

# Leveraging artificial intelligence and software engineering methods in epidemiology for the co-creation of decision-support tools based on mechanistic models

## Supporting information

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## 1 A full example of an PASTE-generated web application

This section presents additional screenshots from the web tool on Bovine Respiratory Disease (main manuscript sections 2.5 and 3.2) with the underlying YAML specification.

### Execution

---

Simulation duration (half days):



Simulation name

contrasted\_isolated

Simulation description

Calves with low and high risk levels, allocated in perfectly isolated batches

first step | prev step

Step 3 of 3

Figure SI1. Input form for simulation execution. The user can indicate the duration of the period to simulate, associated with a simulation name and comments. The form specifications are defined in the YAML file L80-192 (Fig. SI2).

```

80 input_forms:
167 .....
167 - execution:
168     - total_duration:
169         type: IntegerField
170         label: "Simulation duration (half days)"
171         required: True
172         widget: NumberInput
173         widget_attrs:
174             'data-min': 0
175             'data-step': 2
176             'data-value': 60
177             'data-skin': 'round'
178             'data-label': 'half days'
179             'data-grid': 'true'
180             'data-grid-num': 5
181             'data-max': 100
182     - simulation_name:
183         type: CharField
184         label: "Simulation name"
185         required: True
186         widget: forms.TextInput
187
188     - simulation_description:
189         type: CharField
190         label: "Simulation description"
191         required: False
192         widget: forms.Textarea

```

Figure S12. Specification of the execution input form (Fig. S11)

Mean Clinical signs in all scenarios

comparison dose in all scenarios

### Animals with severe clinical signs

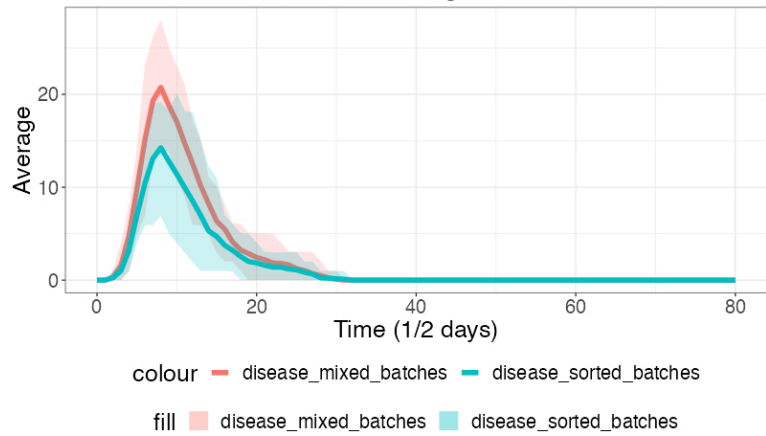


Figure S13. Output page showing results at farm scale over time. The figure presents the number of severely diseased animals (average and 5th-95th percentiles) over time in two scenarios. The graph definition is L255-280, based on the treatment of simulation results specified in L195-207 (Fig. S14).

```

194 statistics:
195   for_each_scenario:
196     - mean_C:
197       - desc: "Animals with severe clinical signs (mean, q05, q95)"
198       - target_variable: [ "metapop_total_C" ]
199       - groupby: [ "step" ]
200       - summarise:
201         - mean
202         - perc_0.5:
203           value: "quantile(..., 0.05)"
204           desc: "5th percentile"
205         - perc_0.95:
206           value: "quantile(..., 0.95)"
207           desc: "95th percentile"
254 .....
254 graphics:
255   plot_mean_C:
256     - data: "mean_C"
257     - on_page: ["Building"]
258     - label: ["Mean Clinical signs in all scenarios"]
259     - single_graph: "yes"
260     - scenario: ["disease_mixed_batches", "disease_sorted_batches"]
261     - plot_variables:
262       x: "step"
263       y: "mean_metapop_total_C"
264     - plot_type:
265       - line:
266         plot_variables:
267           colour: "scenario_name"
268         plot_options:
269           linewidth: "2"
270       - ribbon:
271         plot_variables:
272           ymax: "perc_0.95_metapop_total_C"
273           ymin: "perc_0.5_metapop_total_C"
274           fill: "scenario_name"
275         plot_options:
276           alpha: "0.2"
277     - plot_annotations:
278       title: "Animals with severe clinical signs"
279       x_title: "Time (1/2 days)"
280       y_title: "Average"

```

Figure S14. Specification of the plot (Fig. S13)

Mean Clinical signs in all scenarios  
 comparison dose in all scenarios

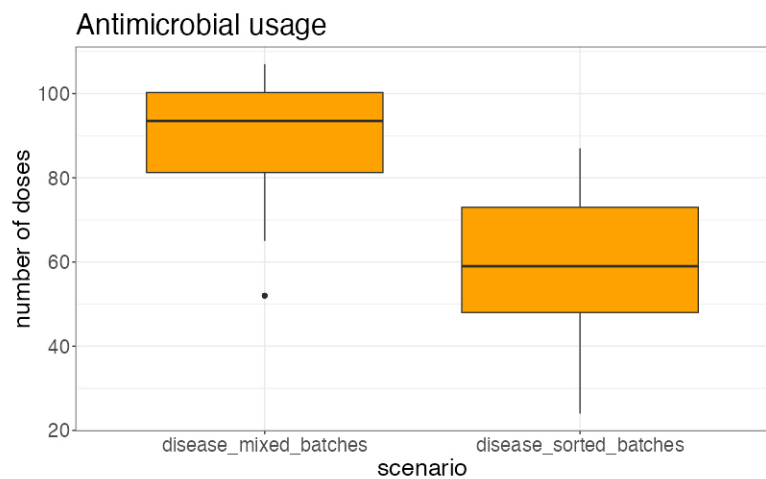


Figure S15. Output page showing AMU at farm scale. The figure presents the number of antimicrobial doses used by all batches (distribution over the stochastic repetitions) in two scenarios (left vs. right). The graph definition is L358-371, based on the treatment of simulation results specified in L208-211 (Fig. S16).

```

194 statistics:
.....
208   - nb_doses:
209     - desc: "Number of doses at farm scale"
210     - target_variable: [ "metapop_nb_doses" ]
211     - condition: [ 'step == MAX.STEP' ]
.....
254 graphics:
.....
358 plot_doses:
359   - data: "nb_doses"
360   - on_page: ["Building"]
361   - label: ["comparison dose in all scenarios"]
362   - single_graph: "yes"
363   - scenario: ["disease_mixed_batches", "disease_sorted_batches"]
364   - plot_variables:
365     y: "metapop_nb_doses"
366   - plot_type:
367     - boxplot:
368       plot_variables:
369         x: "scenario_name"
370       plot_options:
371         fill: "orange"
    
```

Figure S16. Specification of the plot (Fig. S15).

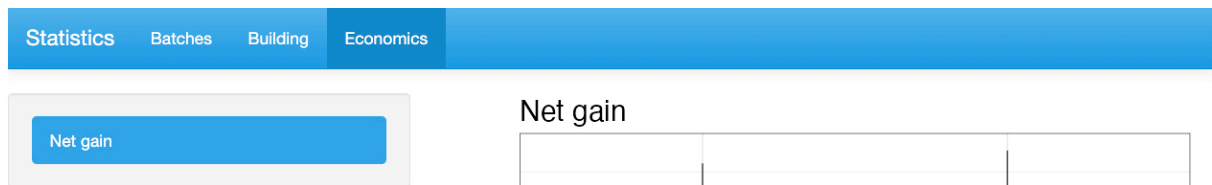


Figure S17. Output page showing economic gain at farm scale. The figure presents the net gain of fattening at farm scale (distribution over the stochastic repetitions) in two scenarios (left vs. right). The graph definition is L388-390, based on the treatment of simulation results specified in L239-246 (Fig. S18).

```

194 statistics:
239 .....
239     - economics:
240         - desc: "Net gain of fattening"
241         - target_variable: ["total_population", "metapop_nb_doses", '
242         - condition: [ 'step == MAX.STEP' ]
243         - add_new_column:
244             gain:
245                 value: "selling_price_bull * total_population - cost_l
246                 desc: "Net gain"
247 .....
254 graphics:
378 .....
378     plot_gains:
379         - data: "economics"
380         - on_page: ["Economics"]
381         - label: ["Net gain"]
382         - single_graph: "yes"
383         - scenario: ["disease_mixed_batches", "disease_sorted_batches"]
384         - plot_variables:
385             y: "gain"
386         - plot_type:
387             - boxplot:
388                 plot_variables:
389                     x: "scenario_name"
390                 plot_options:

```

Figure S18 Specification of the plot (Fig. S17).

## 2 PASTE tool specification (YAML file) for the BRD example

This file is available on the public PASTE GIT repository (<https://forgemia.inra.fr/dynamo/software/PASTE-public-release>), in directory "[PASTE\\_examples/brd\\_example](#)".

```
1  django_project_name: brd_project
2
3  django_app_name: brd_app
4
5  input_files_path:
6    path: brd_tool_specification/input_files
7
8  model_emulsion_file:
9    file_name: brd-svepm-paste.yaml
10
11  emulsion_output_directory:
12    path: outputs/
13
14  emulsion_setup:
15    model_name: BRD
16    number_of_repetitions: 20
17    figure_text_size: 20
18
19    emulsion_syntax:
20      command: 'emulsion run'
21      runs: '-r'
22      outputs: '--output-dir'
23      options: '--silent'
24      params: '-p'
25
26  show_hidden_parameters: no
27
28  calcul_URI: "http://127.0.0.1:8100/"
29
30  input_parameters:
31    - block_values:
32      pathogen:
33        - file_path: "input_files/pathogens.csv"
34      batch_isolation:
35        - file_path: "input_files/biosecurity.csv"
36      risk_level:
37        - file_path: "input_files/risk_level.csv"
38
39    - user_parameters_values:
40      - cost_of_antibiotic_dose: 10
41      - cost_purchase_calf: 950
42      - selling_price_bull: 1330
43      - total_feeding_cost: 312
44      - daily_disease_impact: 0.2
45      - batch_size: 10
46      - number_batches: 3
47
48    - user_parameters_matrices: []
49
50  scenarios_components:
51    - health_conditions:
52      - no_disease:
53        optional: "no"
```

```

54     proportion_carrier_low: 0
55     proportion_carrier_medium: 0
56     proportion_carrier_high: 0
57 - disease:
58     optional: "yes"
59
60 - batch_composition:
61 - mixed_batches:
62     optional: "yes"
63     forms:
64     name:
65         - initial_conditions
66     specific_parameters:
67         - sorted_batches: 0
68
69 - sorted_batches:
70     optional: "yes"
71     forms:
72     name:
73         - initial_conditions
74     specific_parameters:
75         - sorted_batches: 1
76
77 scenarios:
78     - ["health_conditions", "batch_composition"]
79
80 input_forms:
81 - initial_conditions:
82     - risk_level:
83         type: CharField
84         label: "Risk level of calves"
85         required: True
86         help_text: "BRD risk associated with calves at purchase"
87         widget: forms.Select
88
89     - batch_isolation:
90         type: CharField
91         label: "Batch isolation"
92         required: True
93         help_text: "Level of isolation between batches"
94         widget: forms.Select
95
96     - pathogen:
97         type: CharField
98         label: "Main pathogen"
99         required: True
100        help_text: "Pathogen identified as major cause of BRD"
101        widget: forms.Select
102
103     - cost_of_antibiotic_dose:
104         type: IntegerField
105         label: "Cost of antibiotic dose"
106         required: True
107         help_text: "cost_of_antibiotic_dose"
108         widget: NumberInput
109
110     - cost_purchase_calf:
111         type: IntegerField
112         label: "Cost of a 7 month-beef calf"
113         required: True
114         help_text: "Cost of a 7 month-beef calf"

```



```

115         widget: NumberInput
116
117     - selling_price_bull:
118         type: IntegerField
119         label: "Selling price of fattened bull"
120         required: True
121         help_text: "selling_price_bull"
122         widget: NumberInput
123
124     - total_feeding_cost:
125         type: IntegerField
126         label: "Total feeding cost"
127         required: True
128         help_text: "total_feeding_cost"
129         widget: NumberInput
130
131     - daily_disease_impact:
132         type: FloatField
133         label: "Daily disease impact (€)"
134         required: True
135         help_text: "daily_disease_impact"
136         widget: NumberInput
137
138     - number_batches:
139         type: IntegerField
140         label: "Number of simultaneous batches"
141         required: True
142         widget: NumberInput
143         widget_attrs:
144             'data-min': 1
145             'data-step': 1
146             'data-value': 3
147             'data-skin': 'round'
148             'data-label': 'batches'
149             'data-grid': 'true'
150             'data-grid-num': 9
151             'data-max': 10
152
153     - batch_size:
154         type: IntegerField
155         label: "Number of calves per batch"
156         required: True
157         widget: NumberInput
158         widget_attrs:
159             'data-min': 0
160             'data-step': 1
161             'data-value': 10
162             'data-skin': 'round'
163             'data-label': 'animals per batch'
164             'data-grid': 'true'
165             'data-grid-num': 6
166             'data-max': 30
167
168     - execution:
169         - total_duration:
170             type: IntegerField
171             label: "Simulation duration (half days)"
172             required: True
173             widget: NumberInput
174             widget_attrs:
175                 'data-min': 0
176                 'data-step': 2

```

```

176         'data-value': 60
177         'data-skin': 'round'
178         'data-label': 'half days'
179         'data-grid': 'true'
180         'data-grid-num': 5
181         'data-max': 100
182     - simulation_name:
183         type: CharField
184         label: "Simulation name"
185         required: True
186         widget: forms.TextInput
187
188     - simulation_description:
189         type: CharField
190         label: "Simulation description"
191         required: False
192         widget: forms.Textarea
193
194 statistics:
195     for_each_scenario:
196     - mean_C:
197         - desc: "Animals with severe clinical signs (mean, q05, q95)"
198         - target_variable: [ "metapop_total_C" ]
199         - groupby: [ "step" ]
200         - summarise:
201             - mean
202             - perc_0.5:
203                 value: "quantile(..., 0.05)"
204                 desc: "5th percentile"
205             - perc_0.95:
206                 value: "quantile(..., 0.95)"
207                 desc: "95th percentile"
208     - nb_doses:
209         - desc: "Number of doses at farm scale"
210         - target_variable: [ "metapop_nb_doses" ]
211         - condition: [ 'step == MAX.STEP' ]
212
213     - nb_doses_per_batch:
214         - desc: "Number of doses at batch scale"
215         - target_variable: [ "batch_nb_doses" ]
216         - condition: [ 'step == MAX.STEP' ]
217         - add_new_column:
218             batch:
219                 value: "as.factor(population_id + 1)"
220                 desc: "number of the batch"
221
222     - mean_C_per_batch:
223         - desc: "Animals with severe clinical signs (mean, q05, q95)"
224         - target_variable: [ "C" ]
225         - add_new_column:
226             batch:
227                 value: "as.factor(population_id + 1)"
228                 desc: "number of the batch"
229         - groupby: [ "step", "batch" ]
230     - summarise:
231         - mean
232         - perc_0.5:
233             value: "quantile(..., 0.05)"
234             desc: "5th percentile"
235         - perc_0.95:
236             value: "quantile(..., 0.95)"

```

```

237         desc: "95th percentile"
238
239     - economics:
240         - desc: "Net gain of fattening"
241         - target_variable: ["total_population", "metapop_nb_doses",
242 "metapop_clinical_duration"]
243         - condition: [ 'step == MAX.STEP' ]
244         - add_new_column:
245             gain:
246                 value: "selling_price_bull * total_population -
247 cost_purchase_calf * initial_population - total_feeding_cost -
248 cost_of_antibiotic_dose * metapop_nb_doses + daily_disease_impact *
249 metapop_clinical_duration / 24"
250                 desc: "Net gain"
251             comparison_of_scenarios: []
252
253 outputs_pages:
254     - Batches
255     - Building
256     - Economics
257
258 graphics:
259     plot_mean_C:
260         - data: "mean_C"
261         - on_page: ["Building"]
262         - label: ["Mean Clinical signs in all scenarios"]
263         - single_graph: "yes"
264         - scenario: ["disease_mixed_batches", "disease_sorted_batches"]
265         - plot_variables:
266             x: "step"
267             y: "mean_metapop_total_C"
268         - plot_type:
269             - line:
270                 plot_variables:
271                     colour: "scenario_name"
272                 plot_options:
273                     linewidth: "2"
274             - ribbon:
275                 plot_variables:
276                     ymax: "perc_0.95_metapop_total_C"
277                     ymin: "perc_0.5_metapop_total_C"
278                     fill: "scenario_name"
279                 plot_options:
280                     alpha: "0.2"
281         - plot_annotations:
282             title: "Animals with severe clinical signs"
283             x_title: "Time (1/2 days)"
284             y_title: "Average"
285
286     plot_mean_C_disease_mixed_per_batch:
287         - data: "mean_C_per_batch"
288         - on_page: ["Batches"]
289         - label: ["Mean Clinical per batch disease_mixed_batches"]
290         - single_graph: "no"
291         - scenario: ["disease_mixed_batches"]
292         - plot_variables:
293             group: "batch"
294         - plot_type:
295             - line:
296                 plot_variables:
297                     x: "step"

```

```

298         y: "mean_C"
299         colour: "batch"
300     plot_options:
301         linewidth: "2"
302     - ribbon:
303         plot_variables:
304             x: "step"
305             ymax: "perc_0.95_C"
306             ymin: "perc_0.5_C"
307             fill: "batch"
308         plot_options:
309             alpha: "0.2"
310     - plot_annotations:
311         title: "Animals with severe clinical signs (mixed batches)"
312         x_title: "Time (1/2 days)"
313         y_title: "Average"
314
315 plot_mean_C_disease_sorted_per_batch:
316     - data: "mean_C_per_batch"
317     - on_page: ["Batches"]
318     - label: ["Mean Clinical per batch disease_sorted_batches"]
319     - single_graph: "no"
320     - scenario: ["disease_sorted_batches"]
321     - plot_variables:
322         group: "batch"
323     - plot_type:
324         - line:
325             plot_variables:
326                 x: "step"
327                 y: "mean_C"
328                 colour: "batch"
329             plot_options:
330                 linewidth: "2"
331         - ribbon:
332             plot_variables:
333                 x: "step"
334                 ymax: "perc_0.95_C"
335                 ymin: "perc_0.5_C"
336                 fill: "batch"
337             plot_options:
338                 alpha: "0.2"
339     - plot_annotations:
340         title: "Animals with severe clinical signs (sorted batches)"
341         x_title: "Time (1/2 days)"
342         y_title: "Average"
343
344 plot_doses_per_batch:
345     - data: "nb_doses_per_batch"
346     - on_page: ["Batches"]
347     - label: ["Number of doses per batch in all scenarios"]
348     - single_graph: "yes"
349     - scenario: ["disease_mixed_batches", "disease_sorted_batches"]
350     - plot_variables:
351         y: "batch_nb_doses"
352     - plot_type:
353         - boxplot:
354             plot_variables:
355                 x: "scenario_name"
356                 fill: "batch"
357     - plot_annotations:
358         title: "Antimicrobial usage"

```

```

359     x_title: "scenario"
360     y_title: "number of doses"
361
362 plot_doses:
363   - data: "nb_doses"
364   - on_page: ["Building"]
365   - label: ["comparison dose in all scenarios"]
366   - single_graph: "yes"
367   - scenario: ["disease_mixed_batches", "disease_sorted_batches"]
368   - plot_variables:
369     y: "metapop_nb_doses"
370   - plot_type:
371     - boxplot:
372       plot_variables:
373         x: "scenario_name"
374       plot_options:
375         fill: "orange"
376
377   - plot_annotations:
378     title: "Antimicrobial usage"
379     x_title: "scenario"
380     y_title: "number of doses"
381
382 plot_gains:
383   - data: "economics"
384   - on_page: ["Economics"]
385   - label: ["Net gain"]
386   - single_graph: "yes"
387   - scenario: ["disease_mixed_batches", "disease_sorted_batches"]
388   - plot_variables:
389     y: "gain"
390   - plot_type:
391     - boxplot:
392       plot_variables:
393         x: "scenario_name"
394       plot_options:
395         fill: "green"
396   - plot_annotations:
397     title: "Net gain"
398     x_title: "scenario"
399     y_title: "Value"

```