SAND2013-6099C

Using Surrogates to Calculate Sensitivities and Improve Optimization-Based Calibration Routines

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Outline

1. Calibration
2. Surrogates
    1. Traditional role in optimization
    2. Assisting with uncertainty issues
3. The algorithm
4. Some examples
5. Ongoing & future work

Computational Modeling

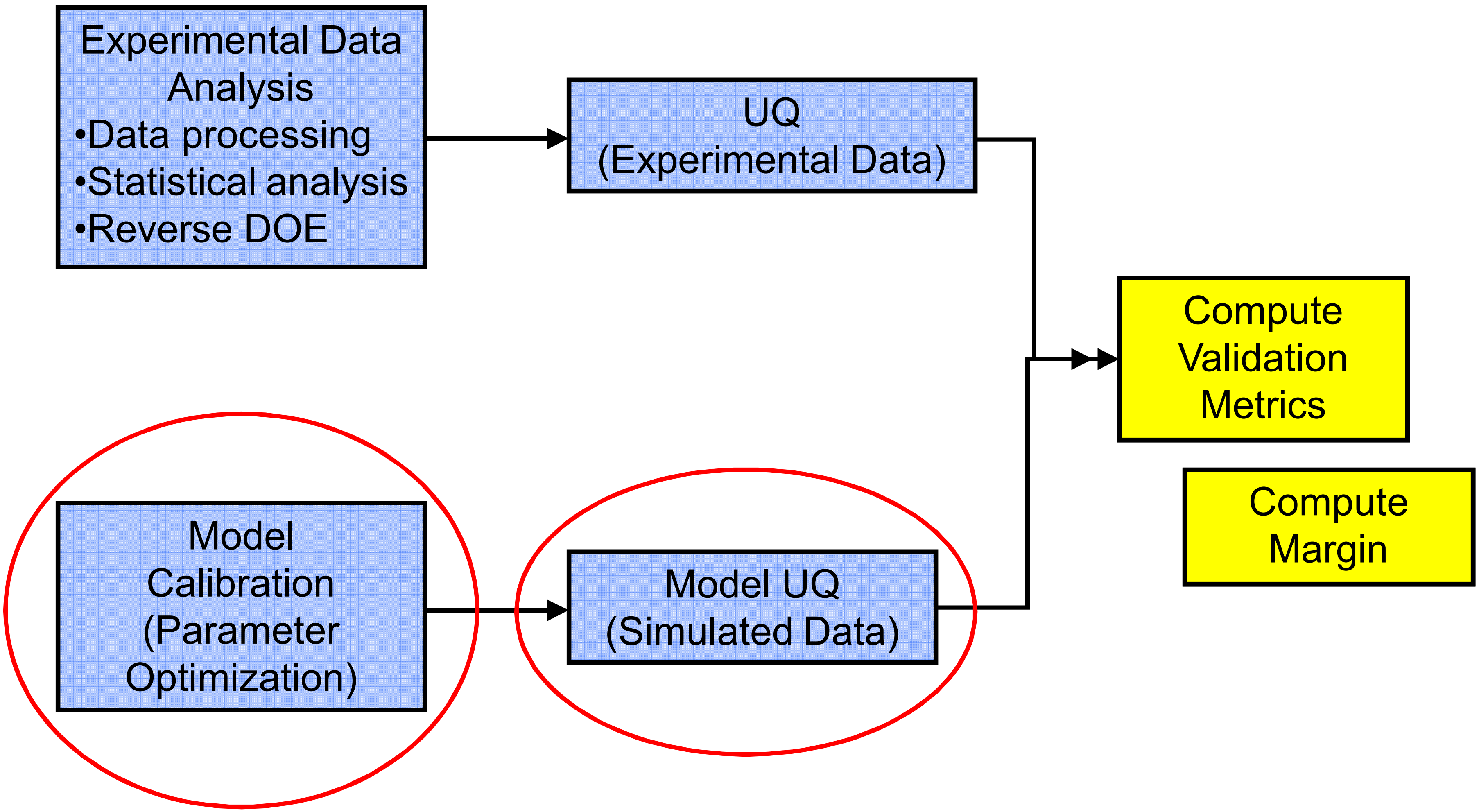
Issue in simulation-based optimization:
Uncertainty in the computational model

Understanding uncertainty: Optimization can play a significant role.

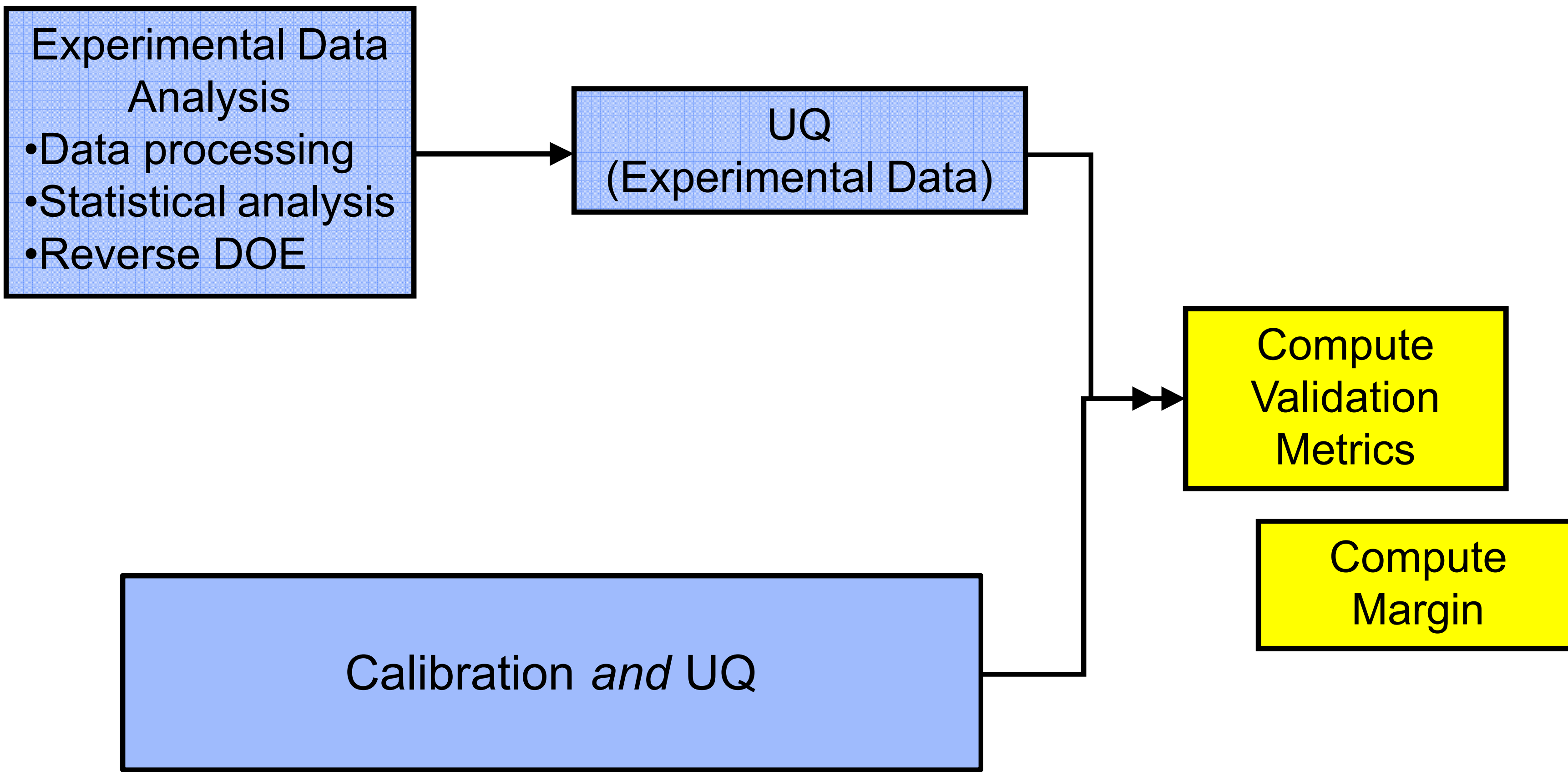
Challenges of Simulation

- Is the simulation correctly solving the underlying equations? (verification)
- Are the physical phenomena being modeled correctly? (validation)
- Can errors be identified? (uncertainty quantification & data analysis)
- How can inaccuracies be quantified? (metrics)
- What inherent model parameters should be used? (model calibration)

(Current) Validation Analysis Process

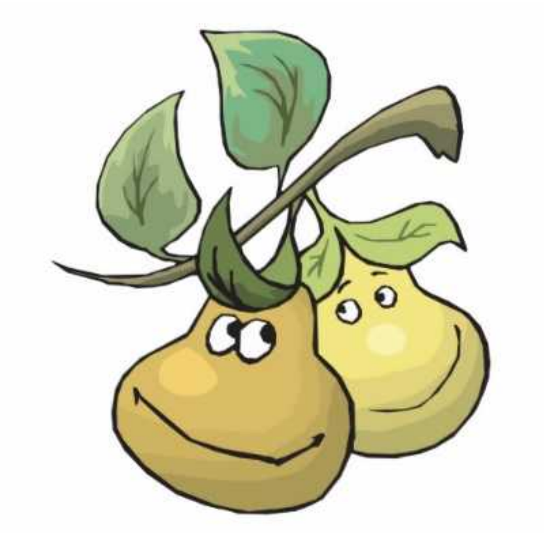


(Goal) Validation Analysis Process



Pairing Calibration & UQ

- **A combined approach doesn't just give the optimized model parameters, but also includes information to help assess their quality.**
- **In validation environments, calibration errors must be understood and should be minimized.**
- **The overall system error in the simulator is often not well understood.**



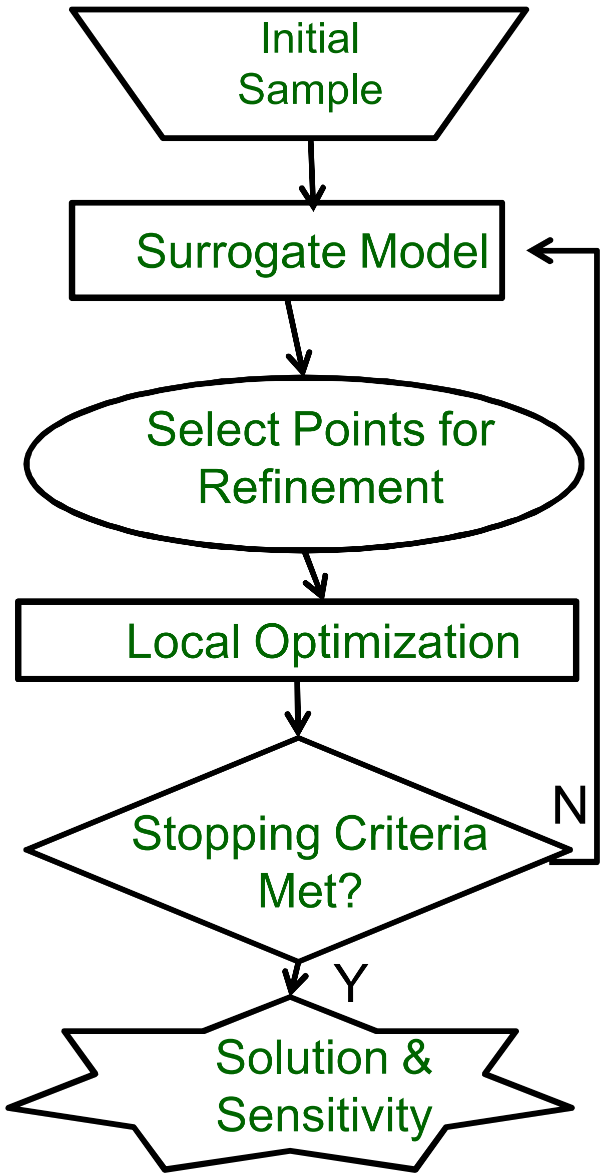
Use of Surrogates in Optimization

- Surrogates (*aka* response surface models, low fidelity models, metamodels, emulators)
  - Estimate true function behavior as close as possible
  - Computationally cheaper
- Surrogate-based optimization utilizes a surrogate in the case of computationally expensive objective functions(See for example Forrester & Keane)
- Many techniques for creating surrogates:
  - Math/stats: Kriging, Gaussian Process, etc.
  - Software options: mesh, model descriptors
- Common approach: Optimize on surrogate using periodic corrections from the true model

Using Surrogates to Estimate Sensitivities

- Explore the design space to understand the global behavior of the entire system.
  - Different goal that that of traditional optimization
  - Way to include behavior requirements without explicit constraints
- Error in the surrogate estimation must be considered
- Bayesian models provide a coherent mechanism for propagating and combining uncertainty
- Examine uncertainty using sensitivity analysis
  - How do code outputs vary due to changes in code inputs?
  - Local sensitivity: code output gradient (derivative) data for a specific set (or sets) of code input parameter values
  - Global sensitivity: the general trends of the code outputs over the full range of code input parameter values (linear, quadratic, etc.)

SQUAC Framework (Simultaneous Quantification of Uncertainty and Calibration)



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SQUAC Run

- Initial points selected via LHS
- Build the surrogate using TGP
- EGO point(s) determined at each iteration
- Local optimization routine initiated at every j-th iteration
- After convergence, all intermediate optimization iterates added to the GP model

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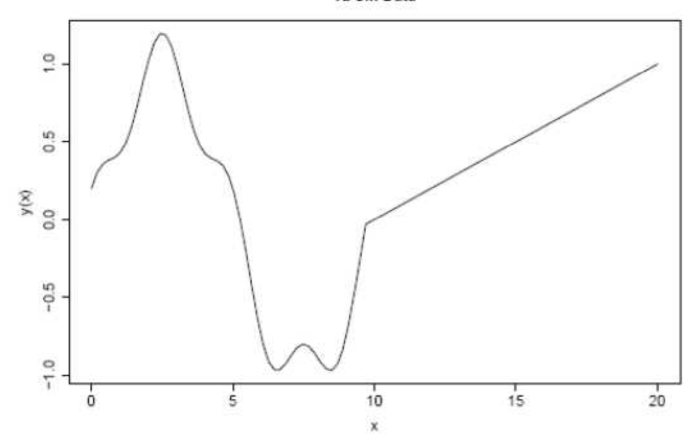
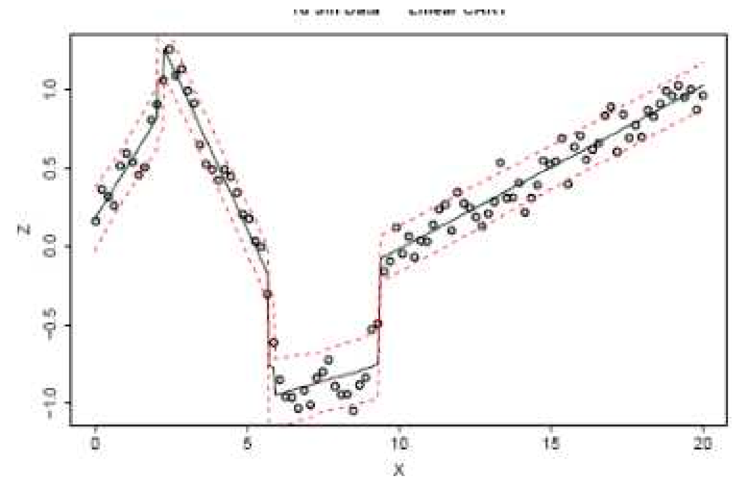
- NOTE: Many algorithm inherent "knobs" that need to be investigated

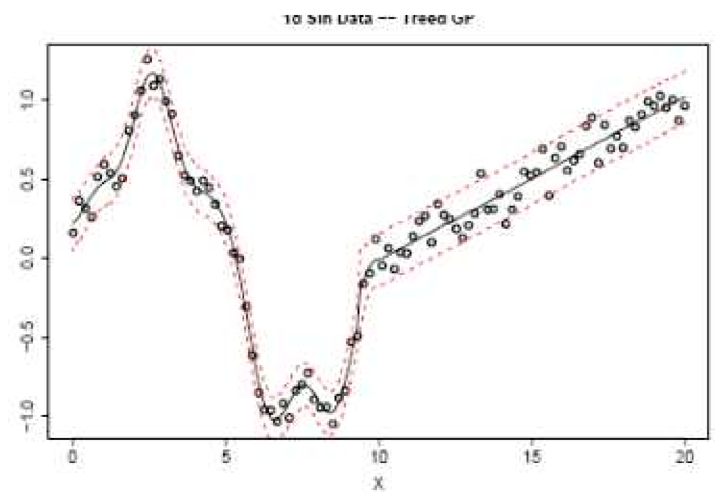
TGP: Treed Gaussian Process

- Non-stationary modeling method that couples stationary Gaussian processes with treed partitioning
- Open source R package, available from the CRAN, L-GPL license

Gramacy, Taddy, Lee







ACRO

- **Supports a variety of optimization capabilities**
  - **Linear programming**
  - **Mixed-integer linear programming**
  - **A rigorous nonlinear global optimization solver**
  - **Derivative-free local search**
  - **Stochastic global optimization methods: multistart local search, evolutionary algorithms**
  - **Parallel branch-and-bound**
  - **Bound-constrained derivative-based local optimization**
- **Open source, BSD license**
- **Available via DAKOTA**

Siirola, Hart

Application Example #1

- Problem: Appropriate design of a bipolar junction transistor (BJT)
- Question: Given certain design variables, does the simulation of the BJT response over time match the experimental response?
- Model/Simulator: Xyce
- Variables: 3 continuous
  - $1.65 \leq var1 \leq 1.95$
  - $1.82e\text{-}4 \leq var2 \leq 1.98e\text{-}4$
  - $2.04e\text{-}04 \leq var3 \leq 2.25e\text{-}4$
- Optimization Objective: Least Squares difference between simulation and experimental data

Paskaleva, Castro, Hembree

Results

- Total Wall Clock Time: ~25 hours
- Number of Function Evaluations: 446
- Results:

	Var1	Var2 * e-4	Var3 * e-4
Lower Bd (defined)	1.65	1.82	2.04
Upper Bd (defined)	1.95	1.98	2.25
Pt w/ Best SD	1.8993759033	1.9548180998	2.1102588309
Pt w/ Best Conf. Bd	1.7492615770	1.9489892813	2.1855684542
Classical Opt Soln	1.8389242337	1.9567873122	2.1567230281

Application Example #2

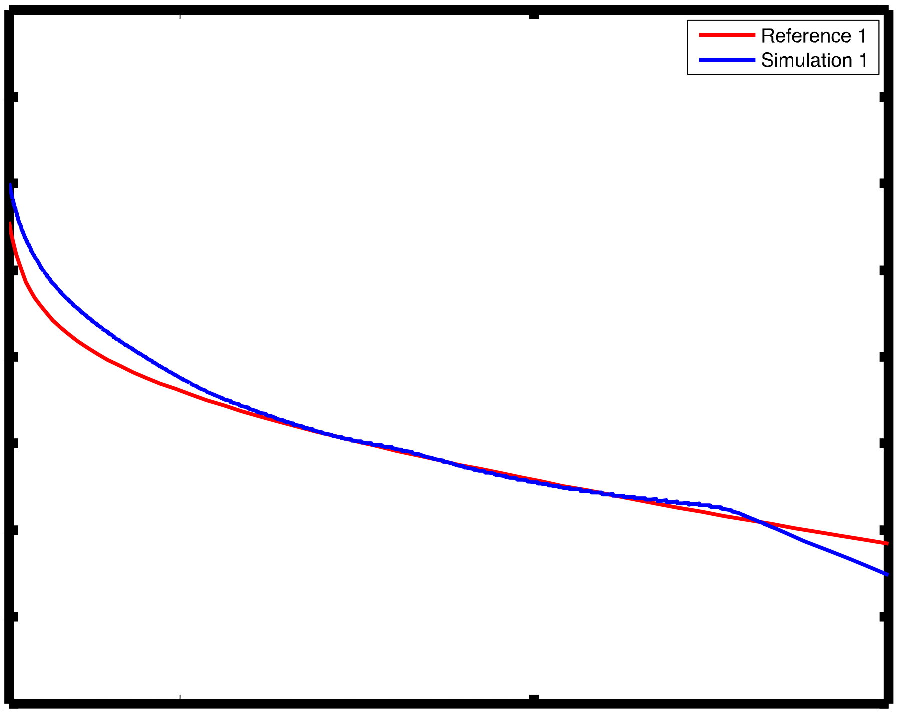
- Problem: Appropriate selection of model parameter values of a heterojunction bipolar transistor (HBT)
- Question to answer: Given design variables, does the simulation of the HBT response to a stimulus over time match the response of reference data?
- Model/Simulator tool: Xyce
- Variables: 2 continuous
  - ✓ $0.5 \leq ua \leq 2.00$
  - ✓ $0.1 \leq ub \leq 1.50$
- Optimization Objective: Least Squares difference between simulation and reference data

Results

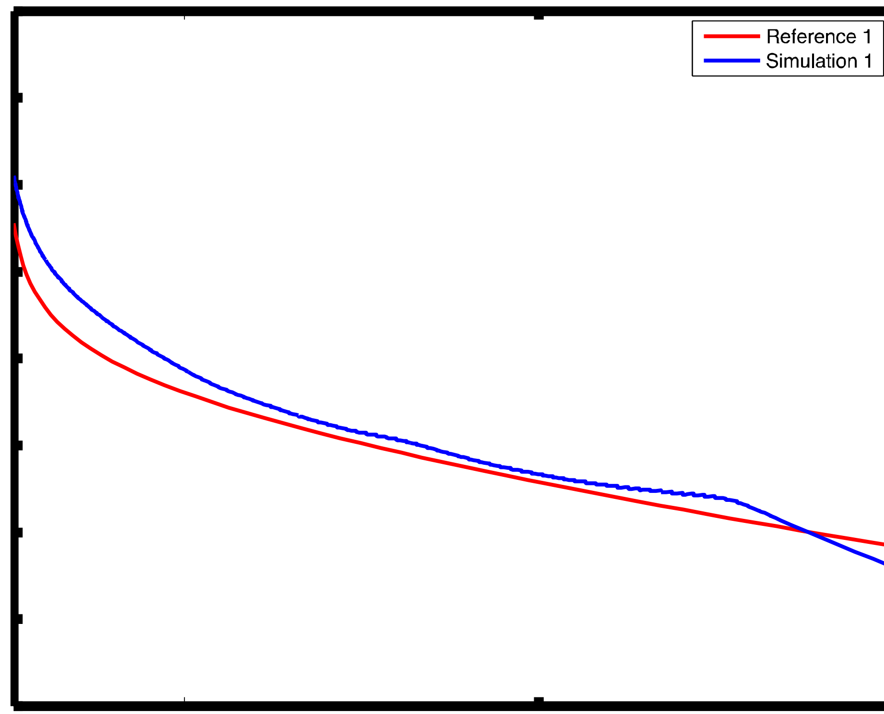
HBT Device	Optimal Solution TGPO	Optimal Solution MOGA	# Fn Evals TGPO	#Fn Evals MOGA	Total Time (Hrs)	SQFIT TGP (10e-03)	SQFIT MOGA (10e-03)
1	1.0661743908 9.0766844773e-01	1.0738527468 9.1629941073e-01	506	219	3.15	3.424	5.487
2	1.0973663353 6.6957300437e-01	1.1306264350 5.9615848134e-01	193	213	1.5	3.608	5.948
3	9.5057394851 7.9797247646e-01	9.3547443903e-01 8.6885081985e-01	193	215	1.49	5.439	8.49
4	1.1633999400 7.5076774351e-01	1.1306264350 8.2046881137e-01	682	219	3.94	3.396	7.146
5	1.1764720238 7.5927475756e-01	1.1519550300 8.5096085321e-01	633	264	3.76	3.693	5.145
6	1.0599146094 7.9311727991e-01	1.0738527468 7.7253641788e-01	222	269	1.63	5.752	6.406

HBT 1

TGP

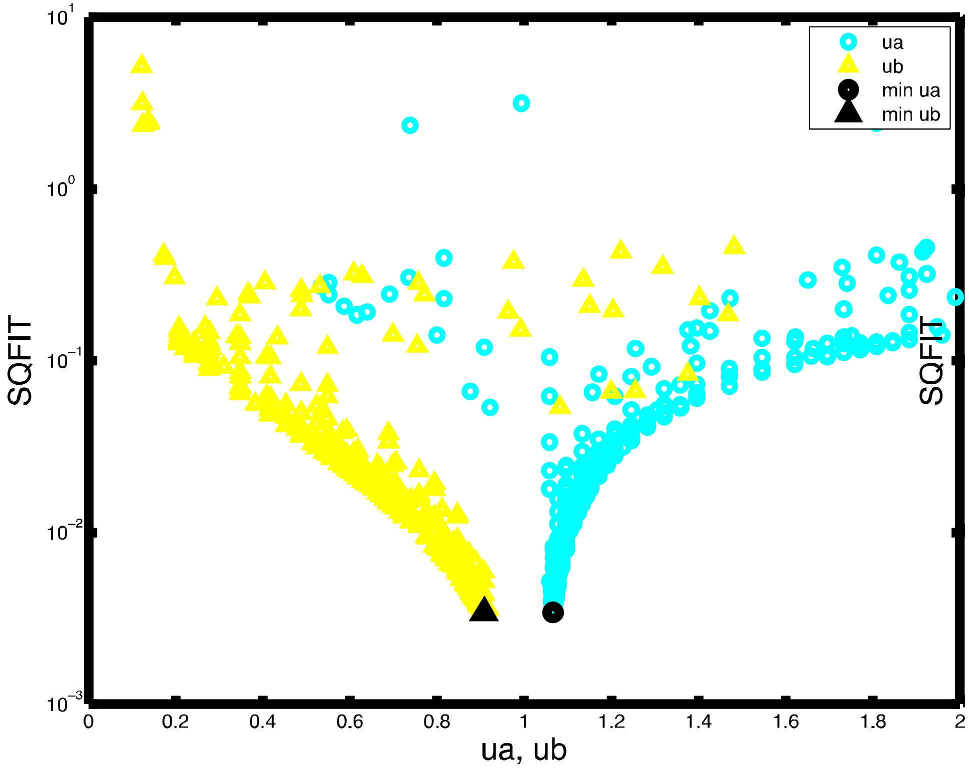


MOGA

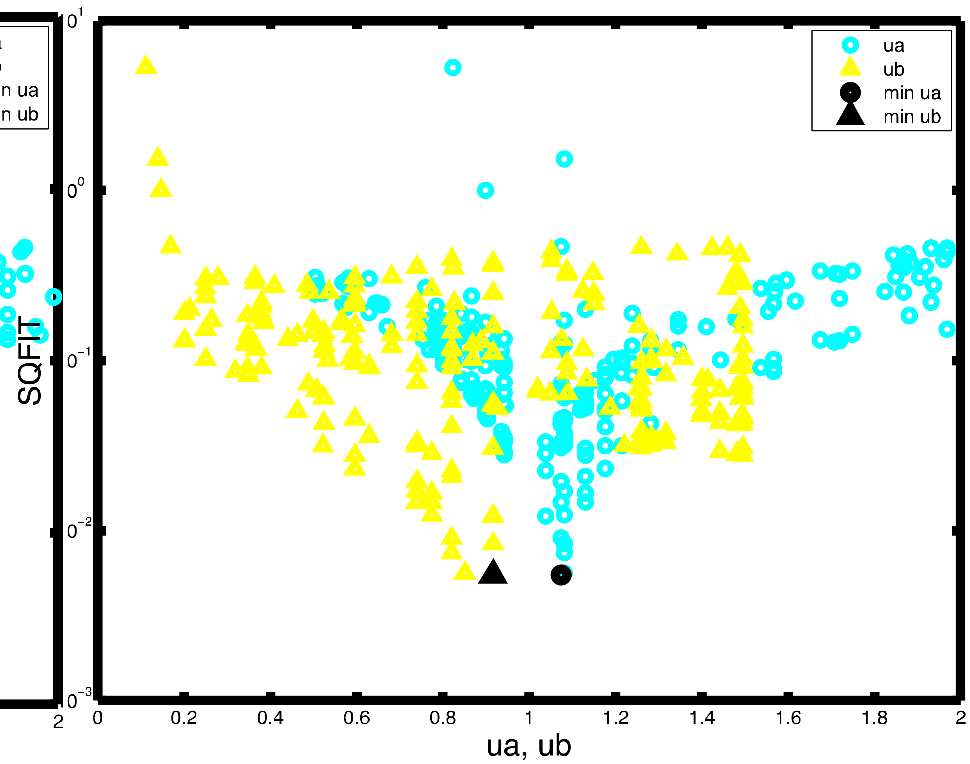


HBT 1

TGP



MOGA



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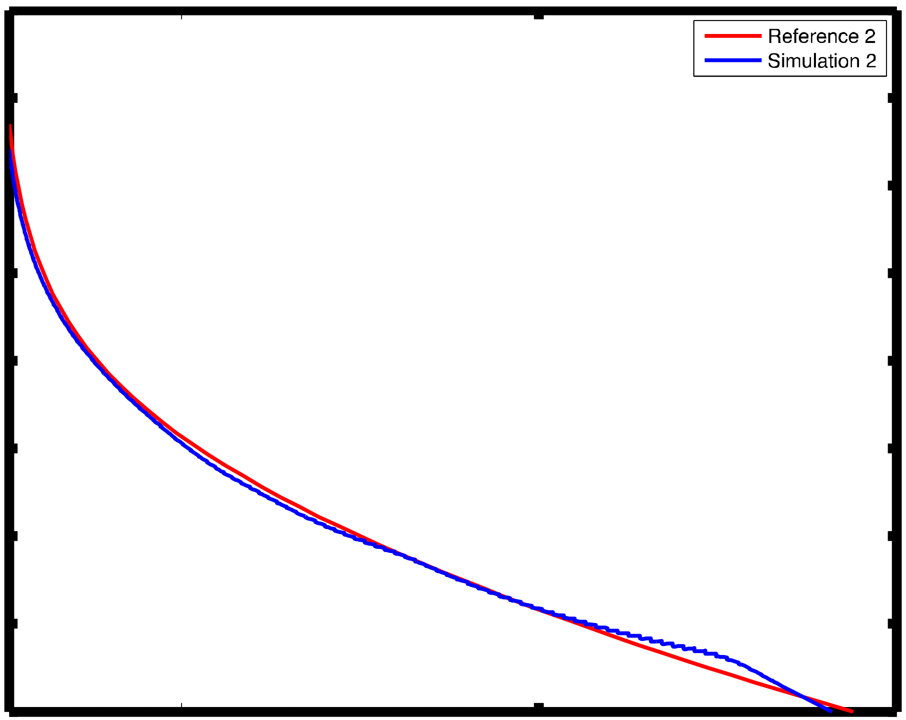
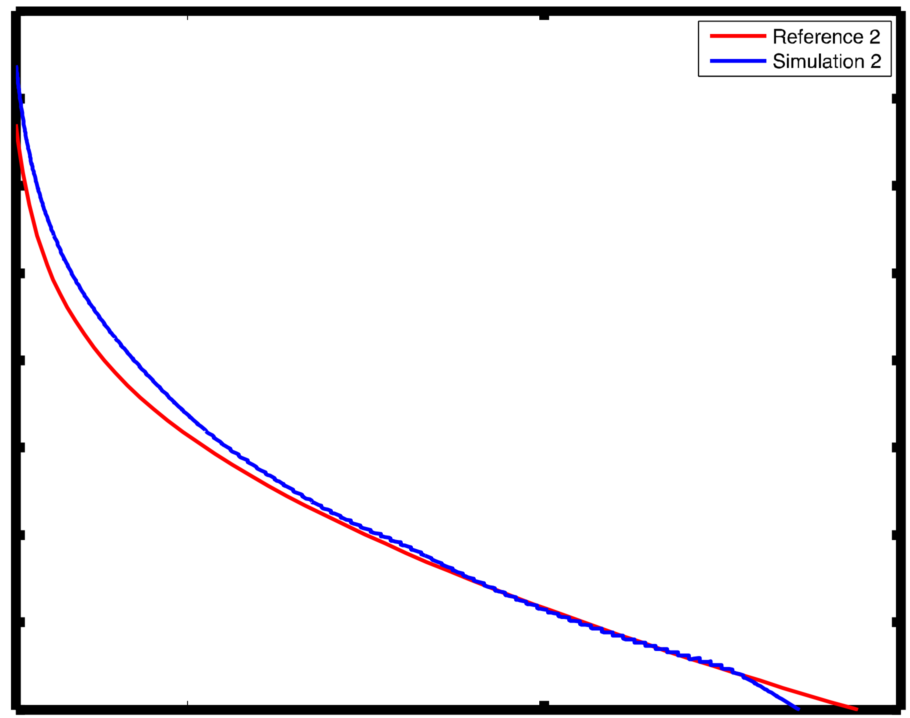
HBT2

TGP



MOGA



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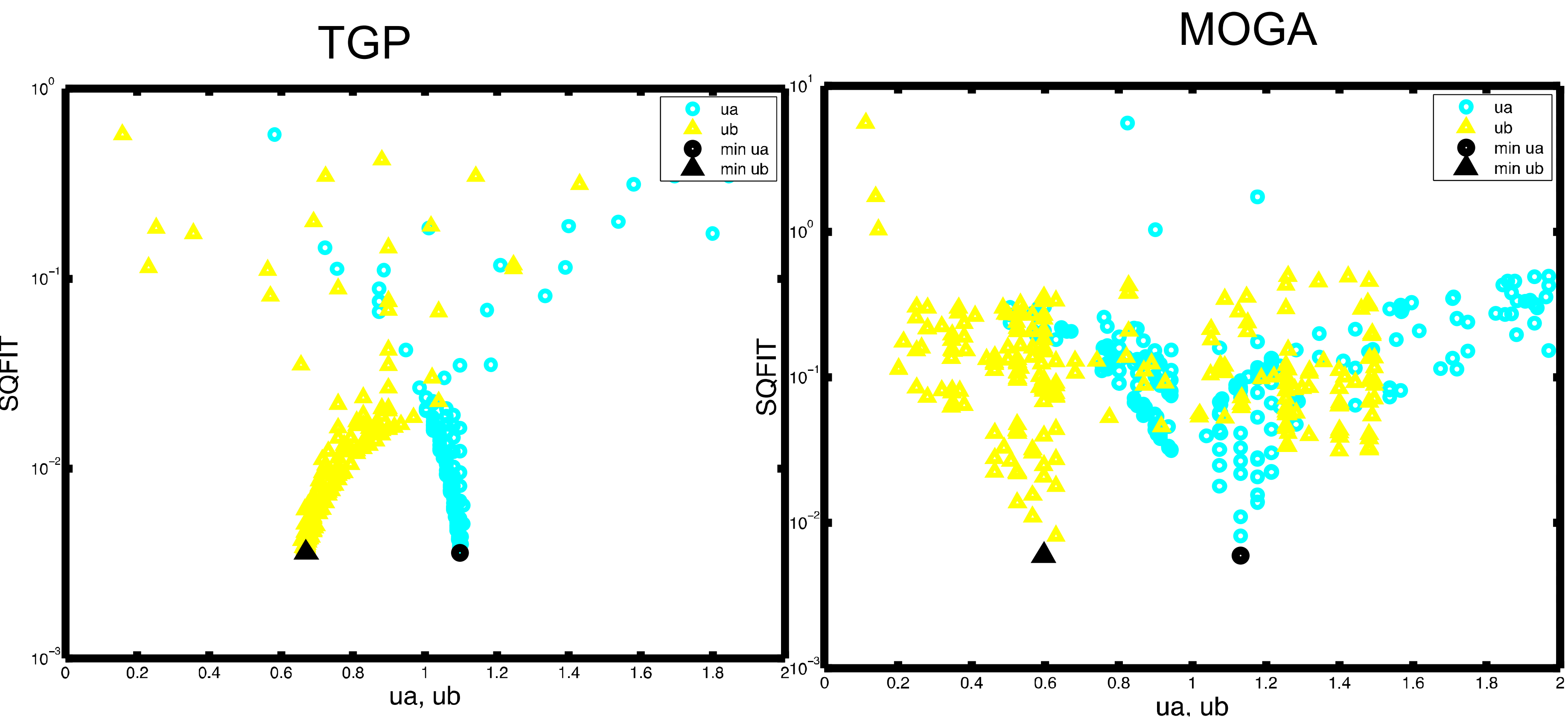
HBT2



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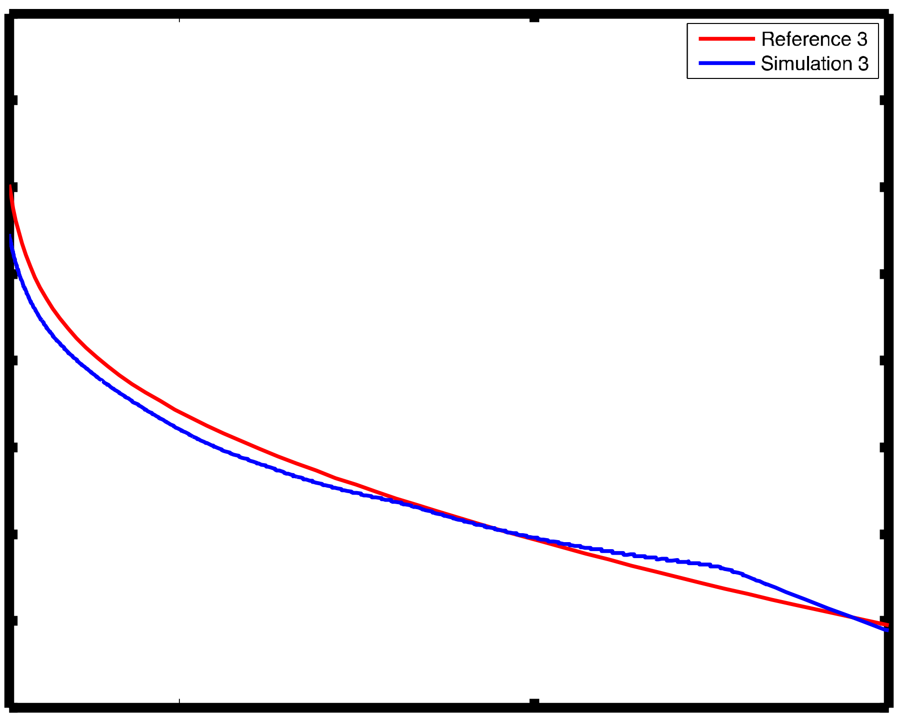
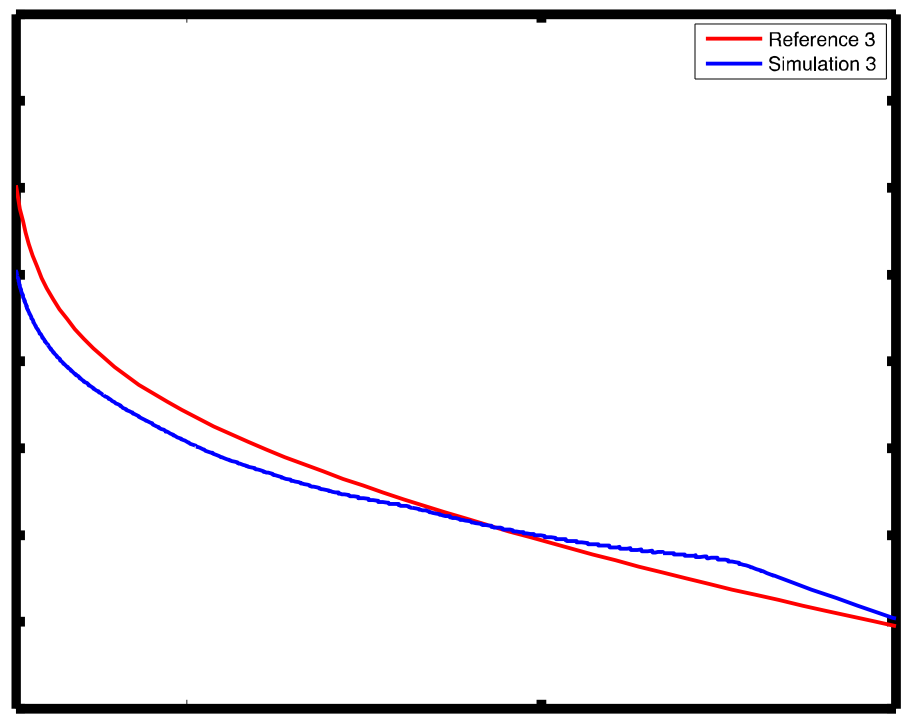
HBT3

TGP

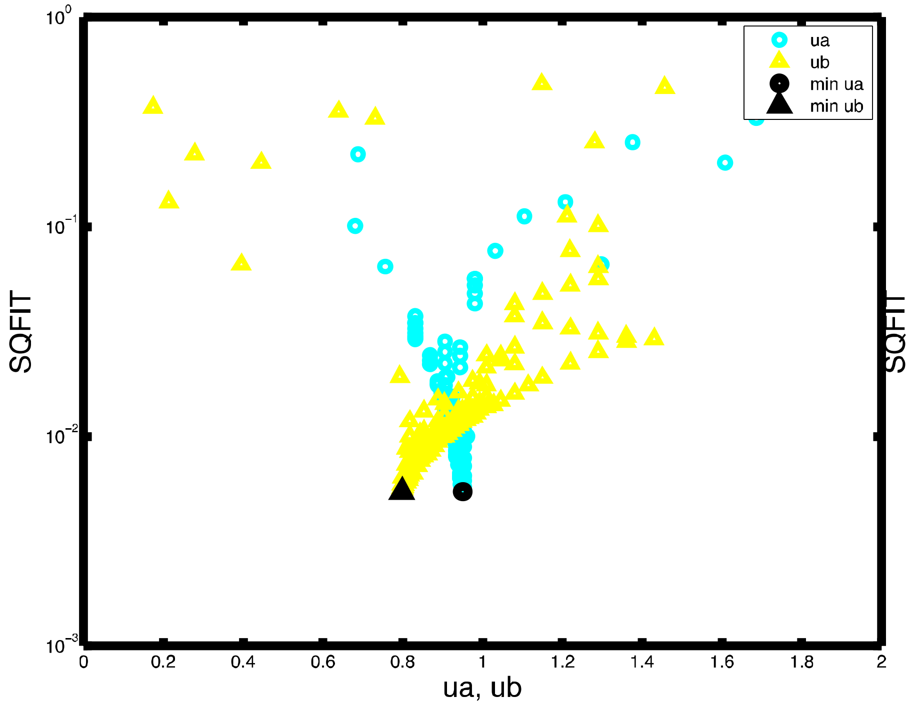


MOGA

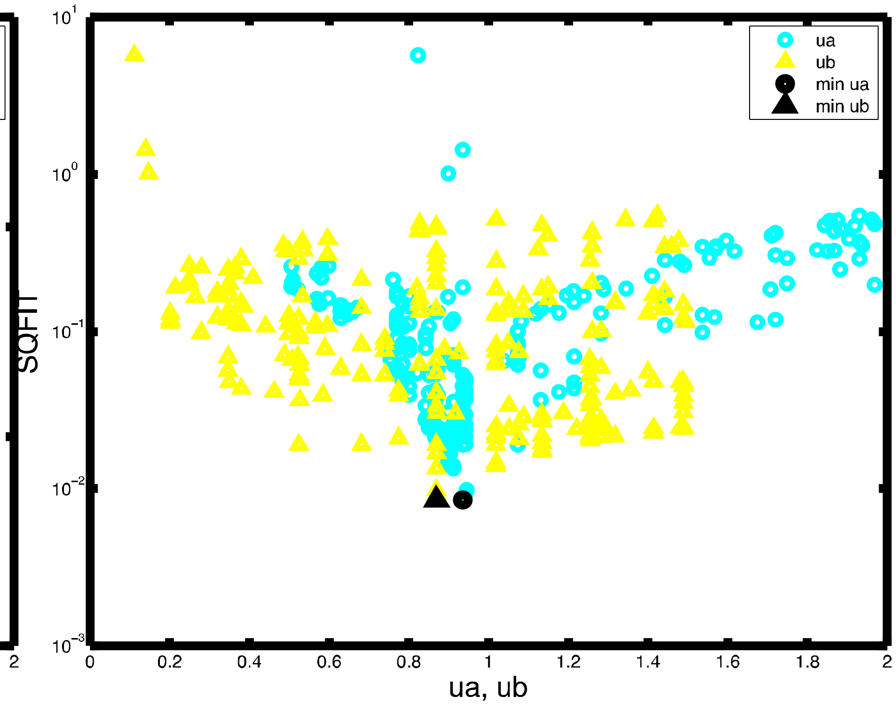


HBT3

TGP

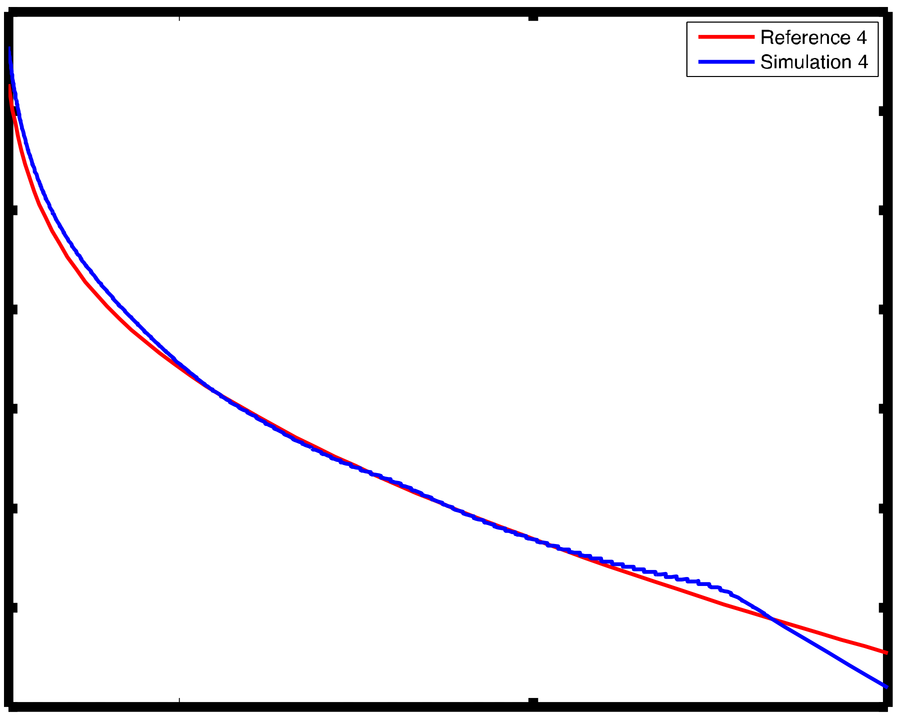


MOGA

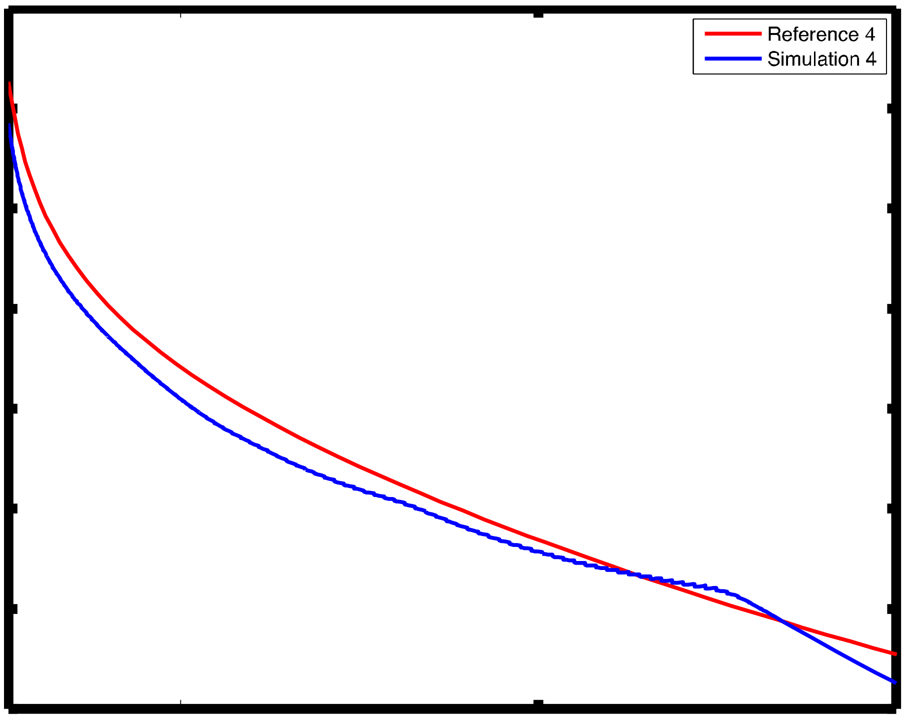


HBT4

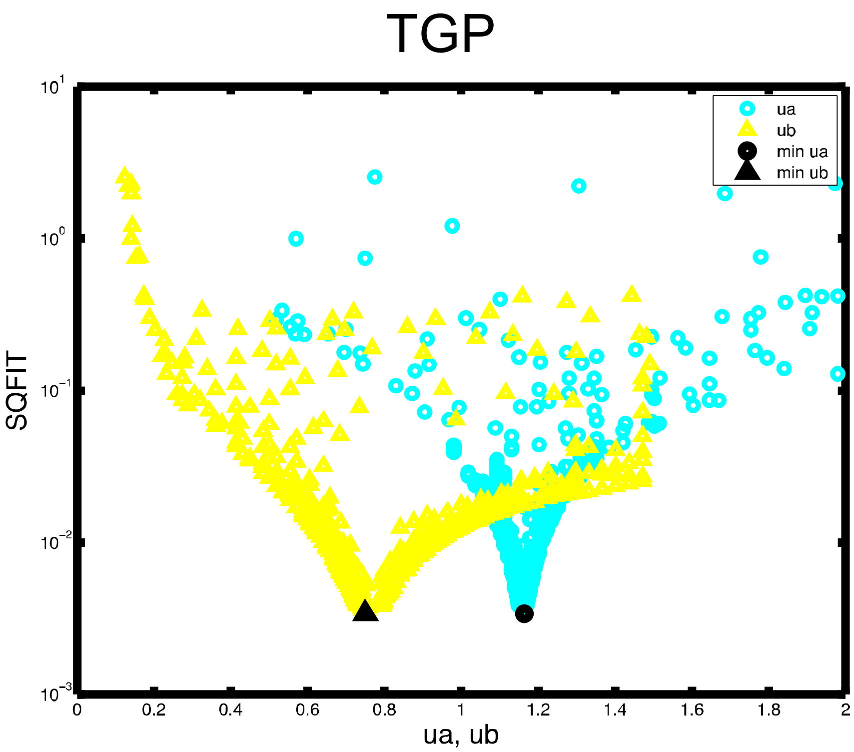
TGP



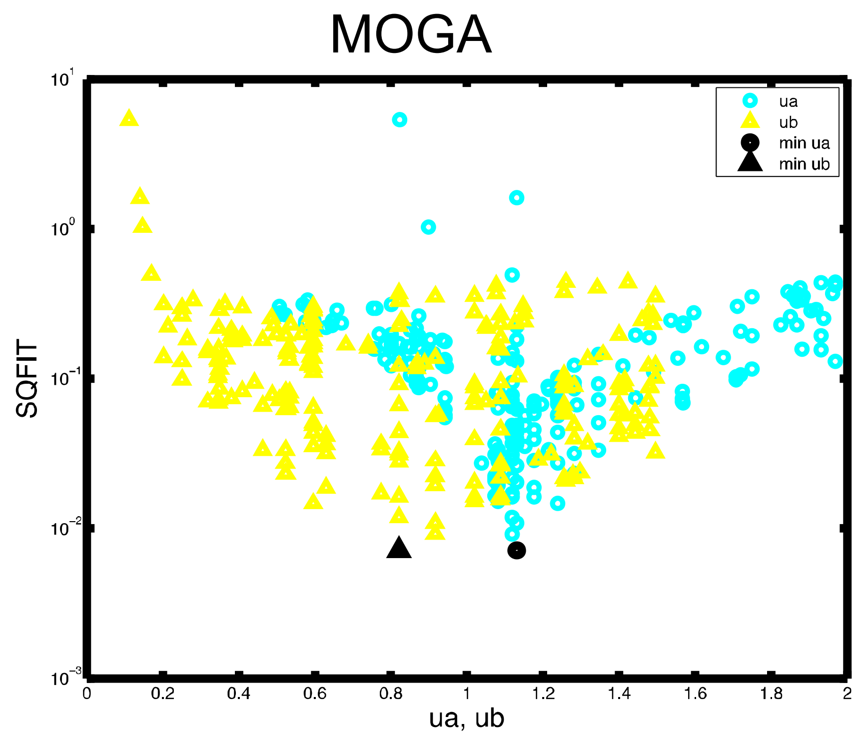
MOGA



HBT4



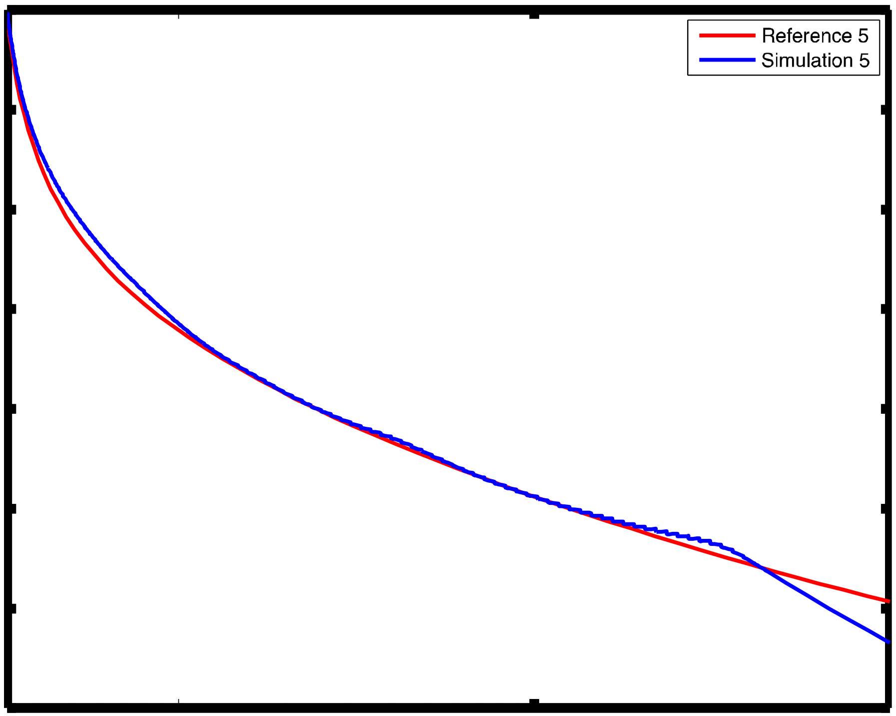
TGP
SQFIT
ua, ub
ua
ub
min ua
min ub
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2



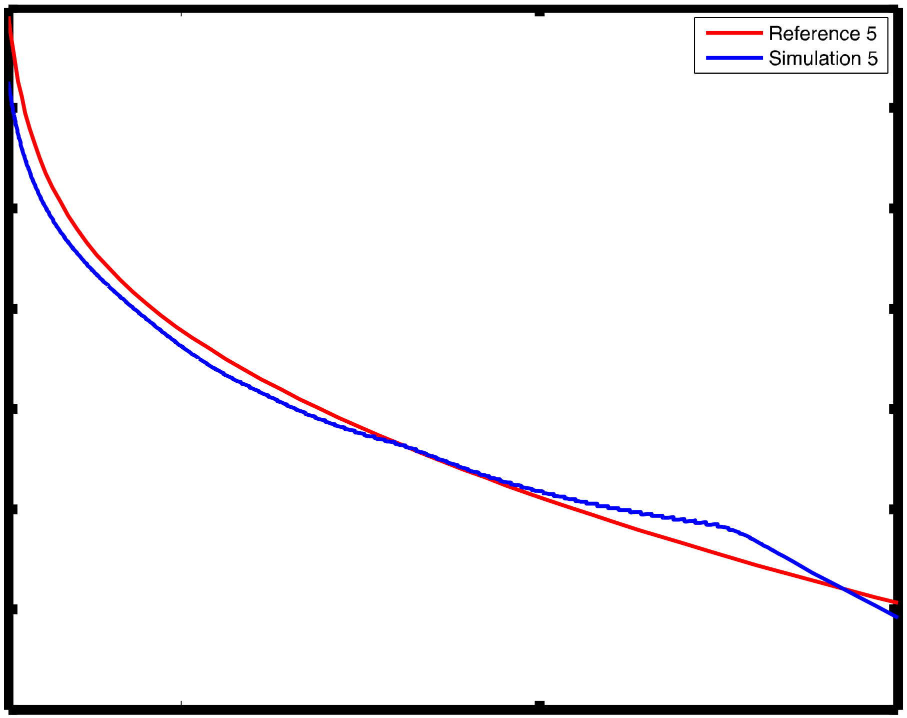
MOGA
SQFIT
ua, ub
ua
ub
min ua
min ub
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2

HBT5

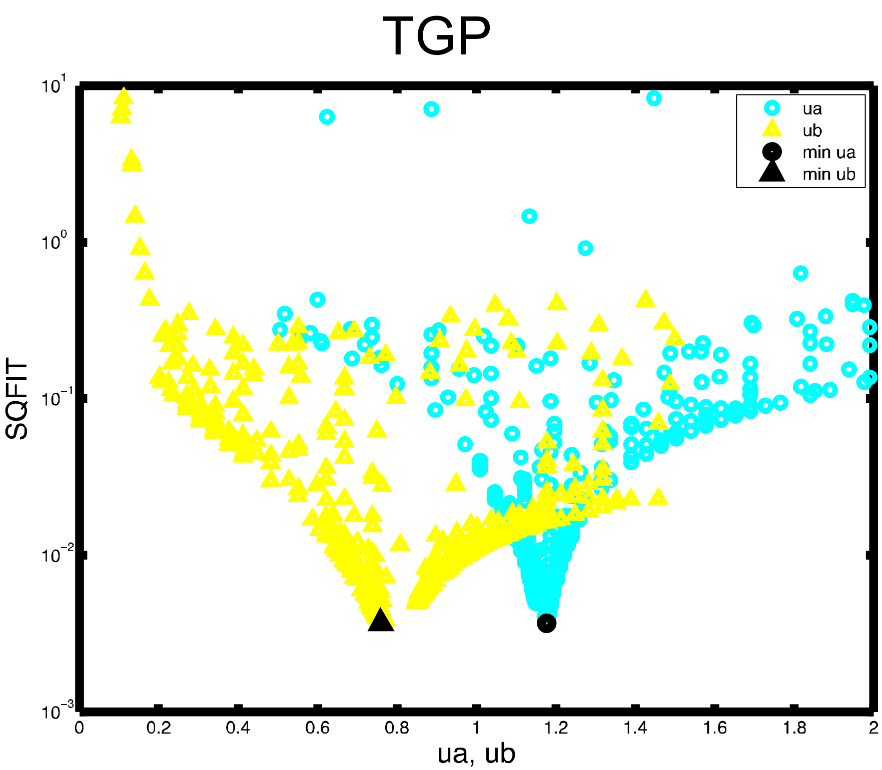
TGP



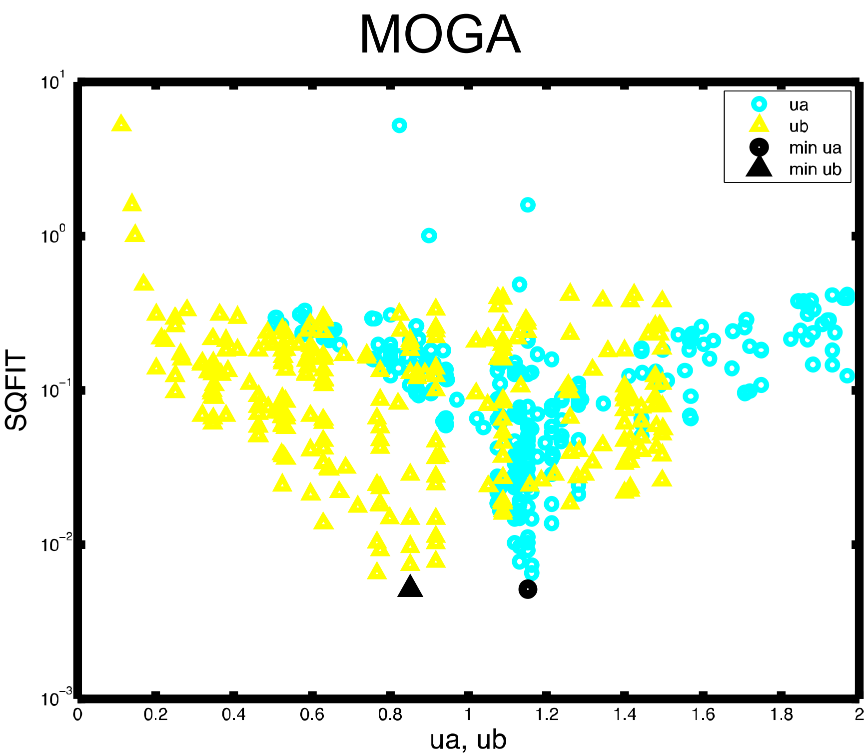
MOGA



HBT5

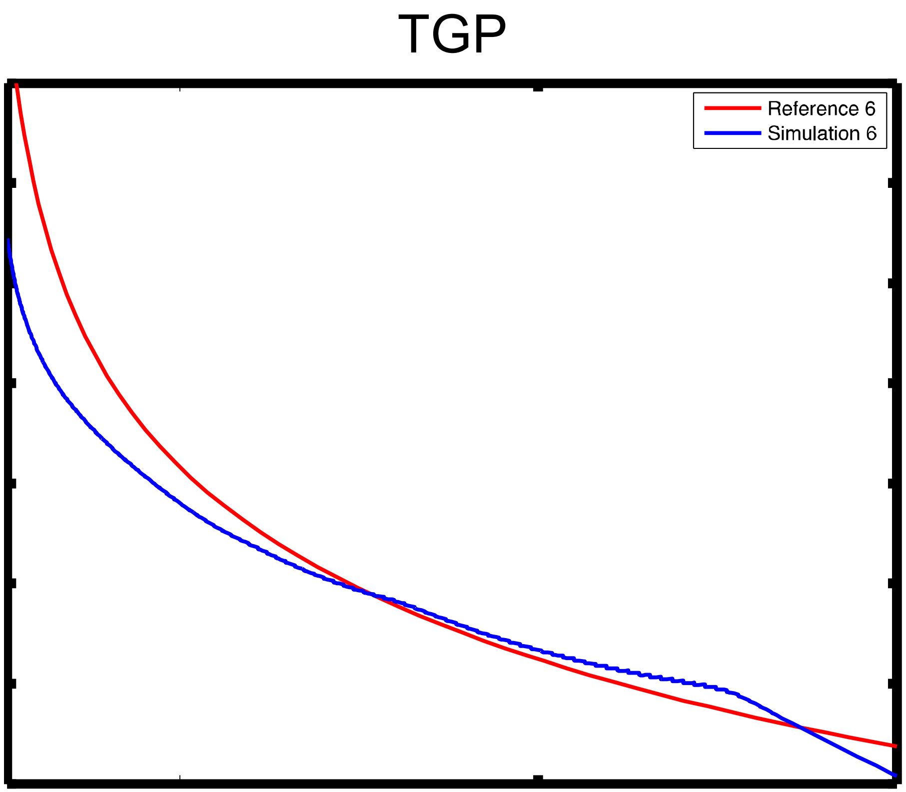


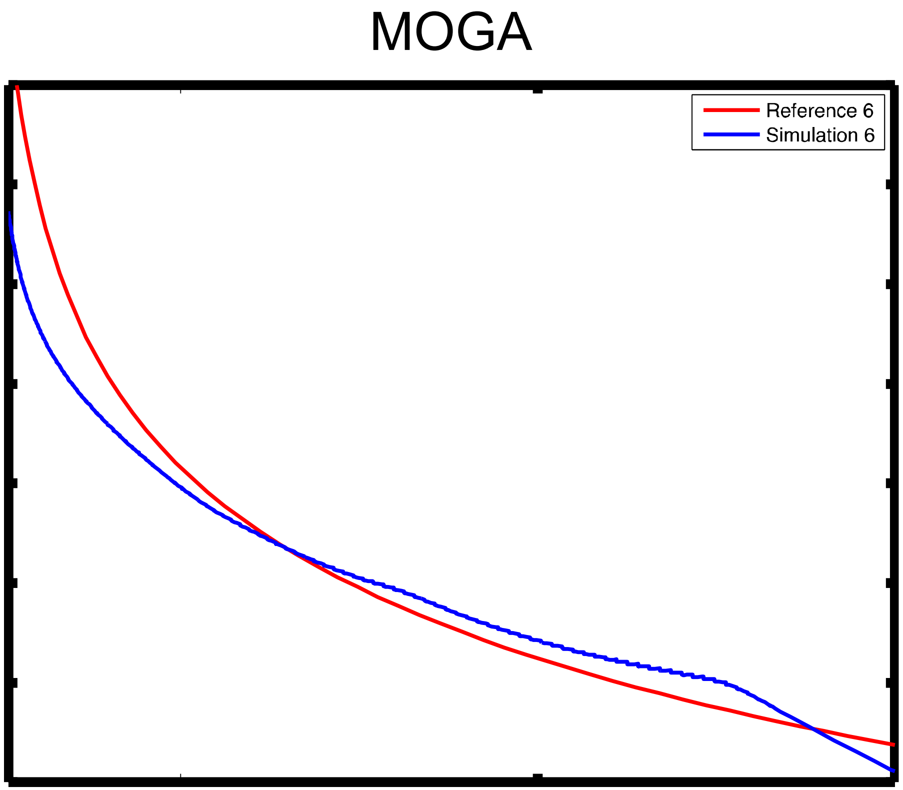
TGP
SQFIT
ua, ub
ua
ub
min ua
min ub



MOGA
SQFIT
ua, ub
ua
ub
min ua
min ub

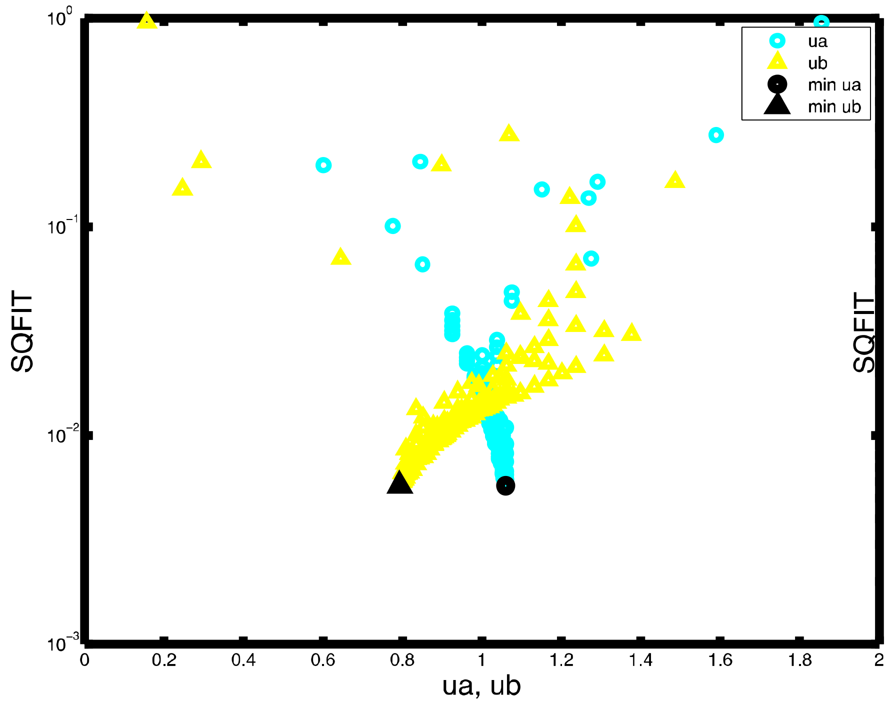
HBT6



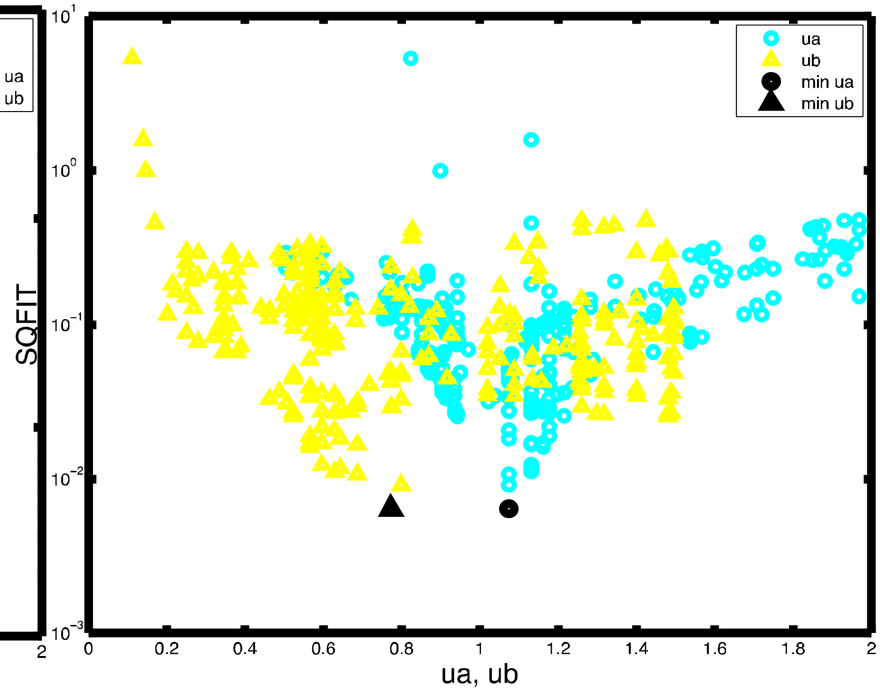


HBT6

TGP



MOGA



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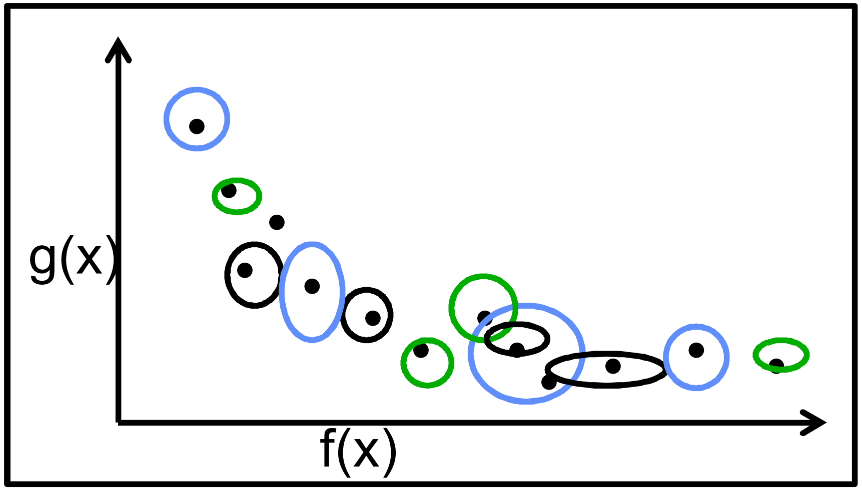
What's Next

- Test alternatives in the framework
  - Optimization methods
  - Sampling methods
  - Surrogate modeling approaches
  - Expected improvement functions
- Include optimization on the surrogate
- Apply to multi-objective problems



Concept of uncertainty on the multi-objective Pareto front.

Collaborators/Contributors

Collaborators:

- Herbie Lee, John Guenter, UCSC
- Bobby Gramacy, University of Chicago
- Peter Bosman, CWI

Funding thanks to:

- American Institute of Mathematics (AIM)
- Sandia ASC & LDRD programs