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Refactor

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Torsten Refactor

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CHAPTER 1

Major components

1. PKEventList

List of PK events as provided by NONMEM, not necessarily ordered, hence refrain using "history" in name.

It describes PK and is facing users. It evoles when Stan provides more friendly types such as tuples.

Example:

time amt rate ii evid cmt addl ss

. . .

• PKSystem: PK parameters as a 1-1 mapping to an ODE system.

2. PKSolver

A PKSolver iterates through PKSystem to solve the ODE using various solution methods.

It solves ODE and is facing developers.

It is orthogonal to PKSystem.

Could be several things:

Named. For built-in models

Matrix exp. For linear ODE model and built-in.

Numerical integration. For all kinds of PKModel.

3. PKPopulation

A list of PKSystem.



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CHAPTER 2

PKModel

A PKModel is what utilizes parameters in PKSystem to describe a PK system, e.g. 2-cpt model. It is ODE and is facing developers.

Could be several things:

- Named: For built-in models such as 1-cpt, 2-cpt, etc.
- \bullet Matrix: For linear ODE model
- Functor: For general ODE model

A PKModel is orthogonal to PKEventList.

1. Implementation

```
template<class... Ts>
struct PKModel {
   // ...
}
```



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CHAPTER 3

PKSystem

PK parameters as a 1-1 mapping to an ODE system, consisting of PKModel and corresponding parameters, ordered in time. It consumes tlag & rate data to re-order and augment the event history. It also incorporates ModelParameterHistory.

It describes ODE and is facing developers & power users. Example:

time parameters(theta, rate, biovar) PKModel

parameters can be backed by std::tuple so that it is a combination of data and var, improving MCMC efficiency.