Introduction

The QUESO library is a collection of parallel statistical algorithms and object-oriented programming constructs supporting research into the uncertainty quantification of mathematical models.

- Quantification of Uncertainty for Estimation, Simulation and Optimization
- Available at https://github.com/libqueso/queso
- Development began in 2008 under the PSAAP program
- Since 2011, QUESO development has been part of the SCIdac3 program as part of the QUEST center
- QUESO is used by Dakota to solve the inverse problem
- QUESO has traditionally focused on the inverse problem but has forward propagation capabilities as well

Why use QUESO?

- Other solutions available: R, PyMC, emcee, MICA, etc
- QUESO solves the same problem but has significantly more CS&E capabilities
- Has been designed to be used with large forward problems
- Has been used with over 10k cores
- Support for finite and infinite dimensional problems
- Can sample multimodal distributions
- Can leverage Dakota for forward propagation (Dakota can use QUESO for the inverse problem)
- Emulation capabilities being developed

HPC Relevance

- Parallel Sampling
- Automatic load-balancing for homogenous systems
- Future load-balancing for heterogeneous systems
- Fault tolerance

Sponsors

- 2008 – 2014: DOE NNSA, PSAAP Program
- 2010 – 2011: DOE SNL-NM, Peridynamics Program
- 2010 – 2012: KAUST, AEA2 Program
- 2011 – 2013: AFSR, RTC, DDDAS Program
- 2011 – 2015: DOE SC, SciDAC3 Program
- 2012 – 2013: DOE LANL and ORNL, CASL Project
- 2012 – 2014: KAUST, AEA2 Program

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Recent Changes in QUESO

- New swanky website: http://libqueso.com
- Version 0.51.0
- A new likelihood for scalar GPMSA use case of Higdon et al
- Add a log-transformed transition kernel for more efficient proposals
- Adding Jeffreys distribution as an available prior distribution
- Adding likelihood value caching to ML sampler
- Version 0.52.0
- A new canned Gaussian likelihood for different full/block diagonal covariance matrices
- Above 428 commits

DAKOTA integration. Ongoing work with Laura Swiler, Brian Adams, Mike Eldred, Brian Williams
- Version 0.53.0
- Add linear interpolation surrogates
- Refactor input options processing
- Refactored existing qeuso errors and asserts
- Add new error checking macros
- Add basic scoped pointer wrappers
- Better error message reporting for bad sample covariance matrices

Parallel Chains in QUESO

Performance improvement with \( \text{logit}(x) = \log(1/(1-x)) \)

This maps \((0, 1) \rightarrow (-\infty, \infty)\). We never propose states out of bounds:

SPNDS recommands

- Parallel chains

QUEST Impact on QUESO

• PAST
  - Documentation and testing
  - Stress integration
  - Dakota integration
  - New example problems

• PRESENT
  - cPUMA
  - More Dakota integration
  - Software quality and usability improvements
  - User community development
  - Infinite dimensional UQ

• FUTURE
  - Further emulation development
  - Continued software engineering improvement
  - Additional options for vector/matrix classes to increase user base
  - Opportunity to be adopted as THE community code for uncertainty quantification

Extended documentation effort!

Questions?

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• QUESO development team

Extended documentation effort!

Questions?