

Simulation and model analysis

Non Linear Dynamics

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as.character(Sys.Date())

LAC Operon Model analysis

Based on Yildirim et al. 2004.

See repository for more information.

Setup

```
library(tidyverse)
library(broom)
```

Scan of appropriate time step size

Loading simulation results

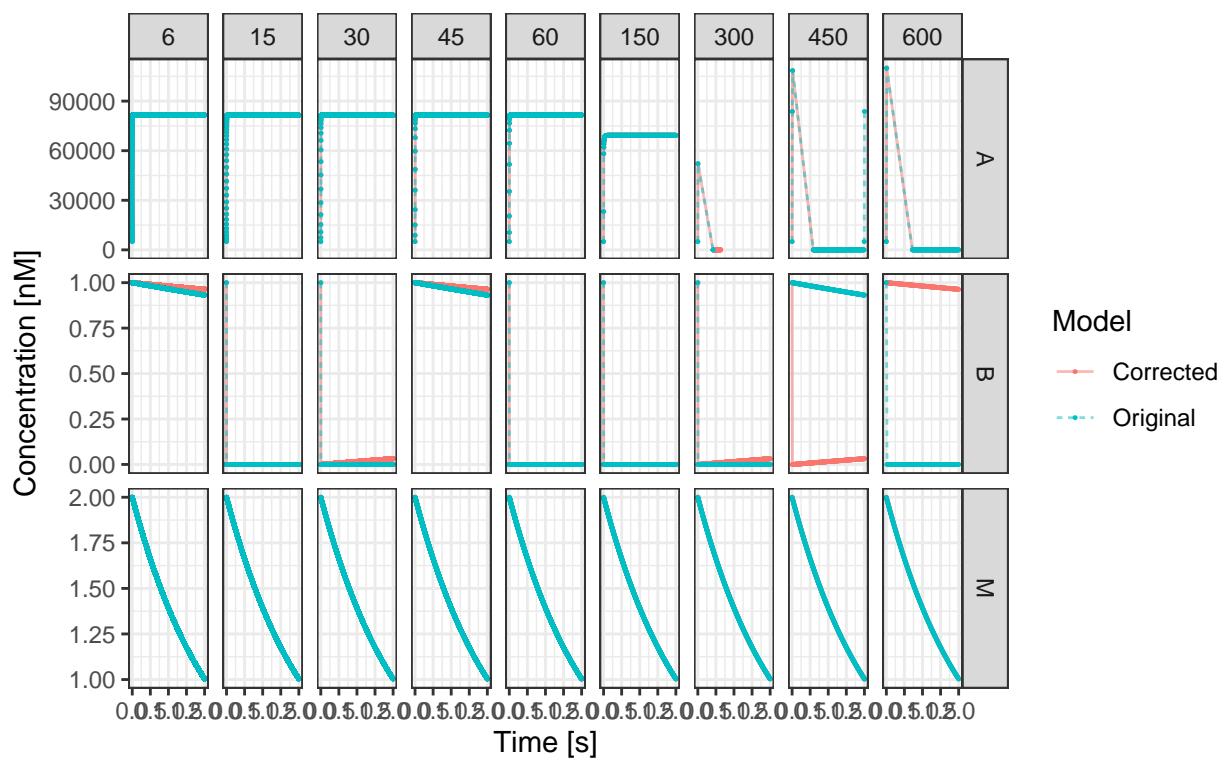
Loading and structuring data:

```
## Rows: 18
## Columns: 3
## $ Model      <chr> "Corrected", "Corrected", "Corrected", "Corrected", "Corrected"
## $ Timestep   <dbl> 0.00010, 0.00025, 0.00050, 0.00075, 0.00100, 0.00250, 0.00500...
## $ Data       <list> [<tbl_df[60003 x 3]>], [<tbl_df[24003 x 3]>], [<tbl_df[12003...
## # A tibble: 6 x 3
##       Time Species Concentration
##   <dbl> <chr>     <dbl>
## 1 0     M          2
## 2 0     B          1
## 3 0     A         5000
## 4 0.0001 M         2.00
## 5 0.0001 B         1.00
## 6 0.0001 A        5419.
```

Visualizing results

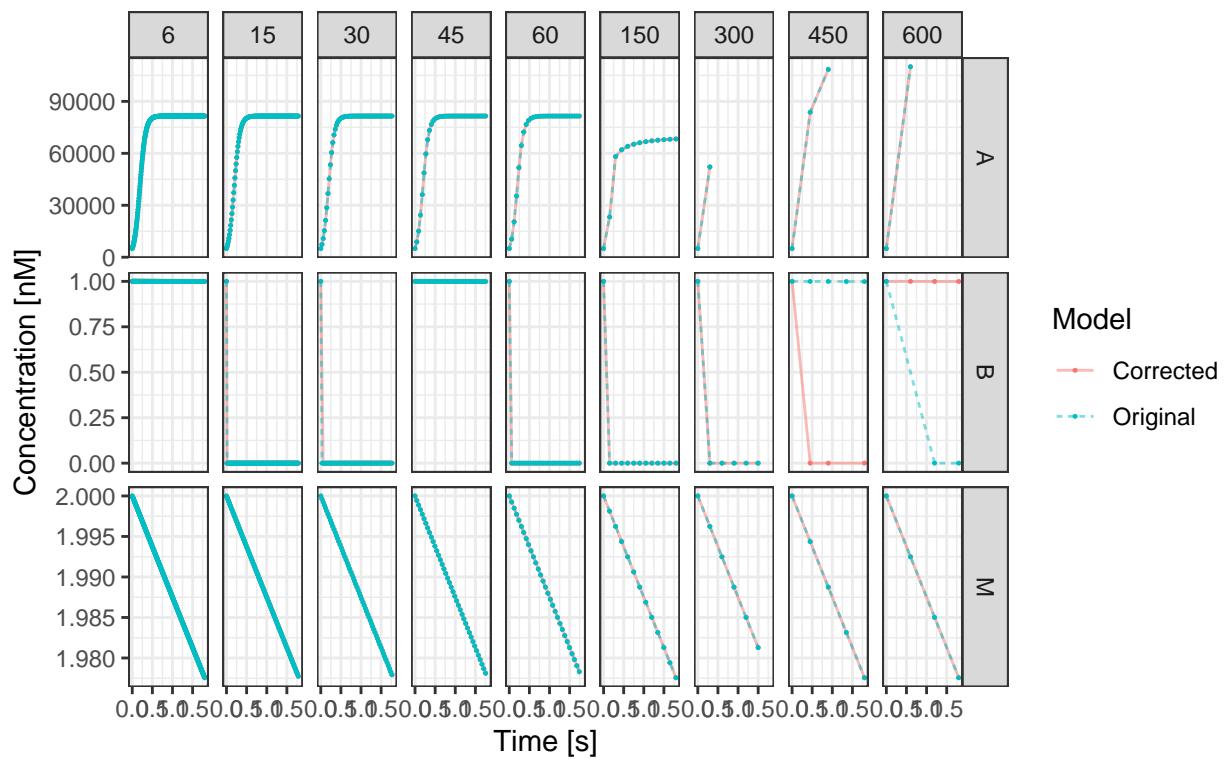
Time course of species by time step size [ms]

Scan of time step size



Time course of species by time step size [ms]

Scan of time step size



Scan of starting conditions

Loading simulation results

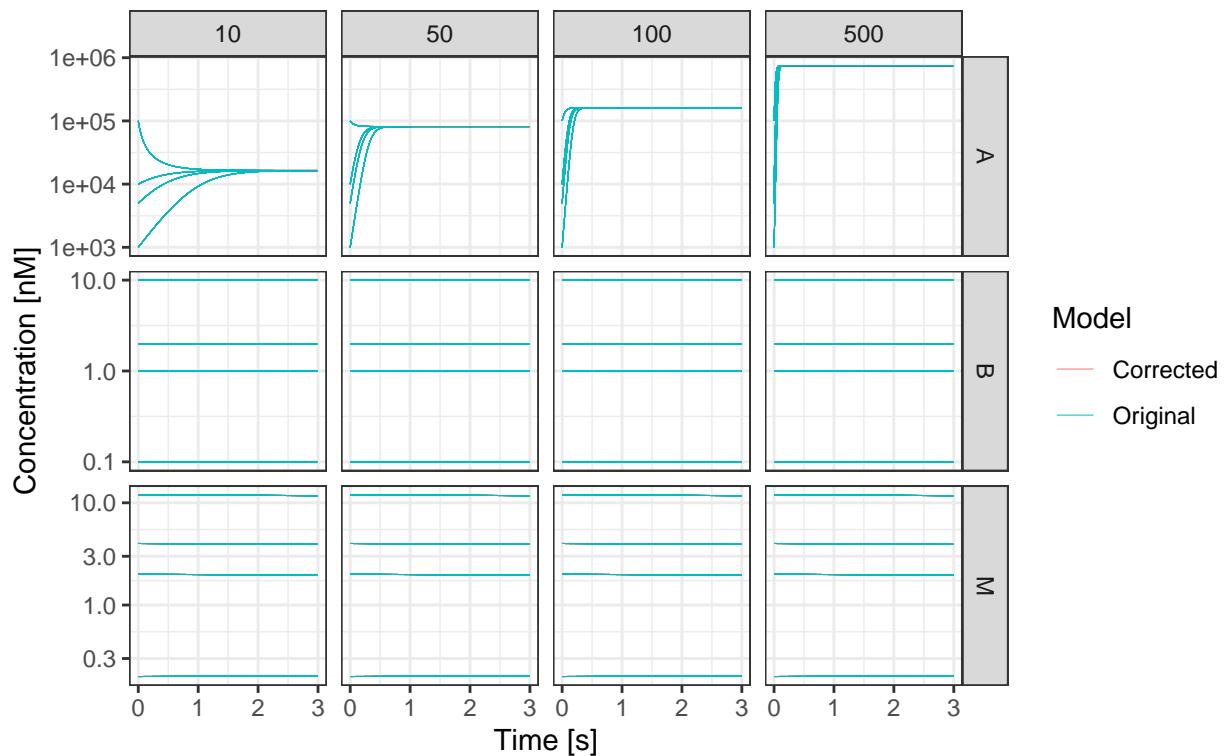
Loading and structuring data:

```
## Rows: 512
## Columns: 6
## $ Model <chr> "Corrected", "Corrected", "Corrected", "Corrected", "Corrected", ~
## $ L      <dbl> 10000, 10000, 10000, 10000, 10000, 10000, 10000, 10000, 1~
## $ M_0    <dbl> 0.2, 0.2, 0.2, 0.2, 0.2, 0.2, 0.2, 0.2, 0.2, 0.2, 0.2, ~
## $ B_0    <dbl> 0.1, 0.1, 0.1, 0.1, 1.0, 1.0, 1.0, 1.0, 10.0, 10.0, 10.0, ~
## $ A_0    <dbl> 1e+03, 1e+04, 1e+05, 5e+03, 1e+03, 1e+04, 1e+05, 5e+03, 1e+03, 1~
## $ Data   <list> [<tbl_df[15003 x 3]>], [<tbl_df[15003 x 3]>], [<tbl_df[15003 x ~
## # A tibble: 6 x 3
##       Time Species Concentration
##     <dbl> <chr>        <dbl>
## 1 0      M            0.2
## 2 0      B            0.1
## 3 0      A           1000
## 4 0.0001 M            0.200
## 5 0.0001 B            0.100
## 6 0.0001 A           1017.
```

Visualizing results

```
conditions_data %>%
  unnest(Data) %>%
  mutate(Time = Time * 60,
         L = L * 1e-3) %>%
  filter(Time < 3) %>%
  ggplot(aes(x=Time, y=Concentration, color=Model, fill=paste0(M_0, B_0, A_0))) +
  geom_line(size=0.1) +
  scale_y_log10() +
  facet_grid(Species~L, scales="free_y") +
  labs(title="Time course of species by lactose concentrations [μM]",
       subtitle="Scan of starting conditions") +
  xlab("Time [s]") +
  ylab("Concentration [nM]") +
  theme_bw()
```

Time course of species by lactose concentrations [μM] Scan of starting conditions



Analysing model differences

Checking null hypothesis: There is no difference between the original and corrected model.

```
conditions_data %>%
  unnest(Data) %>%
  nest(Data=c(Time, Concentration)) %>%
  slice(1)

## # A tibble: 1 x 7
##   Model      L    M_0    B_0    A_0 Species Data
##   <chr>    <dbl> <dbl> <dbl> <dbl> <chr>   <list>
## 1 Corrected 10000    0.2   0.1  1000 M      <tibble [5,001 x 2]>
```