Highlights of QUEST Developments and Partnership Activities

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Outline

1. Introduction
2. FES Edge Plasma Partnership
3. BER Atmospheric Modeling Partnership
4. Closure

Key Elements of our UQ strategy

- Probabilistic framework
  - Uncertainty is represented using probability theory
- Parameter Estimation, Model Calibration
  - Experimental measurements
  - Regression, Bayesian Inference
- Forward propagation of uncertainty
  - Polynomial Chaos (PC) Stochastic Galerkin methods
    - Intrusive/non-intrusive
  - Stochastic Collocation methods
- Model comparison, selection, and validation
- Model averaging
- Experimental design and uncertainty management

QUEST Team

Institution	Participants
SNL	**H. Najm**, M. Eldred, B. Debusschere, J. Jakeman, K. Chowdhary, C. Safta, K. Sargsyan
USC	**R. Ghanem**
Duke	**O. Knio**, O. Le Maître, F. Rizzi, J. Winokur
UT	**O. Ghattas**, R. Moser, E. Prudencio, A. Alexanderian T. Bui-Thanh, K. E.-Hiroms, N. Petra, G. Stadler
LANL	**D. Higdon**, J. Gattiker
MIT	**Y. Marzouk**, P. Conrad, T. Cui, A. Gorodetsky, M. Parno

Team Expertise and Capabilities

Institution	Expertise	Tools
SNL	Forward and inverse UQ methods, design under uncertainty	DAKOTA UQTK
USC	Intrusive UQ methods probabilistic modeling	
Duke	Sparse adaptive forward UQ methods	
UT	Large scale inverse problems validation, inverse UQ	QUESO
LANL	Gaussian process modeling, inverse UQ	GPMSA
MIT	Calibration, adaptive sampling, inverse UQ, experimental design	MUQ

Recent Progress

Software development & integration: SNL, UT, LANL, MIT

DAKOTA, QUESO, UQTk, GPMSA, MUQ

Algorithmic developments:

- Hierarchical sparse grid interpolation SNL
- Adaptive basis & sparse representations USC, Duke, MIT
- Compressive sensing, sparsity, & multifidelity SNL
- Missing data & sparse random fields SNL
- Gradient based optimization and MCMC Duke, MIT
- Conditional polynomial representations USC
- Bayesian additive regression trees for massive data LANL
- Extreme scale Bayesian inverse problems UT
- Kernel approx. & discontinuity detection in hi-D MIT

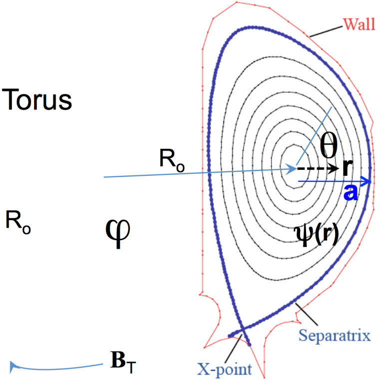
QUEST Partnerships

DOE	Project Title	Lead PI	QUEST
FES	Center for Edge Plasma Physics Simulation (EPSI)	C.S. Chang Princeton	Moser UT
FES	Plasma Surface Interactions: Bridging from the Surface to the Micron Frontier	B. Wirth ORNL	Higdon LANL
BER	Predicting Ice Sheet & Climate Evolution at Extreme Scales (PISCEES)	P. Jones LANL	Eldred, Ghattas SNL, UT
BER	Multiscale Methods for Accurate, Efficient & Scale-Aware Earth System Modeling	B. Collins LBNL	Debusschere SNL
NP	Nuclear Computational Low Energy Initiative (NUCLEI)	J. Carlson LANL	Higdon LANL
HEP	Computation-Driven Discovery for the Dark Universe	S. Habib ANL	Higdon LANL
HEP	Community Project for Accelerator Science & Simulation (ComPASS)	P. Spentzouris FNAL	Prudencio UT

EPSI-QUEST UQ Participants

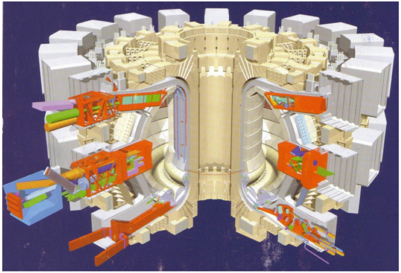
- C.S. Chang, Princeton EPSI PI
- Robert Moser, UT-Austin QUEST Center Lead
- Martin Greenwald, MIT
- Suenghoe Ku, Princeton
- Julian Cummings, Caltech
- Varis Carey, UT-Austin
- Devon Battaglia, Princeton

EPSI Overview — C.S. Chang

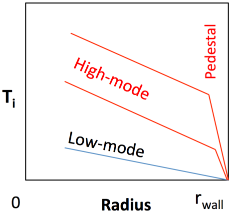


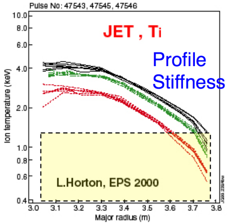
Poloidal cross-section at a constant toroidal angle

Poloidal magnetic flux label $\psi(r)$: 1 at r/a=1, 0 at r/a=0

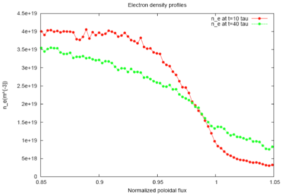


Key Problem: Understanding Edge Physics





- Plasma near material wall must stay cold
- Temperature slope limited by turbulent transport
  - Ion Temperature(T_i) too low if fusion core in L-mode
- ITER based on "H-mode" pedestal
  - experimental, Wagner 1982
- Steep pressure gradient induces edge localized modes
- Underlying physics and inherent uncertainties must be understood



EPSI-QUEST Partnership Plan

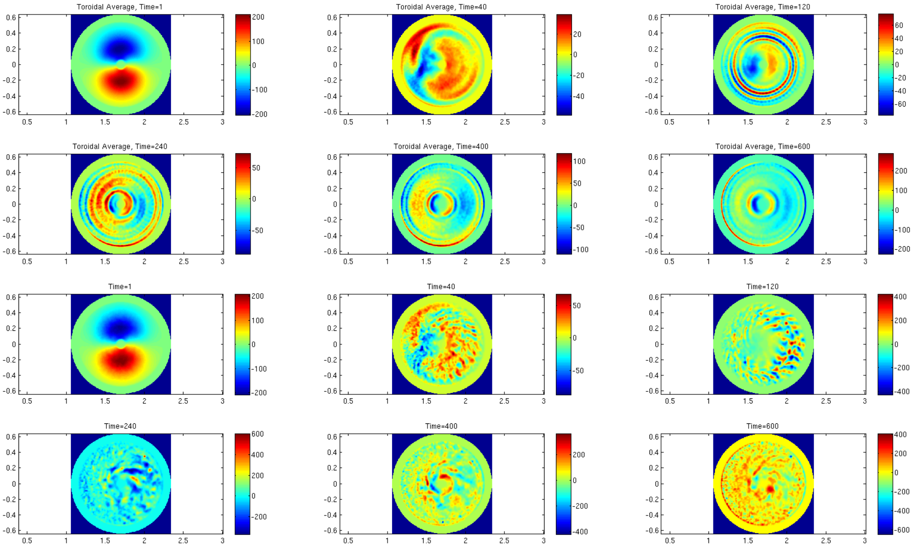
Primary Thrust

1. Identify key model sensitivities for gyrokinetic code XGC-1
2. Validate/invalidate hierarchy of physics in XGC-1
    1. Initial UQ focus: Ion Temperature Gradient (ITG) turbulence
    2. Enrich physics, guided by:
        - Validation studies
        - Edge profiles and fluxes

Secondary Projects: Validation/Reduced Order Modeling

1. Improve uncertainty estimates for derived experimental quantities. (Martin, MIT) (*Provides both input profiles for XGC-1 and validation observables*)
2. Perform calibration exercises for reduced physics model (Battaglia,Princeton). (*Bayesian calibarion using* QUESO)

Diagnostics of ITG Mode



Current Status

- Dedicated UQ branch of XGC-1, with access to richer physics as needed
- Postprocessing tools for 1D XGC-1 diagnostic outputs
- Scripts for XGC-1 interface with DAKOTA
- Initial sensitivity results for heating power, numerical parameters (particles, timestep)

Plans & Challenges

- Development of computationally tractable problems for UQ analysis, with QoI uncertainties that will be represenative of the full problem
- Seconday projects
  - Uncertainty in experimental data analysis
  - Bayesian calibration of reduced models

BER Atmospheric Modeling Partnership

Multiscale Methods for Enabling Scale-Aware Capability in CESM – PI: William Collins (LBNL)

- QUEST: Bert Debusschere & Kenny Chowdhary (SNL)
- Multiscale Project Collaborator: Vincent Larson (UWM)

Project goal is to develop climate modeling capability with high fidelity down to scales of key features of interest: cloud systems and ocean eddies

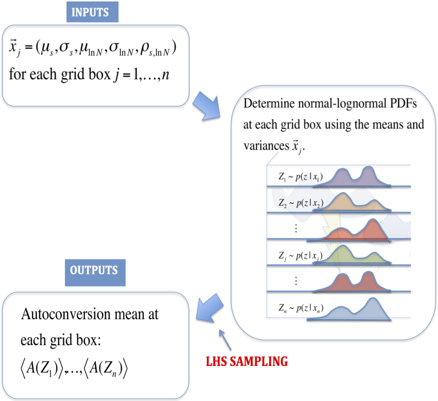
- Variable resolution unstructured grids
- Multiscale parameterizations of microphysics
- Numerics geared to next-generation comp. architectures
- Verification, validation and UQ

QUEST supports project UQ and statistics needs

- Provide expertise and tools for enabling UQ
  - Sensitivity analysis, surrogate modeling, forward UQ, calibration
  - Discussions ongoing regarding the selection of the proper QUEST tools
    - Calibration of CLUBB parameters with DAKOTA
    - GPMSA for multi-fidelity calibration
- Quadrature approaches to account for subgrid variability in microphysics
  - Subgrid variability modeled through assumed distributions for the microphysics parameterization inputs
  - Efficient approaches needed to compute averages of microphysics over grid box

Traditionally, random sampling can be used to account for sub-grid physics variability

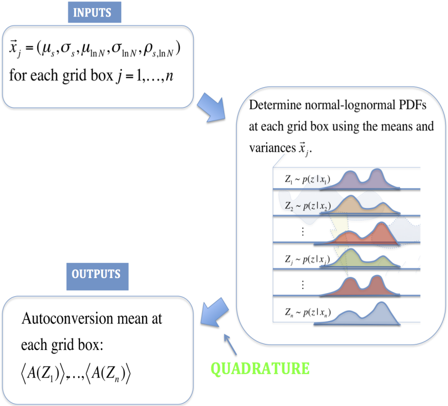
Autoconversion: conversion of cloud droplets to rain droplets
– measured as a rate of mass transfer



- Autoconversion depends on
  - cloud water mixing ratio s
  - cloud droplet number concentration N
- CLUBB model:
  - $s, N|x_j \sim$ joint normal-lognormal PDF
  - $x = (\mu_s, \sigma_s, \mu_{\ln N}, \sigma_{\ln N}, \rho_{s,\ln N})$
- Currently, at each time step, and grid box
  - PDF is sampled using LHS
- Samples used to compute the autoconversion mean, at each grid box and time step.

Quadrature approaches show significant improvement to sub-grid physics calculations

We can replace Latin Hypercube sampling with a quadrature based approach.



Latin Hypercube Sampling vs Quadrature

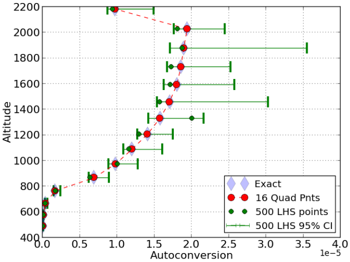


Figure: Using a quadrature approach, we can bypass the random sampling and calculate the Autoconversion mean using far fewer points, with even greater accuracy.

Applying quadrature based approaches to other microphysics processes

- We want to apply this quadrature technique to all microphysics processes with relevant sub-grid variability
- Each process has 1-3 uncertainty parameters
- There are ∼14 uncertainty parameters in total
- Two implementation approaches
  1. Use NCAR's sub-column approach
     - Samples all microphysics simultaneously
     - Would require all microphysics to use the same number of quadrature points
  2. Integrate each microphysics process separately
     - Low-dimensional quadrature tailored to each microphysical process
     - Requires all microphysics to be implemented in separate subroutines

Example Microphysics Processes
Average evaporation/ condensation rate of cloud water and ice
Autoconversion of cloud ice to snow
Accretion of cloud water by snow
Accretion of cloud water by rain
Freezing of cloud droplets and rain
Evaporation/ sublimation of precipitation

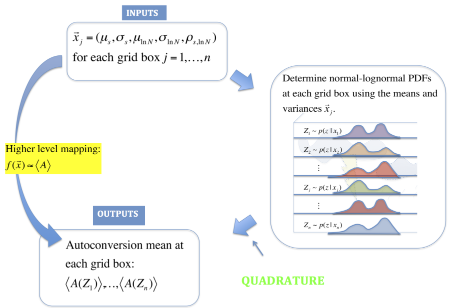
Integrating each microphysics process separately

In many microphysics processes in a global circulation model like CAM, the number of variable sub-grid parameters is a model choice

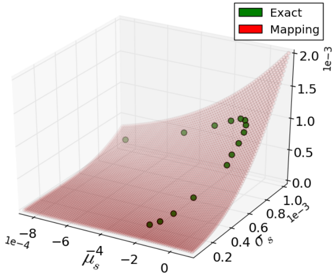
Example Microphysics Processes	# of uncertain sub grid parameters	Likely # of quadrature points needed
Average evaporation/ condensation rate of cloud water and ice	3	$4 \times 4 \times 4$
Autoconversion of cloud ice to snow	1	4
Accretion of cloud water by snow	3	$4 \times 4 \times 4$
Accretion of cloud water by rain	2	4×4
Freezing of cloud droplets and rain	2	4×4
Evaporation/ sublimation of precipitation	3	$4 \times 4 \times 4$

- For calculation of the mean, 4 quadrature points is equivalent to approximating the function of interest with a 7th order polynomial.
- The choice of the number of quadrature points is a trade off between accuracy and cost. However, even a four point quadrature approach shows drastic improvements over Latin Hypercube sampling for the autoconversion mean.
- We are working with Vince Larson (UWM) to prototype this approach in CLUBB.

Creating a higher level function that maps the inputs directly to the sub-grid microphysics quantities



5D Mapping (projected in 2D)



- This higher level mapping would allow us to bypass the on-the-fly calculation of microphysics completely, with potential for improvements in both speed and accuracy.
- The mapping can built from a predetermined set of quadrature points or by a growing set of random samples collected over the course of the simulation.

Figure: We can create a higher level 5D function that maps the means and variances of s and N directly to the autoconversion mean. We can use the same mapping as a proxy for the autoconversion mean at every time step.

UQ algorithms impacting simulation of climate physics

- Quadrature offers a promising approach to account for microphysics subgrid variability with high accuracy and reasonable numbers of samples
- Currently exploring the application of this to all microphysics processes with relevant sub-grid variability
  - CLUBB single column model considered for initial implementation
- Application of QUEST tools in other climate physics areas under discussion

Closure

- Broad range of ongoing work on UQ software and algorithms development
- A number of SciDAC partnership activities
- Highlighted two example partnerships

Partnerships using UQ methods/tools for:

- Global sensitivity analysis
- model calibration and validation
- microphysics modeling
    - Improved accuracy **and** computational performance