

APPLICATION

denim: An R package for deterministic compartmental models with flexible dwell-time distributions

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Abstract

1. Compartmental models are widely used for dynamical systems where states are discrete, such as in infectious disease epidemiology with the so-called Susceptible-Infectious-Recovered (SIR) framework. For mathematical simplicity, rates of transition between compartments are generally assumed to be independent of the dwell time (or secondary timescale in survival analysis): they are either constant or dependent on the epidemiological time (or primary timescale in survival analysis) only, either directly (e.g. environmental or behavioural forcings in epidemiological models) or indirectly through dependence on other variables of the system (e.g. the force of infection in epidemiological models). In some domains of application, this memoryless assumption leads to distributions of dwelling times that are incompatible with those observed in data (e.g. infectious periods for childhood diseases), which can lead to serious problems since the model predictions are highly sensitive to the exact shape of these distributions.
2. Here, we propose a deterministic, continuous-variable, numerical modelling approach that allows full flexibility on the dwell-time distributions. The accompanying denim package provides a user-friendly interface to implement our proposed method through a dedicated language for model definition.
3. The package is open source and available on CRAN. As more detailed data on the clinical process of infections become available, the denim package will be extremely useful for building more realistic epidemiological models that provide more accurate projections.

KEYWORDS

compartmental model, competitive risks, dwell-time distribution, R package, semi-Markovian, sojourn time distribution

Thinh Phuc Ong and Anh Truong Quynh Phan contributed equally to this study.

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1 | INTRODUCTION

Compartmental models are widely used in various domains of application dealing with the dynamics between discrete states. For example, in epidemiology, the population is typically divided into susceptible, infectious and recovered compartments with specified transition rates between them. In their classical and most commonly used form, these models are Markovian (i.e. memoryless), meaning that the rate at which individuals leave a compartment is independent of the duration spent in the compartment (or the secondary timescale in survival analysis). The main motivation for this assumption is tractability, as these models can easily be implemented using ordinary differential equations (ODEs) (Hong et al., 2024). Furthermore, under the Markovian assumption, modelling transitions to multiple compartments as competing risks is straightforward, as the total exit rate from the compartment is simply the sum of the individual transition rates. It also makes it possible to express deterministic systems of ODEs as discrete counting processes, allowing straightforward stochastic simulation (e.g. via the Gillespie algorithm; Zachreson et al., 2022).

The consequence of the Markovian assumption, however, is that it implicitly involves a specific distribution of dwelling time. For example, constant rates of transitions in an epidemiological model imply that the latency/infectious durations follow an exponential distribution. This distribution is characterized by a coefficient of variation of 1 ($CV = 1$) and the mode equal to 0, neither of which is supported by the empirical distributions of these durations, which typically exhibit much lower relative variability (i.e. $CV < 1$) with a mode significantly higher than 0 (Lessler et al., 2009; Nishiura & Eichner, 2006; Wearing et al., 2005). Theoretical analyses also show that the shape of exact dwell-time distributions greatly affects the model's trajectory (Keeling & Grenfell, 1998; Kenah & Miller, 2011; Krylova & Earn, 2013; Lloyd, 2001). For example, Wearing et al. (2005) illustrated that assuming exponential infectious periods always underestimates the basic reproductive ratio.

An easy relaxation of this strong assumption of exponential distribution is to model Erlang-distributed dwell times using ODEs via the linear chain trick (LCT; Hurtado & Kiro Singh, 2019). Even though this two-parameter distribution increases flexibility, there are still many instances where it does not provide a great fit to the data. Instead, recent studies propose incorporating arbitrary parametric distributions by formulating compartmental models as delay integro-differential equations and then solving them numerically (Hernández et al., 2021; Hong et al., 2024). Tallis (1994) laid the theoretical foundation for incorporating competing risks into compartmental models under semi-Markovian assumptions. However, to our knowledge, no prior work or existing tools have introduced a simulation algorithm for compartmental models with arbitrarily distributed competing risks.

In this paper, we provide a semi-Markovian (Korolyuk et al., 1975) modelling framework where transition rates now depend on the time individuals have spent in a compartment (but are still memoryless regarding state, contrary to non-Markovian models that have memory both in time and in state). The framework is implemented in the R package *denim* that allows users to specify any dwell-time distribution, including non-parametric forms, thus enabling direct

integration of empirical data and more realistic modelling of progression and delay. Model structures are easy to define and highly customizable with support for competing risks. The syntax is intuitive and designed for seamless integration with existing workflows using *deSolve* (Soetaert et al., 2008) or *odin* (FitzJohn, 2019), enabling users to adapt their current models with minimal effort.

2 | MODELLING APPROACH

Our framework considers a deterministic, discrete-time, and continuous variable compartmental model in which all compartments are further subdivided into sub-compartments, the values of interest being transition probabilities between sub-compartments.

To demonstrate *denim*'s algorithm, consider a basic compartmental model with three compartments X , Y and Z . Individuals in compartment Y come from X , and will move to Z . The time individuals stay in Y before moving to Z follows a discrete probability distribution $P_Y = p_1, p_2, \dots, p_n$ with $\sum_i p_i = 1$, where n is the maximum number of time steps individuals can stay in compartment Y . Compartment Y is then further split into sub-compartments, where sub-compartment Y_i represents individuals that have been in the Y compartment for i time steps (Figure 1).

At each time step, a proportion q_i of individuals in Y_i (where $1 \leq i \leq n$) move to the Z compartment, while the remaining $1 - q_i$ move to Y_{i+1} . The central problem in this sub-compartment approach is to relate the transition proportion q_i to the target dwell-time distribution p_i .

To derive this relationship, we reformulate our problem within the framework of survival analysis, where the event of interest is 'transitioning from Y to X '. The relationship between compartmental models and survival analysis has been explored in previous studies (Hay et al., 2024; Tallis, 1994) and is discussed in greater detail in [Supporting Information](#). In this setting, the distribution $P_Y = p_1, p_2, \dots, p_n$ can be interpreted as a discrete estimation of a probability density function $f(\tau)$ of dwelling times such that:

$$p_i = \int_{(i-1)\Delta t}^{i\Delta t} f(\tau) d\tau$$

where Δt is the duration of each time step.

q_i (probability of leaving Y , given that individuals have stayed for i time steps, i.e. $P(Z|Y_i)$) is thus an estimation for the hazard rate $h(\tau)$ in survival analysis. The relationship between $h(\tau)$ and $f(\tau)$ is represented by the following formula.

$$h(\tau) = \frac{f(\tau)}{S(\tau)} = \frac{f(\tau)}{1 - \int_0^\tau f(x) dx}$$

In discrete time, q_i can then be estimated using p_i as follows.

$$q_i = P(Z|Y_i) = \int_{(i-1)\Delta t}^{i\Delta t} h(\tau) d\tau = \frac{\int_{(i-1)\Delta t}^{i\Delta t} f(\tau) d\tau}{1 - \int_0^{(i-1)\Delta t} f(\tau) d\tau} \approx \frac{p_i}{1 - \sum_{j=1}^{i-1} p_j}$$

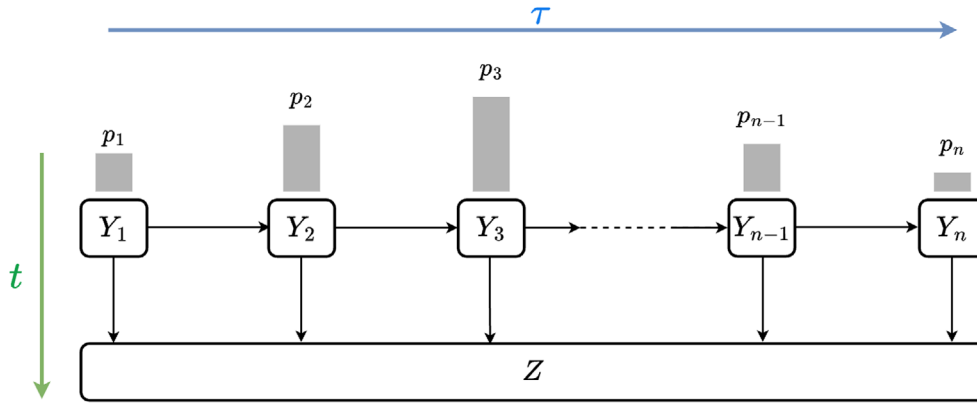


FIGURE 1 Visualization of the sub-compartments in denim. p_i represents the proportion of individuals in Y that transition to Z from each sub-compartment Y_i . Two timelines are presented, where t represents the primary timescale (i.e. calendar time since the start of the simulation) while τ represents the secondary timescale (i.e. dwell time or time since entering compartment Y). Progression along τ indicates remaining in Y for another time step while progression along t indicates the advancement of simulation time, during which individuals may transition to Z .

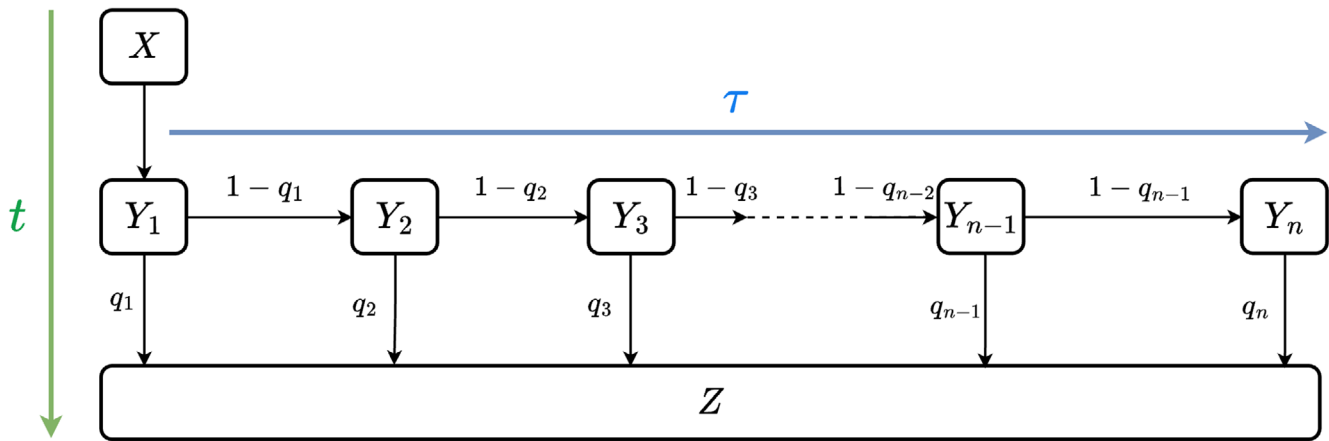


FIGURE 2 Visualization of the transition proportions q_i and $1 - q_i$ of each sub-compartment Y_i . See the legend of [Figure 1](#) for the meaning of τ and t .

A visualization of transitions between sub-compartment Y_i and Z is provided below ([Figure 2](#)).

This sub-compartmental structure can be used as a numerical method to solve the following system of delay integro-differential equations.

$$\begin{cases} \frac{dX(t)}{dt} = -N_Y(t) \\ \frac{dY(t)}{dt} = N_Y(t) - \int_0^{\tau_Y} h(\tau)Y(t, \tau)d\tau \\ \frac{dZ(t)}{dt} = \int_0^{\tau_Y} h(\tau)Y(t, \tau)d\tau \end{cases}$$

where $N_Y(t)$ is the population of X that transitions to Y at time t ; τ_Y denotes the maximal dwell time in the Y compartment; $Y(t, \tau)$ is the sub-population of Y at time t that has been in Y for a duration τ (i.e.

$Y(t, \tau) = S(\tau)N_Y(t - \tau)$). The sub-compartment Y_i can thus be interpreted as $Y_i \approx \int_{(i-1)\Delta t}^{i\Delta t} Y(t, \tau)d\tau$.

When using denim, users only need to specify the dwell-time distributions, and the transition probabilities q_i are computed automatically using the formulation above. The dwell-time distribution could be one of denim's built-in parametric distributions or a vector of values corresponding to the ordered values of a histogram with a bin width equal to the model time step. Currently supported parametric distributions include the discretized versions of the exponential, gamma, log-normal and Weibull distributions.

With the transition probabilities computed, the simulation can be carried out by updating the population of each sub-compartment at every time step based on incoming and outgoing individuals. In the given example, the outgoing population for Y (or the incoming population for Z) is $\sum_{i=1}^n q_i n Y_i$ where $n Y_i$ is the population that has stayed in Y for i time steps (i.e. the population of the Y_i sub-compartment).

2.1 | Transition to multiple outgoing compartments

Transitions from one compartment to multiple downstream compartments can be defined in two ways: (i) as multinomial transitions; or (ii) as competing risks, depending on what information the modellers currently have.

Consider a scenario where individuals in compartment Y can transition to an additional compartment V. The information we may have includes the following:

1. Distribution of the time in which individuals stay in Y, denoted $f_Y(\tau)$.
2. Distributions of the time that individuals in Y transition to Z and to V (denoted $f_{Y \rightarrow Z}(\tau)$ and $f_{Y \rightarrow V}(\tau)$, respectively).
3. Proportion of individuals in the Y compartment that end up in Z and V, denoted w_1 and w_2 , respectively.

If information 2 is available (*Scenario 1*), transitions can be modelled using a competing risks framework. Alternatively, if we have information 2+3 (*Scenario 2*) or 1+3 (*Scenario 3*), the transitions can be modelled using a multinomial framework. In other words, the multinomial approach is used when we want to specify how individuals are distributed across k downstream compartments following a proportion w_m where $\sum_1^{m=k} w_m = 1$ (Figure 3).

The multinomial transition is implemented by having k chains corresponding to k outgoing compartments. Upon entry, a proportion w_m of the population will be allocated to sub-compartment chain m . For example, to implement a scenario where 80% of Y goes to V and the remaining 20% goes to Z, we create two sub-compartment chains for $Y \rightarrow V$ and $Y \rightarrow Z$ transitions. When a population of n enters Y, $0.8 \times n$ goes to $Y \rightarrow V$ chain and $0.2 \times n$ goes to $Y \rightarrow Z$ chain, and the outgoing populations to V and Z are computed from these chains independently. In *Scenario 2*, these are computed using $f_{Y \rightarrow Z}(\tau)$ and $f_{Y \rightarrow V}(\tau)$ while *Scenario 3* is equivalent to setting $f_{Y \rightarrow Z}(\tau) = f_{Y \rightarrow V}(\tau) = f_Y(\tau)$ (see Supporting Information S1 for the proof) (Figure 4).

Outgoing transitions are modelled as competing risks when we have $f_{Y \rightarrow Z}(\tau)$ and $f_{Y \rightarrow V}(\tau)$, but without the knowledge of w_m . We assume that: (i) the individuals in Y are simultaneously susceptible to mutually exclusive events $Y \rightarrow V$ and $Y \rightarrow Z$, of which only the first to occur is realized; and (ii) $f_{Y \rightarrow Z}(\tau)$ and $f_{Y \rightarrow V}(\tau)$ are independent. Under these assumptions, the competing risk scenario can be implemented using a single sub-compartmental chain, where the proportion leaving Y_{*i*} is the sum of $P(V|Y_i)$ and $P(Z|Y_i)$ (see Supporting Information S1). For example, suppose that $Y \rightarrow V$ and $Y \rightarrow Z$ are competing risks, with maximal waiting times n and m ($n > m$). To model this, we create a sub-compartmental chain with length n , then calculate the population that goes to V as $\sum_{i=1}^n P(V|Y_i) * nY_i$ and that of Z is $\sum_{i=1}^n P(Z|Y_i) * nY_i$ (where $P(Z|Y_i) = 0$ when $i > m$) (Figure 5).

A more detailed discussion regarding competing risks and multinomial, along with their corresponding delay-integro differential equation formulations, is provided in Supporting Information S1.

The implementation details and comparisons with the alternative packages are presented in Supporting Information S2.

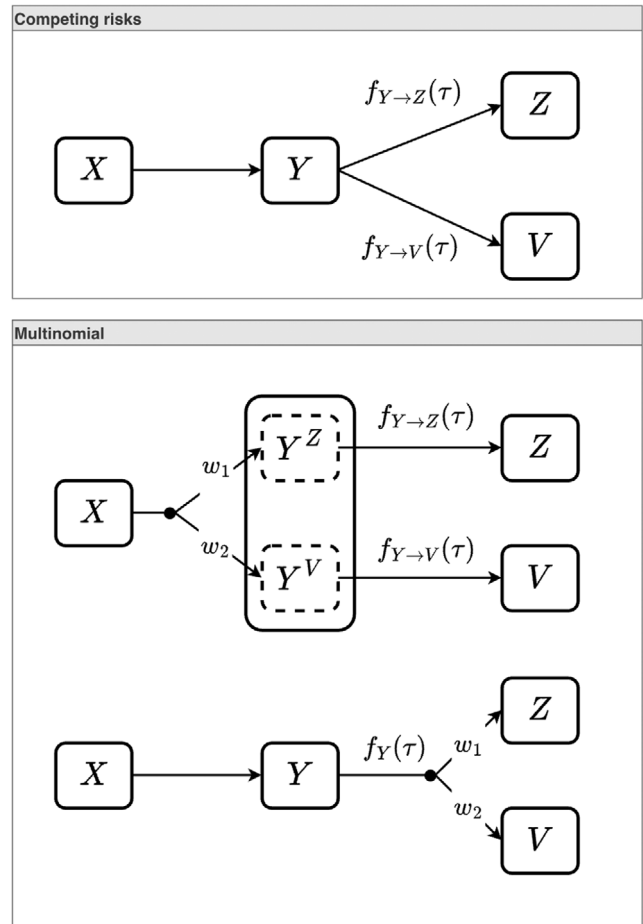


FIGURE 3 Visualization of the three scenarios. The lines extending from the black dot indicate the proportion of individuals that will eventually enter each outgoing compartment at equilibrium.

3 | EXAMPLE APPLICATION

Users can install the package from CRAN by running the following command in R:

```
install.packages("denim")
```

Then load it into R with

```
library(denim)
```

To create a simulation in denim, users need to specify (i) model structure (compartments and the transitions between compartments), (ii) initial state of each compartment and (iii) simulation duration and duration for each time step.

In the following subsections, we will go through a process of building a compartmental model in denim and introduce the core functionalities of the package. A visual representation of the model being built is shown in Figure 6. The example was run using denim version 1.2.2.

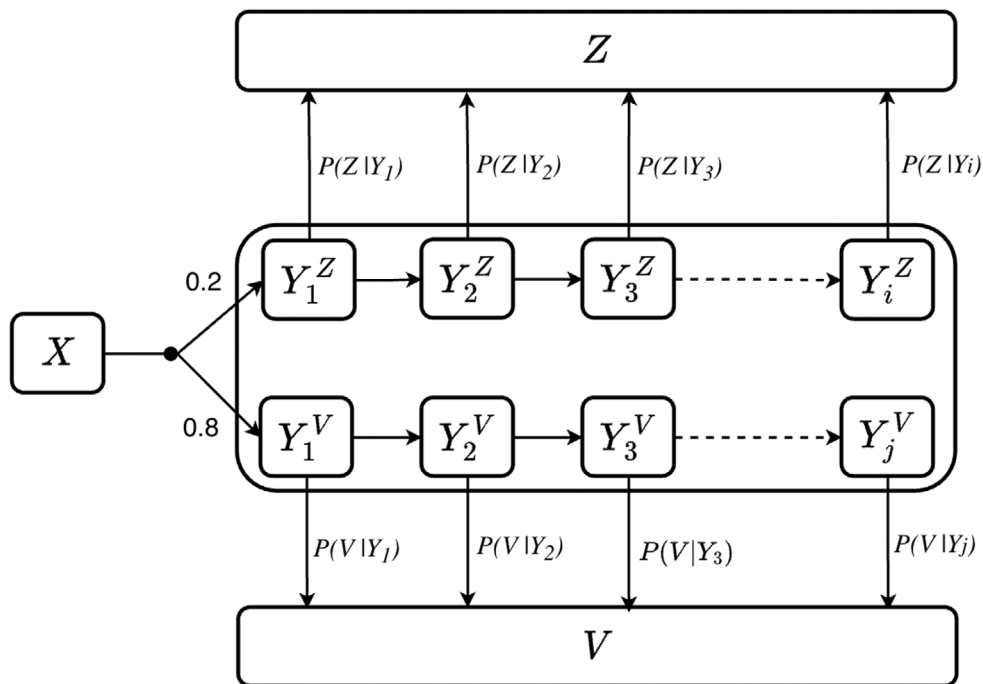


FIGURE 4 Visualization of the sub-compartment chains in multinomial. Y^Z and Y^V denote the sub-populations of Y that will transition to Z and V , respectively. The total population that goes to Z is computed by $\sum_{n=1}^i P(Z|Y_n)Y_n^Z$, and the population that goes to V is $\sum_{n=1}^j P(V|Y_n)Y_n^V$.

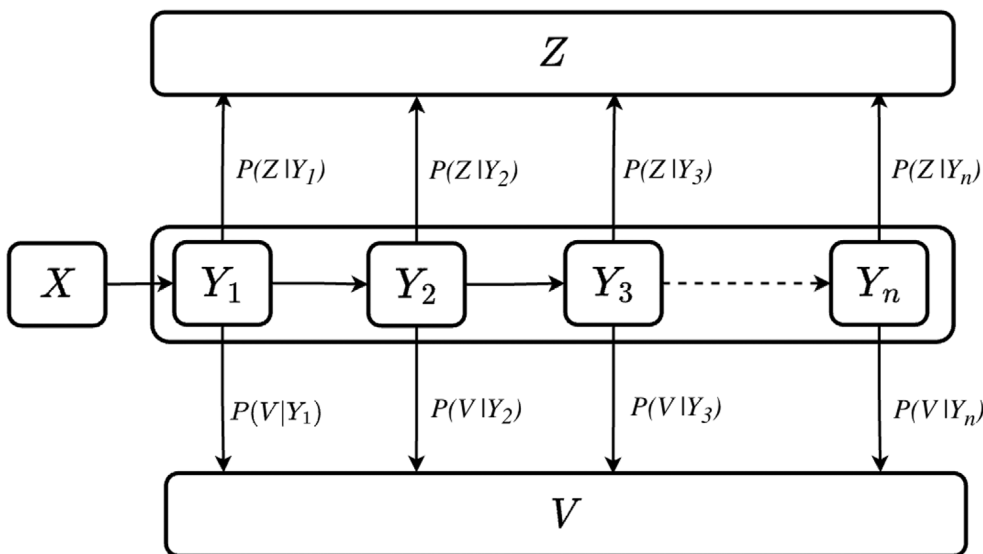


FIGURE 5 Visualization of the sub-compartment chain in a competing risks scenario.

3.1 | Model structure

A compartmental model consists of compartments and transitions between them. In *denim*, the model structure is defined by a set of *key-value* pairs where *key* specifies the direction of population flow between compartments and *value* is a built-in dwell-time distribution function or mathematical expression to describe that transition.

Table 1 lists all the transitions implemented in *denim* and their required parameters.

These *key-value* pairs can be defined in two ways: (i) using *denim* domain-specific language (DSL), or (ii) as a list in R. This paper focuses on the use of *denim* DSL; an R list example is available on the *denim* website (https://drthinkong.com/denim/articles/denim_dsl.html#r-list).

All transitions must be defined in the format `from -> to = transition`, and the code written in *denim* DSL must be parsed

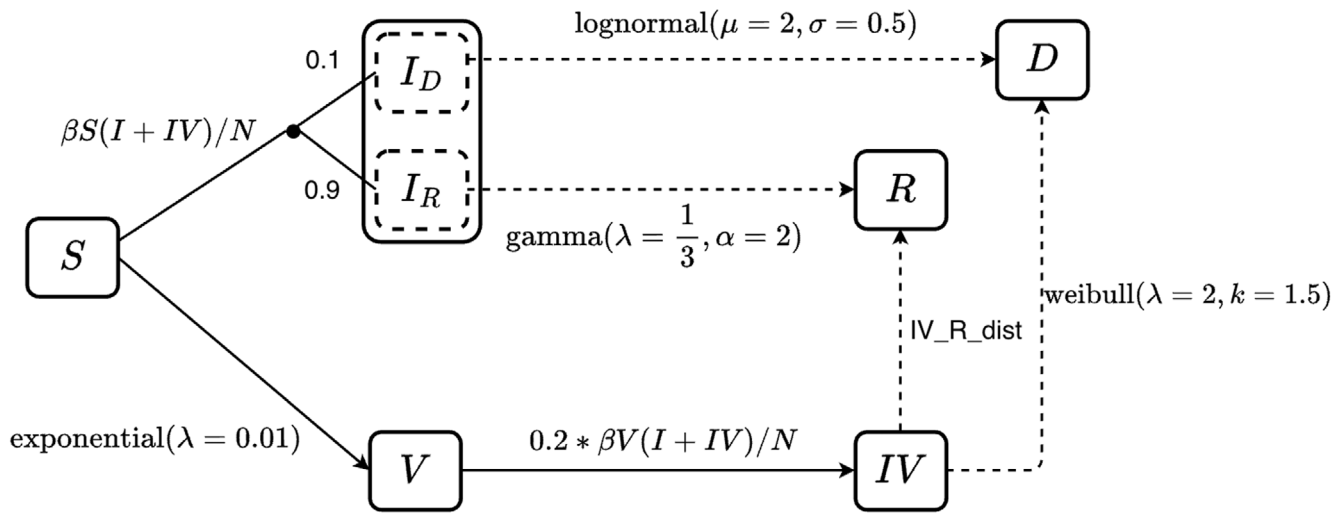


FIGURE 6 An example of a compartmental model. Dashed lines indicate transitions described by dwell-time distributions, while solid lines indicate transition rates. Susceptibles (S) can get infected (I) or vaccinated (V), and these events are treated as competing risks. Among the infected, 90% recover (R) and 10% die (D), with recovery times following a gamma distribution and death times a log-normal distribution. Vaccinated individuals can still be infected (IV), then either recover or die, following a nonparametric distribution (denoted IV_R_dist) and Weibull distribution, respectively.

TABLE 1 Built-in transition functions.

Transition type	Function name	Parameters	Description
Distribution	<code>d_exponential</code>	Rate	For exponentially distributed dwell time
	<code>d_gamma</code>	Rate, shape	For gamma-distributed dwell time
	<code>d_lognormal</code>	Mu, sigma	For lognormal-distributed dwell time
	<code>d_weibull</code>	Scale, shape	For Weibull-distributed dwell time
	<code>nonparametric</code>	Vector of probabilities or numbers	For user-defined dwell-time distribution
Math expression		String for math expressions	For user-defined math expression for transition per time step

by the function `denim_dsl`. The example model is defined as follows:

```
modelStructure <- denim_dsl({
  S -> I = beta * S * (I + IV) / N
  S -> V = d_exponential(0.01)
  0.1 * I -> D = d_lognormal(2, 0.5)
  0.9 * I -> R = d_gamma(1/3, 2)
  V -> IV = 0.2 * beta * V * (I + IV) / N
  IV -> R = nonparametric(iv_r_dist)
  IV -> D = d_weibull(scale=2, shape=1.5)
})
```

The model structure in `denim` can easily be scaled up by adding more transitions, each of which typically requires only a single line of code. Moreover, model structure can include additional arbitrary parameters as variables for mathematical expressions (`beta`, `N`) or distributional parameters (`iv_r_dist`), which allows customizable transitions.

3.2 | Model configurations

The initial values for each compartment can be defined as *key-value* pairs (using an R named list or named vector), where *key* is the compartment name and *value* is its initial population.

Any additional parameters (i.e. variables in the mathematical expressions and distributional parameters) must also be provided in a similar way where *key* is the name of the parameter and *value* is the corresponding value.

The initial states and parameters for the above model can be defined as follows:

```
initialValues <- c(S=999, I=1, R=0, V=0, IV=0, D=0)
parameters <- list(
  beta=0.9,
  N=1000,
  iv_r_dist = c(0, 0.15, 0.15, 0.05, 0.2, 0.2, 0.25)
)
```

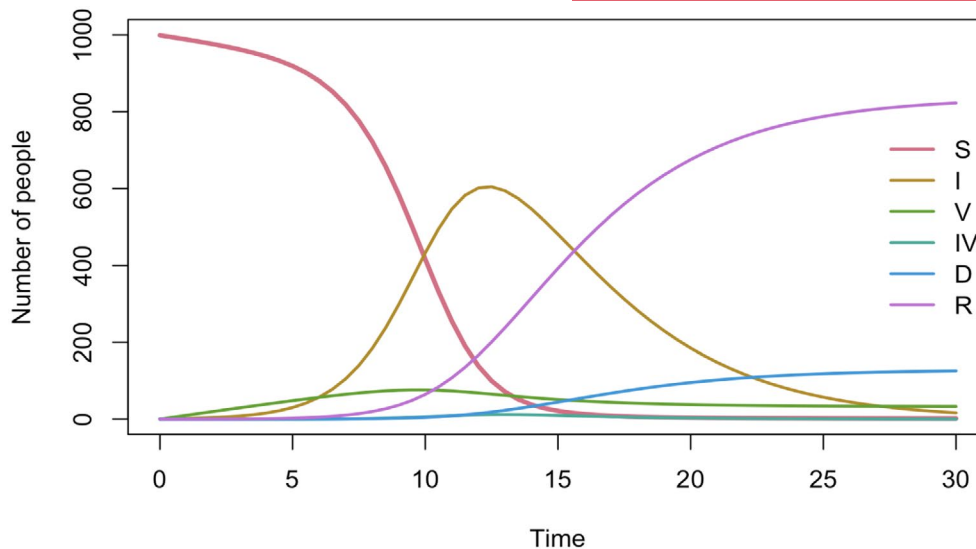


FIGURE 7 Denim plot output for the example model.

By default, the initial population of a compartment is assigned to the first sub-compartment. In this example, denim will internally initialize the first sub-compartment of the $I \rightarrow R$ chain to 0.9, that of the $I \rightarrow D$ chain to 0.1 and the subsequent sub-compartments with a population of 0. Users can also choose to distribute the initial values based on the waiting time distribution by setting the parameter `dist_init` of distribution transitions to `TRUE` as follows:

```
distributeInitVal <- denim_dsl({
  S -> I = beta * S * (I + IV) / N
  S -> V = d_exponential(0.01)
  0.1 * I -> D = d_lognormal(2, 0.5, dist_init =
    TRUE)
  0.9 * I -> R = d_gamma(1/3, 2, dist_init =
    TRUE)
  V -> IV = 0.2 * beta * V * (I + IV) / N
  IV -> R = nonparametric(iv_r_dist)
  IV -> D = d_weibull(scale=2, shape=1.5)
})
```

In a competing risks scenario (i.e. $IV \rightarrow R$ and $IV \rightarrow D$), `dist_init` configuration is ignored and the default behaviour is applied.

3.3 | Simulator

After defining model structure and configuration, a simulation can be created by using the function `sim` of `denim`. To do this, two additional parameters are required: `simDuration` for the simulation time and `timeStep` for the duration of each time step. These configurations will determine the total number of simulated time steps (i.e. `simDuration/timeStep`) and the length of each sub-compartment chain (computed by dividing the maximal dwell time in a compartment by `timeStep`).

To simulate the model defined above with a duration of 30 and a time step size of 0.5, the code in R is as follows:

```
simulation <- sim(transitions = modelStructure,
  initialValues = initialValues,
  parameters = parameters,
  simulationDuration=30,
  timeStep=0.5)
```

3.4 | Output

By default, denim returns an R object of class `denim`, which inherits from `data.frame` and provides additional utilities, such as plotting. The returned object stores the population for each compartment at each time step.

Simply call `print(simulation)` to print the underlying data frame, or call `plot(simulation)` to create a plot for the disease dynamics over time (Figure 7).

4 | DISCUSSION

In this paper, we propose a modelling framework to easily and intuitively render any kind of dwell-time distribution. Accompanying it is the `denim` package, which implements the proposed algorithm, with a user-friendly interface to define the model structure in a clear and concise way. We also demonstrate how a compartmental model can be seamlessly translated into code in `denim`.

We envision that `denim` will be an essential tool for model selection, thanks to the ease of modification from one dwell-time distribution to another. The package `denim` is especially useful for modelling diseases with infectious period distributions that

cannot be formulated using ODEs (e.g. log-normal (Nishiura & Eichner, 2006), Weibull (Hellewell et al., 2020; Kuk & Ma, 2005), gamma with non-integer shape parameter). Additionally, the declarative nature of the package enhances the readability of the model definition, thus promoting reproducibility, and improving the maintainability and reusability of the code.

Compared to existing ODE numerical solvers available in R (e.g. `deSolve` (Soetaert et al., 2008), `diffeqr` (Rackauckas, 2018)), `denim` requires longer run time due to the need to iterate over the sub-compartments to update their populations (see Supporting Information S2, sections 2 and 3). Its discrete-time formulation also implies that the value of time step may have an impact on the output of the model. The use of a fixed time step, as opposed to the adaptive step-size approach employed by ODE solvers, also contributes to the longer run time in `denim`. However, for most practical applications, the longer run time remains manageable. These downsides are also compensated for by several key advantages.

- Concise model definition: Using `denim` DSL, the transition between two compartments can be defined in a single line of code. This simplicity is particularly apparent when comparing the implementation for Erlang-distributed transition using `deSolve` by applying the LCT (refer to https://drthinong.com/denim/articles/deSolve_to_denim.html).
- Flexible dwell-time distribution: Users can easily incorporate any transition distribution shapes, which is essential for assessing the impact of different dwell-time distribution on the disease dynamics. Notably, `denim` is the only package that can handle multiple competing outgoing transitions that are arbitrarily distributed.
- Direct integration of empirical data: The option to provide the distribution as a histogram allows the users to directly use empirical data on dwell time for modelling.

To the best of our knowledge, there is no simulation package tailored for simulating compartmental models with diverse built-in dwell-time distributions. To promote adoption, we also provide a step-by-step migration guide from `deSolve`—a widely used ODE-based modelling package, to `denim` (https://drthinong.com/denim/articles/deSolve_to_denim.html).

For future versions of the package, we plan to extend support for a broader range of parametric distributions, including but not limited to Pareto, inverse Gaussian, Gompertz and log-logistic. Improving the package run time is also one of the priorities, as this can be essential during the model fitting process.

AUTHOR CONTRIBUTIONS

Marc Choisy, Thinh Phuc Ong and Lam Minh Ha conceived the ideas and designed the methodology. Thinh Phuc Ong and Anh Truong Quynh Phan developed the package. Marc Choisy, Thinh Phuc Ong and Anh Truong Quynh Phan led the writing of the manuscript. All authors contributed critically to the drafts and gave final approval for publication.

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CONFLICT OF INTEREST STATEMENT

The authors declare no conflicts of interest.

PEER REVIEW

The peer review history for this article is available at <https://www.webofscience.com/api/gateway/wos/peer-review/10.1111/2041-210x.70256>.

DATA AVAILABILITY STATEMENT

The `denim` package is available on CRAN (<https://cran.r-project.org/package=denim>; Ong et al., 2024). The source code is publicly available via Zenodo (<https://doi.org/10.5281/zenodo.18309307>; Phan et al., 2026) and Github (<https://github.com/thinhong/denim>). No data were used in this study. The anonymized GitHub repository for `denim` is available at <https://anonymous.4open.science/r/denim-72E0/README.md>.

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SUPPORTING INFORMATION

Additional supporting information can be found online in the Supporting Information section at the end of this article.

Data S1: Mathematical formulation of the simulation algorithm implemented in *denim*.

Data S2: *denim* implementation details, benchmarking and performance scaling.

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