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
         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", "Correcte~
## $ timestep <chr> "0.0001", "0.00025", "0.0005", "0.00075", "0.001", "0.0025", ~
## $ data     <list> [<tbl_df[60003 x 3]>], [<tbl_df[24003 x 3]>], [<tbl_df[12003~
```

```
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 & Concentration < 1000000000) %>%
  ggplot(aes(x=Time, y=Concentration, color=timestep, lty=model)) +
    geom_point(size=0.2) +
    facet_grid(Species~timestep, scales="free_y") +
    theme_bw()
```

```
data %>%
  unnest(data) %>%
  filter(Concentration > 0 & Concentration < 1000000000) %>%
  filter(Time < 0.03) %>%
  ggplot(aes(x=Time, y=Concentration, color=timestep, lty=model)) +
    geom_point(size=0.2) +
    facet_grid(Species~timestep, scales="free_y") +
    xlab("Time [< 0.03]") +
    theme_bw()
```

0.0001
0.00025
0.0005
0.00075
0.001
0.0025
0.005
0.0075
0.01
A
B
M
Concentration
90000
60000
30000
0
1.00
0.75
0.50
0.25
0.00
2.000
1.995
1.990
1.985
1.980
Time [< 0.03]
timestep
0.0001
0.00025
0.0005
0.00075
0.001
0.0025
0.005
0.0075
0.01