

Simulation and model analysis

Non Linear Dynamics

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LAC Operon Model analysis

Based on Yildirim et al. 2004.

See repository for more information.

Setup

```
library(tidyverse)
library(broom)
options(scipen=999)
```

Scan of appropriate time step size

Loading simulation results

Loading and structuring data:

```
results_dir = "results/timestep_scan"
data <-
  tibble(filename = list.files(results_dir, pattern=".csv")) %>%
  mutate(model = map_chr(filename, ~ str_split(.x, " ") %>% pluck(1, 1)),
         timestep = map_chr(filename, ~ str_split(.x, " ") %>% pluck(1, 2) %>% str_split("=") %>% pluck(1, 1)),
         data = map(paste(results_dir, filename, sep="/"), read.csv),
         data = map(data, ~ .x %>% pivot_longer(-Time, names_to="Species", values_to="Concentration")))
  select(-filename)
```

```
data %>% glimpse()
```

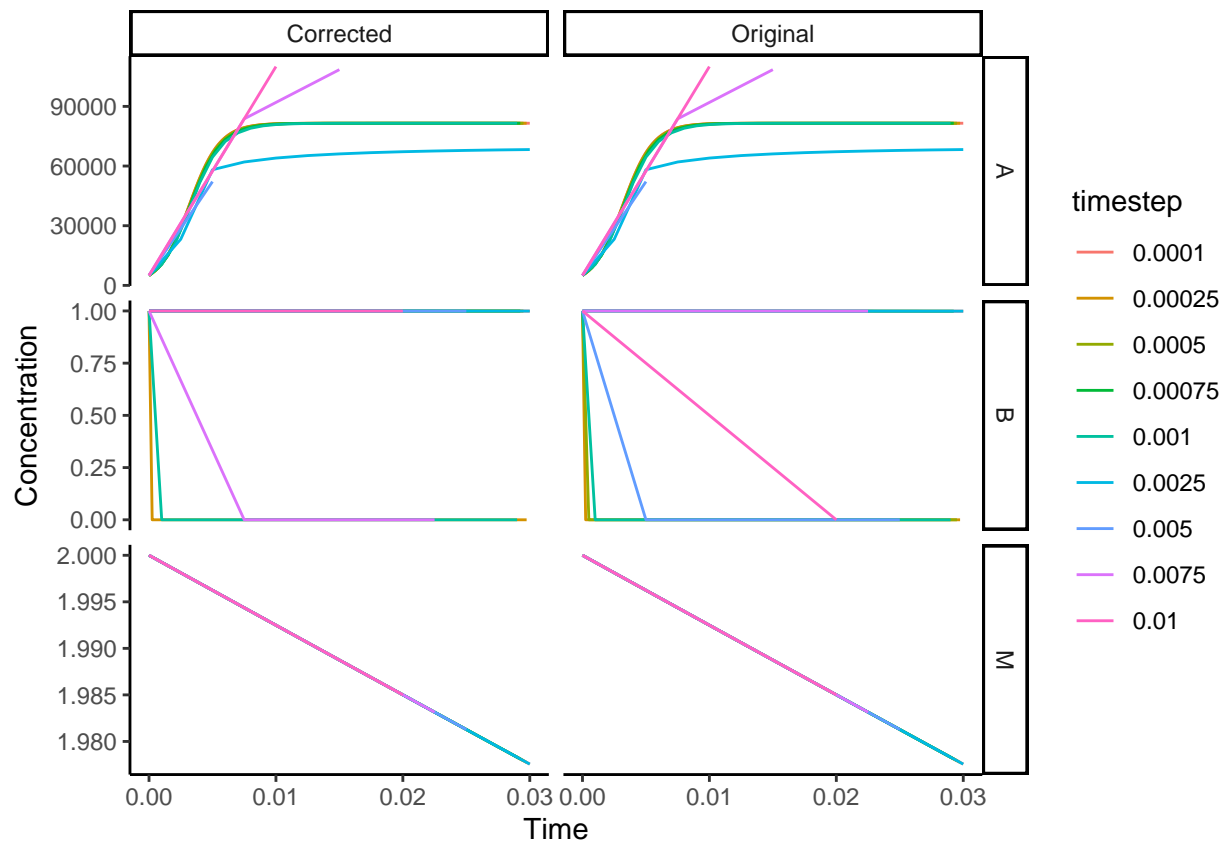
```
## Rows: 18
## Columns: 3
## $ model      <chr> "Corrected", "Corrected", "Corrected", "Corrected", "Corrected", "Corrected", "Corrected", "Corrected", "Corrected", "Corrected", "Corrected", "Corrected", "Corrected", "Corrected", "Corrected", "Corrected", "Corrected"
## $ timestep   <chr> "0.0001", "0.00025", "0.0005", "0.00075", "0.001", "0.0025", "0.005", "0.01", "0.025", "0.05", "0.1", "0.25", "0.5", "1", "2.5", "5"
## $ data       <list> [<tbl_df[60003 x 3]>], [<tbl_df[24003 x 3]>], [<tbl_df[12003 x 3]>], [<tbl_df[60003 x 3]>], [<tbl_df[24003 x 3]>], [<tbl_df[12003 x 3]>], [<tbl_df[60003 x 3]>], [<tbl_df[24003 x 3]>], [<tbl_df[12003 x 3]>], [<tbl_df[60003 x 3]>], [<tbl_df[24003 x 3]>], [<tbl_df[12003 x 3]>], [<tbl_df[60003 x 3]>], [<tbl_df[24003 x 3]>], [<tbl_df[12003 x 3]>], [<tbl_df[60003 x 3]>], [<tbl_df[24003 x 3]>], [<tbl_df[12003 x 3]>]
```

```
data %>% pluck("data", 1) %>% head()
```

```
## # 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

```
data %>%
  unnest(data) %>%
  filter(Concentration > 0) %>%
  filter(Time < 0.03) %>%
  ggplot(aes(x=Time, y=Concentration, color=timestep)) +
  geom_line() +
  facet_grid(Species~model, scales="free_y") +
  theme_classic()
```



Models with a scan of starting conditions

(No data available - still fine tuning simulation parameters like timestep)

Loading simulation results

Loading data into dataframes

```
import_data <- read_csv("results/Starting conditions scan 2022-11-14 00:33:10.csv") %>%
  mutate(across(c(Model, Starting_Conditions_Set, L), as.factor))

import_data %>% head()
import_data %>% glimpse()
```

Transforming data

```
data <-
  import_data %>%
  pivot_longer(cols=c(M, B, A), names_to="Species", values_to="Concentration") %>%
  mutate(Species = as.factor(Species)) %>%
  nest(data=c(Time, Species, Concentration))
```

Visualising results

```
data %>%
  filter(Model == "Corrected") %>%
  unnest(data) %>%
  ggplot(aes(x=Time, y=Concentration, color=Starting_Conditions_Set)) +
    geom_line(show.legend=F) +
    facet_grid(Species~L, scales="free_y") +
    #scale_y_log10() +
    labs(title="Time progression curves for the three species for different Lactose concentrations [nM]
  xlab("Time [min]") +
  ylab("Concentration [nM]") +
  theme_classic()
```

Model analysis

Checking hypothesis: There is no significant difference between the data measured with either model.

```
data %>%
  unnest(data) %>%
  group_by(Species) %>%
  nest() %>%
  mutate(F_test = map(data, ~ aov(Concentration ~ Model + Time + L + Starting_Conditions_Set, data = .x))
  unnest(F_test)
```