

Numerical ODE group/population integrators in Torsten

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ODE group integrators

Single ODE system

```
pmx_integrate_ode_rk45  
pmx_integrate_ode_bdf  
pmx_integrate_ode_adams
```

ODE group

```
pmx_integrate_ode_group_rk45  
pmx_integrate_ode_group_bdf  
pmx_integrate_ode_group_adams
```

Single ODE system

```
real[,]  
pmx_integrate_ode_xxx(  
    f,  
    real[] y0, real t0,  
    real[] ts,  
    real[] theta,  
    real[] x_r, int[] x_i,  
    ...);
```

ODE group

```
matrix  
pmx_integrate_ode_group_xxx(  
    f,  
    real[ , ] y0, real t0,  
    int[] len, real[] ts,  
    real[ , ] theta,  
    real[ , ] x_r, int[ , ] x_i,  
    ...);
```

ODE group integrators

Single ODE system

```
real[ , ]  
pmx_integrate_ode_xxx(  
    f,  
    real[] y0, real t0,  
    real[] ts,  
    real[] theta,  
    real[] x_r, int[] x_i,  
    ...);
```

ODE group

```
matrix  
pmx_integrate_ode_group_xxx(  
    f,  
    real[ , ] y0, real t0,  
    int[] len, real[] ts,  
    real[ , ] theta,  
    real[ , ] x_r, int[ , ] x_i,  
    ...);
```

- ▶ `len` specifies the length of data for each subject within the above ragged arrays, and the size of `len` is the size of the population.
- ▶ The group integrators return a single matrix ragged column-wise. The number of rows equals to the size of ODE system.

Exercise

autocatalytic reaction model: ODE group version

- ▶ Change the loop with the numerical integrator to use group integrator.
- ▶ Edit/Add cmdstan/make/local

```
TORSTEN_MPI = 1  # flag on torsten's MPI solvers  
CXXFLAGS += -isystem /usr/local/include      # path to MPI  
↪ library's headers
```

- ▶ Build in cmdstan

```
make ../example-models/ttpn2/ttpn2_group
```

- ▶ Run

```
mpiexec -n 2 -l ./chem_group sample adapt delta=0.95 random  
↪ seed=1104508041 data file=chem.data.R init=chem.init.R
```

Exercise

- ▶ What does output say?
- ▶ How many cores can you use until performance saturates? Why?
- ▶ Can you do it using Stan's `map_rect`? Is there a difference in style, output, and performance?