public access to LLMs has been made possible by general-purpose Chatbot AI tools such as Open AI’s ChatGPT,³ Perplexity. AI’s Sonar,⁴ Anthropic’s Claude,⁵ DeepSeek-R1 (DeepSeek et al., 2025) and Google’s Gemini.⁶ The underlying LLMs are trained on large amounts of curated web data (including code from sources such as StackOverFlow and GitHub) and fine-tuned for chat-based human interaction. In general, the tools have been shown to understand and generate human-like text (and code) across a wide range of tasks. The overall architecture and training of these models is complex and for most models is not fully known given the commercial nature of the companies that create and operate them at substantial cost. As a general rule, however, LLMs such as GPT-3.5 or 4 are not used as is; instead, a new round of training is undertaken using a curated question and answer dataset. This process of fine tuning produces an Assistant Model that provides chat like responses to a human prompt. A further round of training employs reinforcement

learning from human feedback (RLHF) where a human workforce reviews and rates responses output by the model (Casper et al., 2023). RLHF aims to help Chatbot AI's tools align responses with the human values and the intentions of their prompts (the so-called "alignment problem"). This process attempts to filter out inappropriate or offensive content while enhancing the models' ability to provide a relevant response.

Human interaction with these models is *via* a user-friendly chat interface. The underpinning LLM in use varies by free and paid tiers (e.g., at the time of writing ChatGPT offers a free GPT-3.5 or paid GPT-4/4.5 tier). While the LLM architectures have no memory of prior prompts, a Chatbot AI tool has a context window allowing a user to interact iteratively with an LLM within a larger history/context of prompts and responses. There are size restrictions on these context windows that vary with each Chatbot AI tool and underlying model.

2.7. Generative AI in software engineering

LLMs have also been fine-tuned for software engineering and coding tasks such as code generation and code completion. Contemporary tools include GitHub Copilot⁷ and Meta Code Llama.⁸ Research in this area has been extensive with the vast majority spread across software development and maintenance (Hou et al., 2024).

Code generation has used a mix of general LLM tools such as GPT-3.5/4.0 (Dou et al., 2024; Yetiştiren et al., 2023) and fine-tuned models such as GPT-3's codex (Chen et al., 2021). Performance of LLMs in code generation in these studies typically makes use of a curated benchmark dataset of programming problems and their solutions such as the *Mostly Basic Python Problems Dataset*⁹ (Austin et al., 2021). LLM solution performance against these datasets are evaluated using various standard metrics.

Prompt engineering to reduce ambiguity of intent has emerged as a key challenge for code generation as LLMs, which may struggle to reliably generate code reflecting the users' requirements. To date the majority of studies have employed zero- or few-shot prompt engineering to maximise LLM effectiveness (Hou et al., 2024); a smaller number have explored novel approaches such as prompting LLMs to include a planning phase before generating solutions (Jiang et al., 2024).

2.8. Generative AI and computer simulation

2.8.1. Automated code generation

Recent research has explored the integration of generative AI with computer simulation, yielding

promising hybrid approaches. Several pioneering studies have investigated small-scale applications and conceptual frameworks across DES, system dynamics, conceptual modelling, and documentation (Akhavan & Jalali, 2024; Giabbanelli, 2024; Jackson et al., 2024; Plooy & Oosthuizen, 2023; Shrestha et al., 2022).

Jackson et al. (2024) explored the potential of using GPT-based models to produce simulation models for inventory and process control in logistics systems. Their research focused on the concept of an "NLP Shortcut," where simulation models are generated from a textual description of the model passed to a language model. The study used the OpenAI Davinci Codex (a code-based Application Programming Interface (API) to the GPT-3 model) to successfully generate simple Python-based simulations of logistics systems (e.g., a single-product inventory-control system). The LLM outputs consist of 20–30 lines of Python code implementing simple DES model logic and code to plot the model output. Their framework incorporated dynamic execution of the generated code with human expert oversight, demonstrating the potential for AI-assisted simulation development.

Akhavan and Jalali (2024) and Plooy and Oosthuizen (2023) investigated the application of ChatGPT in system dynamics modelling. Both studies take the position that generative AI should not replace a modeller but rather serve as a tool to facilitate the research process, review content, and enhance idea implementation in simulation modelling. Akhavan and Jalali (2024) develop a simple System Dynamics model of COVID-19's impact on economic growth. Their approach first prompts ChatGPT (GPT-4) in an iterative manner to support conceptual modelling and decisions about methods. The authors *manually code* a small Python model (40 lines of code) and provide this along with prompts to ChatGPT to generate suggestions for code optimisations, additional plotting code, and improvements to model documentation.

Plooy and Oosthuizen (2023) focused on using ChatGPT (GPT-4) to generate Python code implementing a simple system dynamics model of a resource-bound population in equilibrium. They outline a six-step approach to iteratively generate a model with ChatGPT's help. Early steps focus on textual information describing equations for stocks and flows that are first manually implemented in the commercial simulation package iSee Systems Stella Architect.¹⁰ The final step converts the generated equations into 32 lines of Python code with outputs verified by comparing the manually created and generated models. Extending this, Frydenlund et al. (2024) attempted to generate working

simulation models from narratives across different languages and simulation libraries for agent-based modelling, System Dynamics, and DES. While small models were produced for each (up to around 35 lines of code), ChatGPT failed to produce concise or fully executable code in all three paradigms, which the authors highlight as evidence of current LLM limitations in generating robust simulation models directly from narrative descriptions.

2.8.2. Conceptual modelling

Shrestha et al. (2022) proposed a method where generative AI is used to explain simulation models, by creating simple conceptual model descriptions from more complex causal maps. Their approach involved decomposing large conceptual models into smaller parts and then performing Natural Language Generation (NLG) using a fine-tuned GPT-3 model. Giabbanelli (2024) published a conceptual study that hypothesised the potential of LLM application across common simulation tasks. The study focused on four key areas: structuring conceptual models, summarising simulation outputs, improving accessibility to simulation platforms, and explaining simulation errors with guidance for resolution. For example, the potential to use the emerging capability of LLMs to convert images to text to provide automated explanations of charts of simulation output could benefit both non-experts and people with visual impairments. Building on this work, Giabbanelli et al. (2025) argued for a more structured and reliable role for LLMs to support conceptual modelling—not as standalone problem-solvers, but as middleware that connects specialised modelling and simulation tools. They emphasised the importance of maintaining human oversight and domain expertise. To mitigate hallucinations and ensure logical correctness, the authors proposed integrating LLMs with formal verification tools and adopting validation loops in which the LLM iteratively refines its output based on tool feedback.

2.9. Summary of lessons from the literature

The application of generative AI to practical domains, including computer simulation modelling, is an emerging and rapidly evolving field of research. Our study has been designed to account for the following lessons and challenges identified in the existing literature:

- **User Expertise:** The effectiveness of generative AI can depend on the expertise and skill level of the user.
- **Mitigating Hallucination:** Generative AI models are prone to hallucination (producing incorrect

or fabricated outputs). This risk can be reduced through strategies such as prompt engineering, retrieval-augmented generation (RAG), and iterative refinement during interactions.

- **Model Validation:** AI-generated models require thorough testing and validation at each stage of development to ensure reliability and accuracy.
- **Selection of Test Data:** The choice of test data is critical to avoid data leakage, which can compromise the validity of results in generative AI studies.
- **Model Complexity:** Current research has predominantly focused on applying generative AI to relatively simple models, leaving its performance with more complex systems largely unexplored.

3. Methods overview

Our study followed four stages: setup and model design (Stage 0); prompt engineering and code generation (Stage 1); internal replication (Stage 2); and evaluation and preservation (Stage 3). Figure 1 illustrates these stages and the activities carried out in each. For model generation, we used Perplexity.AI's standard model (free tier) that includes RAG from internet sources. The RAG functionality provides the model with up-to-date and new online sources about simulation and *SimPy*.

3.1. Stage 0: Setup and model design

For the two chosen case studies, we read the academic paper and wrote down a design for a simulation model organised by the *Strengthening The Reporting of Empirical Simulation Studies* (STRESS) guideline format for reporting models (Monks et al., 2019). Previous studies of replicating models from journal articles have been challenging due to reporting ambiguities (McManus et al., 2019; Schwander et al., 2021). We therefore document any simplifications or additional assumptions (e.g., undocumented parameters or logic or removal of a feature) that were made to enable us to design a functioning version of the model reported in the journal article. We designed a common Python 3.10 software environment (implemented as a conda¹¹ environment) that could be used in stages 1 to 3 to run the generated code.

3.2. Stage 1: Prompt engineering and code generation

In Stage 1, we created a prompt database that stored all prompts given to the LLM and for what purpose. We then proceeded to generate the design of the model as reported in the paper for Case Study 1.

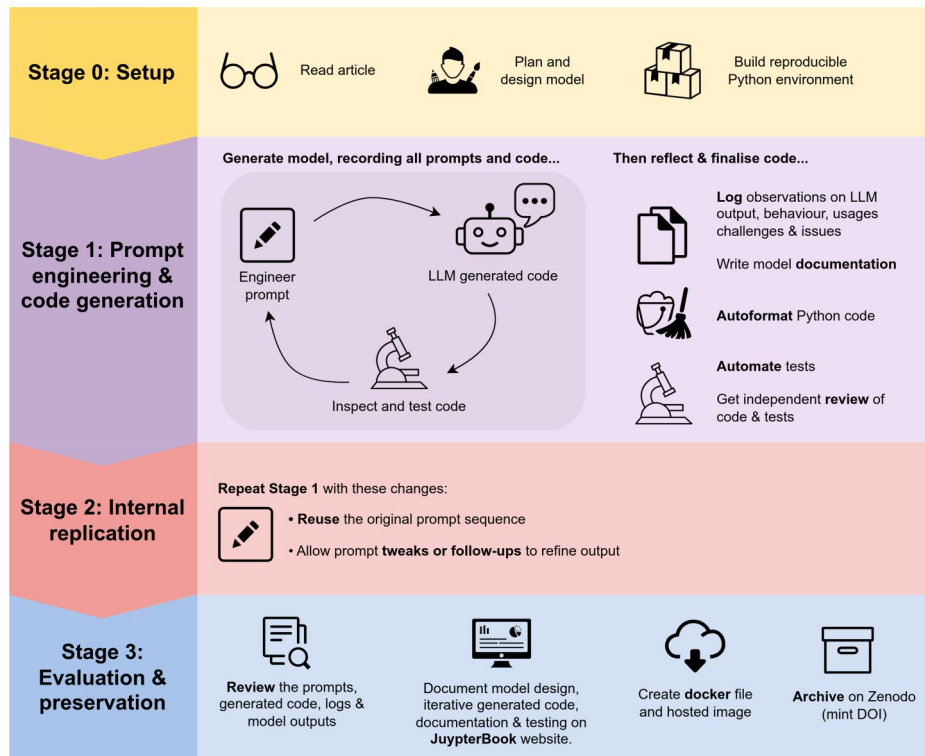


Figure 1. Overview of approach to model recreation using generative AI.

Abbreviations: AI, artificial intelligence; DOI, digital object identifier; LLM, large language model.

When complete, we recreated Case Study 2. Where appropriate we reused or adapted prompts from Case Study 1 when recreating the model for Case Study 2. All case study prompts were stored in the database in sequence of use. After the models were complete we created a research compendium consisting of a STRESS report for the design, formatted model code (using the tool 'black'), a script to run the model, documentation for the user interface, and an automated model test suite. A second modeller then reviewed the research compendium and identified any Stage 1 modifications required before proceeding to Stage 2.

3.3. Stage 2: Internal reproduction

In Stage 2, a second modeller reproduced the process from Stage 1 by attempting to recreate the models using the original sequence of prompts. Given the stochastic nature of creative LLM output (i.e., the same input prompt may not produce the same output), we allowed for the re-engineering of prompts in the replication phase. This included direct modification of the original prompts and additional follow-up prompts to refine the output. We also allowed for structural differences between the original and replicated models, for example, the use of different Python data structures, and class/function designs. Stage 2 was added to the research compendium and independently checked in an identical manner to Stage 1.

3.4. Stage 3: Evaluation and preservation

3.4.1. Evaluation

In Stage 3, we compared the artefacts generated and experience of working with the LLM to create the *SimPy* models in Stages 1 and 2. We defined a successful internal replication to be when Stages 1 and 2 models produced the same results. As we designed the models to use the same seeds and random number generators we aimed for identical results; however, we allowed a small tolerance of 5% in line with other replication studies (McManus et al., 2019; Schwander et al., 2021). To evaluate the use of the LLM for generating the models, the modellers from Stages 1 and 2 synthesised their experience of prompting the LLM: identifying common successes/failings, general challenges, coding mistakes, and opportunities.

3.4.2. Model preservation

The final step in Stage 3 was to preserve the models we had recreated, ensuring that they are available to others to inspect or use long term. We structured all of our materials into a research compendium – a website compiled using the tool JupyterBook.¹² The compendium consists of the code, data, and documentation needed to understand and reproduce our study. We then deposited the research compendium in the Zenodo open science archive¹³ and obtained a Digital Object Identifier (DOI).

4. Case study selection

We selected two published healthcare DES case studies. Prior LLM simulation coding studies had focused on very simple coding tasks comprising 20–30 lines of code (Akhavan & Jalali, 2024; Jackson et al., 2024; Plooy & Oosthuizen, 2023). We aimed to increase the complexity of the coding task for the LLM in our study. We selected DES models that consisted of multiple classes of patients (e.g., multiple arrival sources and differing sampling distributions for length of stay), and at least two activities (delays). From experience, we estimated that design of such models would require between 200 and 500 lines of Python code. We would still classify these as simple DES models.

A threat to the external validity of our study is selecting a DES study where the exact or a very similar model is available within the training data of the LLM. The risk is that the LLM simply outputs the training data when prompted. The exact training data of commercial LLMs is unknown, but we assumed it would include popular code repositories such as GitHub¹⁴ and coding question-and-answer sites such as Stack Overflow.¹⁵ As we are using Python, one way to reduce this risk is to select a DES study where the model has been reported to be developed in a commercial simulation package interface such as Simul8,¹⁶ Arena,¹⁷ or Excel.¹⁸ The majority of such models are contained within a bespoke proprietary format and not the natural (or coding) language that a LLM is typically trained on. Our hypothesis was that, even if these commercial models were available online in a location we did not know about, they were unlikely to be translatable directly to Python.

4.1. Case 1: Critical care unit model

The first case study was published in the Journal of Simulation (J D Griffiths et al., 2010). The model

was coded in VBA and has never been published online to our knowledge. The description of the model was published before any reporting guidelines for DES, but the paper contains a detailed description of the model and its parameters, although in some areas they are not reported in a manner that allows full replication of quantitative results reported in the paper (for example, an empirical distribution was used, but not detailed); although some obvious simplifications were available based on descriptions in the paper (e.g., use of a statistical distribution for elective inter-arrival time instead of an unreported empirical distribution).

The model represents a Critical (Intensive) Care Unit (CCU); we provide our interpretation of the process described in the article in Figure 2. It consists of six classes of entities that arrive following varying static distributions. These arrivals are either unplanned (emergency) or planned (elective surgery), and share a total of 24 beds. Unplanned emergency patients are prioritised for critical care beds. Elective patient balk (a cancelled elective operations) if no beds are available. Patient classes have their own treatment time distributions (length of stay in the CCU). After discharge a deterministic bed turnaround time is included to allow for intensive cleaning. The study aimed to explore capacity requirements and related scenarios and their impact on the number of cancelled operations. A warm-up period and multiple replications are employed.

4.2. Case 2: Stroke pathway capacity planning model

The second case study was published in BMC Health Services Research (Monks et al., 2016). The model was coded in the Simul8 simulation package and has never been published online. The authors present a simple generic model to support health services to plan the capacity of an acute stroke ward, rehabilitation ward, and (optionally), early

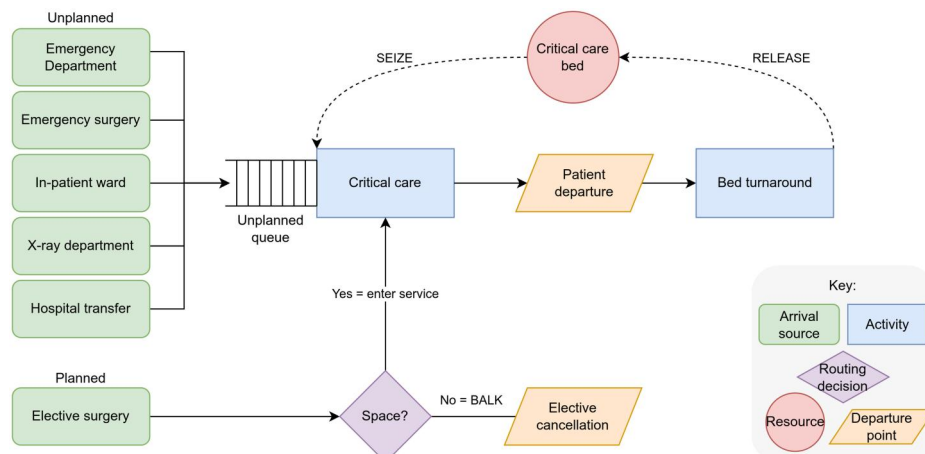


Figure 2. Logic diagram for the design of the CCU model.

support discharge capacity (ESD). The model was published before reporting guidelines for DES, but contains a detailed [online appendix](#), supplementary materials allowing for recreation of the model (and uses simple parameters and equations).

The model allows users to specify a population of stroke, transient ischaemic attack (TIA), complex neurological, and other patient types who use acute and rehabilitation services. We provide our interpretation of the process described in the article in [Figure 3](#). The patient classes have their own external inter-arrival distributions to acute and rehabilitation services, transfer probabilities between services, and length of stay distributions (where first sub-division occurs to model ESD versus non-ESD patients). The model takes an infinite capacity approach to capacity planning and estimates the probability of delay. A warm-up period and multiple replications are employed. It has a clear logic diagram and documentation of parameters in the main article and an online appendix. The ESD modelling is not used or documented in the article; we therefore chose to simplify the design and focus on the acute stroke and rehabilitation units, although we aimed for model setup to be simple to extend for ESD capacity modelling.

5. Model design

5.1. *SimPy* models

All generated models were built in *SimPy* (Team SimPy, 2024): a process-based DES package

implemented in Python that is available under a permissive MIT license. DES models are built by defining Python generator functions and logic to request and return resources. The package *SimPy* is lightweight and provides a full event scheduling engine. Statistical distributions for sampling, common random number streams, output analysis tools, user interfaces, and model animation are not included. The implementation of all of these tools are available in the general and scientific Python stack. For example, *NumPy* and *pandas* for sampling and output analysis, and *Matplotlib* for visualising results. For those unfamiliar with *SimPy* we provide some sample code in online [Appendix A Listing 5](#).

5.2. Model coding plan

The number of modelling iterations needed to recreate the models was not known in advance. Instead, we read the publications reporting the model designs and constructed a general plan that ordered and batched iterations into 12 aims of model recreation (e.g., each aim might take 2–3 prompts and code iterations to achieve). [Table 2](#) details the ordered aims of the model recreation process along with a description and examples of changes to the model that could be expected. Our aims took us from modelling of arrivals of patients and patient classes (e.g., types of stroke, or unplanned emergencies versus elective patients) through to a user

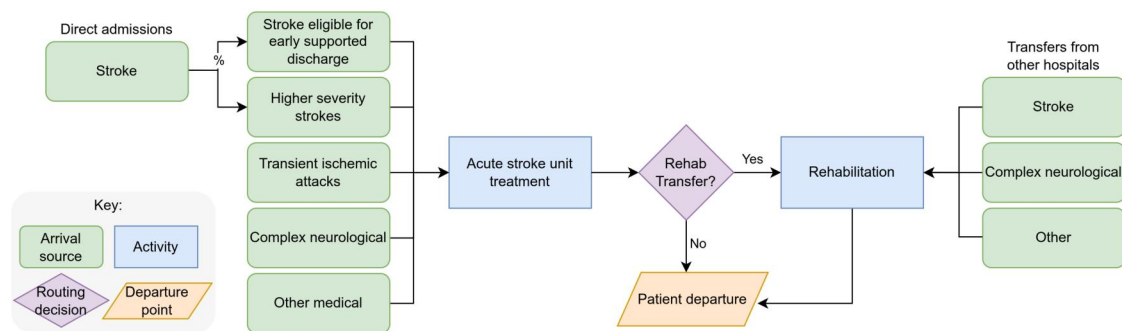


Figure 3. Logic diagram for design of the acute stroke and community rehabilitation capacity planning model.

Table 2. Ordered aims of the model recreation process.

Aim	Description	Example additions to model
1	Arrival processes and logic	Single and multiple classes of patients
2	Initial queuing logic and activities (delays)	Reneging, patient class dependent length of stay in a ward
3	Separation of parameters from model logic	A configurable Experiment class to hold all model parameters.
4	Simulated trace control	Functionality to hide and display simulated events
4	Patient routing	Sampling to determine post-ward destinations and activities
5	Additional queuing and activities	Additional treatment in a different hospital/ward
6	Results collection	Audit and calculate ward occupancy, bed utilisation, waiting times etc.
7	Warm-up period	Split the model run length into warm-up and results collection, reset all KPIs, introduce auditing processes.
8	Multiple replications	Multiple unique runs of the model.
9	Output analysis procedures	Charts and summary tables
10	Common random numbers	Allocate unique random number stream to each distribution
11	User interface	A web browser-based interface for the model.
12	Final bug fixes	Patch any remaining bugs identified by a 2nd modeller

interface allowing for basic experimentation. We believe this mirrors how the recreation of a DES model would take place regardless of whether an LLM was used.

To optimise the organisation and usability of the *SimPy* simulation model we adopted the approach of Monks and Harper (2023b, 2023c) in aims 3, 8 and 11. The result is that model logic is separated from parameters using an `Experiment` class (used to set up “what-if” experiments). The `Experiment` class is used in combination with a multiple replications wrapper function to generate results. This simple organisation enables quick integration with Python web app frameworks such as *Streamlit* to make models usable by a wider group of people.

To enable both repeatable replications and variance reduction between experiments, we chose to implement common random number (CRN) streams in our models; i.e., each random statistical distribution used for sampling has its own unique controllable pseudorandom number stream (Davies & Brooks, 2007). This is in line with Case Study 2 which used *Simul8* and implemented CRN. However, we note that Case Study 1 was implemented in VBA and it is unclear if CRN streams were implemented by the authors. We aimed to manage all random sampling through the *numpy.random* module and the PCG-64 pseudorandom number generator (Harris et al., 2020). We followed a simple approach where the replication number was used to spawn n independent random number streams.

6. Prompt engineering

6.1. Prompts versus academic article write-up

Although it might seem that directly copying the published model description into an LLM would guarantee fidelity to the original, in practice academic narratives often contain ambiguities, implicit assumptions, or imprecise language that can be misinterpreted by an LLM. In contrast, prompt engineering, when done systematically, enables the modeler to clarify intent, resolve ambiguities, and specify requirements in a way that guides the LLM toward a faithful implementation of the original model logic. Our approach involved iterative refinement of prompts, use of consistent terminology, and explicit instructions to minimize the risk of unintentionally introducing modifications or solving a different problem. By documenting all prompt iterations and decisions, we make transparent any assumptions or clarifications introduced during the process.

Box 1. Example of prompt engineering. Excerpt taken from section 2.1 (Griffiths et al., 2010).

Excerpt from journal article: *If an arriving patient finds that all beds are occupied, they are sent to a queue. There are two queues built into the model, the ‘Unplanned Admissions’ queue and the ‘Planned Admissions’ queue. The patients in the ‘Planned Admissions’ queue—that is the Elective surgery patients—have their surgery cancelled and are then sent home. The patients in the ‘Unplanned Admissions’ queue wait until a bed becomes available.*

Engineered Prompt:

Add a new arrival source to the CCU: Elective surgery patients. Elective surgery patients are modelled as a separate process from the unplanned admissions but share the critical care bed resources.

As an elective patient arrives at the CCU, a check is made on the number of critical care beds available. There are two outcomes from this check:

- **Outcome 1:** The number of beds in use is equal to the total number of beds available. In this case, the elective patient leaves the model immediately. This is called a “cancelled operation” event and should be reported to the user.
- **Outcome 2:** The number of beds in use is less than the total number of beds available. In this case, the elective patient requests a critical care bed, is treated, and is then discharged.

As a simple example, consider [Box 1](#) where the first paragraph is an excerpt from [section 2.1](#) of the CCU case study (J D Griffiths et al., 2010) that describes balking of elective patients in a CCU. A human reader of this text may understand the context and logic of this text exactly; especially if they have viewed a logic diagram of the model beforehand. On the other hand, an LLM prompted using this text is less likely to produce consistent models due to the mixing of patient types in the discussion and lack of precision in the language.

The second half of [Box 1](#) constructs (engineers) a prompt for the LLM with the aim of being more precise. Instead of a discursive prose, we re-frame the natural language to:

1. Instruct the LLM to add a new arrival source to the model for elective surgery patients;
2. Precisely define which resources are used by the elective patients on arrival and if these are shared with other types of patients;
3. Identify the outcome logic if all beds are in use versus if they are not all in use.

6.2. Common tokens

In a healthcare simulation study, stakeholders and modellers may use multiple terms to refer to the same concept. For example, the terms “treatment time” and “length of stay” may be used interchangeably in a conversation or a written article. We aimed to make our prompts as specific as possible to obtain the iteration of the model that met our

design. We therefore attempted to use a common token throughout an individual prompt and across iterations. We did allow for the shortening of tokens within prompts. For example, if we had introduced the concept of “critical care bed” resources and the model had no other ambiguous resource names, we allowed our prompts to refer to “beds.”

6.3. Initial prompts

In both cases our initial prompts were designed to generate a simple working simulation model in *SimPy* that generated patient arrivals only. Our hypothesis was that the level of detail and scope could then be expanded in further iterations. Our initial prompt was one of the most detailed provided. We broke it down into four sections.

- **Main command:** Specified the context (e.g., a critical care unit DES model), programming language, simulation package and that this was a code generating task.
- **General model logic:** Including time units, arrival sources, model boundaries and run length.
- **Simulation inputs:** For the first iteration this was always inter-arrival distributions and parameters.
- **Simulation methodology:** Underlying sampling tools and how this should be implemented.

To illustrate this method we include [Box 2](#): the initial prompt from the CCU case study.

6.4. Refactoring prompts

Within an iteration, we occasionally made use of subsequent short prompts to refactor the code closer to our requirements or expectations. For example, if the code generated a set of functions when we preferred classes we would issue the follow-up prompt: “re-factor the functions into a CCU class.”

6.5. One-shot prompt engineering

When refactoring of code was judged to be complex we chose to provide a short example of the refactoring in the prompt for the LLM to mimic (so-called “1-shot prompt engineering”).

An excerpt from a prompt given to the LLM from the stroke case study is provided in [Box 3](#) where we are refactoring the code to use random sampling that follows best practice. The LLM must modify the code in multiple methods and also count

Box 2. Initial prompt example: CCU case study.

Main command: Code a discrete-event simulation model of a critical care unit (CCU) in Python 3.10 and *SimPy* 4. Code the full model specified. Do not return a simplified version. Show all code.

General model logic:

- All time units in the model are in hours.
- Each patient in the model has a unique identifier. The first patient to arrive has an identifier of 0. For each subsequent patient increment the identifier by 1.
- Patients to arrive at the CCU from five different sources: Accident and Emergency, the Wards, Emergency surgery, other hospitals, or the X-Ray department.
- Each source has a different inter-arrival time distribution.
- After patients arrive they immediately leave the model.
- All patient types must have their own generator function
- The model should print out useful information after each event.
- The model should include a user-settable run length. This defaults to 12 months.

Simulation inputs: The inter-arrival time distributions and parameters of patients are dependent on patient type. For each distribution, time is measured in hours.

- Accident and Emergency = Exponential: 22.72
- The Wards = Exponential: 26.0
- Emergency surgery = Exponential: 37.0
- Other hospitals = Exponential: 47.2
- The X-Ray department = Exponential: 575.0

Simulation methodology: NumPy should be used for sampling. Each inter-arrival distribution should have its own `numpy.random.Generator` object.

Box 3. Example of one-shot prompt engineering to guide code refactoring.

Modify the `acute_treatment` functions in `AcuteStrokeUnit` class. Do not modify the functions.

Code that uses `numpy.random`, must be replaced with a call to a unique stream in the `Experiment` list `streams`. Select the stream using a hard-coded integer.

Start from zero and increment by 1 each time to allocate a unique number to each stream. **E.g.**, In `stroke_acute_treatment` the first instance of `length_of_stay=np.random.lognormal(mu, sigma)` becomes `length_of_stay=self.experiment.streams[0](mu, sigma)`; the second instance uses index 1 and the third uses index 2 and so on.

from 0 to the number of random streams implemented. We therefore provide an example of how this should be implemented.

6.6. Numbered steps

Many simple functions in programming are a series of steps to be followed by the Python interpreter.

Box 4. Example of specify a prompt using numbered steps.

Write python code that creates an interactive user interface using the package Streamlit. The interface should include a main window. The main window contains a button labelled “Simulate.” After the button is pressed the following logic is implemented:

1. Display a spinner with the text “please wait for results.”
2. Run the python code included below *[not shown]*.
3. Display a Streamlit table for `df_acute` and `df_rehab` results.
4. Display all plots. Plotting functions return a tuple of figure, axis.

All **classes** and functions should be imported from a module called `stroke_rehab_model`.

Where they were very clear, we specified them as a number-ordered list of natural language instructions that the LLM could follow. **Box 4** illustrates such a prompt applied to create an initial iteration of a Streamlit interface for the stroke case study model.

6.7. Restrictive clauses in prompts

We appended restrictive clauses to our prompts to avoid changes to parts of the code that were not part of our design. For example, when specifying a modification to the treatment of patients we could append “Do not modify the `patient_generator` functions at all” to ensure these were not modified in the same way. Similarly, if we were interested in refactoring the `Experiment` class to add new variables we might specify “only modify the `Experiment` class” or “do not modify the `CCU` class” to avoid small changes to the design between iterations.

7. Testing of generated code

A structured four-stage testing process was implemented for each model iteration. Initial visual inspection used JupyterLab but was later enhanced in Case 2 (Iteration 11) with *nbdime* to highlight code differences (see online [Appendix B](#) Listing 6). A second modeller independently reviewed modifications to ensure accuracy and consistency.

Classical verification involved systematic experiments, including extreme value tests, parameter

variations, and component-level validation (e.g., testing the Acute Stroke Unit separately from the Rehabilitation Ward). Testing evolved iteratively with model development.

Automated and manual tests were formalised post-development, using *pytest* for automated checks and visual trace inspection for manual verification. These tests were stored in dedicated Python modules to ensure reproducibility. We provide a more detailed account of testing in online [Appendix B](#) and a list of the types of test conducted in [Tables B1](#) and [B2](#).

8. Results

[Table 3](#) links to all of the research artefacts generated in the study. To preserve the outputs we have archived each artefact at Zenodo and provide a DOI. [Figure 4](#) is a screenshot of the study’s online research compendium. The compendium organises the generated model code, testing, and prompts by the case study and stage. We have deployed usable versions of the generated models as a web app to GitHub Pages.

For each model we report the outputs generated by the model; the results of the internal replication test; describe the code generated, and provide a screenshot of the user interface. The full code listings are available in the research compendium; here we provide short excerpts of the code in Listings.

8.1. Case 1: Critical care unit model

8.1.1. Model outputs

The simulation models generated in Stages 1 and 2 produced identical results to one another (to two decimal places), as in [Table 4](#). The table summarises the number of patient arrivals to the models, the four output measures in the design and how these vary across six experiments with the model. To formally assess the equivalence of the Stage 1 and Stage 2 models, we conducted paired t-tests for each key output metric across all experimental scenarios. In every case, the mean difference was zero and the standard deviation of the differences was also zero, resulting in an undefined t-statistic and p-value. This outcome is expected given that both models used identical random number streams for all stochastic elements. The absence of any difference

Table 3. Links to research artefacts and generated models.

Research compendium	
Deployment	https://pythonhealthdatascience.github.io/llm_simpy
DOI	https://doi.org/10.5281/zenodo.15090962
GitHub	https://github.com/pythonhealthdatascience/llm_simpy
Generated models as a web app	
Deployment	https://pythonhealthdatascience.github.io/llm_simpy_models
DOI	https://doi.org/10.5281/zenodo.15082494
GitHub	https://github.com/pythonhealthdatascience/llm_simpy_models

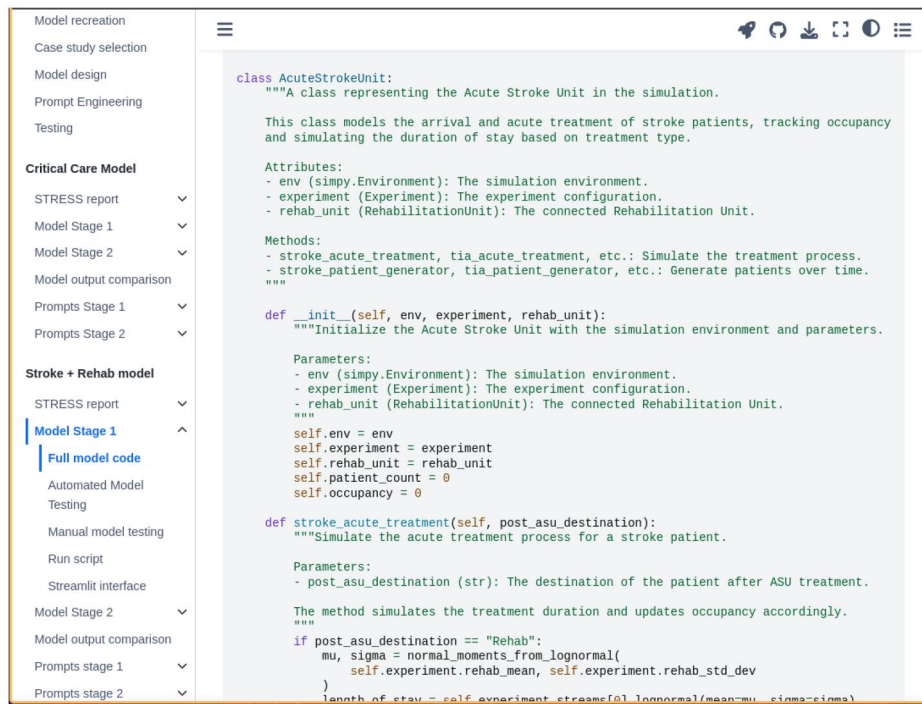


Figure 4. Screenshot of the study's research compendium. Model code, testing, and prompt archive are organised by case study and stage.

Table 4. Comparison of critical care model outputs: Stage 1 versus Stage 2 (internal replication). Figures are mean (standard deviation).

Study stage	Metric	23 beds	24 beds	25 beds	26 beds	27 beds	28 beds
Stage 1	0. Patient Count	1,650.4 (17.83)	1,650.4 (17.83)	1,650.4 (17.83)	1,650.4 (17.83)	1,650.4 (17.83)	1,650.4 (17.83)
	1. Cancelled Elective Operations	390.6 (30.57)	337.8 (38.75)	279.0 (39.13)	231.4 (33.83)	178.4 (32.46)	139.8 (27.58)
	2. Bed Utilization	0.9 (0.02)	0.9 (0.02)	0.9 (0.02)	0.9 (0.02)	0.8 (0.02)	0.8 (0.02)
	3. Bed Occupancy	21.3 (0.49)	21.8 (0.50)	22.3 (0.54)	22.6 (0.56)	23.0 (0.58)	23.3 (0.62)
	4. Mean Unplanned Admission Waiting Time (hours)	103.8 (72.08)	62.5 (55.23)	35.0 (29.28)	20.8 (15.59)	12.0 (7.66)	7.0 (3.76)
Stage 2	0. Patient Count	1,650.4 (17.83)	1,650.4 (17.83)	1,650.4 (17.83)	1,650.4 (17.83)	1,650.4 (17.83)	1,650.4 (17.83)
	1. Cancelled Elective Operations	390.6 (30.57)	337.8 (38.75)	279.0 (39.13)	231.4 (33.83)	178.4 (32.46)	139.8 (27.58)
	2. Bed Utilization	0.9 (0.02)	0.9 (0.02)	0.9 (0.02)	0.9 (0.02)	0.8 (0.02)	0.8 (0.02)
	3. Bed Occupancy	21.3 (0.49)	21.8 (0.50)	22.3 (0.54)	22.6 (0.56)	23.0 (0.58)	23.3 (0.62)
	4. Mean Unplanned Admission Waiting Time (hours)	103.8 (72.08)	62.5 (55.23)	35.0 (29.28)	20.8 (15.59)	12.0 (7.66)	7.0 (3.76)

confirms that the models are functionally identical under internal replication.

The model results did not replicate those reported in J D Griffiths et al. (2010). Our results have a higher arrival rate overall and higher occupancy of the CCU. The explanation would appear to be that we did not have access to information about the empirical distributions used for elective patients in the original article and the alternative distribution recommended in the article is not representative. To test the robustness of our findings, we conducted sensitivity analyses varying key uncertain parameters by $\pm 30\%$ and testing alternative distributional assumptions. These analyses confirmed that parameter uncertainty does not explain the replication gap—our model remained unable to reproduce the original results across all tested scenarios. Full sensitivity analysis results are available in our online research compendium.

8.1.2. Model code

Disregarding comments and documentation, Stage 1 generated a model consisting of 262 lines of code and Stage 2 generated 355 lines of code. Both models passed the same batch of 35 verification tests with 100% code coverage (i.e., all lines of code were executed in our tests). The difference in the design of the Python classes representing an experiment and CCU model logic can be seen in the number of class attributes and methods in Table 5.

The final code files from Stages 1 and Stage 2 (our internal replication) for the critical care unit model and its interface were overall very similar. For example, code Listings 1 and 2 illustrate the similarities in code generated to model emergency department arrivals. Minor differences included the naming of variables, functions and classes. Another minor difference was the setup of random number generators for each activity in the

model. However, both approaches in Stage 1 and 2 were acceptable.

A more substantial difference is that the Stage 2 code is arguably easier to understand for a new user than Stage 1 code. For example, the LLM in Stage 2 generated an `Experiment` class where each parameter used in a statistical distribution (e.g., the mean inter-arrival times) was implemented as a named variable. Whereas in Stage 1 code the LLM generated an `Experiment` class where inter-arrival means were set *via* a list of unnamed parameter

values. This increased clarity resulted in more lines of code in Stage 2 than in Stage 1; although we do not consider this a good or bad outcome.

A similar difference in clarity can be seen in the code to convert the mean and standard deviation of a log-normal into scale and shape parameters (suitable for the *numpy* log-normal functions). In Stage 2 the logic was (optimally) implemented in a reusable function. In Stage 1 the conversion logic is coded directly into each process and is harder to follow and test.

Example code generated in Stage 1 and Stage 2 (Critical Care Model)

```

1 class CCUModel:
2     def __init__(self, env, experiment):
3         self.env = env
4         self.experiment = experiment
5         self.patient_count = 0
6         self.critical_care_beds = simpy.Resource(
7             env, capacity=experiment.num_critical_care_beds
8         )
9
10    def patient_arrival_AE(self):
11        while True:
12            yield self.env.timeout(
13                self.experiment.streams[0].exponential(
14                    self.experiment.interarrival_means[0]
15                )
16            )
17            self.patient_count += 1
18            if self.experiment.trace:
19                print(
20                    f"Patient {self.patient_count} ... time {self.env.now}"
21                )
22            self.env.process(
23                self.unplanned_admission(
24                    self.experiment.stay_distributions[0]
25                )
26            )

```

Listing 1: Example CCU code from Stage 1

```

1 class CCU:
2     def __init__(self, env, experiment):
3         self.env = env
4         self.experiment = experiment
5         self.patient_id_counter = 0
6         # ...
7         self.critical_care_beds = simpy.Resource(
8             env, capacity=self.experiment.num_critical_care_beds
9         )
10
11    def accident_emergency_arrivals(self):
12        while True:
13            yield self.env.timeout(
14                self.experiment.rng_accident_emergency.exponential(
15                    self.experiment.accident_emergency_arrival_rate
16                )
17            )
18            self.patient_id_counter += 1
19            if self.experiment.trace:
20                print(
21                    f"Patient {self.patient_id_counter} ...{self.env.now:.2f}"
22                )
23            self.env.process(
24                self.unplanned_admissions_process(
25                    "Accident and Emergency"
26                )
27            )

```

Listing 2: Example CCU code from Stage 2

8.1.3. Prompts

In total, 22 iterations of the model were used to build the model and interface. We report the number of prompts by iteration and stage in online Appendix D Table D1. In Stage 1 there were 26 prompts passed to the LLM. The number of prompts increased to 36 in Stage 2. Five of the 10 extra prompts occurred in the first two iterations of the model. Some minor additional prompting was needed to ensure comparable performance measures. The final iteration of the model was a bug fix that was only relevant to Stage 1; therefore Stage 2 saved one prompt. Our approach to prompt engineering, along with all prompts, is available in our online research compendium.

8.2. Case 2: Stroke pathway capacity planning model

8.2.1. Model outputs

We again confirmed that the results of the two generated simulation models were identical using a paired-t test. The results for the Stage 1 and Stage 2 models are reported and compared graphically in Figure 5 and Figure E1 (in online Appendix E). The

Table 5. Count of CCU model code components comparing Stages 1 and 2.

Component	Number of attributes		Number of methods/ functions	
	Stage 1	Stage 2	Stage 1	Stage 2
Experiment class	13	27	3	2
CCU model logic class	4	9	10	12
Functions	N/A	N/A	6	6

figures show that the probability of delay and ward occupancy match across the acute and rehabilitation wards within the 2 models.

The outputs from the generated models results replicated the results reported in the original article (Monks et al., 2016); although we note that we did not run all of the experiments reported in the article.

8.2.2. Model code

Disregarding comments, documentation and the Streamlit interface, Stage 1 generated a *SimPy* model consisting of 436 lines of code and Stage 2 generated 531 lines of code. Both models passed the same batch of 39 verification tests, with the Stage 2 model including 3 extra tests to ensure 100% code coverage.

The final code files from Stage 1 and Stage 2 for the stroke capacity planning model have some substantial differences. Table 6 summarises the difference in implementation. Notable differences included an additional `PatientType` class in the Stage 2 model; and a six-fold difference in the number of member attributes of the `Experiment` class.

The difference in the code led to a difference in the how each model was setup to run an experiment. For example, in the stage 1 model the code to setup an experiment that simulated a 5% increase in stroke patients, and then check the parameter value is shown in Listing 3. The equivalent code in stage 2, shown in Listing 4 involved an additional line of code to create a Python dictionary and a collection data-structure to access the internal parameters.

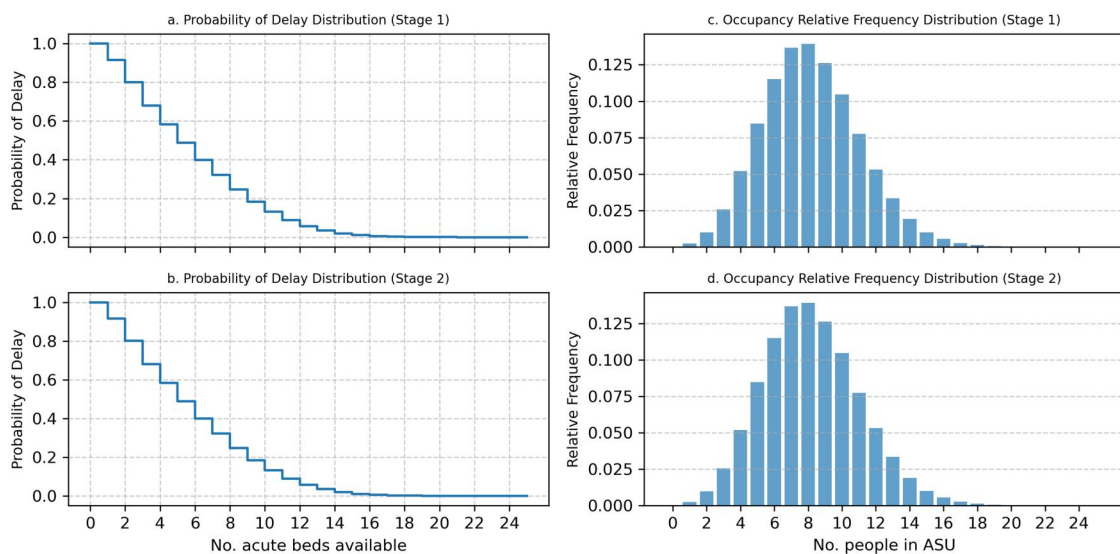


Figure 5. Acute stroke unit (ASU) outputs: comparison of Stage 1 and Stage 2 models.

Comparison of Python code to setup Experiments in Stages 1 and 2

```

1 # setup experiment
2 default_experiment = Experiment(stroke_mean=1.2*1.05)
3
4 # access and check parameter value
5 print(default_experiment.stroke_mean)

```

Listing 3: Setup a stroke model experiment in Stage 1

```

1 # setup parameter dictionary
2 experiment_params = {
3     "patient_types": {"Stroke": {"interarrival_time": 1.2 * 1.05}}
4 }
5
6 # pass to Experiment. LLM provided code that updates internal parameter dicts
7 demand_experiment = Experiment(experiment_params)
8
9 # access and check parameter value
10 print(
11     demand_experiment.params['patient_types']['Stroke']['interarrival_time']
12 )

```

Listing 4: Setup a stroke model experiment in Stage 2

Table 6. Count of stroke capacity planning model code components comparing Stages 1 and 2.

Component	Number of attributes		Number of methods/functions	
	Stage 1	Stage 2	Stage 1	Stage 2
Experiment class	36	5	3	5
PatientType class	N/A	6	N/A	3
AcuteStrokeUnit model logic class	5	7	6	7
RehabilitationUnit model logic class	6	18	7	9
Functions (excluding classes)	N/A	N/A	11	10

We do not argue that either of the approaches generated by the LLM is optimal. Rather that there are pro's and con's to their implementations. Stage 1 code offers a simple code interface, but does not choose a clear naming convention (i.e., `stroke_mean` is not specific to inter-arrival time). Stage 1 also does not clearly separate model parameters from the outputs of the experiment. Stage 2 code requires more code and requires a user to understand Python dictionaries. Stage 2's hierarchy to access parameters is more complex than stage 1's (including the internal workings of `Experiment`), but it uses clear specific naming conventions for patients types and their different parameters configurations.

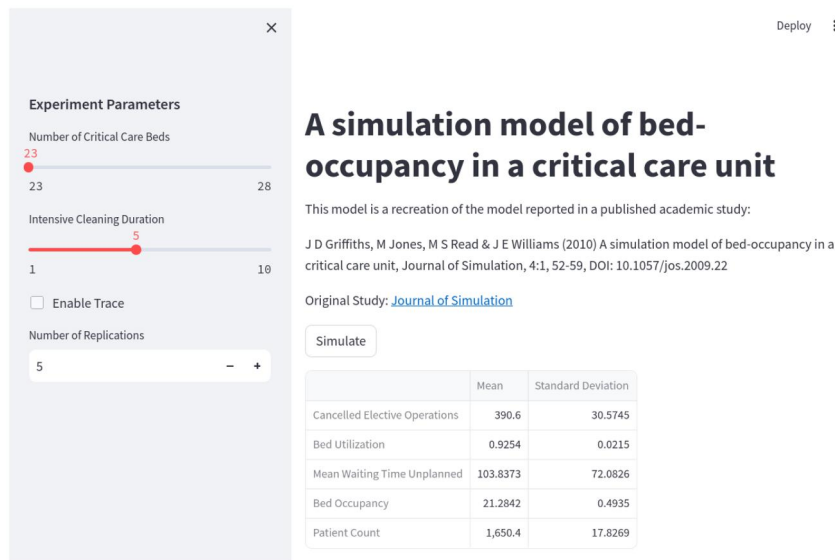
8.2.3. Prompts

In total 31 iterations of the model were used to build the model and interface. In Stage 1 this consisted of 41 prompts passed to the LLM. The number of prompts increased to 57 in Stage 2. An additional prompt was needed in Stage 2 to fix a variable type bug introduced by the LLM for representing "patient type" across the acute and rehab sections of the model. Stage 2 required 4 additional

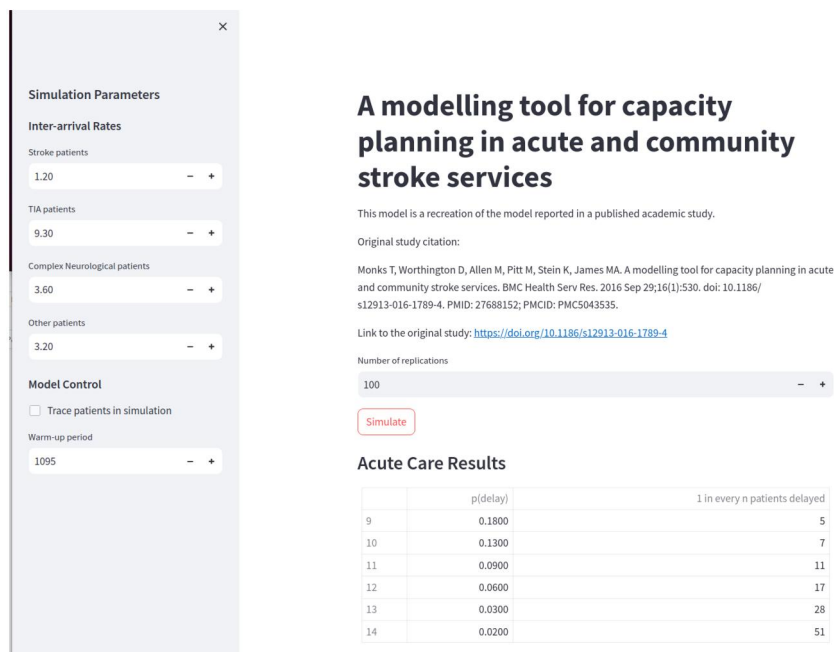
prompts for introducing common random numbers streams to the LLM struggling to assign streams across model activities. The number of prompts are report in online [Appendix D Table D2](#).

8.3. Model interfaces

In both case studies, we were successful in generating model interfaces using the streamlit Python package. [Figure 6](#) depicts the model interfaces from stage 1 (we include stage 2 figures in the online [Appendix C Figure C1](#)). The generated interfaces were largely consistent across stage 1 and 2. This was possibly due to the simplicity of our requirements. A minor difference was observed between stage 1 and 2 in the second case study. In [Figure 6b](#) Perplexity generated input widgets used to manipulate the model input parameters. In Stage 1 "numeric boxes" were used where-as in stage 2 "sliders" are used. The former allowed the input parameters to take negative values – that result in a model error (as you cannot have a negative inter-arrival arrival rate) – where-as sliders prevented this unacceptable setting with a minimum value



(a) Generated streamlit interface for Critical Care Unit



(b) Generated interface for the stroke capacity planning model

Figure 6. Model interfaces from stage 1.

(although still allowed 0). This result suggests that prompts should specify valid ranges for input widgets.

9. Discussion

Our objective was to test if we could recreate a version of published healthcare DES models in FOSS using generative AI. We selected two DES models from the literature where the coded model was not available and the original model was reported to have been implemented in commercial software that could not have formed part of the internet training data for a LLM. We read the natural language

description of models in these papers and formed a model design. Based on model designs, we engineered prompts for the free tier of a generative AI tool (Perplexity) to code a Python and *SimPy* model and a basic *Streamlit* browser interface. We found that using our iterative approach to coding the model we were able to generate relatively sophisticated versions of two DES models. By sophisticated we mean:

- The model logic was represented by up to 600 lines of Python code representing a queuing network in healthcare; this is relatively sophisticated compared to simulation models generated by

others, for example, models were only represented by 20–30 lines of Python code (Frydenlund et al., 2024; Jackson et al., 2024; Plooy & Oosthuizen, 2023);

- The generated model design followed best practice recommendations (Monks & Harper, 2023b) i.e., we separated model parameters from logic to enable simple experimentation, automated model testing, and linkage to a user interface;
- Between the two models we included multiple arrival sources and entity classes, balking, sampling mechanisms, queuing network routing, and calculation of multiple performance measures;
- The models' run length and output calculation were split into warm-up and data collection periods;
- Sampling in the models was implemented using streaming (common random numbers) and results across replications were repeatable.

We were able to reproduce our findings internally using the original prompts and several additional smaller prompts. In each case, the model code generated was different but produced consistent results. Given our ambition to preserve the time and effort put into coded models reported in the literature, we have archived all of our generated models in the Zenodo open science archive. This provides a guarantee on the persistence of the coded models – as long as the European Organization for Nuclear Research (CERN) exists. The models are MIT-licensed and available for others to download, inspect, reuse, adapt and redistribute with citation.

We would emphasise that, although successful in both stages of the study (the original recreation of a model design and its internal reproduction), neither were straightforward and provided several prompt engineering, model testing, and usage challenges for generative AI. We argue that we were only successful due to the process we followed: our use of iterations to add model detail and scope, our approach to differencing and testing code, and our use of modellers experienced in DES, healthcare, and FOSS. We do not believe it would have been achievable without all of these elements. In the following section, we describe the challenges and opportunities of generative AI for recreating model designs.

9.1. Challenges generating models

9.1.1. Lazy generation

We quickly found that Perplexity used a strategy to reduce the amount of Python code it had to generate when prompted to modify code. For example, Python classes were partially generated with sections of code replaced by comments such as “remaining

functions go here” or “original method code continues here.” We can only speculate why the tool behaved this way given our prompts, but we might assume that less text generated required less computation and cost for the provider. We were able to by-pass this undesirable behaviour by a.) appending the clause “Show all of the model code”; b.) prompting for specific(s) part of the model to be generated e.g., “Show the full `RehabilitationUnit` including all patient generator and treatment functions” (e.g., Stage 1 iterations 15 and 27 of the stroke model); c.) using a restrictive clause to only generate functions and classes that were modified e.g., “only show the code for these three functions” (e.g., Stage 1 iteration 18 of the CCU model).

9.1.2. Hitting the maximum context size

For the stroke model, both modellers found that the context size was not large enough to generate the full model. The effects of this manifested in three ways:

- Perplexity, for all intents and purposes, “forgot” a section of model code. For example, it could no longer output the `Experiment` class code and hence could not perform the required modifications (e.g., iteration 18 of Stage 1).
- Incorrect code indentation at the end of the generated output (this is important because Python is whitespace sensitive; e.g., iteration 24 of stage 1).
- Introduction of small errors at the end of the generated text. For example, in a Python class, the ‘self’ keyword was omitted when referring to member attributes.

We solved this problem and were able to get the correct output by switching to a new context window (i.e., a new chat prompt with no history). This meant that we were required to include code snippets (e.g., functions, classes or scripts) in the prompt to fill in the missing context.

9.1.3. Time-consuming prompt engineering

We used a mix of prompt types to generate the models. The time to design these prompts and their complexity varied significantly. For some difficult tasks, we were required to use one-shot or few-shot prompt engineering. An example of this was to modify code when allocating seeds across the model's random number generators (where the LLM had to both modify code and count). This meant we explicitly included Python code examples of what we wanted from the prompt. For this specific example we found, in both stages, that a prompt needed to be split in two to achieve what we wanted

with Perplexity. Informally, we tested the same prompt with OpenAI's ChatGPT and found that it could generate the desired seed allocation from our single prompt. We conclude two things from this example. The first is that if few-shot prompt engineering requires a modeller to write Python code then it is likely cost effective to simply make the changes manually and then reprompt the LLM (including the modified code). The second is that a user may wish to try multiple AI tools when they encounter a difficulty.

9.1.4. Changing nature of tools

We found that the behaviour and performance of Perplexity varied during our study. During the construction of Stage 1's CCU model, Perplexity provided sources with each prompt, meaning that retrieval-augmented generation was used to provide additional context before code generation. This behaviour changed over subsequent models and stages: for example, we found that Perplexity's sources appeared for the first two iterations of the stroke capacity planning model and then no further sources were used (displayed to the user) even when we started a new context window. We re-tested this in early 2025 to find the functionality restored.

During each stage, we also found that the speed and performance of Perplexity's generation varied. In particular, the rate at which new code was generated would drop significantly and potentially would not fully generate the code we required. We did not include a formal investigation of this aspect in our study plan but note that this typically occurred in the afternoon in the UK. We cannot explain this conclusively but speculate that this could have been related to the rapidly growing user base of tools like Perplexity, time difference with the US, and the prioritisation of limited GPU capacity to paying customers. This finding may have also been compounded by the large contexts we were creating and passing to Perplexity over multiple iterations of the models. We handled this problem by pausing the study and re-prompting the following morning.

9.1.5. Internal reproduction, randomness and preservation

We expected that our internal test of reproducibility would be inherently challenging, due to the way generative AI makes use of random noise. In other words, we expected that given the same prompts, any AI tool would generate Python code with subtle to substantial differences. As the model code in Stage 2 deviated from Stage 1 across iterations, the original prompts became less specific to the Stage 2 model implementation. As such (with the current generative AI capability) it seems unlikely that a

general set of sequenced prompts could be expected to reliably regenerate a specific Python simulation model. This finding emphasises the importance of preservation of simulation model artefacts for the long term (so regeneration is unnecessary).

9.2. Wider opportunities presented by LLM for coding python models

We found in all cases that our approach to recreating a version of the published models was successful. We propose the following wider opportunities for the modelling and simulation community.

9.2.1. Reuse of prompts

For simpler tasks, we found that some prompts were fairly generic and can work well if a user takes a "lift and adapt approach." One example of this is generating a basic user interface to the model that we split over three iterations. We provided the interface prompt for the stroke capacity planning model in [Box 4](#); this was a minor adaptation of the prompt used for the CCU model (see iteration 19). These are simple prompts that begin the same and then are tailored to the specifics of the results summary for each model.

9.2.2. Describing models

At the end of the study we also explored the use of generative AI to describe model code. We used the persona pattern (Olea et al., 2024) from prompt engineering and asked the AI tool to take the role of an elective surgery patient. We provided a prompt including all the CCU model code and asked for a description of potential journeys through the model. We found that the routing through the model was described accurately. We provide an excerpt from the response in [Box 5](#).

9.2.3. Documenting model code

We informally tested the ability of LLM's to generate code documentation for stage 1 models. Specifically we issued the prompt "Write PEP257 compliant docstrings for all functions, classes and methods. Provide a brief description of the purpose of the code, document parameter and return values." The generated output was promising and likely warrants further investigation. We provide an example output in online [Appendix F](#).

9.3. General risks presented by LLM for coding python models

As we have already outlined, LLMs make mistakes when coding. For the immediate future, we caution

Box 5. Generated description of the critical care unit model (using the persona pattern for an Elective Patient).

Summary of potential journeys

As an elective surgery patient, my journey through the simulation model can either result in successful admission, surgery, recovery, and discharge, or in the cancellation of my surgery due to a lack of available beds. Here's a condensed view of both paths:

Successful admission and treatment

- Arrival → Bed Request → Bed Available → Admission → Surgery and Recovery → Discharge and Cleaning

Surgery cancellation

- Arrival → Bed Request → No Bed Available → Surgery Cancellation

Implications for the simulation

These paths are critical in understanding the performance of the critical care unit. My journey as an elective surgery patient affects:

- **Bed Utilization:** The time I spend in the bed contributes to overall bed utilization metrics.
- **Bed Occupancy:** My admission impacts bed occupancy rates.
- **Surgery Cancellations:** If my surgery is cancelled, it adds to the count of cancelled elective operations, providing insight into the hospital's capacity challenges.

all users that no code generated by an AI tool should be trusted at face value. Our testing and code differencing procedures were essential to identify these errors, as they could be subtle and easily missed with casual inspection. For example, a critical line of stroke patient routing logic was removed in Stage 1 iteration 3 (fixed *via* a prompt in iteration 11). Although verification is recommended in all DES textbooks as a hallmark of study quality, formal verification of model code is rarely reported in the DES literature (Zhang et al., 2020). Our findings reinforce this message and we recommend all authors who make use of Generative AI write and publish formal tests of their models alongside their model.

A secondary recommendation for users building or generating FOSS models is to make use of simple user interfaces for informal testing. We recognise that the time to test models in a real simulation study is limited. In our study we found that the generation of a basic *streamlit* user interface in addition to our formal design of tests was productive. Specifically, this provided a quick way to conduct combinations of extreme value tests. As an example, this allowed us to identify an error in the logic to generate result charts from the stroke model (fixed in Stage 1 iteration 30).

9.4. The replicability of the reported models

Generative AI is most suitable for model development when (a) a clear, structured conceptual model exists, (b) the modelling task can be decomposed into well-

defined, promptable steps, and (c) the user possesses sufficient domain and technical expertise to iteratively test, validate, and refine the generated code. It is less suitable when model requirements are highly ambiguous, require extensive engagement and/or tacit knowledge, or when high-stakes, safety-critical validation is needed. This theoretical framework aligns with established decision-making models for AI adoption in operational research contexts (Frydenlund et al., 2024; Jackson et al., 2024) and provides explicit guidance for practitioners considering generative AI for simulation model development. Just like our two selected academic papers, the vast majority of DES healthcare models published in the academic literature take the form of a natural language description (with diagrams in some cases) and no coded model is available (Monks & Harper, 2023a). The ability to replicate computer models and results reported in the literature (DES and from other related methods) has long been a concern for the community (Grimm et al., 2020; McManus et al., 2019; Schwander et al., 2021). We found that we were unable to fully replicate the reported results of one of the models. The primary reason for the difference we believe is straightforward: we did not have access to the empirical distributions used in the original study and we were forced to make an assumption (albeit one alluded to as an alternative in the original paper). We believe that the design of the recreated model is still faithful to the original work and if the original parameters were reported, we hypothesise that replication of the experiments we tested would have been successful. While this may seem a minor discrepancy, we note that we cannot fully verify the model is a recreation of the original work without this data. To improve replication success, our recommendation is therefore that authors provide full verification data to support narrative descriptions of their models. Formal guidance on documenting models exists elsewhere (Monks et al., 2019; Zhang et al., 2020). A specific example reporting continuous and discrete empirical distribution functions can be seen in the [online supplementary material](#) that accompanies Lahr et al. (2013).

9.5. Limitations and further work

A limitation of our study is that we only investigated coding models in Python and *SimPy* and further limited this to two simulation models. This narrow focus allowed us to increase the complexity of simulation coding tasks in a way that was above prior studies and to include an internal repetition to investigate reproducibility. A natural extension to this work would be to investigate generation of models in the other popular FOSS language for DES: R and RSimmer.

The study was also limited to two modellers that tested an iterative process to model coding. Although the prompt engineering process we followed was successful, other modellers may not wish to design their models in such an iterative manner. We did not formally test an all-in-one prompt approach but, given the challenges in catching hallucinations and mistakes, we would caution against such a strategy in practice.

Finally, we limited our formal investigation to the free tier of a single AI tool – Perplexity.AI’s standard model – during a period in 2024 and cannot evidence generalisability to other popular tools. Our informal testing leads us to speculate that our findings should translate to paid tiers of services such as Perplexity that offer access to larger models or recent models with reasoning capabilities (e.g., GPT-4.5, Claude 3.7 or DeepSeek-R1). We expect these larger models to be at least as good as the tool we used and still advise rigorous testing of any simulation code they generate.

Looking to the future, we note that the growing presence of AI-generated content on the internet is of increasing concern (Xing et al., 2025). The potential challenges it poses, especially concerning the training of LLMs on AI-generated content, raise concerns about “model collapse,” a degenerative process where models trained predominantly on synthetic data experience performance degradation. This occurs because models recursively learn from outputs that may contain errors or biases, leading to a decline in quality over successive training iterations (Shumailov et al., 2024; Wenger, 2024). Future work for the modelling and simulation community may have to consider the need for careful curation of quality simulation training datasets to maintain integrity and performance.

10. Conclusions

This study explored the feasibility of using generative AI to recreate published DES models in healthcare. Our findings suggest that it is possible to generate DES models in FOSS using engineered prompts derived from narrative descriptions, as demonstrated by our recreation of two published healthcare models in Python. These models passed human-developed verification tests and incorporated simple user interfaces. This study also revealed notable challenges associated with generative AI, including issues with prompt engineering, code generation, and model testing. While we successfully generated, validated, and reproduced these models, our experience underscores the importance of iterative refinement, systematic approaches to model differencing and code testing, and domain expertise in

DES modelling, FOSS, and healthcare. These findings provide valuable insight into the promise and limitations of generative AI for healthcare modelling, but further research is needed to fully understand its broader applicability and scalability.

Notes

1. <https://book.fosteropenscience.eu/>
2. <https://chatgpt.com/>
3. <https://chatgpt.com/>
4. <http://perplexity.ai/>
5. <https://claude.ai>
6. <https://gemini.google.com/>
7. <https://copilot.github.com>
8. <https://llama.meta.com/code-llama>
9. <https://github.com/google-research/google-research/tree/master/mbpp>
10. <https://iseesystems.com>
11. <https://anaconda.org/anaconda/conda>
12. <https://jupyterbook.org>
13. <http://zenodo.org/>
14. <http://github.com/>
15. <https://stackoverflow.com/>
16. <https://www.simul8.com/>
17. <https://www.rockwellautomation.com/en-gb/products/software/arena-simulation.html>
18. <https://www.microsoft.com/en-gb/microsoft-365/excel>

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Data availability statement

All prompts, code and other artefacts used in this study have been archived on Zenodo. Links to artefacts are provided in Table 3.

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