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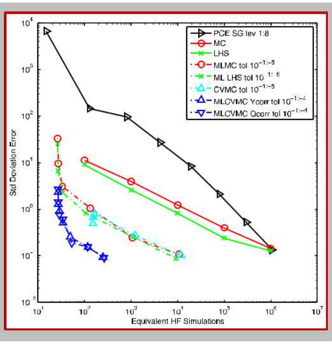
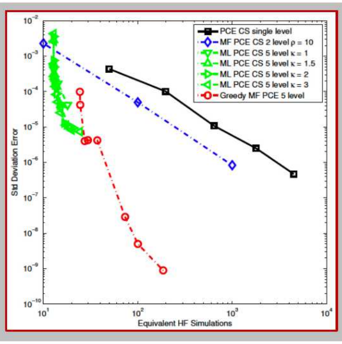
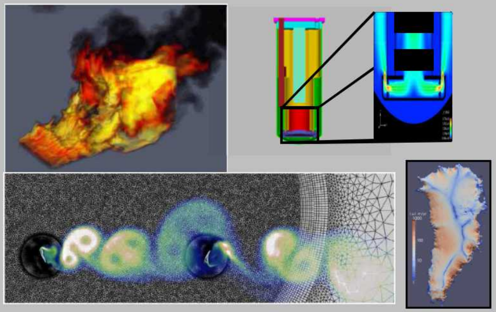




DAKOTA

Explore and predict with confidence



Milestone: Develop multilevel emulator-based Bayesian inference capabilities and demonstrate data assimilation for SWiFT configuration

Tom Seidl, Friedrich Menhorn, Gianluca Geraci, Michael Eldred (SNL 1463)
Tommy Herges, Alan Hsieh, David Maniaci (SNL 8821)
Ryan King (NREL)
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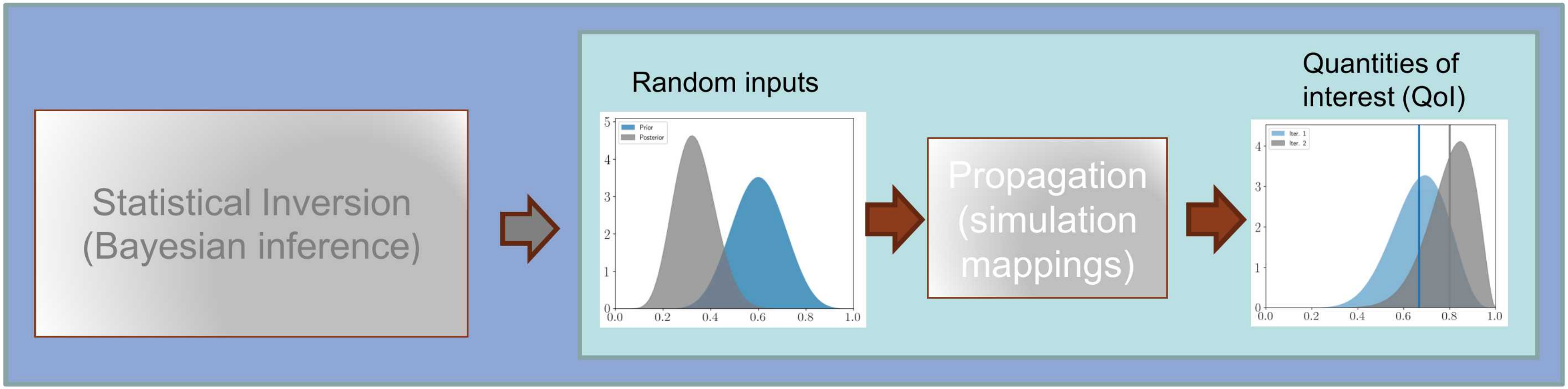
Uncertainty Quantification Workflow

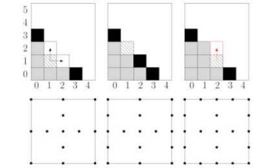
Forward propagation of input uncertainties (Part 1)

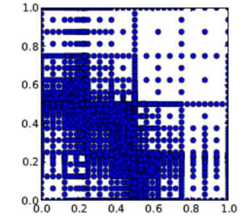
- Push forward of distributions from input variables to output QoI
- Compute statistics that reflect design/analysis goals (e.g., moments, failure probabilities)



Characterization of input uncertainties through data assimilation (Part 2)

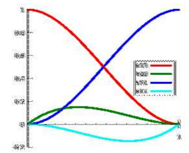
Research Thrusts for UQ



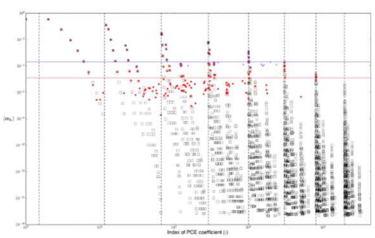


- *Key challenge:* DOE programs are pushing SOA in high fidelity M&S w/ HPC
  - Severe simulation budget constraints (e.g., a handful of runs)
  - Significant dimensionality, driven by model complexity (multi-physics, multiscale)
- *Focus:* Compute dominant uncertainty effects despite key challenge of high–{D,Fidelity}
- *Foundational:* Emphasize scalability through exploitation of special structure
  - *Adaptivity:* p- and h- refinement of stochastic expansions
  - *Adjoints:* gradient enhancement for PCE / SC / GP
  - *Sparsity:* compressed sensing
  - *Low Rank:* tensor / function train (w/ UMich)
  - *Dimension reduction:* active subspaces (w/ CU Boulder), adapted basis PCE (w/ USC)

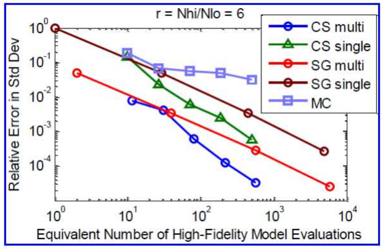
$$\begin{bmatrix} \vdots & \vdots & & \vdots \\ \pi_{0,j}(\vec{\xi}_i) & \pi_{1,j}(\vec{\xi}_i) & \cdots & \pi_{P,j}(\vec{\xi}_i) \\ \frac{\partial \pi_{0,j}}{\partial \xi_1}(\vec{\xi}_i) & \frac{\partial \pi_{1,j}}{\partial \xi_1}(\vec{\xi}_i) & \cdots & \frac{\partial \pi_{P,j}}{\partial \xi_1}(\vec{\xi}_i) \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial \pi_{0,j}}{\partial \xi_{n_\xi}}(\vec{\xi}_i) & \frac{\partial \pi_{1,j}}{\partial \xi_{n_\xi}}(\vec{\xi}_i) & \cdots & \frac{\partial \pi_{P,j}}{\partial \xi_{n_\xi}}(\vec{\xi}_i) \\ \vdots & \vdots & & \vdots \end{bmatrix} \begin{pmatrix} \vdots \\ \vec{u}^{(m,j)} \\ \vec{u}^{(m+1,j)} \\ \vdots \\ \vec{u}^{(m+n_\xi,j)} \\ \vdots \end{pmatrix} = \begin{pmatrix} \vdots \\ \vec{u}_i \\ \frac{\partial \vec{u}_i}{\partial \xi_1} \\ \vdots \\ \frac{\partial \vec{u}_i}{\partial \xi_{n_\xi}} \\ \vdots \end{pmatrix}$$



- Compound efficiencies
  - Multilevel-Multifidelity with sampling & CS/FT surrogates (new: ROM, NN)
  - Active subspaces: subspace quadrature, enhance MF control variates



- Address complex workflows through component-based approach
  - Emulator-based Bayesian inference, Mixed aleatory-epistemic UQ, Optimization under uncertainty (new: Optimal experimental design)



- Position UQ for next generation architectures
  - *Current (imperative):* multilevel parallelism (MPI + local async)
  - *Future (declarative):* exploit DAG + AMT for ensemble workflows (w/ Stanford)

Multiple Model Forms in UQ & Opt

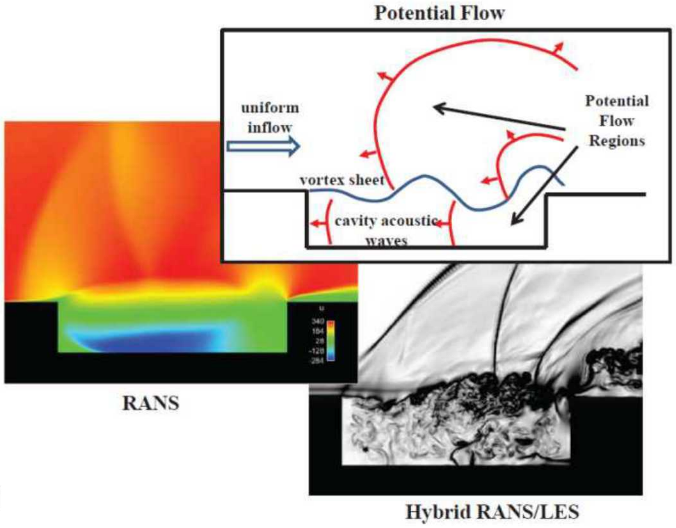
Discrete model choices for simulation of same physics

A clear hierarchy of fidelity (from low to high)

- Exploit less expensive models to render HF practical
    - *Multifidelity Opt, UQ, inference*
- Support general case of discrete model forms
    - Discrepancy does not go to 0 under refinement

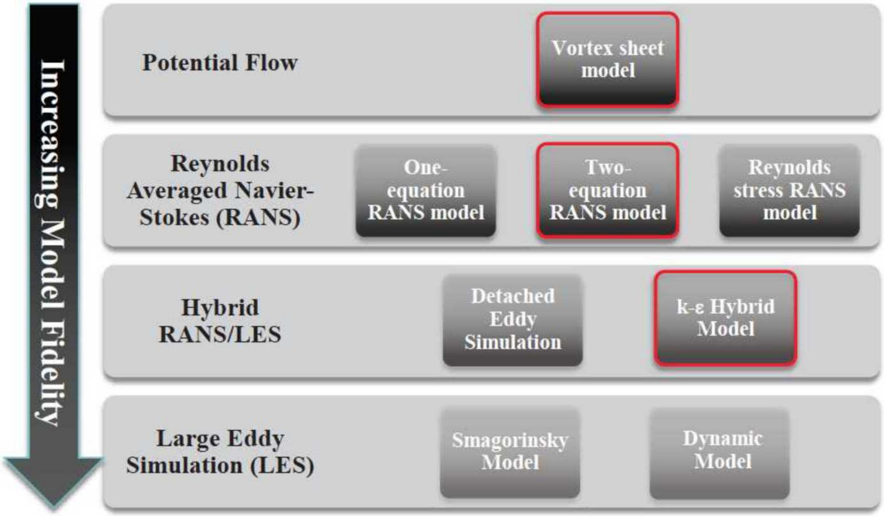
An ensemble of peer models lacking clear preference structure / cost separation: e.g., SGS models

- *With data:* model selection, inadequacy characterization
    - Criteria: predictivity, discrepancy complexity
- *Without (adequate) data:* epistemic model form uncertainty propagation
    - Intrusive, nonintrusive
- *Within MF context:* CV correlation



Discretization levels / resolution controls

- Exploit special structure: discrepancy → 0 at order of spatial/temporal convergence

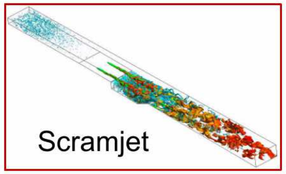


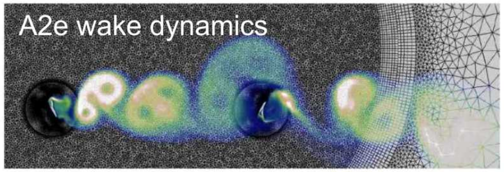
Combinations for multiphysics, multiscale

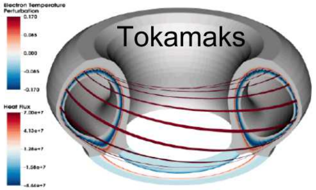
Research & Development in Multifidelity Methods

Recurring R&D theme: couple scalable algorithms with exploiting a (multi-dimensional) model hierarchy

- address scale and expense for high fidelity M&S applications in defense, energy, and climate
- render UQ / optimization / OUU tractable for cases where only a handful of HF runs are possible



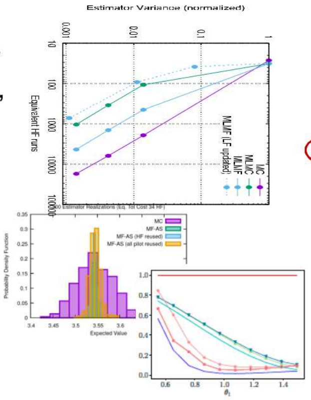




Emerging mission areas: abnormal thermal, Z-pinch MagLIF, quantum chemistry

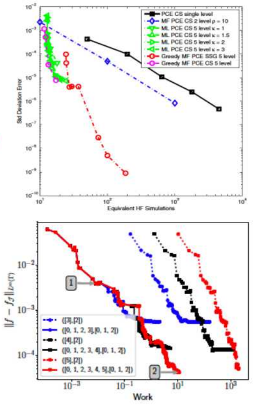
Monte Carlo UQ Methods

- *Production:* optimal resource allocation for multilevel, multifidelity, combined (DARPA x 2, Wind, Cardiovascular)
- *Emerging:* active dimensions ('18 EE LDRD), generalized fmwk for approx control variates (ASC V&V Methods)
- *On the horizon:* control of time avg; tail prob. estimation; learning latent var relationships (CIS LDRD); model tuning / selection (CIS LDRD, DOE BES)



Surrogate UQ Methods (PCE, SC)

- *Production (v6.10):* ML PCE w/ projection & regression; ML SC w/ nodal/hierarchical interp; greedy ML adaptation (DARPA SEQUOIA)
- *Emerging:* multi-index stoch. collocation, ML fn train; multiphysics / multiscale integration (ASC V&V Methods)
- *On the horizon:* new surrogates (GP, ROM, deep NN) with error mgmt ('19 EE LDRD, DOE BES); unification of surrogate + sampling approaches (CIS LDRD)



Optimization Under Uncertainty

- *Production:* manage simulation and/or stochastic fidelity

- *Emerging:*
  Derivative-based methods (DARPA SEQUOIA)
  - Multigrid optimization (MG/Opt)
  - Recursive trust-region model mgmt.: extend TRMM to deep hierarchies

  Derivative-free methods (DARPA ScramjetUQ)
  - SNOWPAC (w/ MIT, TUM) w/ MLMC error estimates
- *On the horizon:* Gaussian process-based approaches: multifidelity EGO (FASTMath OUU); Optimal experimental design (OED) (A2e)

Background: Polynomial Chaos & Stochastic Collocation

Polynomial chaos: spectral projection using orthogonal polynomial basis fns

$$R = \sum_{j=0}^{\infty} \alpha_j \Psi_j(\boldsymbol{\xi})$$ using

$$\begin{aligned}
\Psi_0(\boldsymbol{\xi}) &= \psi_0(\xi_1)\,\psi_0(\xi_2) &= 1\\
\Psi_1(\boldsymbol{\xi}) &= \psi_1(\xi_1)\,\psi_0(\xi_2) &= \xi_1\\
\Psi_2(\boldsymbol{\xi}) &= \psi_0(\xi_1)\,\psi_1(\xi_2) &= \xi_2\\
\Psi_3(\boldsymbol{\xi}) &= \psi_2(\xi_1)\,\psi_0(\xi_2) &= \xi_1^2 - 1\\
\Psi_4(\boldsymbol{\xi}) &= \psi_1(\xi_1)\,\psi_1(\xi_2) &= \xi_1\xi_2\\
\Psi_5(\boldsymbol{\xi}) &= \psi_0(\xi_1)\,\psi_2(\xi_2) &= \xi_2^2 - 1
\end{aligned}$$

Distribution	Density function	Polynomial	Weight function	Support range
Normal	$\frac{1}{\sqrt{2\pi}}e^{\frac{-x^2}{2}}$	Hermite $He_n(x)$	$e^{\frac{-x^2}{2}}$	$[-\infty,\infty]$
Uniform	$\frac{1}{2}$	Legendre $P_n(x)$	1	$[-1,1]$
Beta	$\frac{(1-x)^{\alpha}(1+x)^{\beta}}{2^{\alpha+\beta+1}B(\alpha+1,\beta+1)}$	Jacobi $P_n^{(\alpha,\beta)}(x)$	$(1-x)^{\alpha}(1+x)^{\beta}$	$[-1,1]$
Exponential	e^{-x}	Laguerre $L_n(x)$	e^{-x}	$[0,\infty]$
Gamma	$\frac{x^{\alpha}e^{-x}}{\Gamma(\alpha+1)}$	Generalized Laguerre $L_n^{(\alpha)}(x)$	$x^{\alpha}e^{-x}$	$[0,\infty]$

- Estimate α_j using regression or numerical integration: sampling, tensor quadrature, sparse grids, or cubature

$$\alpha_j = \frac{\langle R, \Psi_j \rangle}{\langle \Psi_j^2 \rangle} = \frac{1}{\langle \Psi_j^2 \rangle} \int_{\Omega} R\,\Psi_j\,\varrho(\boldsymbol{\xi})\,d\boldsymbol{\xi}$$

Stochastic collocation: instead of estimating coefficients for known basis functions, form interpolants for known coefficients

$$R(\boldsymbol{\xi}) \cong \sum_{j=1}^{N_p} r_j \boldsymbol{L}_j(\boldsymbol{\xi})$$

- ***Global:*** Lagrange (values) or Hermite (values+derivatives)
- ***Local:*** linear (values) or cubic (values+gradients) splines
- ***Nodal*** or ***Hierarchical*** interpolants

$$L_j = \prod_{\substack{k=1\\k\neq j}}^{m} \frac{\xi - \xi_k}{\xi_j - \xi_k} \Rightarrow R(\boldsymbol{\xi}) \cong \sum_{j_1=1}^{m_{i_1}} \cdots \sum_{j_n=1}^{m_{i_n}} r\left(\xi_{j_1}^{i_1}, \ldots, \xi_{j_n}^{i_n}\right) \left(L_{j_1}^{i_1} \otimes \cdots \otimes L_{j_n}^{i_n}\right)$$

Sparse interpolants formed using Σ of tensor interpolants

- Tailor expansion form:
  - p-refinement: anisotropic tensor/sparse, generalized sparse
  - h-refinement: local bases with dimension & local refinement
- Method selection: requirements for fault tolerance, decay, sparsity, error estimation

Surrogate approaches: Greedy multilevel refinement

$$\boxed{\hat{Q}_L \approx \hat{Q}_0 + \sum_{l=1}^{L} \hat{\Delta}_L, \text{ for } \Delta_l \equiv Q_l - Q_{l-1}}$$

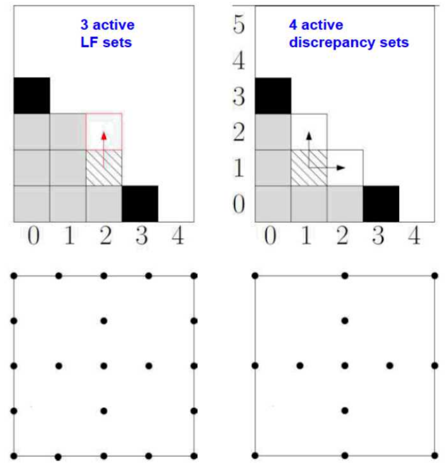
<u>Compete refinement candidates across model levels:</u> max induced change / cost

- 1 or more refinement candidates per model level
- Measure impact on final QoI statistics (roll up multilevel estimates)
  - norm of change in response covariance (default)
  - norm of change in level mappings (goal-oriented: *z/p/β/β**)

  normalized by relative cost of level increment (# new points * cost / point)
- Greedy selection of best candidate, which then generates new candidates for this model level

<u>Level candidate generators:</u>

- *Uniform refinement:* 1 exp order / grid level candidate per model level
  - Tensor / sparse grids: projection PCE, nodal/hierarchical SC
  - Regression PCE: least squares / compressed sensing
- *Anisotropic refinement:* 1 exp order / grid level candidate per model level
  - Tensor / sparse grids
- *Index-set refinement:* many candidates per level
  - Generalized sparse grids: projection PCE, nodal/hierarch SC
  - Regression PCE
- *Adapted candidate basis:* ~3 frontier advancements per model level
  - Regression PCE (Jakeman, E., Sargsyan, “Enhancing ℓ1-minimization estimates of polynomial chaos expansions using basis selection,” *J. Comp. Phys.,* Vol. 289, May 2015.)



Multilevel / Multi-index PCE: greedy competition across models

Model problem results

Steady state diffusion

$$-\frac{d}{dx}\left[a(x,\boldsymbol{\xi})\frac{du}{dx}(x,\boldsymbol{\xi})\right] = 10, \quad (x,\boldsymbol{\xi}) \in (0,1)\times I_{\boldsymbol{\xi}}$$

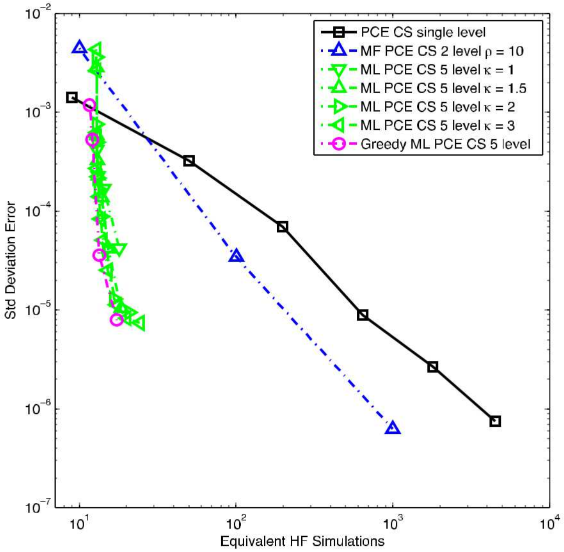
$$u(0,\boldsymbol{\xi}) = 0, \quad u(1,\boldsymbol{\xi}) = 0.$$

Advection diffusion

$$\frac{du}{dt}(x_1,t,Z) + a\frac{du}{dx}(x_1,t,Z) - \frac{d}{dx}\left[k(x_1,Z)\frac{du}{dx}(x_1,t,Z)\right] = g(x_1,t,Z) \qquad (x_1,Z)\in(0,1)\times\Gamma$$

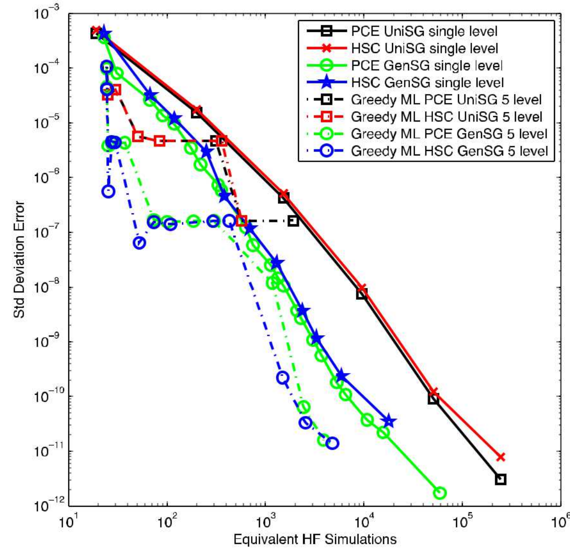
$$u(0,t,Z)=0 \quad u(1,t,Z)=0 \quad u(x_1,0,Z)=0,$$

Greedy ML PCE: compressed sensing with uniform candidate refinement



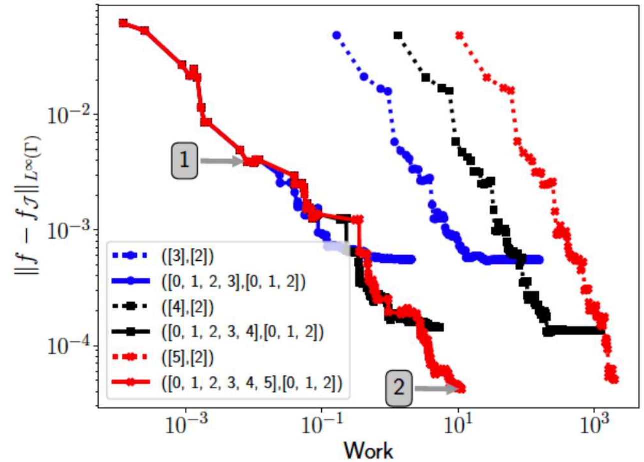
Conv Tol	N_1	N_2	N_3	N_4	N_5
1.e-1	198	9	9	9	9
1.e-2	644	198	9	9	9
1.e-3	1802	644	9	9	9
1.e-4	4505	1802	50	9	9

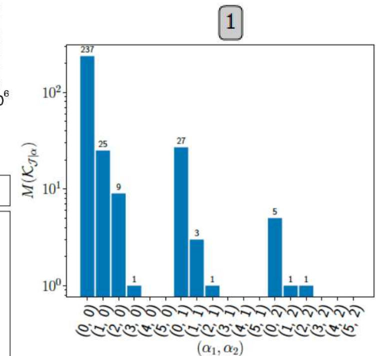
Greedy ML PCE: sparse grids with uniform / generalized refinement

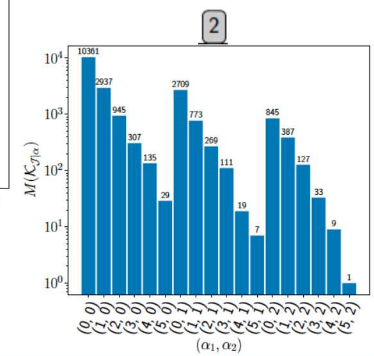


Conv Tol	N_1	N_2	N_3	N_4	N_5
1.e-2	43	23	19	19	19
1.e-4	211	83	19	19	19
1.e-6	391	271	156	19	19
1.e-8	1359	743	327	59	19
1.e-10	3535	2311	1039	391	19
1.e-12	10319	5783	2783	1343	43
1.e-14	26655	14991	8063	3703	1535

Greedy multi-index PCE: sparse grids with generalized refinement





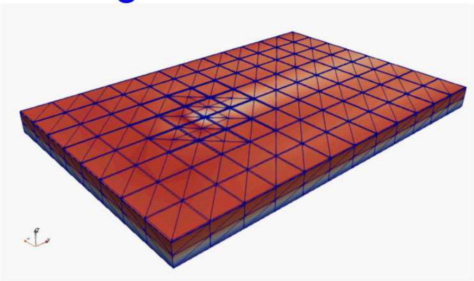


WindSE (RANS) Forward UQ Formulation

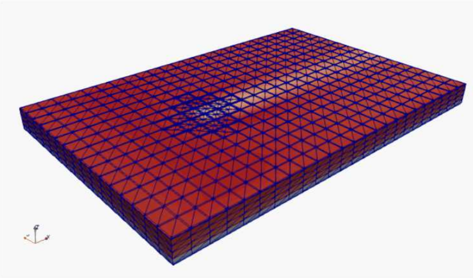
- 6 random input variables

Parameter	Meaning	Uniform lower and upper bound	
HH_vel	Velocity at hub [m/s]	6.0	10.0
power	Exponent for inflow velocity profile	0.11	0.25
wind_angle	Angle of wind direction [deg]	-7.5	7.5
eff_thickness	Effective Thickness of rotor plate	2.4	3.0
axial_induction_factor	Ratio of air velocity reduction due to turbine	0.25	0.5
lmax	Parameter for RANS turbulence model	10	20

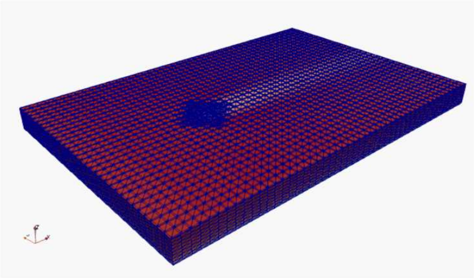
- 3 grid resolutions: coarse, medium and fine



DoF: 5480, Cost: 1 (~ 8.5 s)



DoF: 33952, Cost: 7 (~ 1 min)

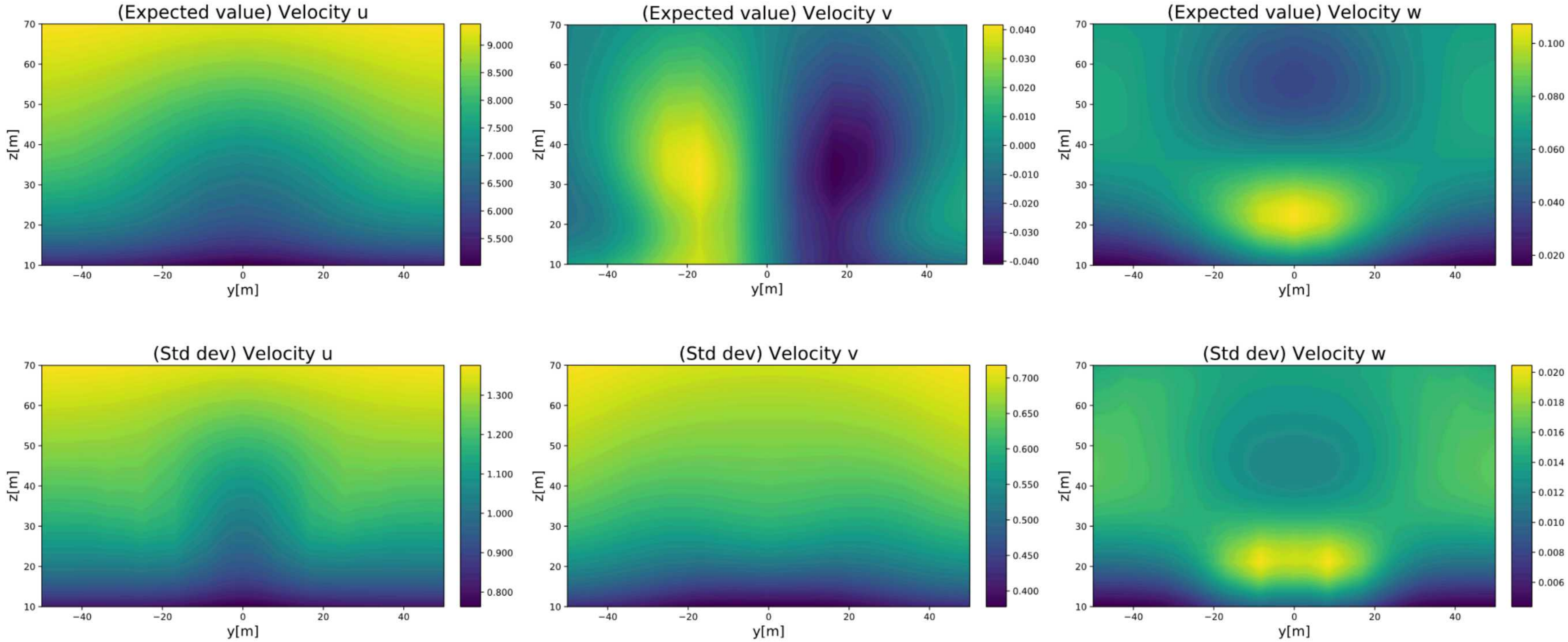


DoF: 229928, Cost: 150 (~21 min)

- 46851 QoI: velocities u,v and w of slice over y and z at distance x = 5 RD

WindSE (RANS) Forward UQ Results

PCE results for mean and variance for u, v and w:



Accuracy tolerance set to 1e-7

Multilevel sample profile:

- Coarse – 641 + 377 = **1018**
- Medium – 377 + 193 = **570**
- Fine – 193 = **193**

Equivalent Fine = **226**

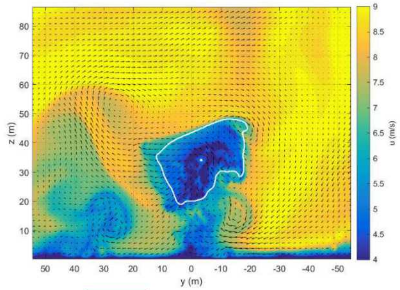
Comparison to single level greedy sparse grid refinement at tol = 1e-7:

- Fine – 1009
- **Factor of 4.5 lower cost**

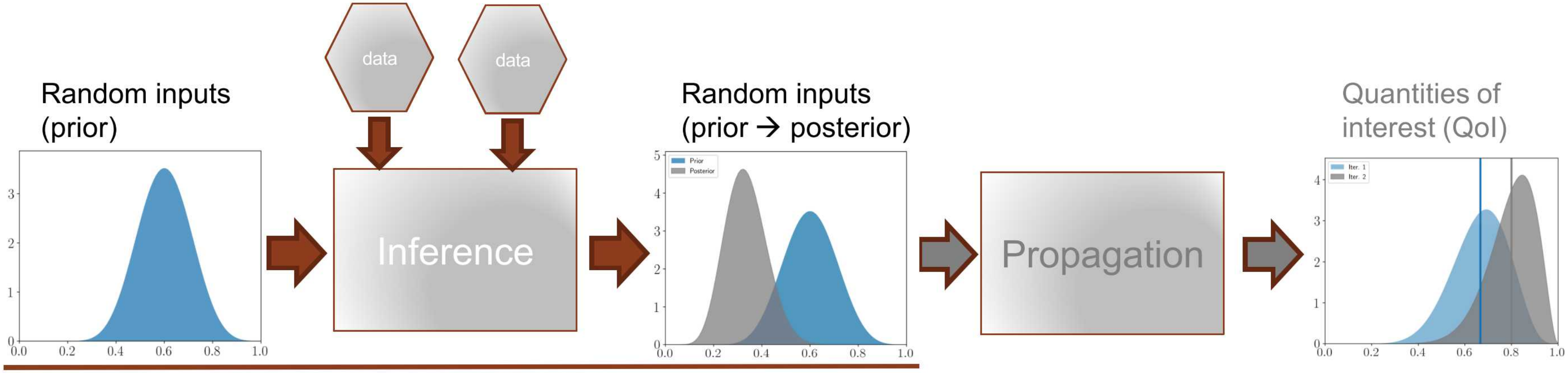
Uncertainty Quantification Workflow

Characterization of input uncertainties through data assimilation (Part 2)

- Prior distributions based on *a priori* knowledge
- Observational data (experiments, reference solns.) → infer posterior distributions via Bayes rule
  - Use of data can reduce uncertainty in parameter to QoI mapping (priors are constrained)
  - Design using prior uncertainties can be overly conservative
  - Reduced uncertainty of data-informed UQ can produce designs with greater performance



Nalu-Wind simulated wake data 5D downwind (inference target is averaged over 600 sec; no lidar processing; zero deg yaw; Nalu coarse mesh)



(ML-MF) Emulator-based Bayesian inference

MCMC sampling performed on emulator, leveraging differentiable emulator structure

- Pre-solve for MAP (maximum a posteriori probability) point: full Newton min of –log(posterior)
- Accurate MCMC proposal: emulator derivatives → Hessian of misfit → MVN proposal covariance
  - mitigates sample rejection in high D: for 10D Rosenbrock test, 98% rejection rate reduced to 30%

$$\boxed{p(\mathbf{d}|\xi) = \exp\left[-\frac{1}{2}(f(\xi)-\mathbf{d})^T\Gamma_{\mathbf{d}}^{-1}(f(\xi)-\mathbf{d})\right]}$$

Gaussian Likelihood

$$\boxed{-\log\left[p(\mathbf{d}|\xi)\right] = \frac{1}{2}(f(\xi)-\mathbf{d})^T\Gamma_{\mathbf{d}}^{-1}(f(\xi)-\mathbf{d}) = M(\xi)}$$

Negative Log Likelihood = Misfit

$$\boxed{\nabla^2_{\xi}M(\xi) = \underbrace{\nabla_{\xi}f(\xi)^T\,\Gamma_{\mathbf{d}}^{-1}\nabla_{\xi}f(\xi)}_{\text{Gauss-Newton approx. Hessian (if only emulator grads)}} + \nabla^2_{\xi}f(\xi)\cdot\left[\Gamma_{\mathbf{d}}^{-1}\,(f(\xi)-\mathbf{d})\right]}$$

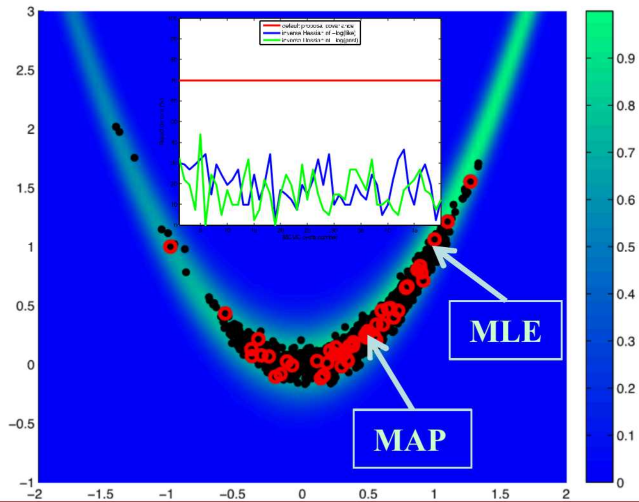
Hessian of Misfit

Laplace approx.: MVN proposal covariance defined by inverse Hessian of negative log posterior

$$\boxed{-\log\pi_d(\xi) = M(\xi) - \log\pi_0(\xi)}$$

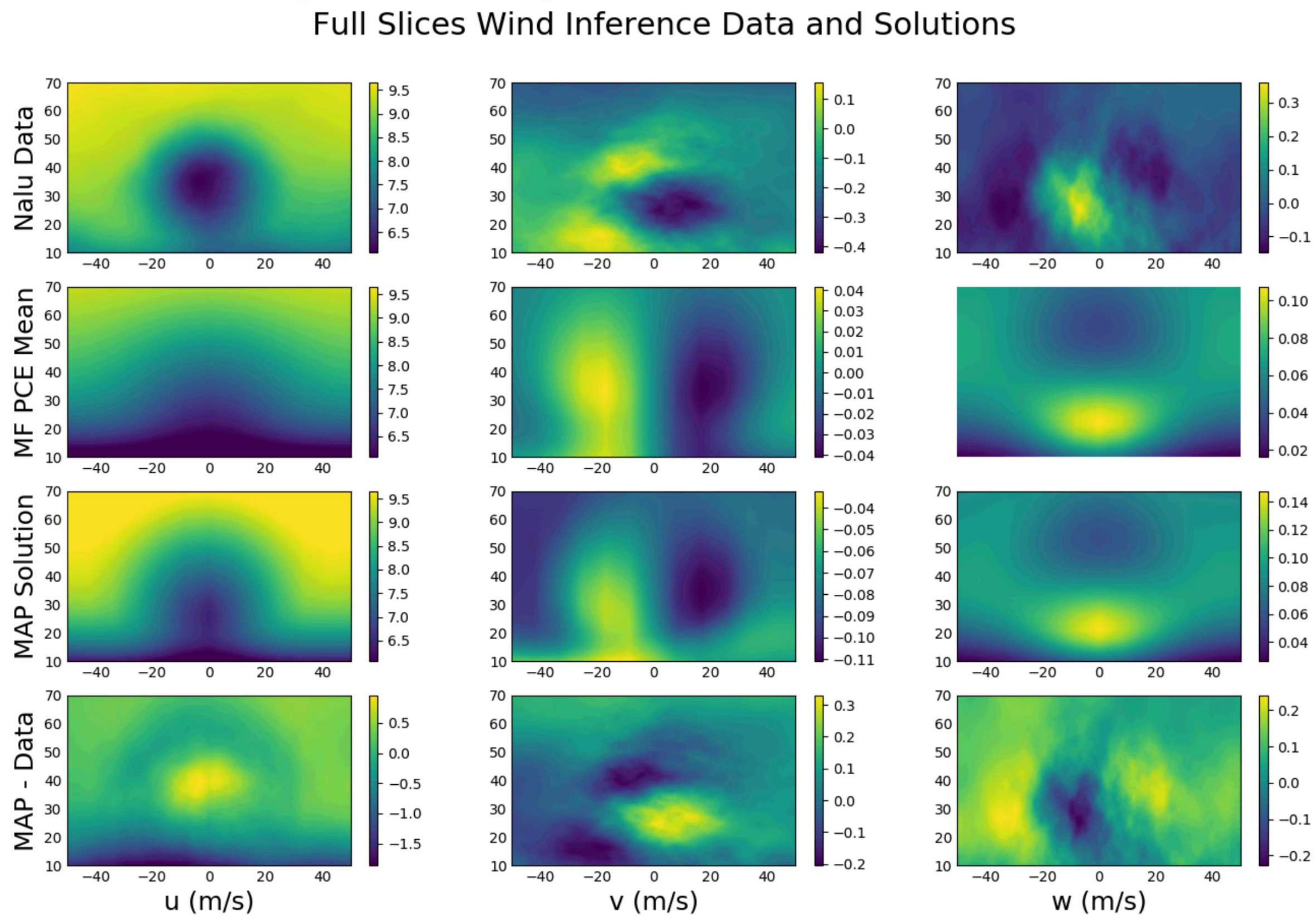
- augmenting misfit: Hessian of negative log prior provides regularization for priors w/ curvature (normal, beta, gamma)
- Posterior Hessian-based proposal balances likelihood and prior, performing better than either alone

Rosenbrock Problem; Prior ~ N(0,1)



WindSE (RANS) Inference UQ Results

Inference results for u, v and w compared to Nalu Data:



WindSE (RANS) Inference UQ Results

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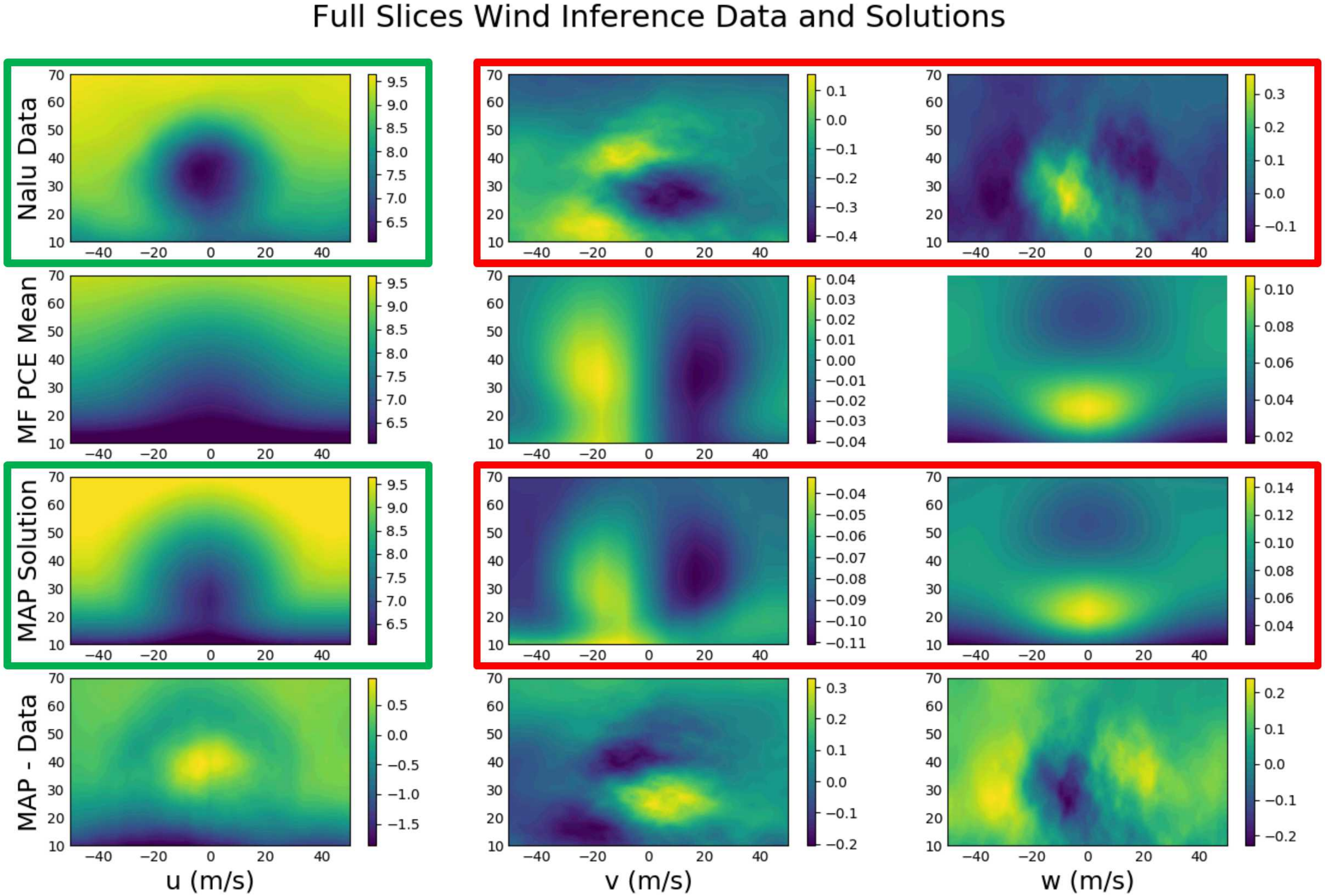

WindSE (RANS) Inference UQ Results

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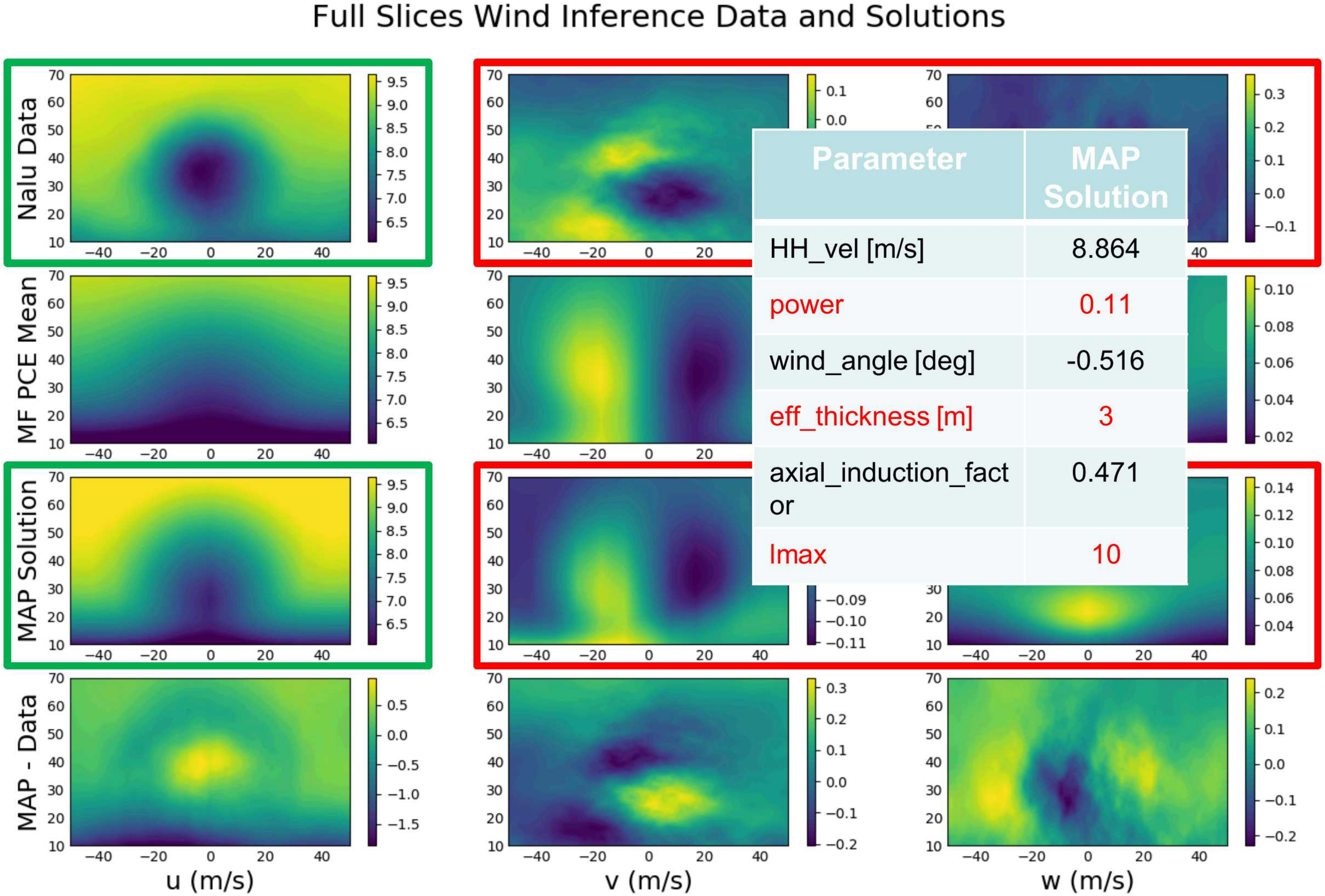
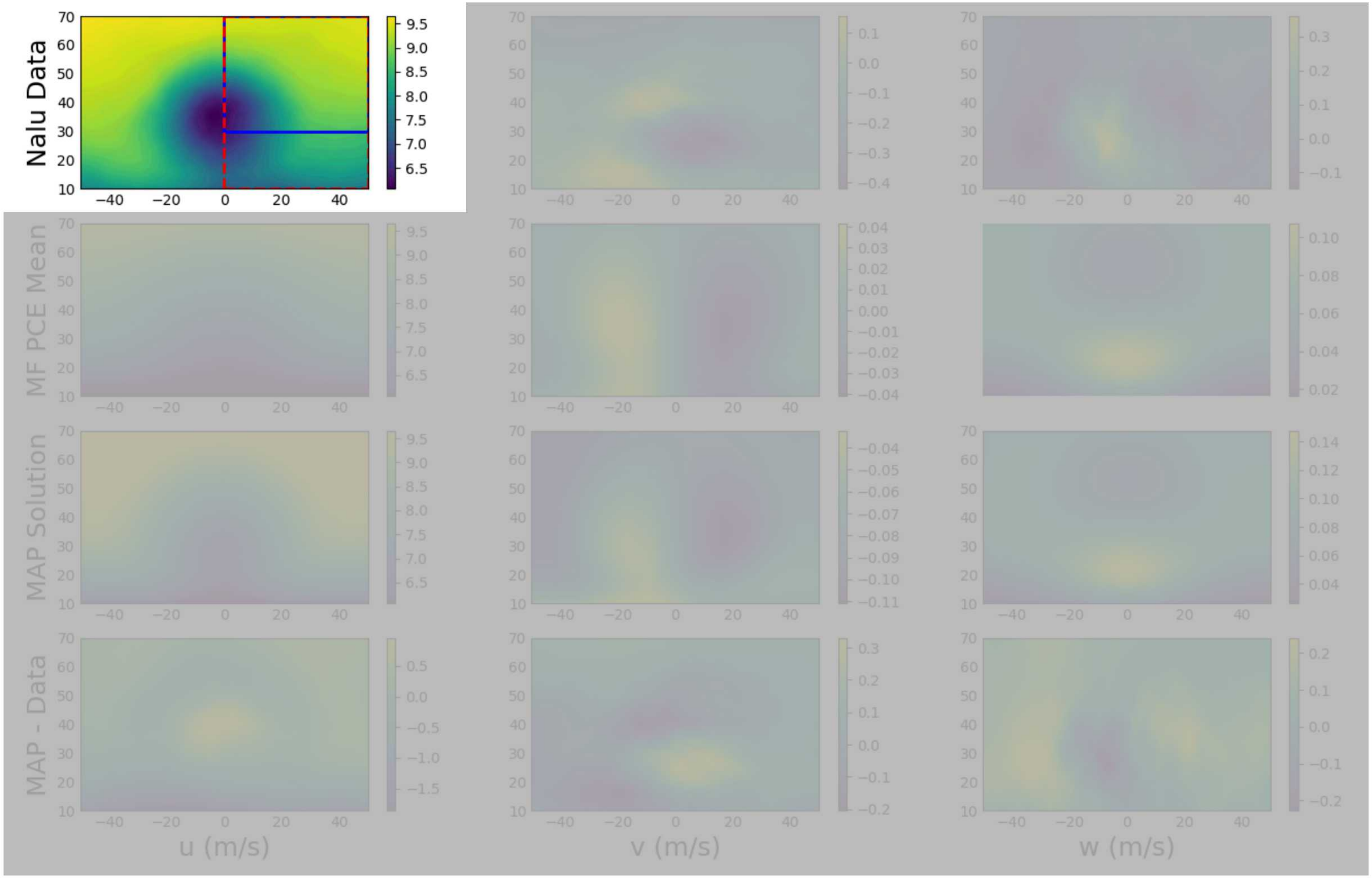


Parameter	MAP Solution
HH_vel [m/s]	8.864
power	0.11
wind_angle [deg]	-0.516
eff_thickness [m]	3
axial_induction_factor	0.471
lmax	10

WindSE (RANS) Inference UQ Results

Inference results for u, v and w compared to Nalu Data:

Full Slices Wind Inference Data and Solutions

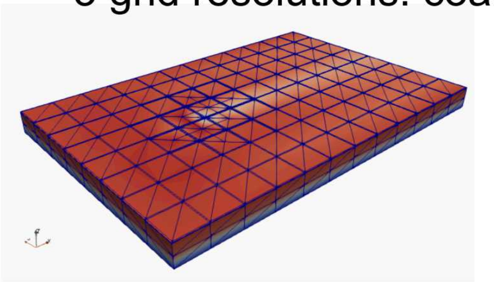


WindSE (RANS) Forward UQ Formulation

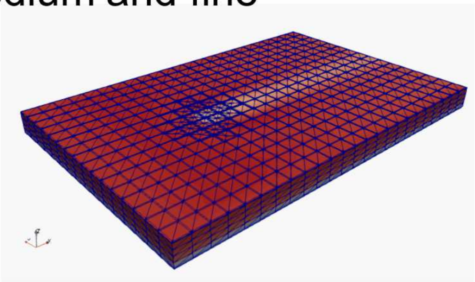
- Updated 6 random input variables:

Parameter	Meaning	Uniform lower and upper bound	
HH_vel	Velocity at hub [m/s]	6.0	10.0
power	Exponent for inflow velocity profile	~~0.11~~ 0.0055	0.25
wind_angle	Angle of wind direction [deg]	-7.5	7.5
eff_thickness	Effective Thickness of rotor plate	2.4	~~3.0~~ 6.0
axial_induction_factor	Ratio of air velocity reduction due to turbine	0.25	~~0.5~~ 0.8
lmax	Parameter for RANS turbulence model	~~10~~ 5	20

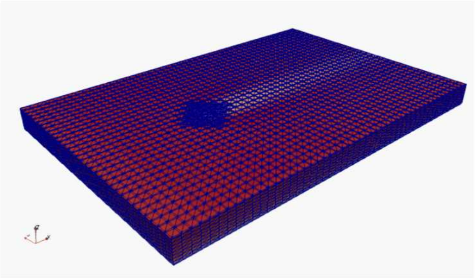
- 3 grid resolutions: coarse, medium and fine



DoF: 5480, Cost: 1 (~8.5 sec)



DoF: 33952, Cost: 7 (~1 min)



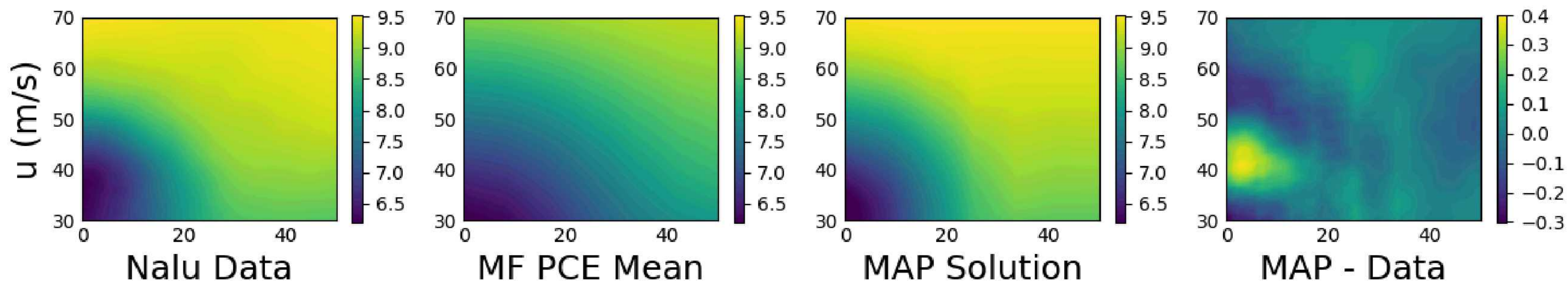
DoF: 229928, Cost: 150 (~21 min)

- ~~46851~~ 5265 QoI: velocities u ~~,v and w~~ of quarter slice over y and z at distance x = 5 RD

WindSE (RANS) Inference UQ Results

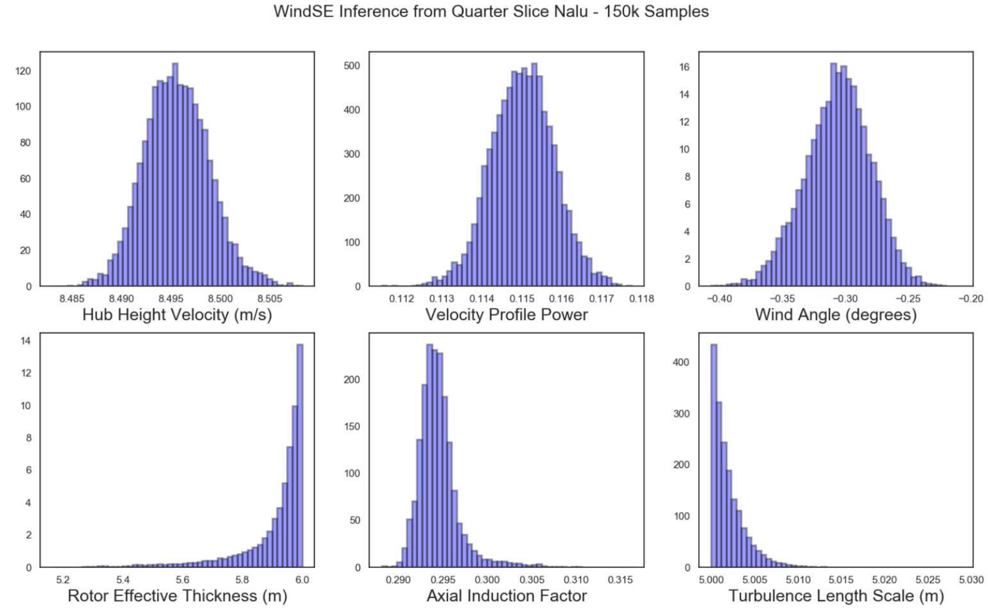
Sandia National Laboratories

Updated Inference results for u compared to Nalu Data:



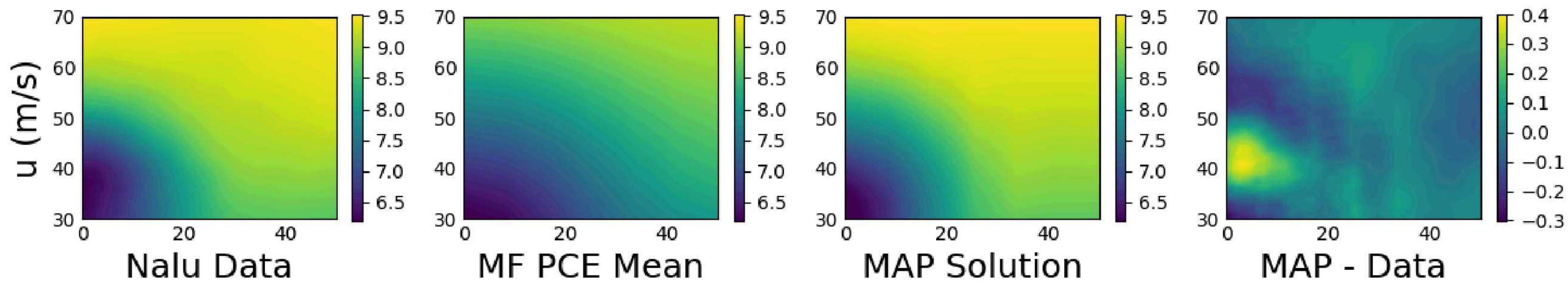
- MCMC chain of 150k samples → effective sample sizes of 10^3 – 10^4
- Only eff thickness, l_{max} at bounds; Axial induction factor closer to 0.33
- MAP soln shows significant improvement in wake capturing relative to mean soln
- Data is informative, especially for bottom 3 params: significant info gain w.r.t. uniform priors

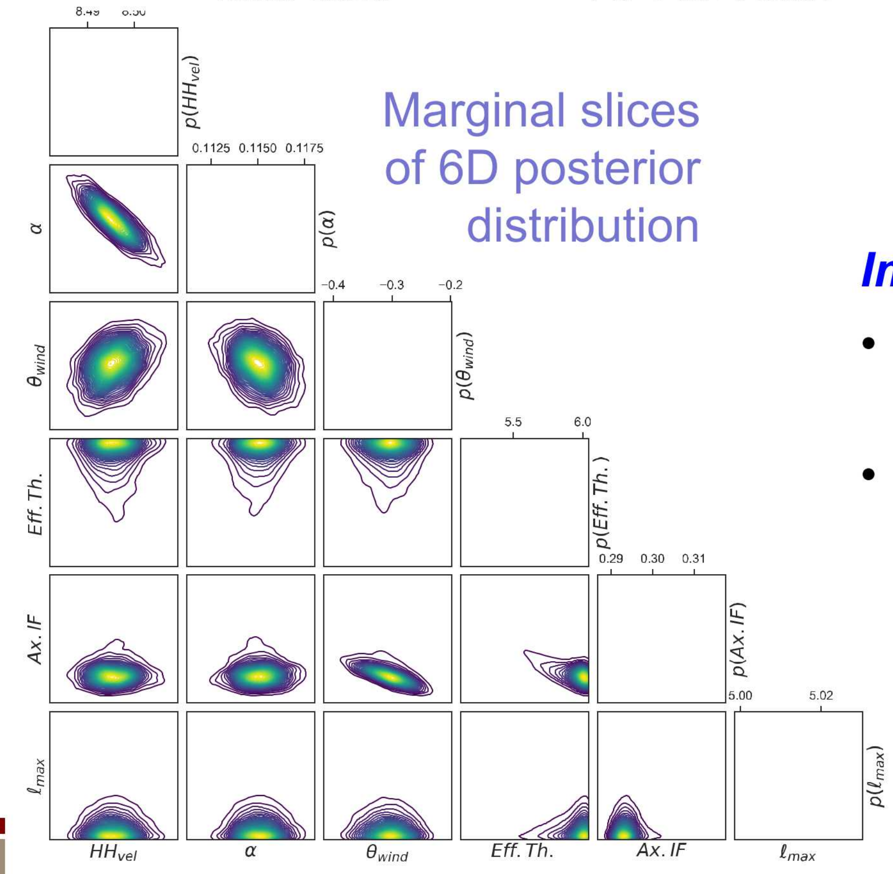
Parameter	MAP Solution
HH_vel [m/s]	8.496
power	0.115
wind_angle [deg]	-0.309
eff_thickness [m]	6
axial_induction_factor	0.295
lmax	5



WindSE (RANS) Inference UQ Results

***Updated** Inference results for u compared to Nalu Data:*





Marginal slices of 6D posterior distribution

Impact

- Reduction of epistemic uncertainty through assimilation of data
- Subsequent push forward of this updated 6D posterior enables more predictive UQ
  - RANS UQ results that are consistent with reference data (Nalu LES, in this case)

Summary Remarks

Key Milestone Results

- Multilevel PCE for forward UQ: RANS in WindSE with Coarse / Medium / Fine meshes
- This emulator admits efficient Bayesian inference, calibrating RANS to LES data for SWiFT case
- Capability enhancements for Dakota and WindSE

This fall: AIAA SciTech 2020 Papers (4)

- GG: MF strategies for forward / inverse UQ
- RK: Annual energy prod. w/ Bayesian quad.
- FM: MF OUU for wind plants
- AH: ML UQ w/ CFD + OpenFAST

Near-term refinements (for papers above)

- Expand model hierarchy + truth reference:
  - Add U-RANS (under dev. in WindSE) to hierarchy as highest fidelity
  - Shift calibration target from Nalu LES to SWiFT experimental data
- Problem formulation: QoI inference targets
  - Revisit v & w data given models with wake rotation

Maximize expected utility from new data $d^{(i)}$, e.g. D-optimal: max information gain / relative entropy / Kullback-Leibler (KL) divergence from $\pi_0 \rightarrow \pi_{post}^{(i)}$

Longer term topics

- Adaptive PCE emulation → posterior accuracy
- Adaptive data collection → optimal experimental design (OED)