SAND2005-7491C

Using APPSPACK to Identify Optimal Model Parameters

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Outline

1. Discussion of Simulation
2. Parameter Extraction via Optimization
3. Example from Circuits
4. Numerical Results
5. Response Surfaces
6. Future Work

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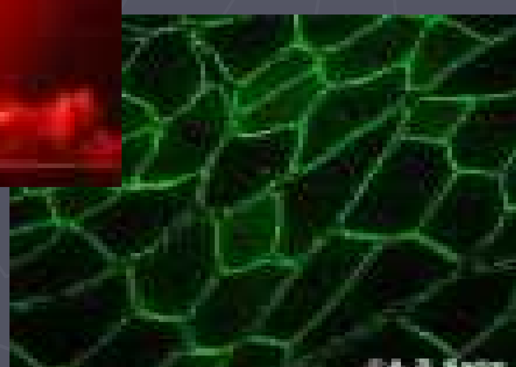
Use of Computer Simulation



- Physical experiments are often expensive.
- Some experiments are impossible.
- The behavior of many physical systems can be imitated by a computer model.
- Computer experiments or simulations are a viable alternative.

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Challenges of Simulation

- Is the physical phenomena being modeled correctly? (validation)
- Is the simulation correctly solving the equations? (verification)
- How can inaccuracies be quantified? (metrics)
- What inherent model parameters should be used?

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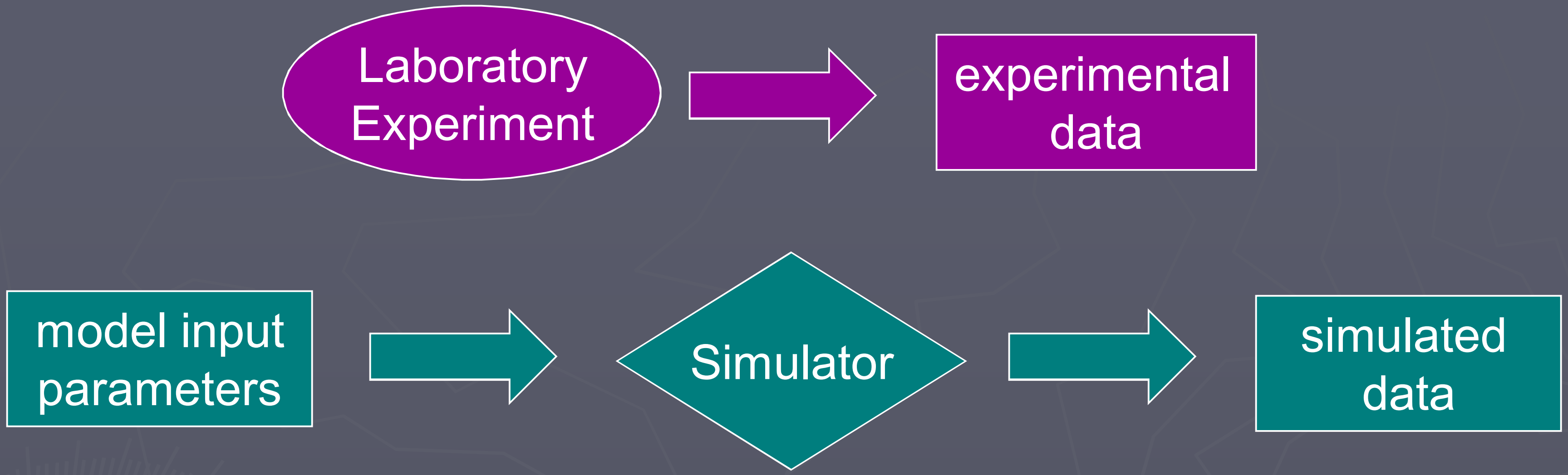
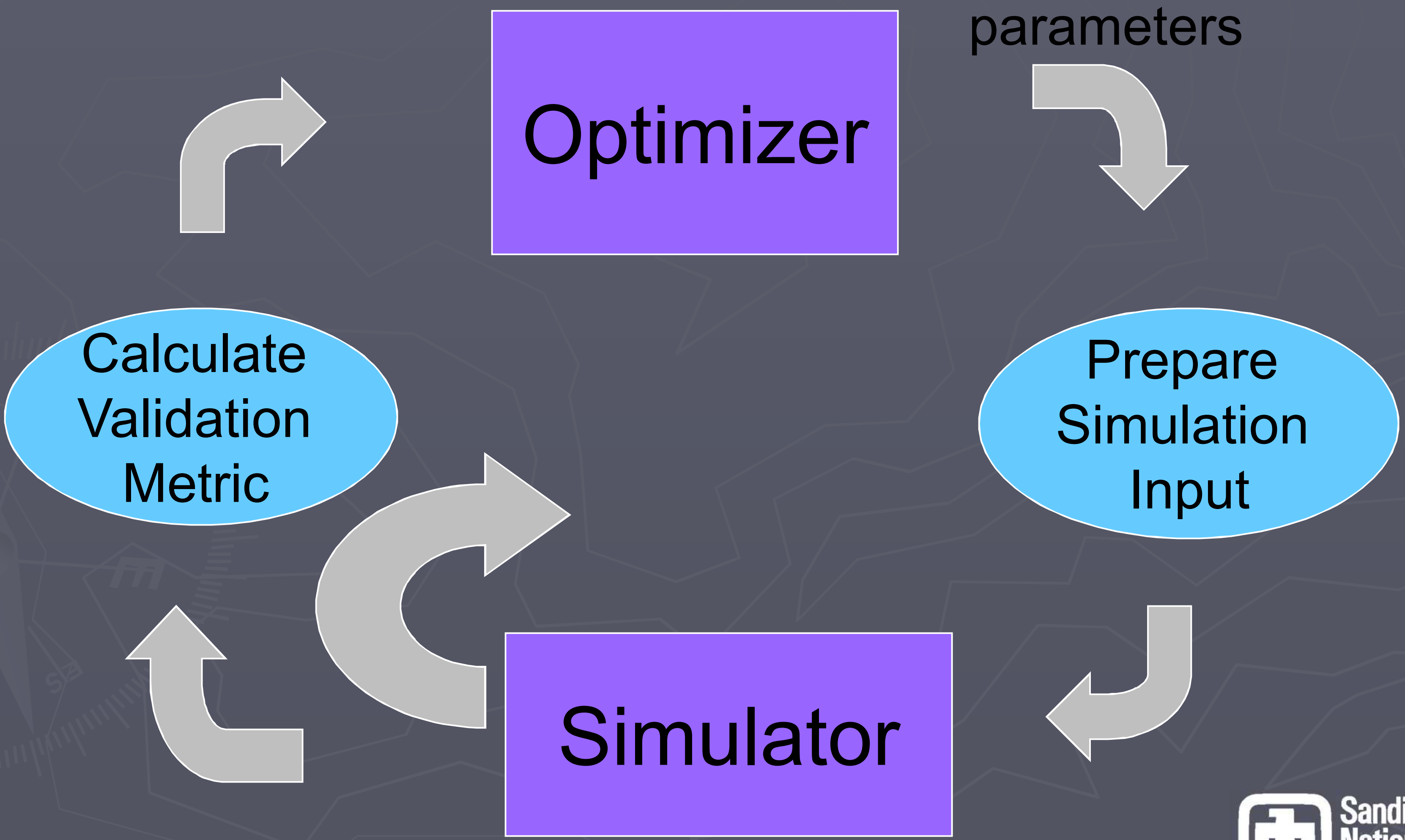
Goal of Parameter Extraction



Find the model input parameters that result in simulated data that is “the same” as some given experimental data.

Parameter Extraction via Optimization



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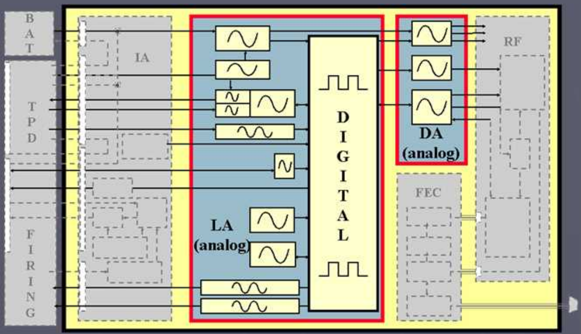
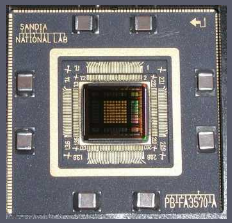
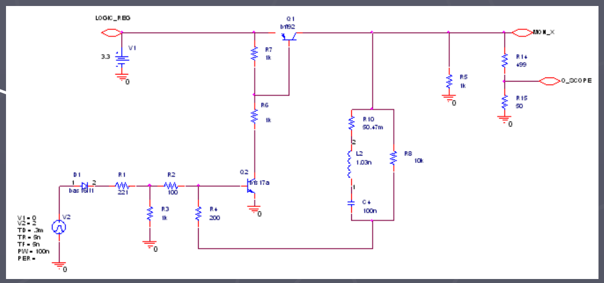
Electrical Hierarchical Validation



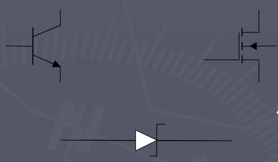
Circuit Board



Single ASIC



Subcircuit



Single Device

- Gain higher visibility into circuits (internal measures not available in test)
- Verify design margins → Provide increased (simulation-based) confidence in design

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Xyce™

- Parallel electronic simulator code for simulating electrical circuits
- Enhanced version of Berkeley SPICE 3f5 that uses physics based models (instead of empirical based models)
- Written at Sandia to support simulations needs of Sandia electrical designers
- Under constant development (version 3 just released)

Hutchinson, Keiter, Hoekstra, Rankin, Waters, Russo, Wix, Ballard, …

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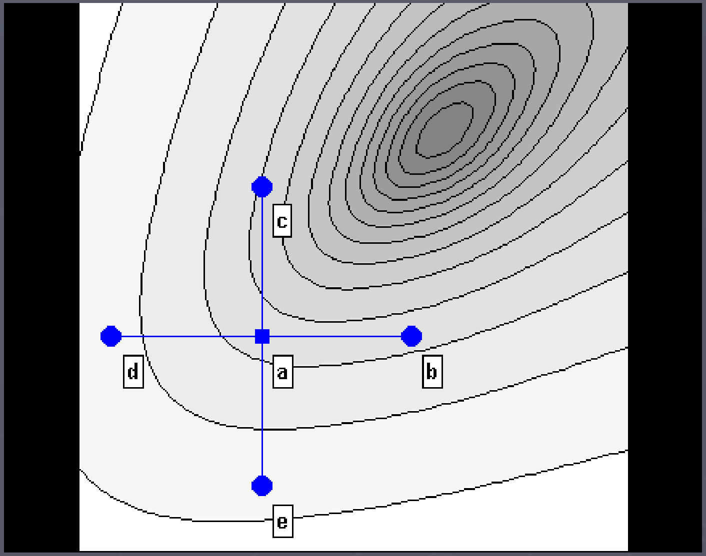
Parameters

- Device model has ~25 parameters
- Parameters ranked by engineers
  - How much does the model rely on the parameter being chosen correctly?
  - How uncertain are we about the current value being used?
- Selected 8 parameters
- Bounds and starting points provided by an engineering "hand tuning" process

Optimizer: APPSPACK

- Direct method → no derivatives required
- Pattern of search directions drives search and determines new trial points for evaluation



- Objective function can be an entirely separate program
- Achieves parallelism by assigning function evaluations to different processors
- Freely available software under the GNU public license (APPSPACK)

http://software.sandia.gov/appspack/version4.0/index.html

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Device Data

- Existing data from two different test facilities
  - Facility 1: 24 tests
  - Facility 2: 4 tests
- Selected 5 representative test results for optimization
- Used remaining test results for validation

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Optimization: Determine the Weights

$$\min \sum_{i=1}^{N} w_i(T_i) \sum_{t=1}^{T_i} (s_i(t;x) - e_i(t))^2$$

N = number of tests

T_i = (relevant) number of experimental values for test i

$w_i(T_i)$ = weighting factor (depends on number of experimental points)

$S_i(t;x)$ = simulated value, calculated with parameters x, corresponding to experimental point t for experiment i

$e_i(t)$ = test value of point t in test i

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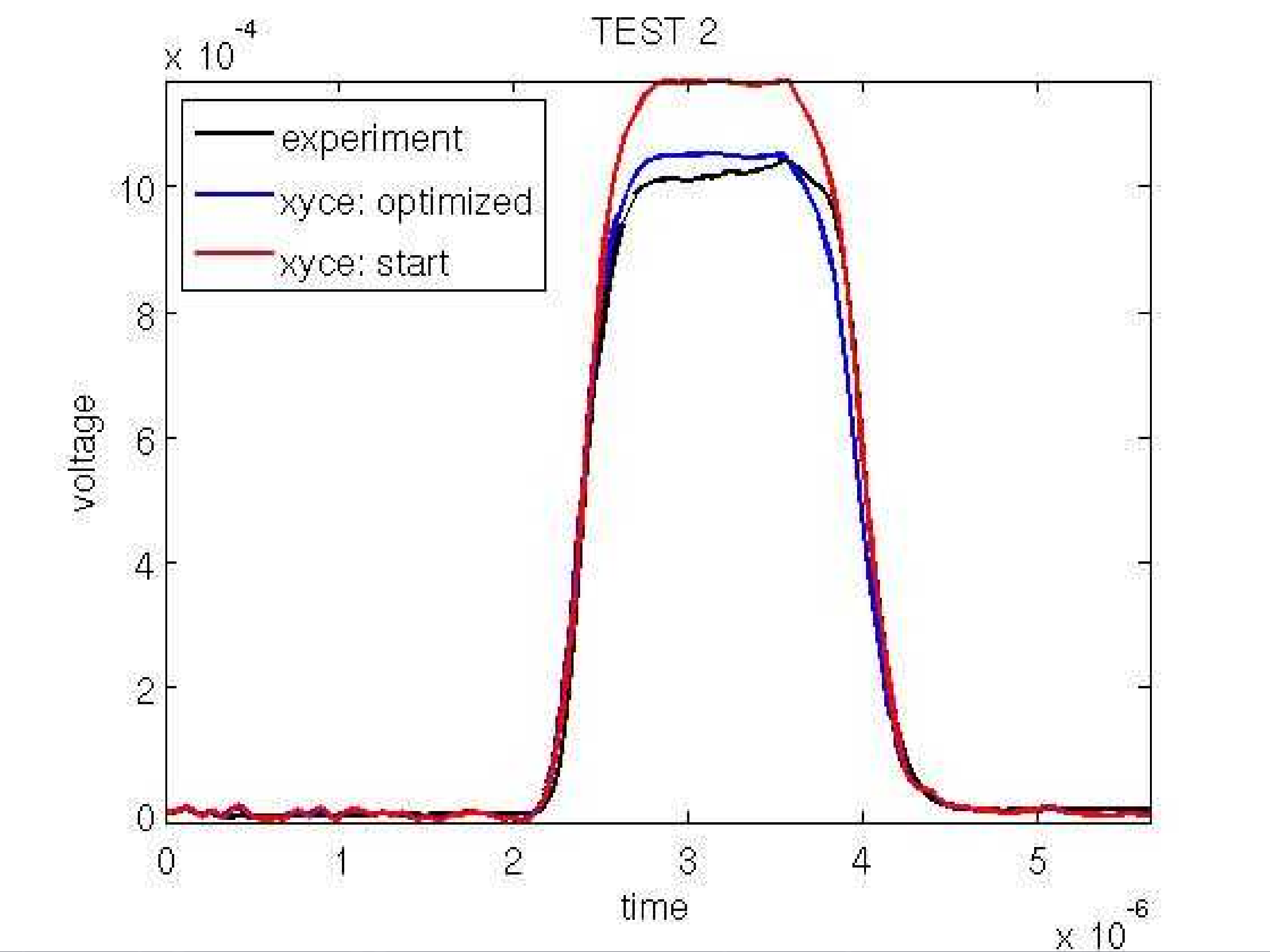
Optimization Results



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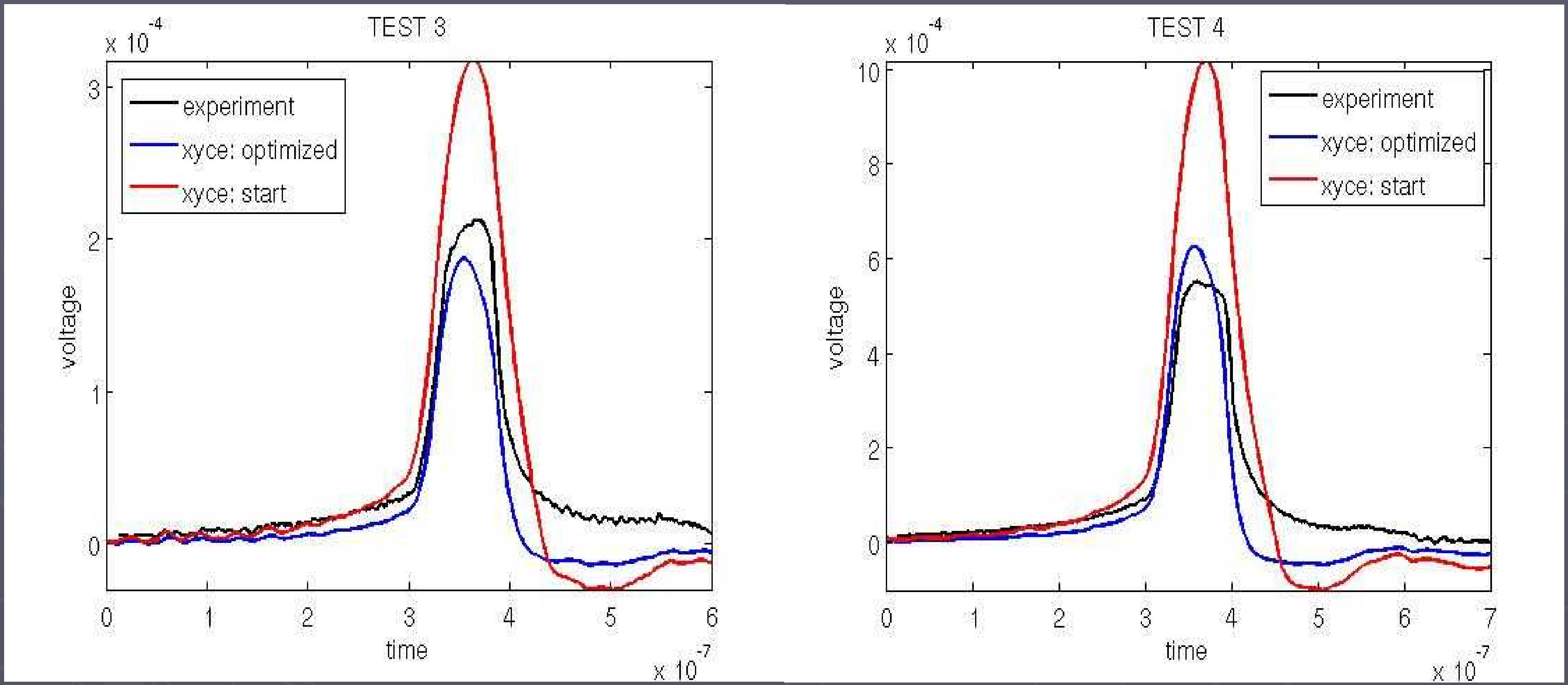
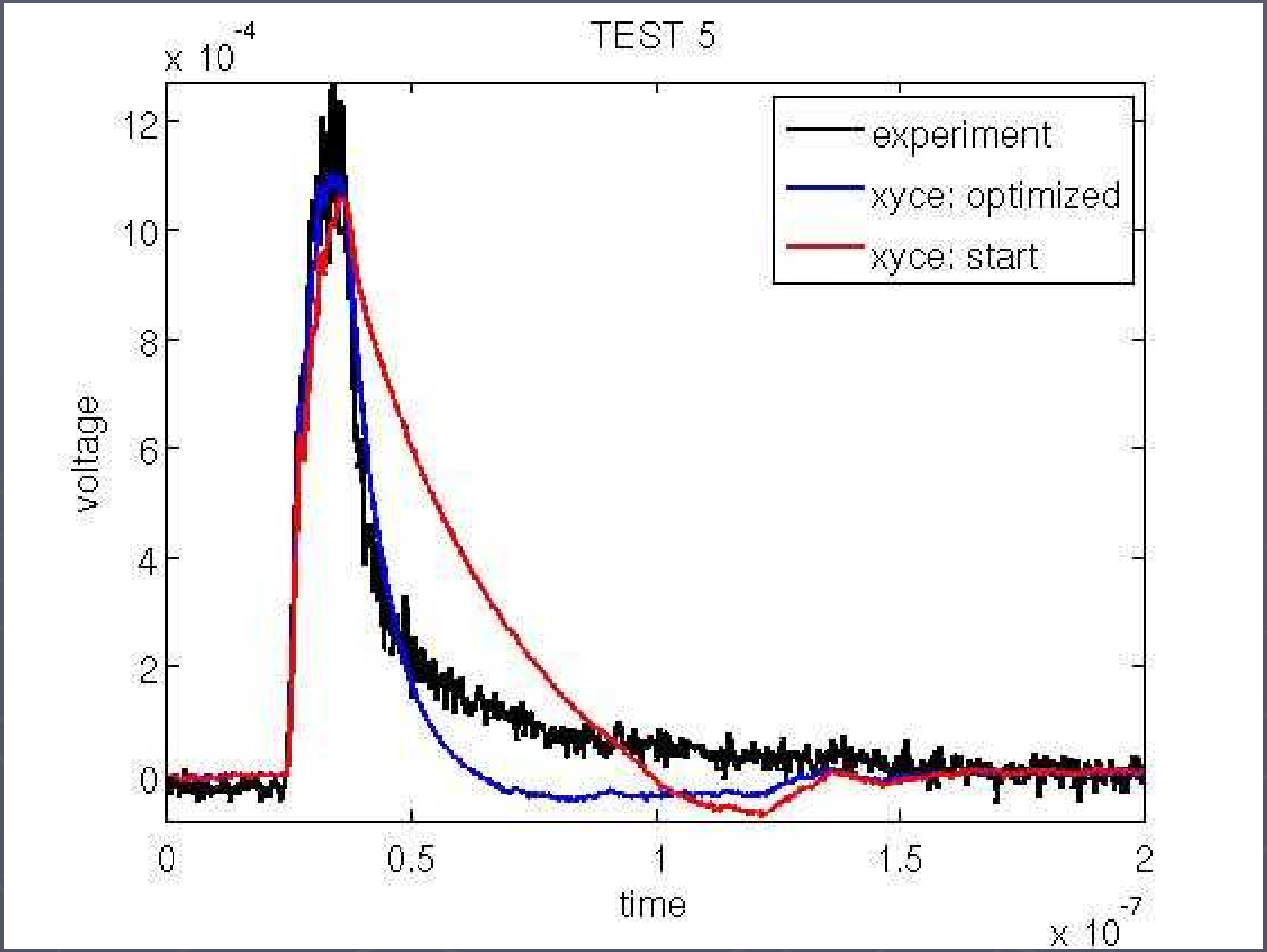
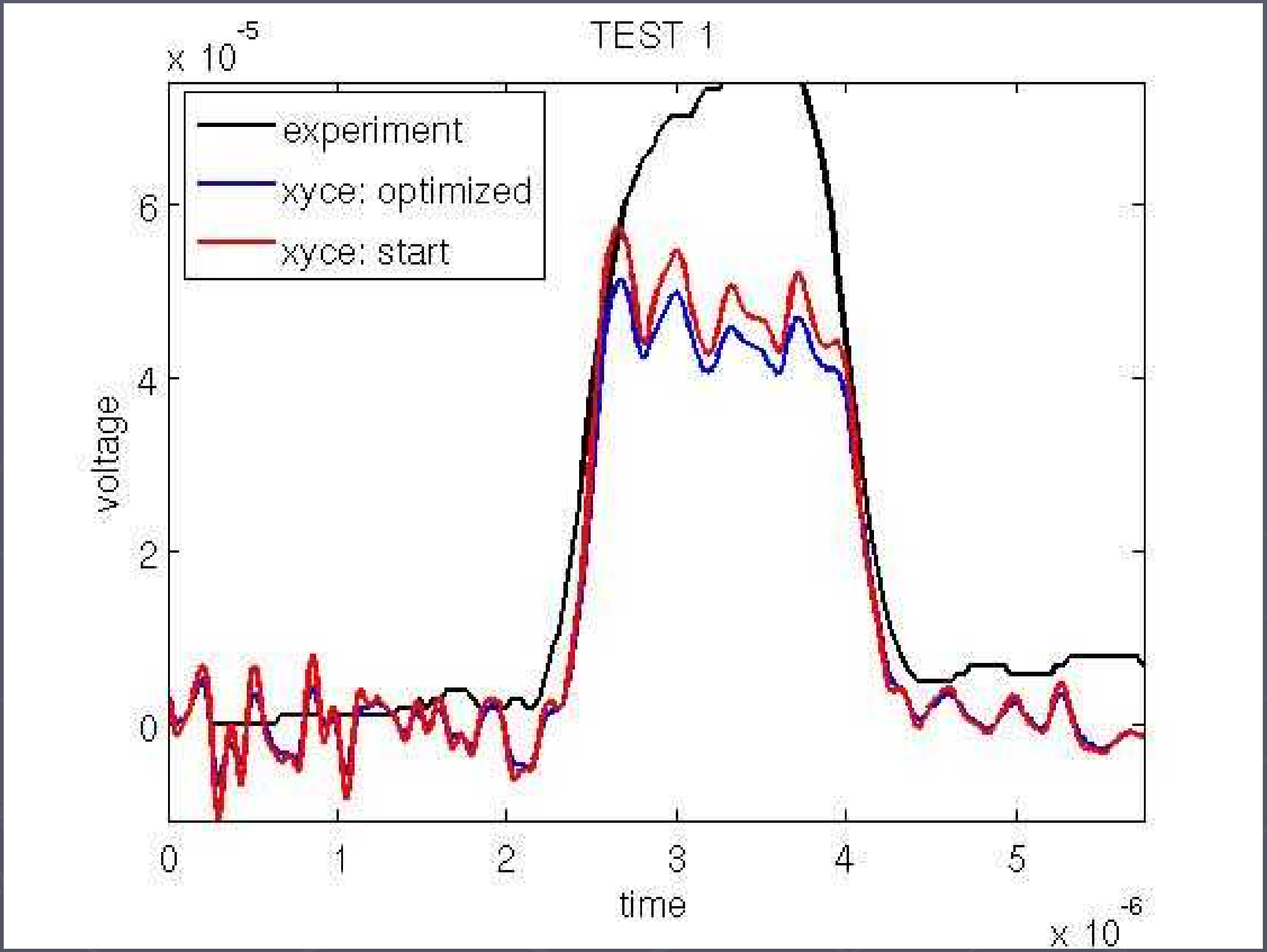
Optimization Results



Optimization Results



Optimization Results



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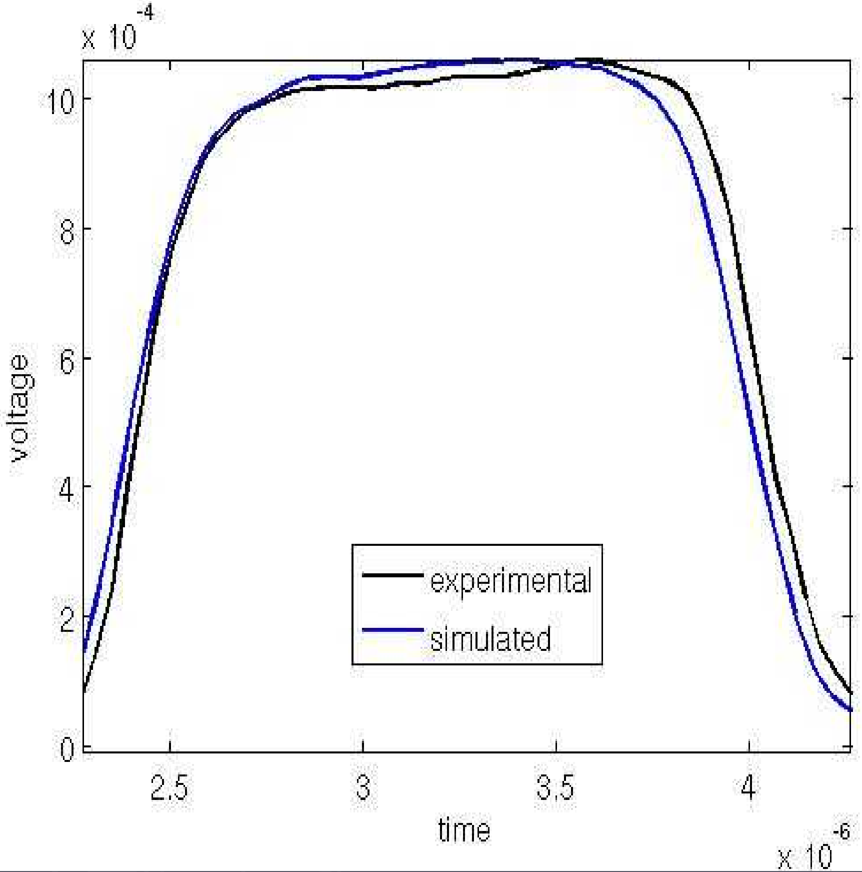
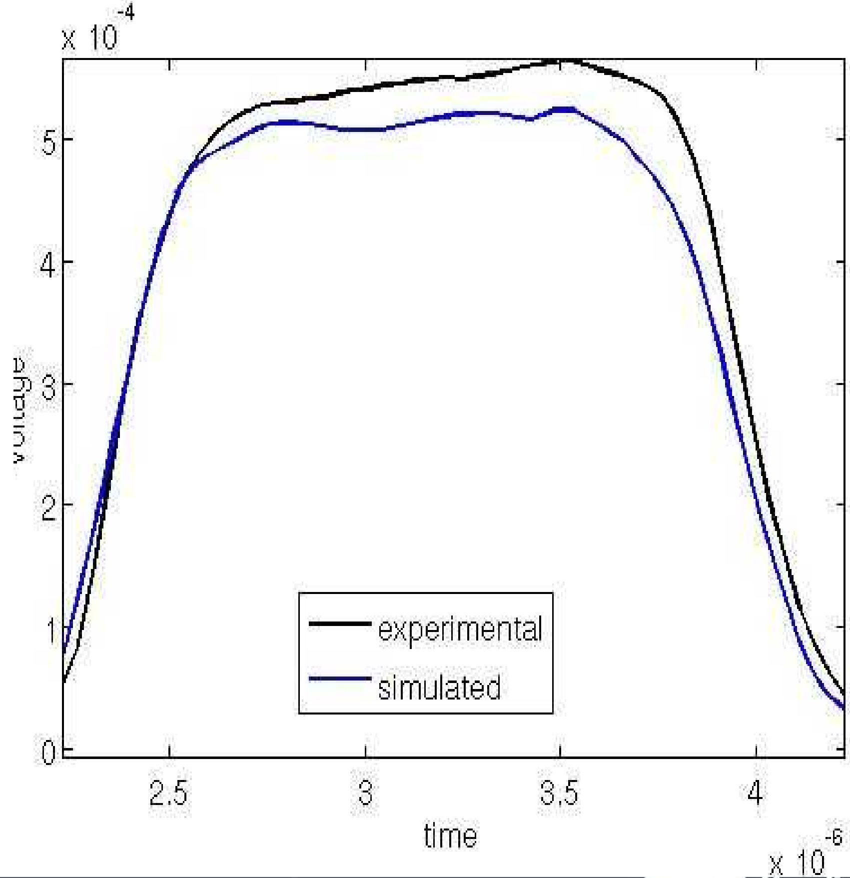
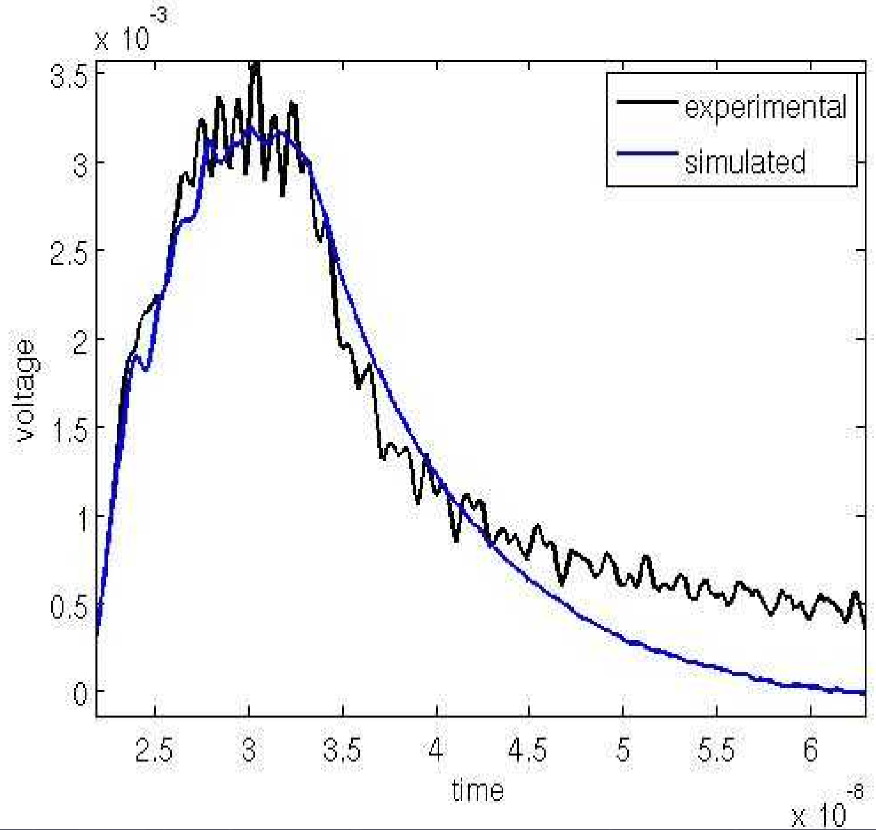
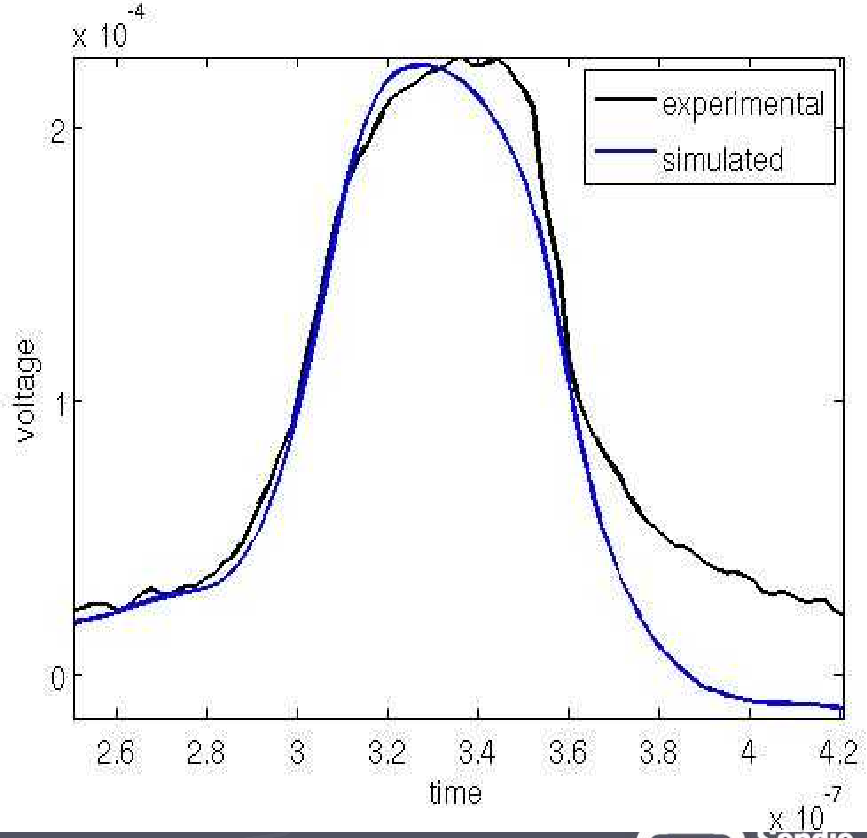
Validation Results





Validation Results





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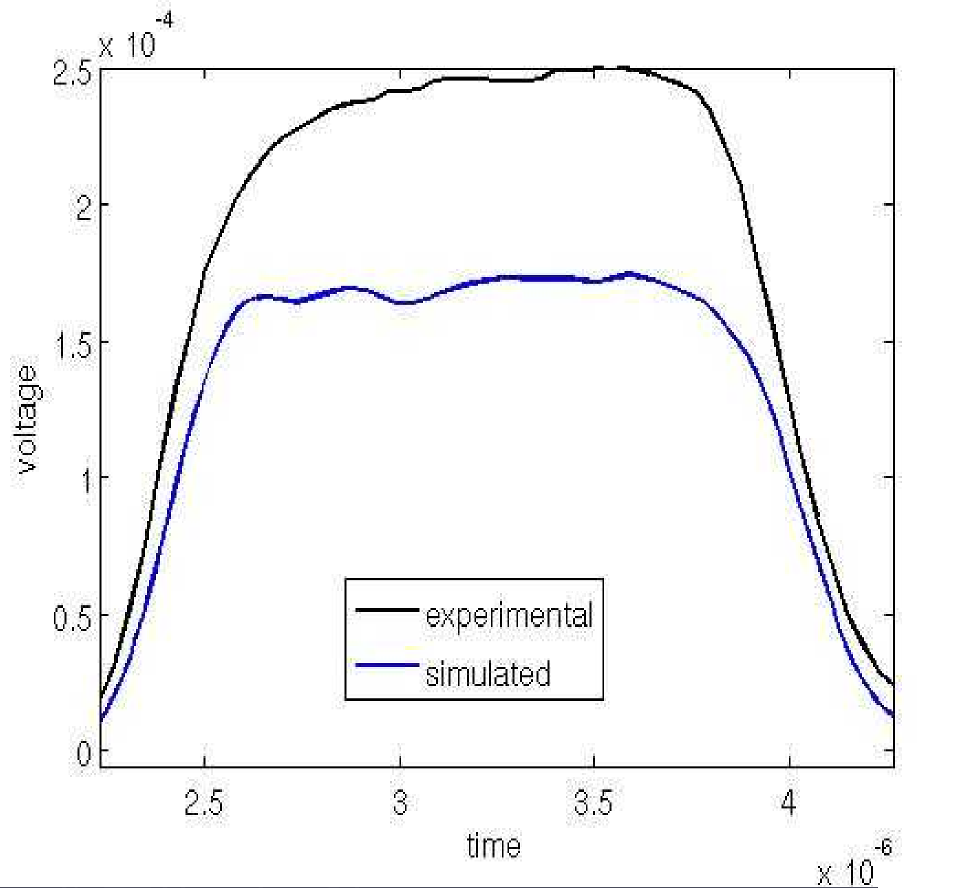

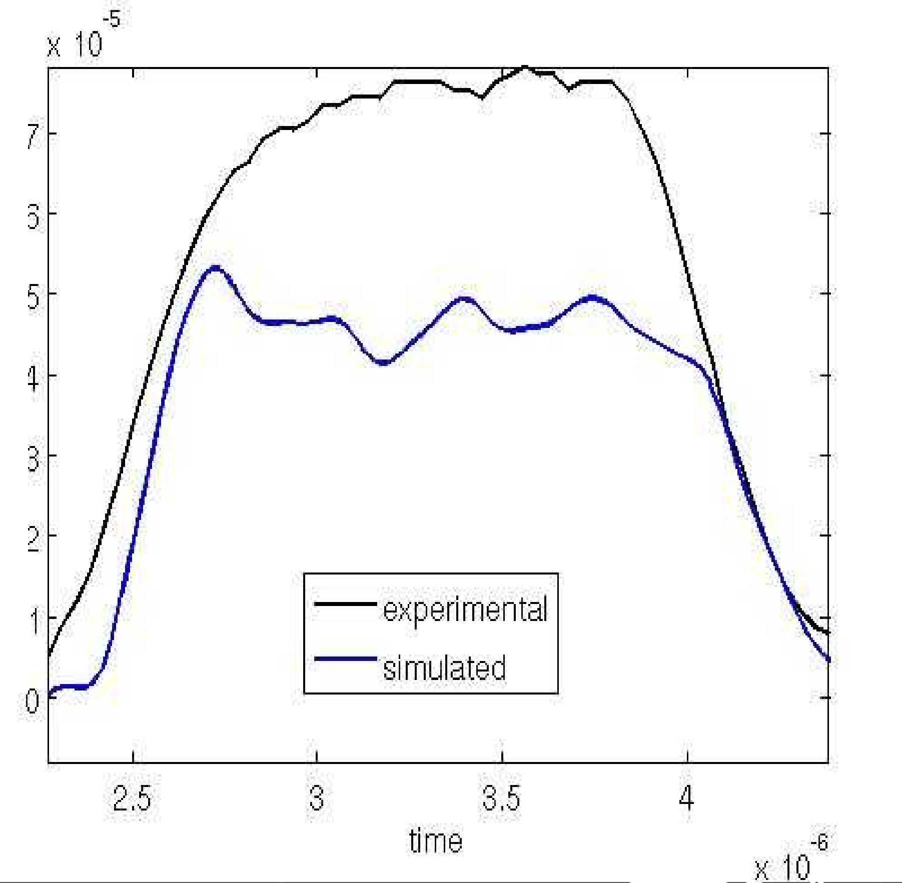

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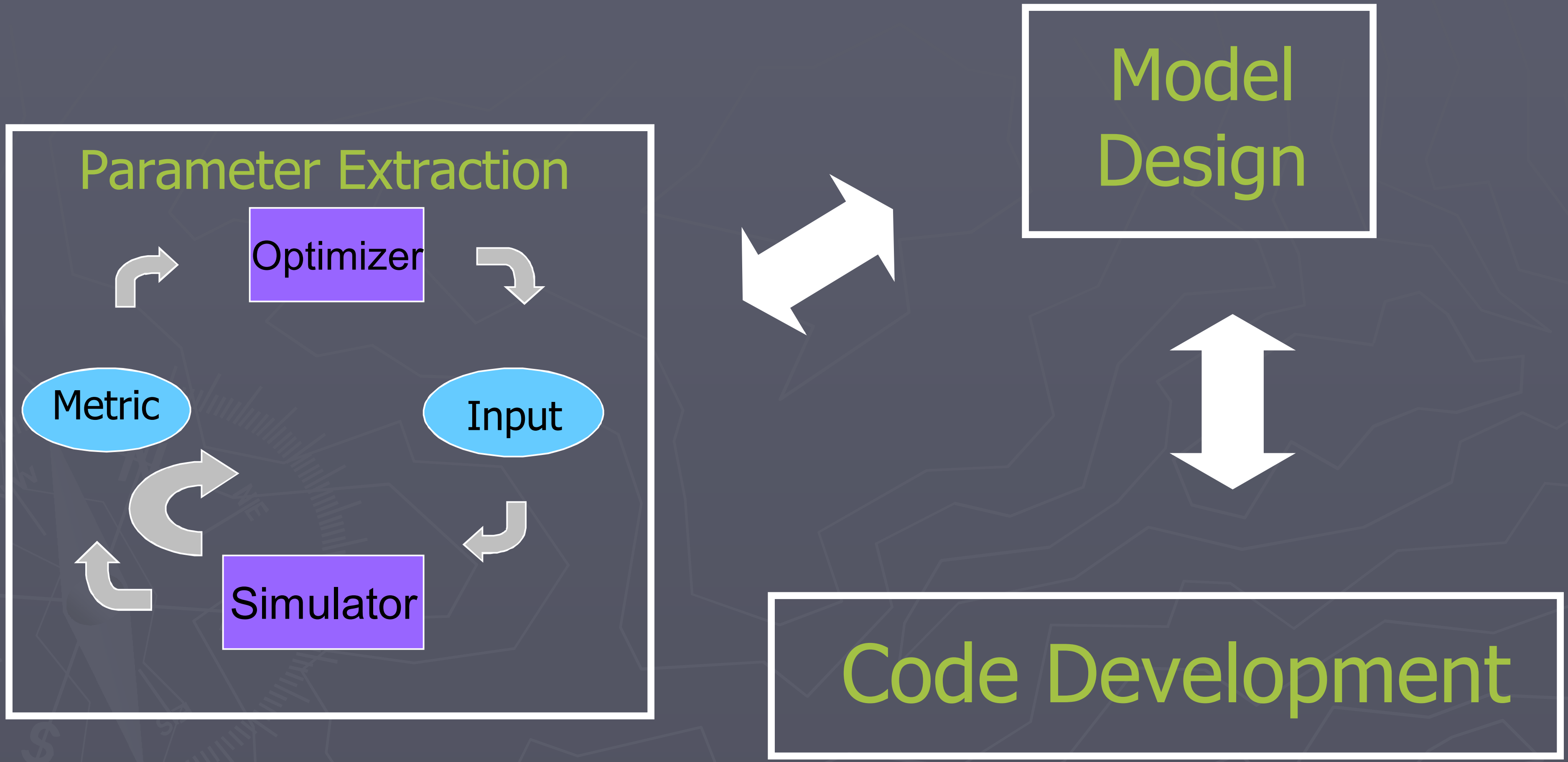
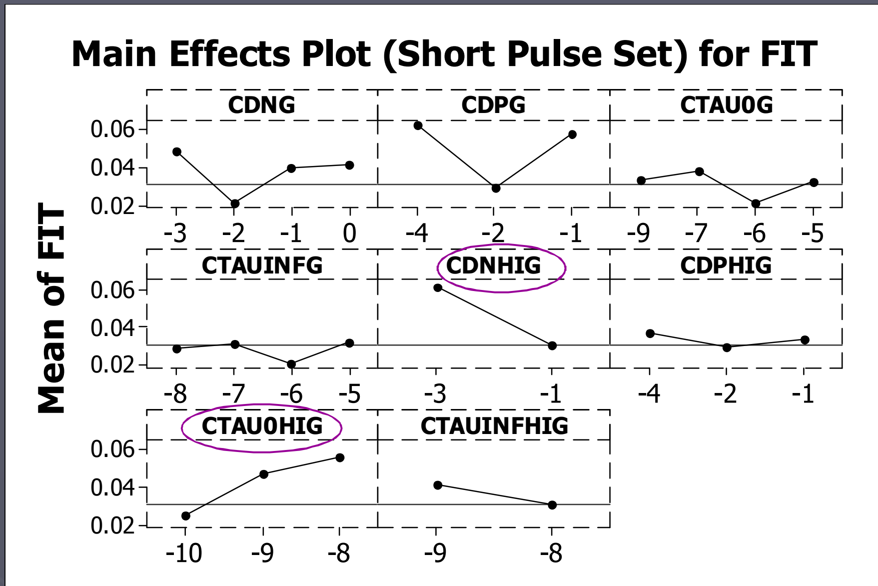
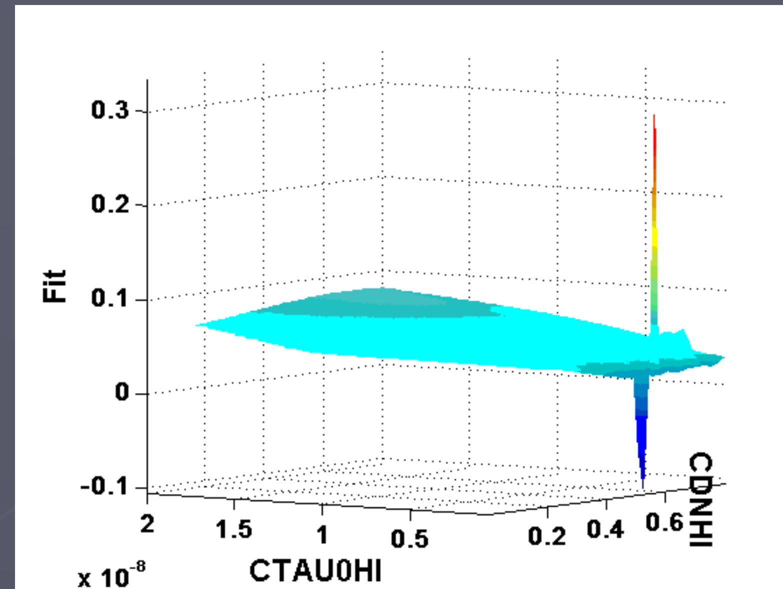
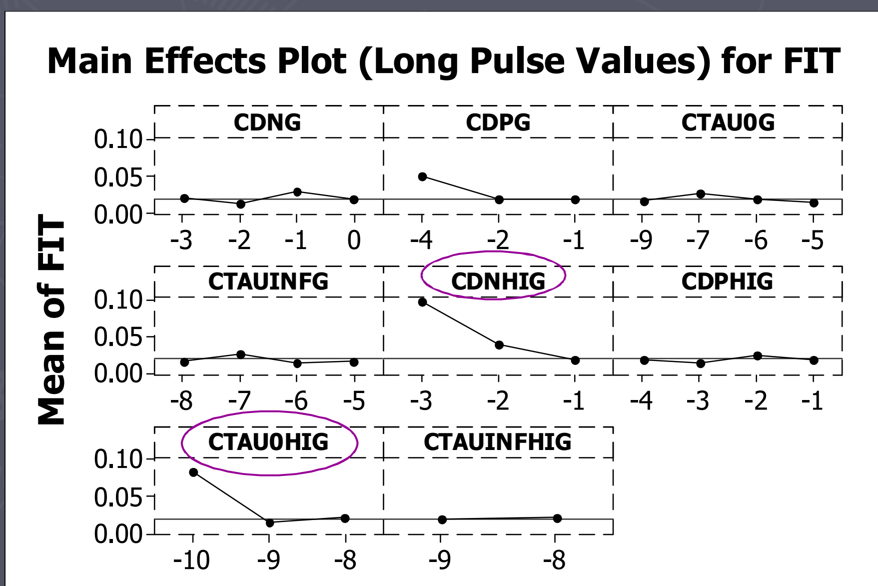
Effect on Model Design and Code Development

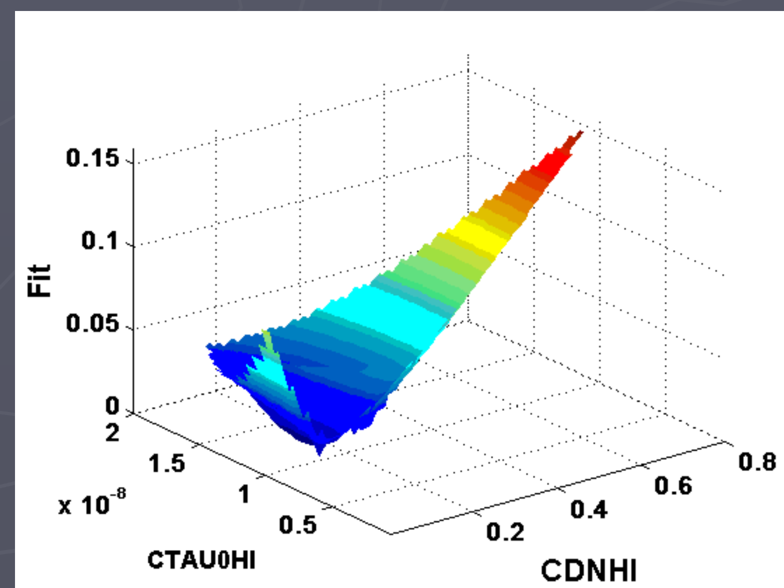


Fit Response Main Effects and Response Surfaces

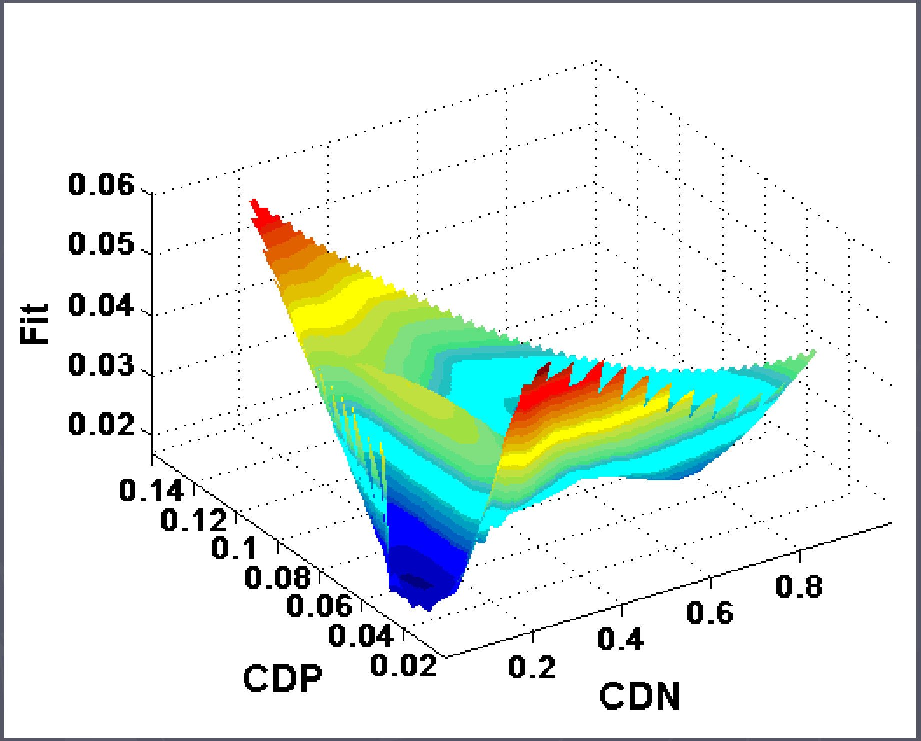


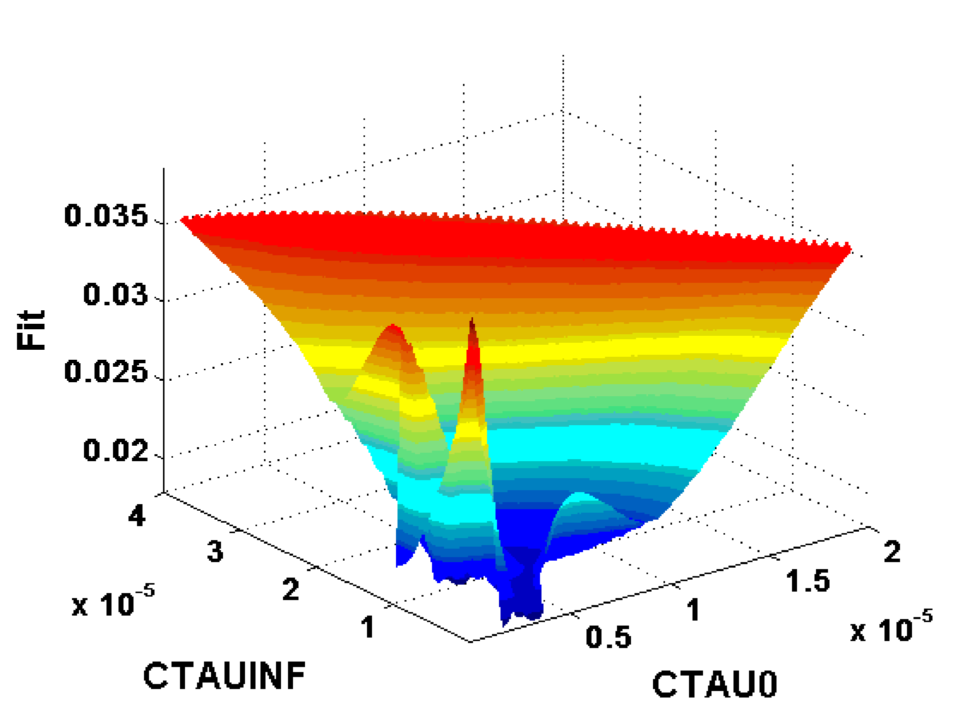






Fit Response Surfaces





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Ongoing & Future Work

- Investigate alternative metrics
  - based on data characteristics
  - application dependent
- Incorporate additional analysis
  - Consider sensitivity/robustness of optimum
  - Include response characterization
  - Differentiate the global optima or between multiple optima
  - Efficiently explore the space (particularly when given a small computing budget)
  - Try adaptive scaling

Collaborators

- Cheryl Lam
- Brian Owens
- Robert Mariano
- Travis Deyle
- Chuck Embree

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