pyPESTO

A Python Package for Parameter Estimation and Uncertainty Quantification

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+ pyPESTO developers

UNIVERSITÄT BONN

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What is the focus of pyPESTO?

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- Optimization and uncertainty quantification
- Simple & unified interface to various optimizers/samplers

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- Jupyter notebook & slides : / jvanhoefer

Modularity as Design Principle

- objective function
  - user defined as python code
  - AMICI
- key parts of analysis/algorithms are interchanageable
- code object oriented and modular

Objective Functions in pyPESTO

User Defined Objective Functions

```python
# define objective function
def f(x: np.array):
    return x[0]**2 + x[1]**2

# define gradient
def grad(x: np.array):
    return 2*x

# define objective
custom_objective = pypesto.Objective(fun=f, grad=grad)
```

Objective = negative-log-likelihood/posterior

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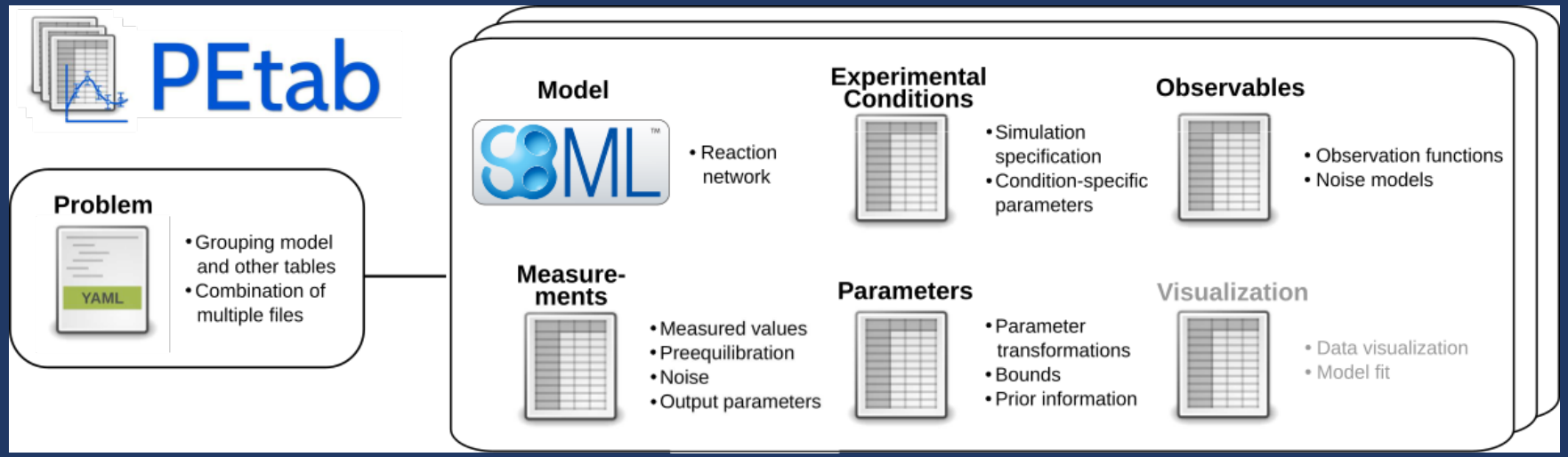
Objective Functions from PEtab

- data format for specifying parameter estimation problems



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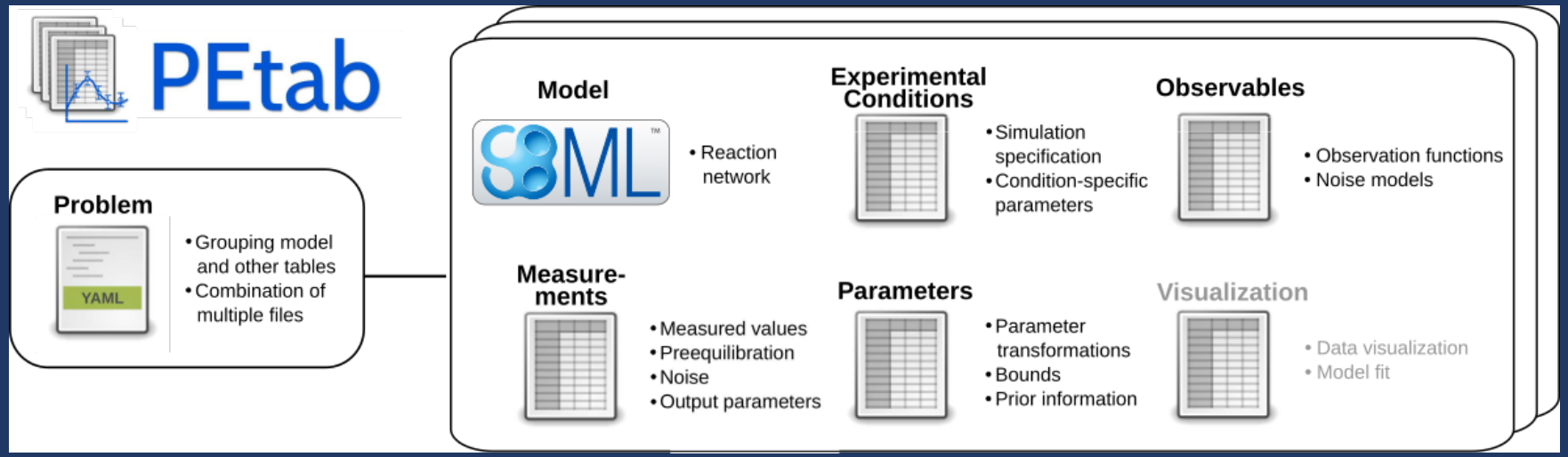
Objective Functions from PEtab

- data format for specifying parameter estimation problems



- PEtab-dev/PEtab
- Objective = negative log-likelihood/log-posterior
- Model simulation → AMICI

Talk by Daniel Weindl
Thu 21:45

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Model Import and Optimization via PEtab

Import

```
# directory of the PEtab problem
petab_yaml = './Boehm_JProteomeRes2014/Boehm_JProteomeRes2014.yaml'

importer = pypesto.petab.PetabImporter.from_yaml(petab_yaml)
problem = importer.create_problem()
```

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```

Optimize

```
optimizer = optimize.ScipyOptimizer()

# do the optimization
result = optimize.minimize(problem=problem,
                           optimizer=optimizer,
                           n_starts=10)
```

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Optimization in pyPESTO

Which optimizers can I use in pyPESTO?

- pyPESTO provides a unified interface to
  - All SciPy-optimizers
  - IpOpt
  - Dlib
  - Particle swarm (pyswarm)
  - CMA-ES

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  - IpOpt
  - Dlib
  - Particle swarm (pyswarm)
  - CMA-ES

- Change optimizer = one line of code:

```
optimizer = optimize.PyswarmOptimizer()
```

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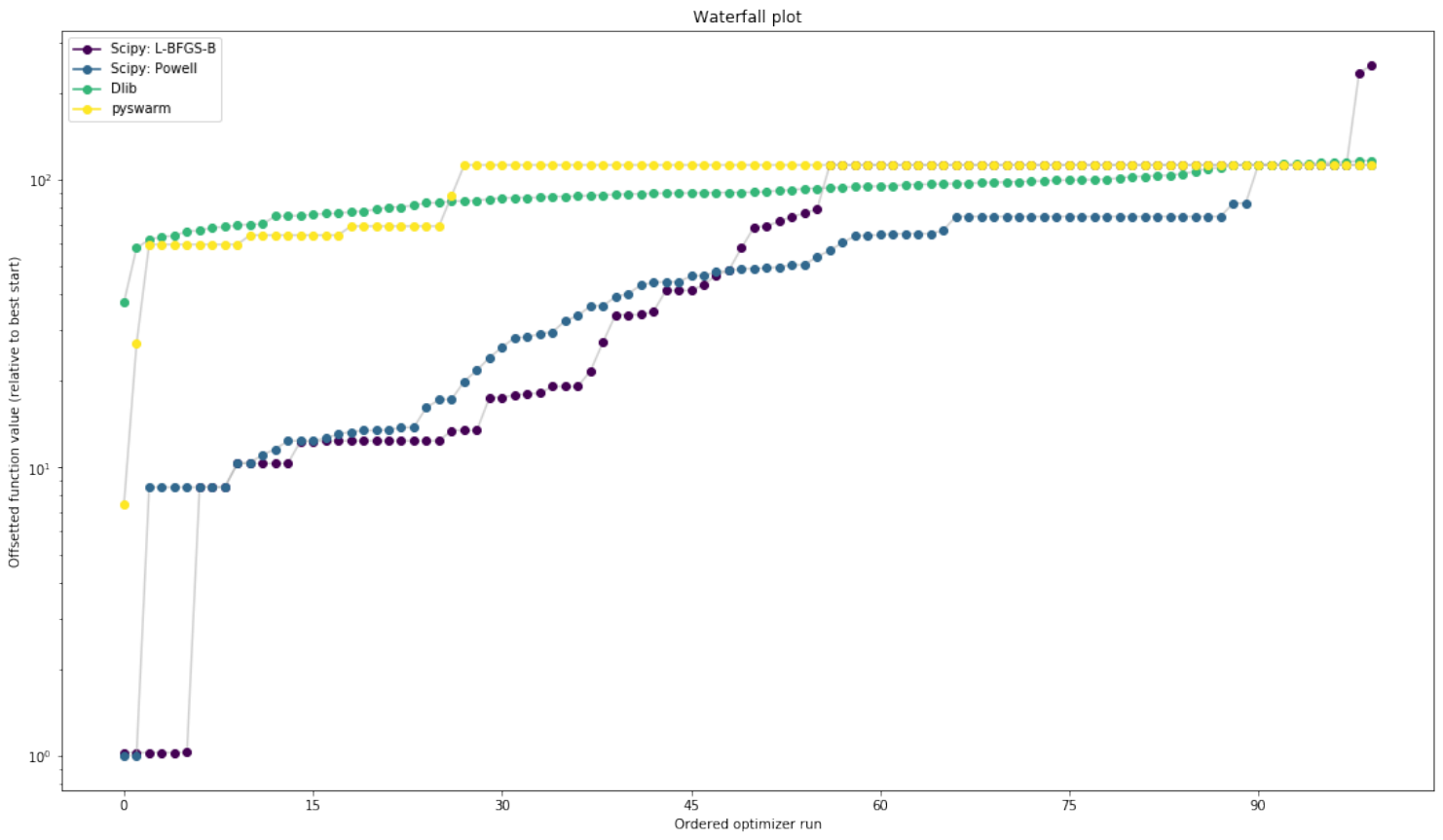
Optimizer Performance




```
Average Run time per start:
--------------------
Scipy: L-BFGS-B: 3.327784 s
Scipy: Powell: 18.523545 s
Dlib: 114.969435 s
pyswarm: 26.666935 s
```

```
pypesto.visualize.waterfall(optimizer_results, legends = optimizer_names)
```

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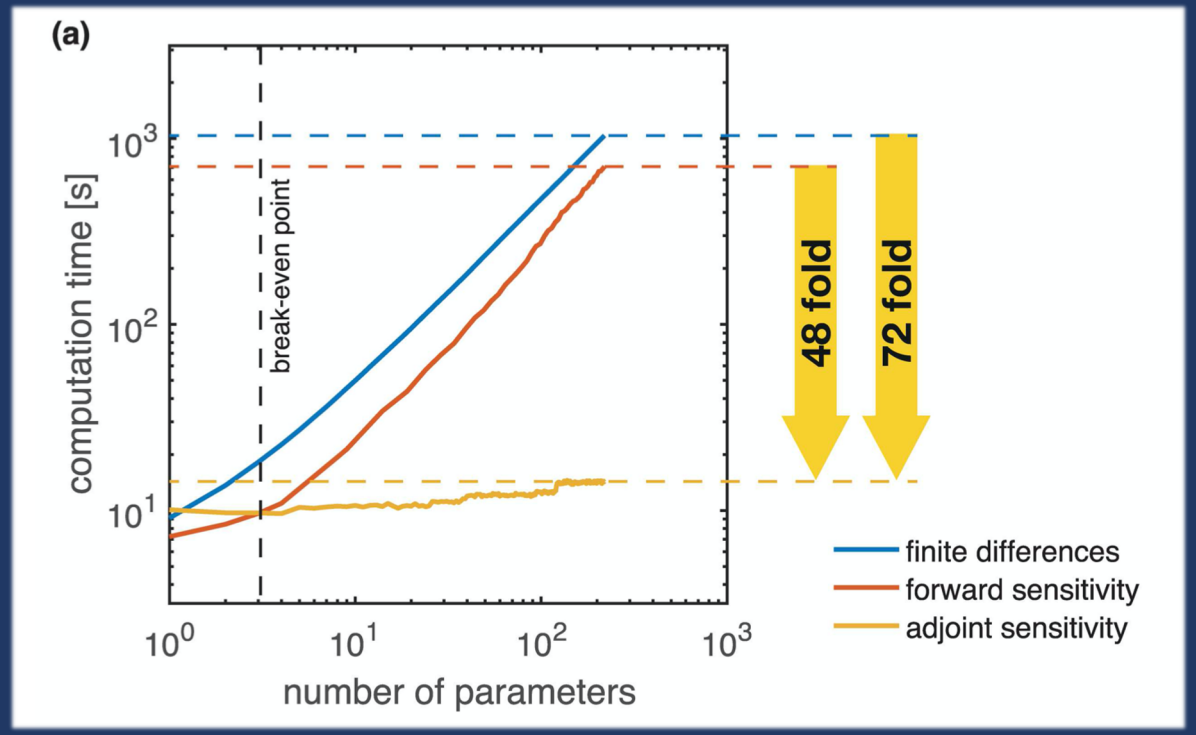
Large Scale Models in pyPESTO

- Fast and reliable gradient computation is key!

  $\Longrightarrow$ **Adjoint sensitivities** (AMICI)
- AMICI lightning Talk by Paul Stapor

- Parallelization



Fröhlich et al. PlosCB 2017

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Large Scale Models in pyPESTO: Code

```
# Set gradient computation method to adjoint
problem.objective.amici_solver.setSensitivityMethod(amici.SensitivityMethod.adjoint)

# Parallelize
engine = pypesto.engine.MultiProcessEngine()

# Optimize
result = optimize.minimize(problem=problem,
                           optimizer=optimizer_scipy_lbfgsb,
                           engine=engine,
                           n_starts=100)
```

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Uncertainty Quantification in pyPESTO

Profile Likelihoods

- Method to compute confidence intervals
- Maximum projection + likelihood ratio test

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- Method to compute confidence intervals
- Maximum projection + likelihood ratio test

```
import pypesto.profile as profile

result = profile.parameter_profile(problem=problem,
                                   result=result,
                                   optimizer=optimizer_scipy_lbfgsb)
```

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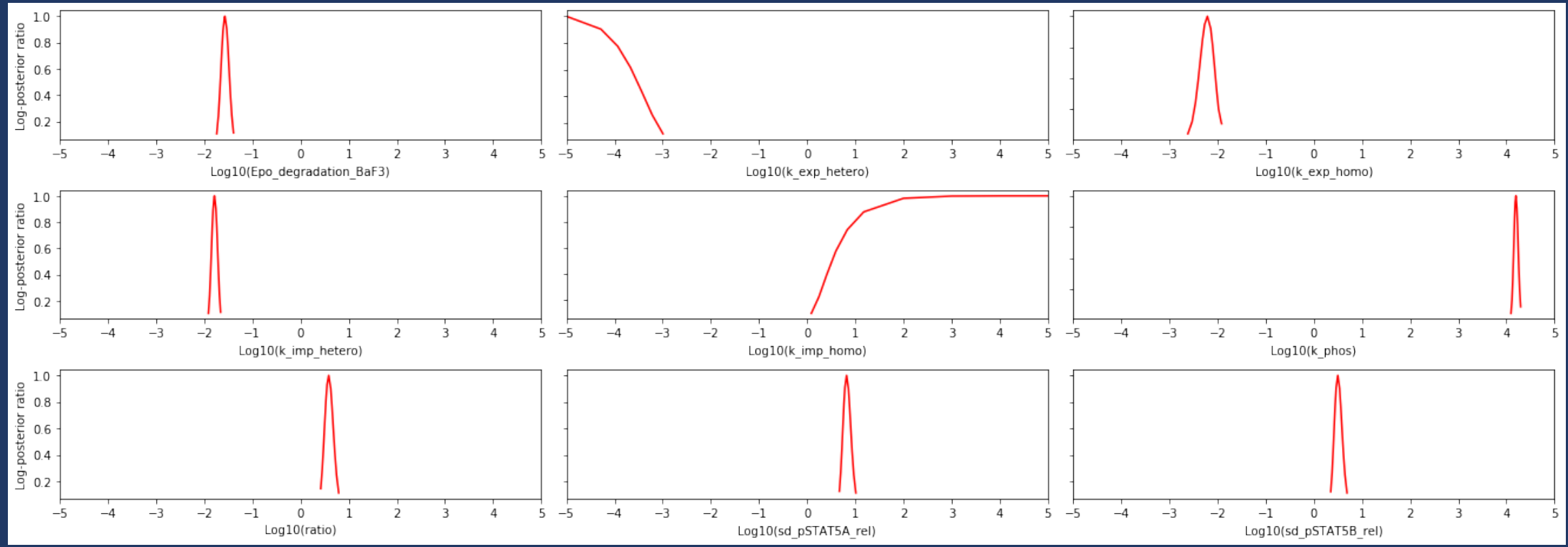
Profile Likelihoods: Projections




```
visualize.profiles(result, x_labels = x_labels, show_bounds=True)
```

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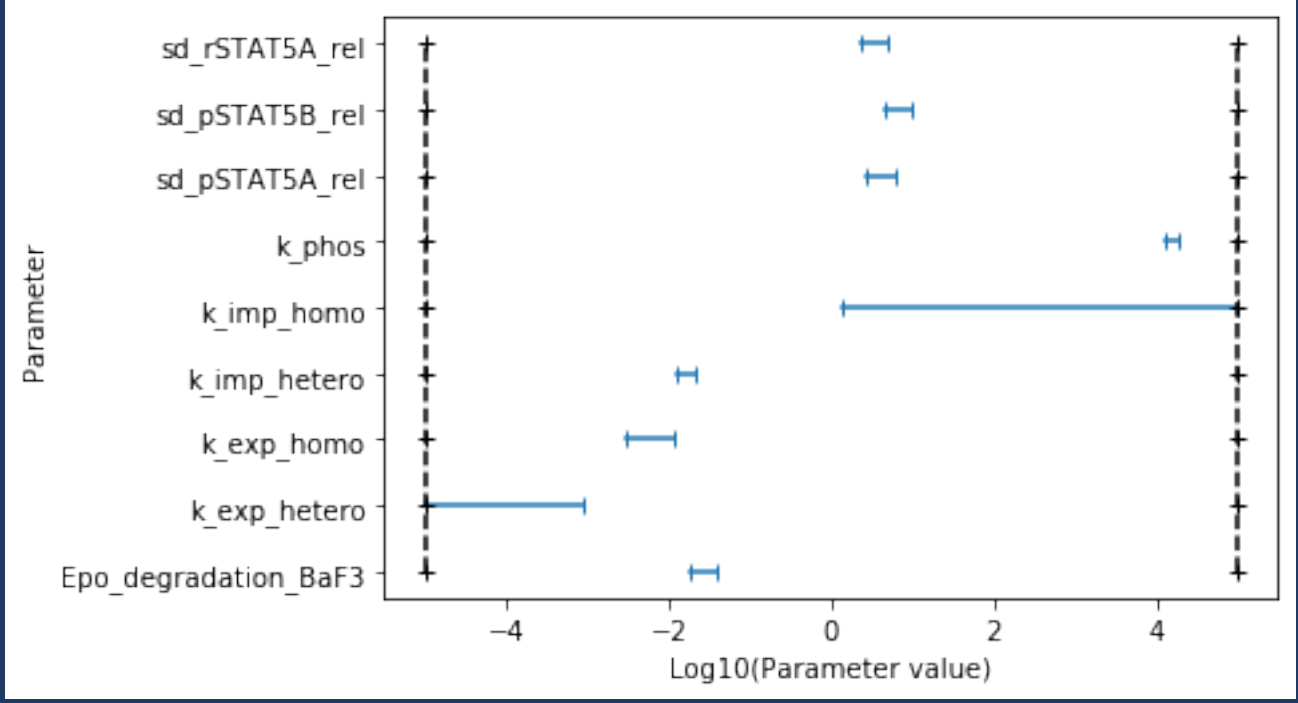
Profile Likelihoods: 95% Confidence Intervals




```
pypesto.visualize.profile_cis(result, confidence_level=0.95)
```

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(MCMC) Sampling

```python
import pypesto.sample as sample

n_samples = 10000

sampler = sample.AdaptiveMetropolisSampler()

result = sample.sample(problem,
                       n_samples=n_samples,
                       sampler=sampler,
                       result=result)
```

```
100%|██████████| 10000/10000 [00:17<00:00, 561.75it/s]
```

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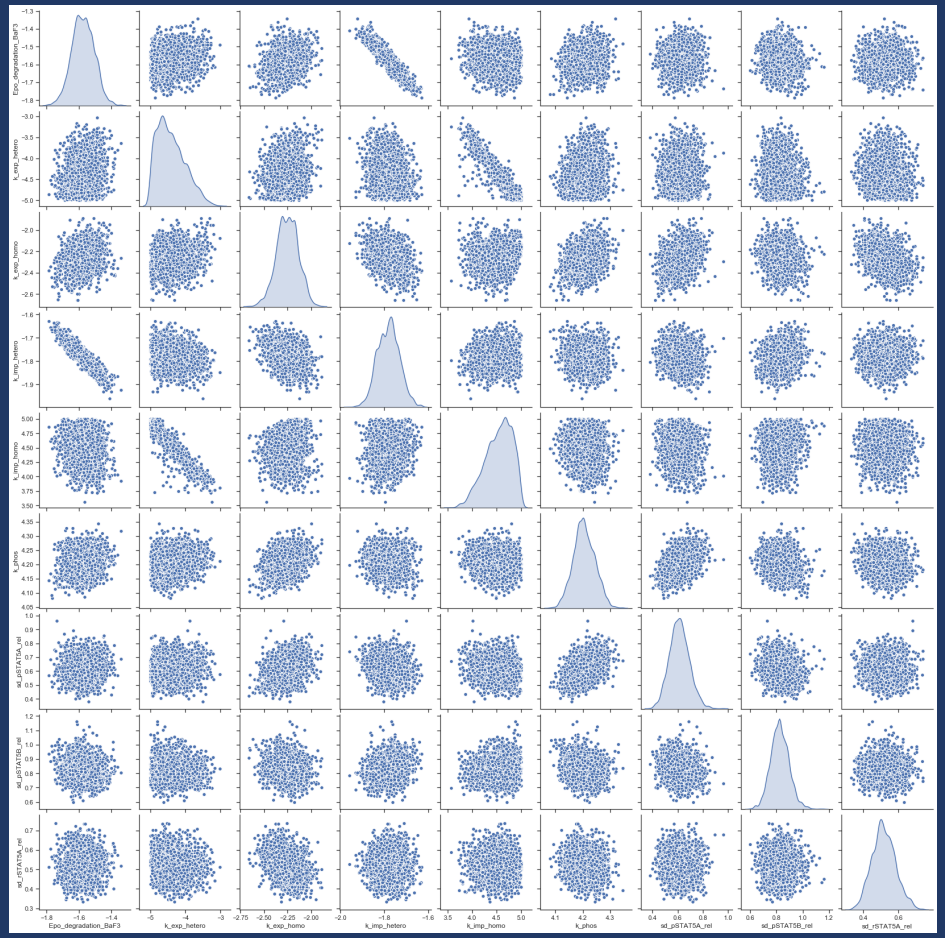
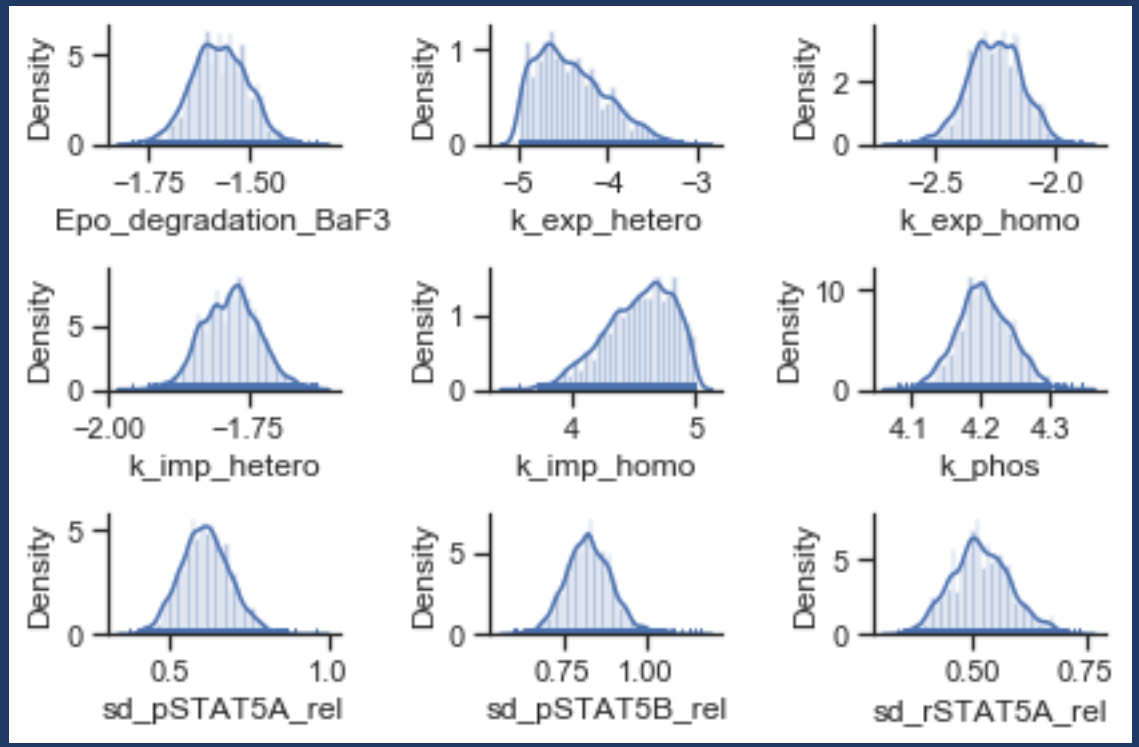
Sampling: Visualization



```
visualize.sampling_scatter(result)
```




```
visualize.sampling_1d_marginals(result)
```

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Which samplers can I use in pyPESTO?

- pyPESTO implements/interfaces
  - Adaptive Metropolis
  - Adaptive parallel Tempering
  - Interfaces pymc3

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- Sampling diagnostics
  - Geweke test
  - effective sample size
  - …

Development & Availability

- Open Source: ICB-DCM/pyPESTO
- `pip install pypesto`
- Docu (RTD) + example notebooks
- Continuous integration + testing via travis

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- 5 – 10 people using, extending and maintaining pyPESTO
- Contributions and feature requests welcome

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Currently under Development

- More Optimizer/Sampler
- Model Selection
- Experimental Design
- Hierarchical optimization of scaling/noise parameters
- Ordinal data

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