Compare mrgsolve and Torsten for EVID=4

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1 Background

This report summarizes steps to simulate a reset & dose(EVID=4) event using `mrgsolve` and `Torsten`.

2 `Torsten` model

First download the repo with

```
git clone -b reset_test git@github.com:metrumresearchgroup/Torsten.git
```

Then make the model

```
make -j4 examples/pk2cpt_reset/reset
```

To run the model, do

```
cd examples/pk2cpt_reset/
./reset sample algorithm=fixed_param num_warmup=1 num_samples=1 data
 ↪  file=reset.data.json init=reset.init.R
```

The above run produces deterministic ODE solutions for a two-compartment PK model based on parameters in `reset.init.R` and data `reset.data.json`.

One can use `cmdstanr` package in `R` to extract the concentration in central compartment

```
fit <- cmdstanr::read_cmdstan_csv("output.csv", variables=c("cHat"))
draws <- fit$post_warmup_draws
torsten.cp <- as.numeric(as.data.frame(draws)[1,])
```

3 mrgsolve model

```
library("mrgsolve")

code <- '
$PARAM CL = 5, Q = 8, V2 = 20, V3 = 70, KA = 1.2

$CMT GUT CENT PERI

$GLOBAL
#define CP (CENT/V2)

$PKMODEL ncmt = 2, depot = TRUE

## $SIGMA 0.01  // variance

$TABLE
capture DV = CP * exp(EPS(1));

$CAPTURE CP
'

mod <- mcode("accum", code) %>% Req(CP) %>% update(end=480,delta=0.1)

data <- rbind(data.frame("time" = 0, "amt" = 10000, "ii" = 24, "addl"=1,
 ↪  cmt=1, evid=1),data.frame("time" = 18, "amt" = 8000, "ii"=0, "addl"=0,
 ↪  cmt=1, evid=4))
data$ID=1
mrgsol <- mod %>% data_set(data) %>% mrgsim(end=50)
```

4 Compare results

```
## first we import Torsten's data file
torsten.data <- jsonlite::read_json("reset.data.json", simplifyVector =
 ↪  TRUE)

## plot
par(mfrow=c(1,2))
plot(torsten.data$time, torsten.cp, type="l", col="red")
plot(mrgsol$time, mrgsol$CP, type="l", col="green")
## or overlay with
## lines(res$time,res$CP,col="green")
```

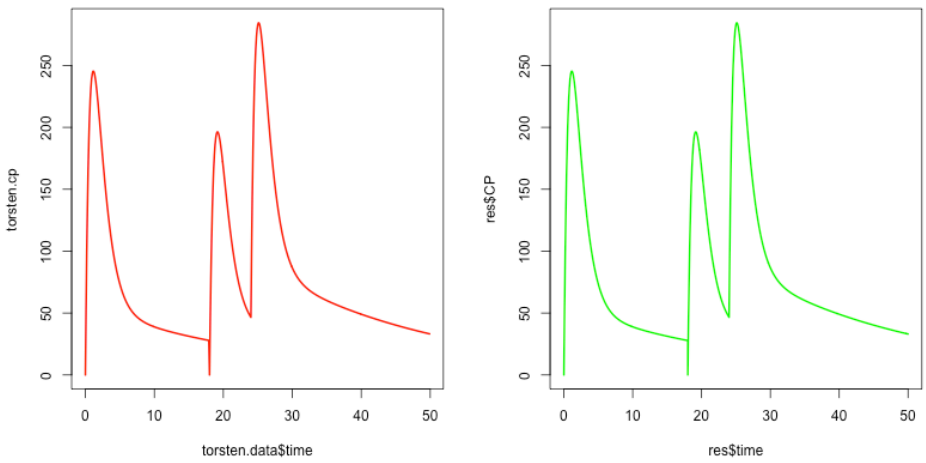

Figure 1: Compare `Torsten` (left) & `mrgsolve` (right) central compartment solution