METRUM
RESEARCH GROUP

mrgsolve: Some ideas

mrgsolve Workshop
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Decide which updates to make persistent

Sometimes you want to do this:

```
mod %<>% update(end=2400)
out <- mod %>% mrgsim
```

Other times this:

```
out <- mod %>%  mrgsim(end=2400)
```

Parallelize your simulation

- Most frequently we parallelize across posterior draws
  - Each posterior draw or bootstrap sample goes to a different worker
- When the data set is large, you can split it on an appropriate factor
  - Study
  - Treatment arm
  - Treatment duration
- Use `mclapply` in Mac/Unix and `doParallel` in Windows
  - Only utilizes cores on the master node
- We use a `qapply` package that will send jobs to all nodes in a cluster via Grid Engine

Save simulated output in serialized format (if needed)

```
out <- mod %>% mrgsim
saveRDS(file="mysim.RDS", out)
```

```
out <- readRDS(file="mysim.RDS")
```

Summarize the simulation prior to returning from the worker

Helpful when memory is limited

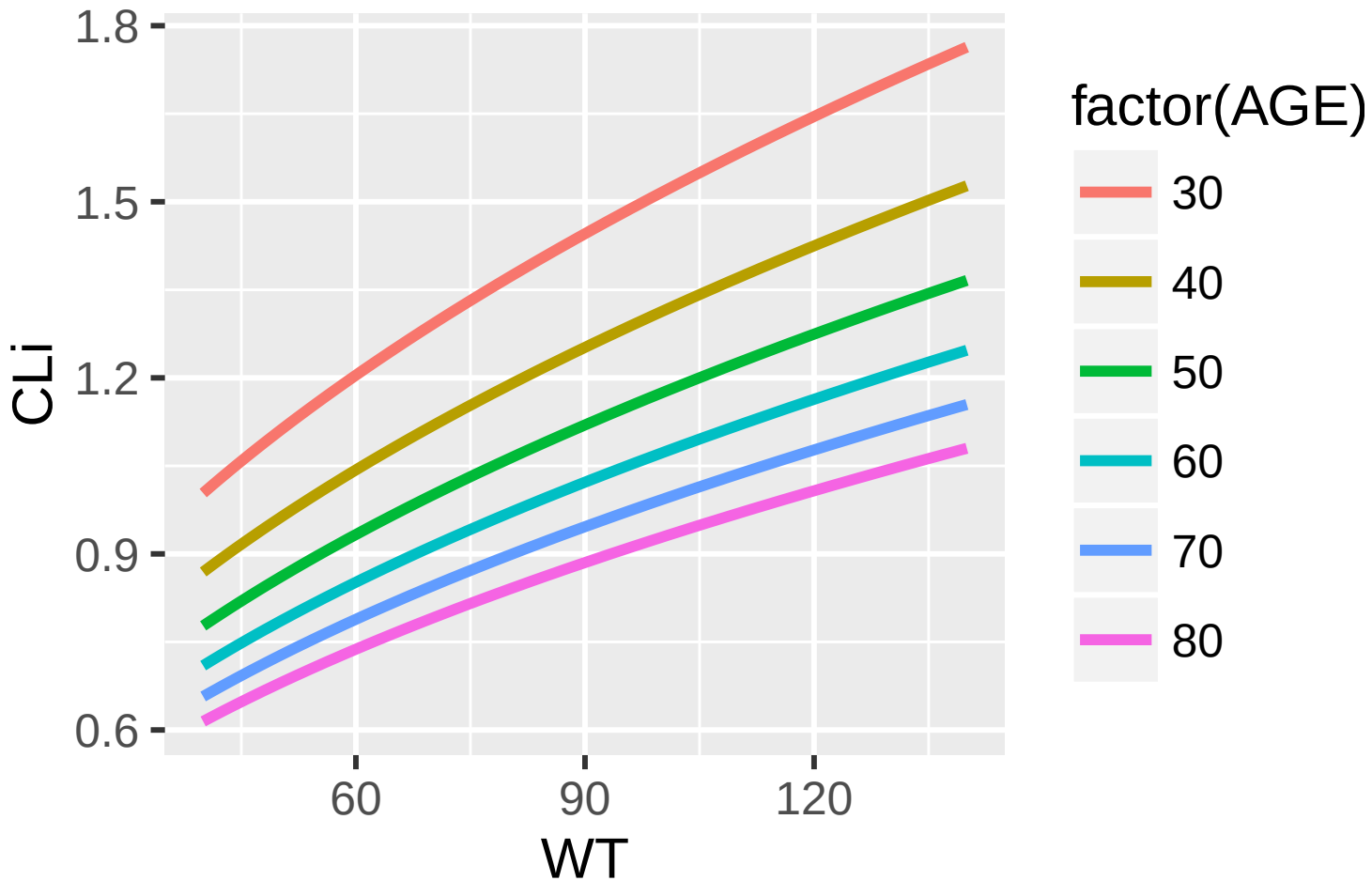
```
out <- mclapply(1:1000, function(i) {

  mod %>%
    data_set(...) %>%
    mrgsim %>%
    mutate(irep=i) %>%
    filter(time > 168) %>%
    group_by(ID,DOSE) %>%
    summarise(Cmax=max(DV))

}) %>% bind_rows
```

Take advantage of the covariate model

```
code <- '
$PARAM TVCL=1, TVVC=20, WT=70, AGE=50

$MAIN
double CLi = TVCL*pow(WT/70,0.45)*pow(AGE/50,-0.5)*exp(ETA

$CAPTURE CLi WT AGE

// Other stuff here....
'

mod <- mread("covmodel", tempdir(),code,warn=FALSE)
```

CL vs WT by AGE

```
idata <- expand.idata(WT=seq(40,140),AGE=seq(30,80,10))
out <- mod %>% idata_set(idata) %>% mrgsim(end=-1)
```



Extend mrgsolve

```
doseA <- function(x,amt,mw=1.23,ii=12,cmt=2,...) {
  x %>% ev(amt=amt/mw/1000,cmt=cmt,ii=ii,...)
}
```

```
mod %>%
  doseA(45,addl=23) %>%
  mrgsim(Req="CENT") %>% head(n=2)
```

```
. Model:  housemodel

.      ID time        CENT
. [1,]  1    0 0.00000000
. [2,]  1    0 0.03658537
```

Start developing the simulation model early

- Don't wait until the end of the project to translate the model to `mrgsolve` so you can simulate all of the different regimens
- When you start simulating early, you will use / re-use the model more