

S1 Appendix – Comparison of modelling paradigms

Supporting Information for Picault *et al.*, “EMULSION: transparent and flexible multiscale stochastic models in human, animal or plant epidemiology”

This document illustrates how two classical models (SIR, section A and SIR with birth and death processes, section B) are implemented using EMULSION using the three modelling paradigms provided by the software: compartment-based, hybrid and individual-based. For each modelling paradigm and each model, EMULSION outputs are also compared with outputs produced for the same model using the R library SimInf (Widgren *et al.* 2016), which is compartment-based.

A comparison of execution times for each modelling paradigm and each model, based on 500 stochastic repetitions for each EMULSION model, is given in table A. Simulations were run on a MacBook Pro (3.3 GHz Intel Core i5, 16 Gb RAM, MacOS 10.14). Memory usage was about 140 Mb in each case.

		compartment	hybrid	IBM
SIR model	duration (s)	84	130	167
	<i>relative</i>	<i>1</i>	<i>1.5</i>	<i>2.0</i>
SIR model + birth/death	duration (s)	120	191	387
	<i>relative</i>	<i>1</i>	<i>1.6</i>	<i>3.2</i>
	<i>relative to SIR</i>	<i>1.4</i>	<i>2.3</i>	<i>4.6</i>

Table A: Execution time (s) for the 500 stochastic repetitions with each modelling paradigm and each model

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A SIR model

This section compares how a classical SIR model is implemented in EMULSION as compartment-based, hybrid and individual-based models (respectively, `compartment_SIR.yaml`, `hybrid_SIR.yaml` and `IBM_SIR.yaml`).

All files correspond to the same epidemiological model, represented by the state machine diagram on Figure A. This diagram can be produced with the following command:

```
emulsion diagrams compartment_SIR.yaml
```

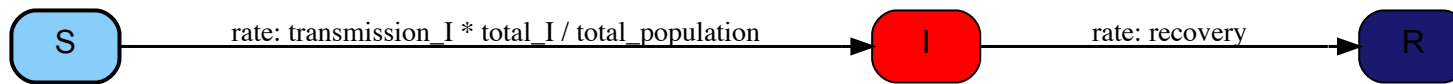


Figure A: State machine diagram associated with a classical SIR model.

The deterministic version of this model can be described through the following Ordinary Differential Equation (ODE) system, where β denotes the transmission rate (parameter `transmission_I`), γ the recovery rate (`recovery`), and $N = S + I + R$ the total population (`total_population`), and S, I, R the amount of individuals in each health state (resp. susceptible, infectious, resistant).

$$\begin{cases} \frac{dS}{dt} = -S\frac{\beta I}{N} \\ \frac{dI}{dt} = S\frac{\beta I}{N} - \gamma I \\ \frac{dR}{dt} = \gamma I \end{cases}$$

Figure B presents simulation outputs produced by EMULSION for each paradigm and by the compartment-based R library `SimInf`, with 500 stochastic repetitions. The dynamics of the deterministic model was added to each of them.

Figure C (resp. D) shows the differences between the files used to represent the SIR in EMULSION as a compartment-based model and as a hybrid model (resp. as a hybrid model and as an individual-based model).

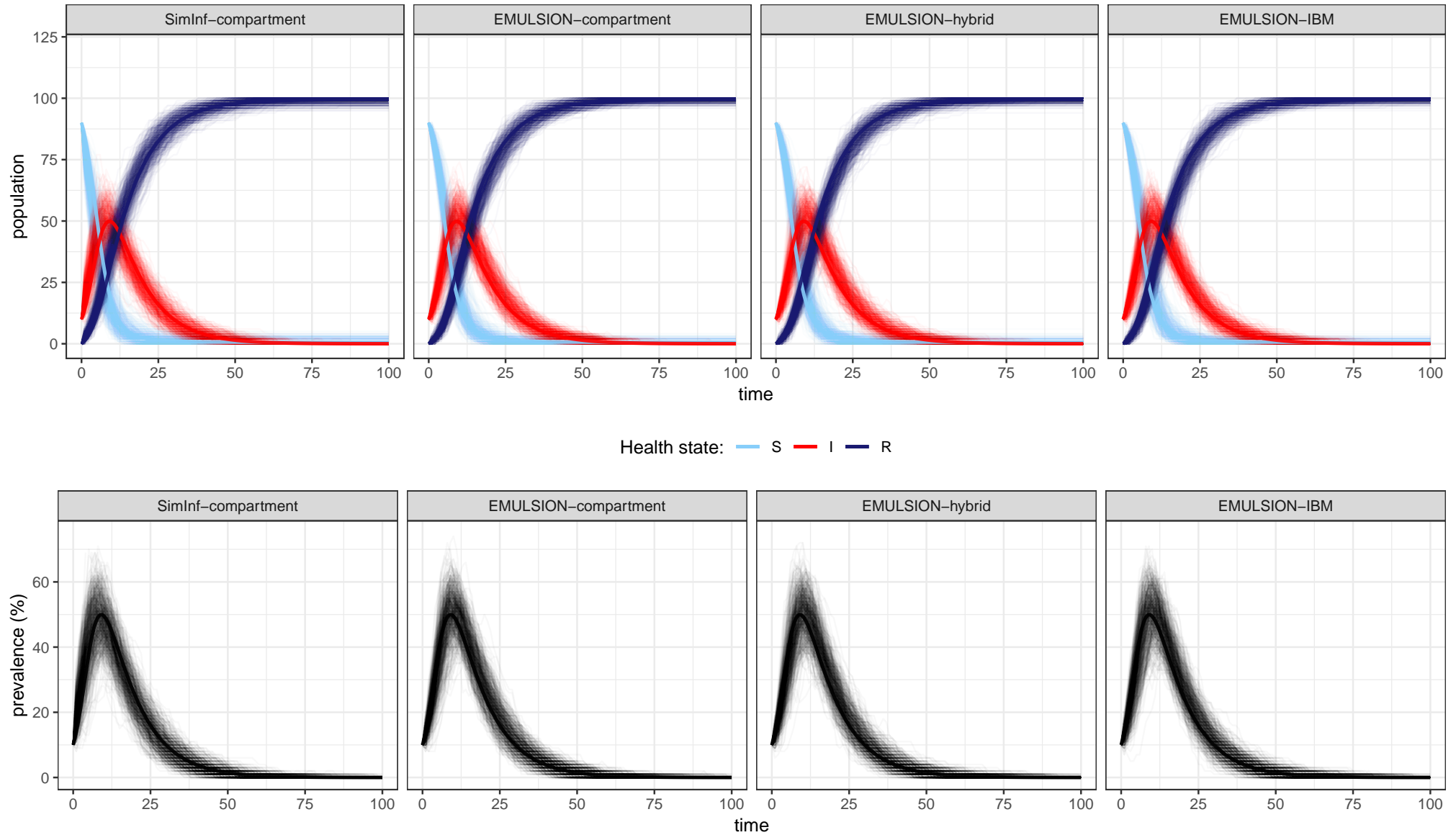


Figure B: Simulation outputs produced for the SIR model (500 stochastic repetitions) with the compartment-based R library SimInf (column 1) and in each modelling paradigm with EMULSION (columns 2-4). Strong lines represent the deterministic version of the model, which corresponds to the average behaviour when infection persists. Parameters: $\text{transmission_I} = 0.5$; $\text{recovery} = 0.1$; $\text{initial_population_size} = 100$; $\text{initial_prevalence} = 0.1$

```

compartment_SIR.yaml
1 # general information
2 model_name: compart_SIR
3
4 model_info:
5 abstract: 'This model is a simple discrete-time, stochastic,
6 compartment-based SIR model.'
7 author: 'Sebastien Picault (sebastien.picault@inra.fr)'
8
---
15 # definition of modelling paradigm, processes and scales
16 levels:
17 population:
18 desc: 'level of the population'
19 aggregation_type: 'compartment'
20
---
72 percentage_prevalence:
73 desc: 'proportion of infectious individuals (%)'
74 value: '100 * total_I / total_population'
75
76 # initial conditions
77 initial_conditions:
78 population:
79 - population:
80 - total: 'initial_population_size'
81 - vars: [I]
82 amount: 'initial_population_size * initial_prevalence'
83
---
hybrid_SIR.yaml
1 # general information
2 model_name: hybrid_SIR
3
4 model_info:
5 abstract: 'This model is a simple discrete-time, stochastic,
6 hybrid SIR model (with individuals grouped automatically).'
7 author: 'Sebastien Picault (sebastien.picault@inra.fr)'
8
---
15 # definition of modelling paradigm, processes and scales
16 levels:
17 population:
18 desc: 'level of the population'
19 aggregation_type: 'hybrid'
20 contains:
21 - individuals
22 individuals:
23 desc: 'level of the individuals'
24
---
76 percentage_prevalence:
77 desc: 'proportion of infectious individuals (%)'
78 value: '100 * total_I / total_population'
79
80 # prototypes = examples of typical agents for each level,
81 # characterized by specific variable values
82 prototypes:
83 individuals:
84 - healthy:
85 desc: 'healthy individuals'
86 health_state: S
87 - infected:
88 desc: 'infected individuals'
89 health_state: I
90
91 # initial conditions
92 initial_conditions:
93 population:
94 - prototype: healthy
95 amount: 'initial_population_size * (1 - initial_prevalence)'
96 - prototype: infected
97 amount: 'initial_population_size * initial_prevalence'
98

```

Figure C: Differences between the compartment-based (`compartment_SIR.yaml`) and the hybrid (`hybrid_SIR.yaml`) versions of the SIR model in EMULSION, presented side-by-side and highlighted (in bold; red: parts removed, green: parts added; yellow: parts modified; dashes: skipped identical lines).

hybrid_SIR.yaml

```

1 # general information
2 model_name: hybrid_SIR
3
4 model_info:
5 abstract: 'This model is a simple discrete-time, stochastic,
6 hybrid SIR model (with individuals grouped automatically).'

```

IBM_SIR.yaml

```

1 # general information
2 model_name: IBM_SIR
3
4 model_info:
5 abstract: 'This model is a simple discrete-time, stochastic,
6 individual-based SIR model (with fully autonomous individuals).'

```

Figure D: Differences between the hybrid (hybrid_SIR.yaml) and the individual-based (IBM_SIR.yaml) versions of the SIR model in EMULSION, presented side-by-side and highlighted (in bold; red: parts removed, green: parts added; yellow: parts modified; dashes: skipped identical lines).

B SIR model with births and deaths

This section compares how a classical SIR model with birth and death processes is implemented in EMULSION as compartment-based, hybrid and individual-based models (respectively, `compartment_SIR_demo.yaml`, `hybrid_SIR_demo.yaml` and `IBM_SIR_demo.yaml`).

All files correspond to the same epidemiological model, represented by the state machine diagram on Figure E. This diagram can be produced with the following command:

```
emulsion diagrams compartment_SIR_demo.yaml
```

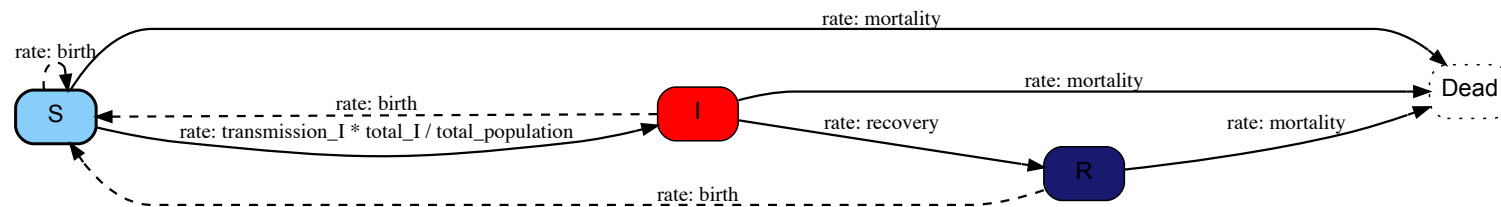


Figure E: State machine diagram associated with a SIR model with birth and death processes. The “Dead” state surrounded by dots is intended to represent individuals removed from the system; dashed arrows represent production links, i.e. how individuals produce new individuals.

The deterministic version of this model can be described through the following Ordinary Differential Equation (ODE) system, where β denotes the transmission rate (parameter `transmission_I`), γ the recovery rate (`recovery`), b the birth rate (`birth`), μ the mortality rate (`mortality`), and $N = S + I + R$ the total population (`total_population`), and S, I, R the amount of individuals in each health state (resp. susceptible, infectious, resistant).

$$\begin{cases} \frac{dS}{dt} = -S\frac{\beta I}{N} + bN - \mu S \\ \frac{dI}{dt} = S\frac{\beta I}{N} - \gamma I - \mu I \\ \frac{dR}{dt} = \gamma I - \mu R \end{cases}$$

Figure F presents simulation outputs produced by EMULSION for each paradigm and by the compartment-based R library `SimInf`, with 500 stochastic repetitions. The dynamics of the deterministic model was added to each of them.

Figure G (resp. H) shows the differences between the files used to represent the SIR in EMULSION as a compartment-based model and as a hybrid model (resp. as a hybrid model and as an individual-based model).

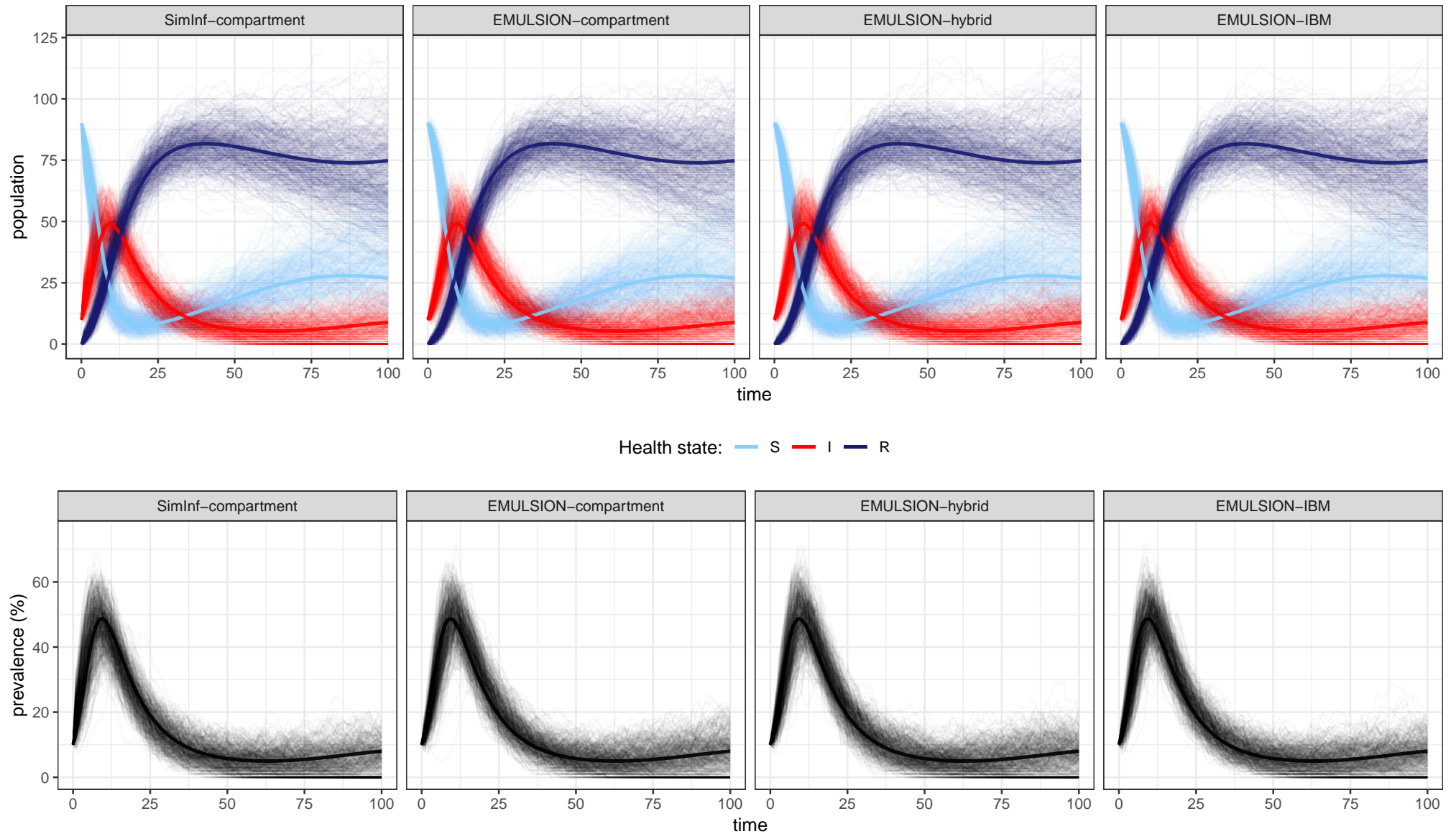


Figure F: Simulation outputs produced for the SIR model with birth/death (500 stochastic repetitions) with the compartment-based R library SimInf (column 1) and in each modelling paradigm with EMULSION (columns 2–4). Strong lines represent the deterministic version of the model, which corresponds to the average behaviour when infection persists. Parameters: $\text{transmission}_I = 0.5$; $\text{recovery} = 0.1$; $\text{birth} = 0.011$; $\text{mortality} = 0.01$; $\text{initial_population_size} = 100$; $\text{initial_prevalence} = 0.1$

```

compartment_SIR_demo.yaml
1 # general information
2 model_name: compart_SIR_demo
3
4 model_info:
5 abstract: 'This model is a simple discrete-time, stochastic,
6 compartment-based SIR model with births and deaths.'
7
8 author: 'Sebastien Picault (sebastien.picault@inra.fr)'
9
---
15 # definition of modelling paradigm, processes and scales
16 levels:
17 population:
18 desc: 'level of the population'
19 aggregation_type: 'compartment'
20
---
65 productions:
66 - {from: S, to: S, rate: 'birth'}
67 - {from: I, to: S, rate: 'birth'}
68 - {from: R, to: S, rate: 'birth'}
69
---
90 mortality:
91 desc: 'mortality rate (/day)'
92 value: 0.01
93
94 # initial conditions
95 initial_conditions:
96 population:
97 - population:
98 - total: 'initial_population_size'
99 - vars: [I]
100 amount: 'initial_population_size * initial_prevalence'
101

hybrid_SIR_demo.yaml
1 # general information
2 model_name: hybrid_SIR_demo
3
4 model_info:
5 abstract: 'This model is a simple discrete-time, stochastic,
6 hybrid SIR model (with individuals grouped automatically),
7 with births and deaths.'
8 author: 'Sebastien Picault (sebastien.picault@inra.fr)'
9
---
16 # definition of modelling paradigm, processes and scales
17 levels:
18 population:
19 desc: 'level of the population'
20 aggregation_type: 'hybrid'
21 contains:
22 - individuals
23 individuals:
24 desc: 'level of the individuals'
25
---
70 productions:
71 - {from: S, to: S, rate: 'birth', prototype: 'healthy'}
72 - {from: I, to: S, rate: 'birth', prototype: 'healthy'}
73 - {from: R, to: S, rate: 'birth', prototype: 'healthy'}
74
---
95 mortality:
96 desc: 'mortality rate (/day)'
97 value: 0.01
98
99 # prototypes = examples of typical agents for each level,
100 # characterized by specific variable values
101 prototypes:
102 individuals:
103 - healthy:
104 desc: 'healthy individuals'
105 health_state: S
106 - infected:
107 desc: 'infected individuals'
108 health_state: I
109
110 # initial conditions
111 initial_conditions:
112 population:
113 - prototype: healthy
114 amount: 'initial_population_size * (1 - initial_prevalence)'
115 - prototype: infected
116 amount: 'initial_population_size * initial_prevalence'
117

```

Figure G: Differences between the compartment-based (`compartment_SIR_demo.yaml`) and the hybrid (`hybrid_SIR_demo.yaml`) versions of the SIR model with birth/death in EMULSION, presented side-by-side and highlighted (in bold; red: parts removed, green: parts added; yellow: parts modified; dashes: skipped identical lines).

hybrid_SIR_demo.yaml

```

1 # general information
2 model_name: hybrid_SIR_demo
3
4 model_info:
5   abstract: 'This model is a simple discrete-time, stochastic,
6   hybrid SIR model (with individuals grouped automatically),
7   with births and deaths.'
8   author: 'Sebastien Picault (sebastien.picault@inra.fr)'
9
---
16 # definition of modelling paradigm, processes and scales
17 levels:
18   population:
19     desc: 'level of the population'
20     aggregation_type: 'hybrid'
21     contains:
22       - individuals
23   individuals:
24     desc: 'level of the individuals'
25
26 processes:
27 # only one process, at population level
28   population:
29     - infection
30
31 grouping:
32   population:
33     infection:
34       # process "infection" relies on the health_state state machine
35       machine_name: health_state
36       # and on the grouping of all "individuals" in the same health state
37       key_variables: [health_state]
38

```

IBM_SIR_demo.yaml

```

1 # general information
2 model_name: IBM_SIR_demo
3
4 model_info:
5   abstract: 'This model is a simple discrete-time, stochastic,
6   individual-based SIR model (with fully autonomous individuals),
7   with births and deaths.'
8   author: 'Sebastien Picault (sebastien.picault@inra.fr)'
9
---
16 # definition of modelling paradigm, processes and scales
17 levels:
18   population:
19     desc: 'level of the population'
20     aggregation_type: 'IBM'
21     contains:
22       - individuals
23   individuals:
24     desc: 'level of the individuals'
25
26 processes:
27 # only one process, at individuals level, driven directly by state machines
28   individuals:
29     - health_state

```

30

Figure H: Differences between the hybrid (hybrid_SIR_demo.yaml) and the individual-based (IBM_SIR_demo.yaml) versions of the SIR model with birth/death in EMULSION, presented side-by-side and highlighted (in bold; red: parts removed, green: parts added; yellow: parts modified; dashes: skipped identical lines).