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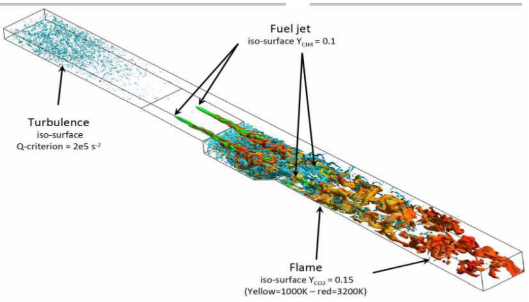

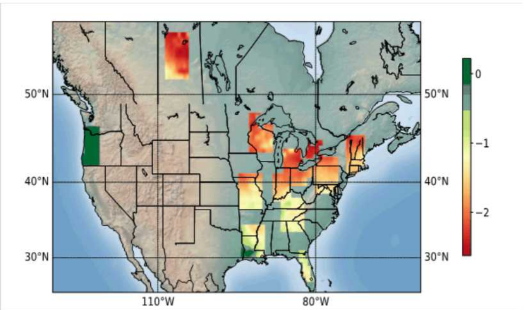

Uncertainty Quantification and Machine Learning Algorithms for Physical Models: Tackling Computational Expense and High-Dimensionality

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with

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UC Merced, October 8, 2019

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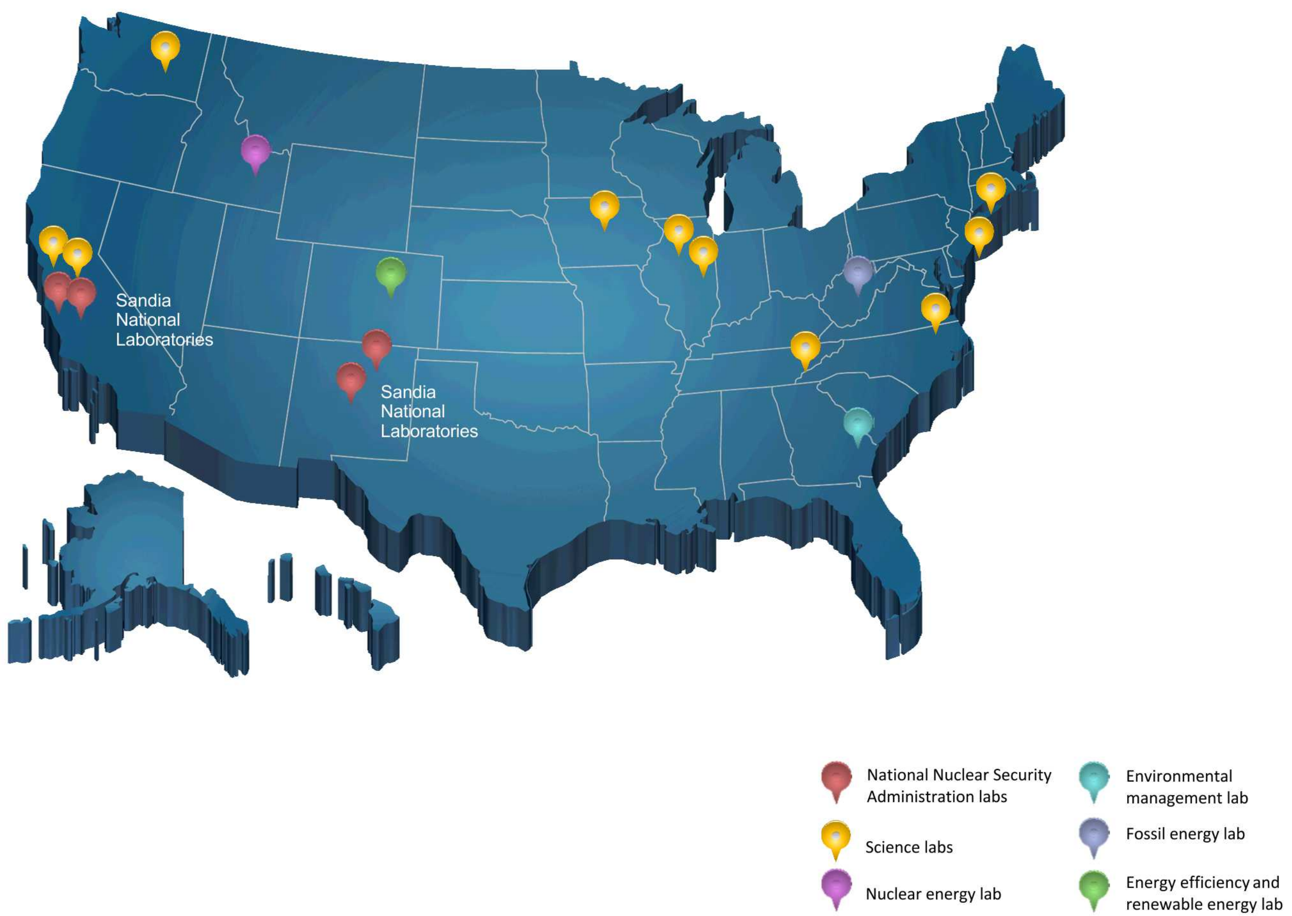
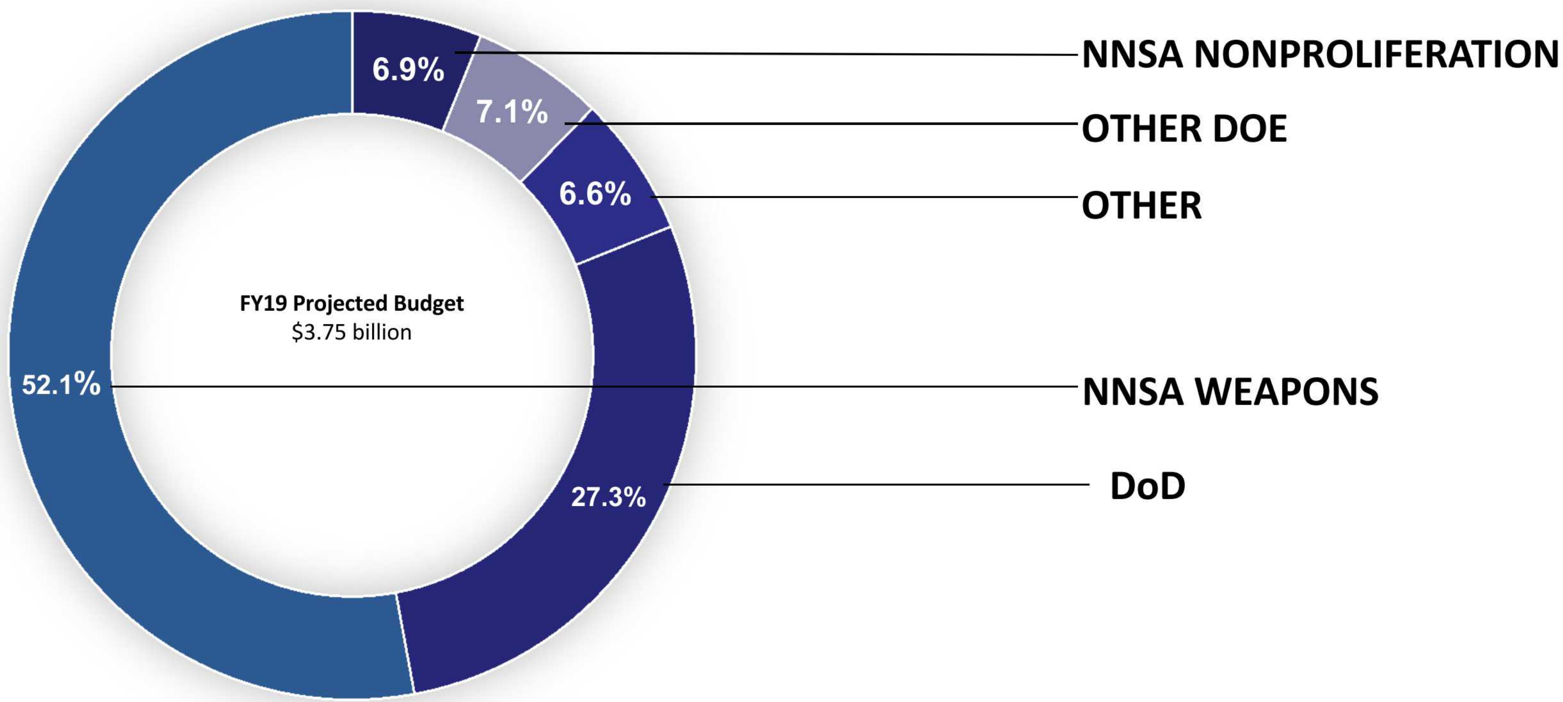
Outline

- Sandia Overview and Employment Opportunities
- Motivation and Context
  - Scramjet Engine
    - **optimize design under uncertainty**
  - Energy Exascale Earth System Model – [illegible] Component
    - **model parameterization and optimal sensor placement**
  - Analysis workflows
- Algorithms: Supervised and Unsupervised Learning
  - Overview
  - Relevant results and impact
- Outcome

Sandia Has Two Main Locations



Sandia's Funding ~ $3.75 Billion

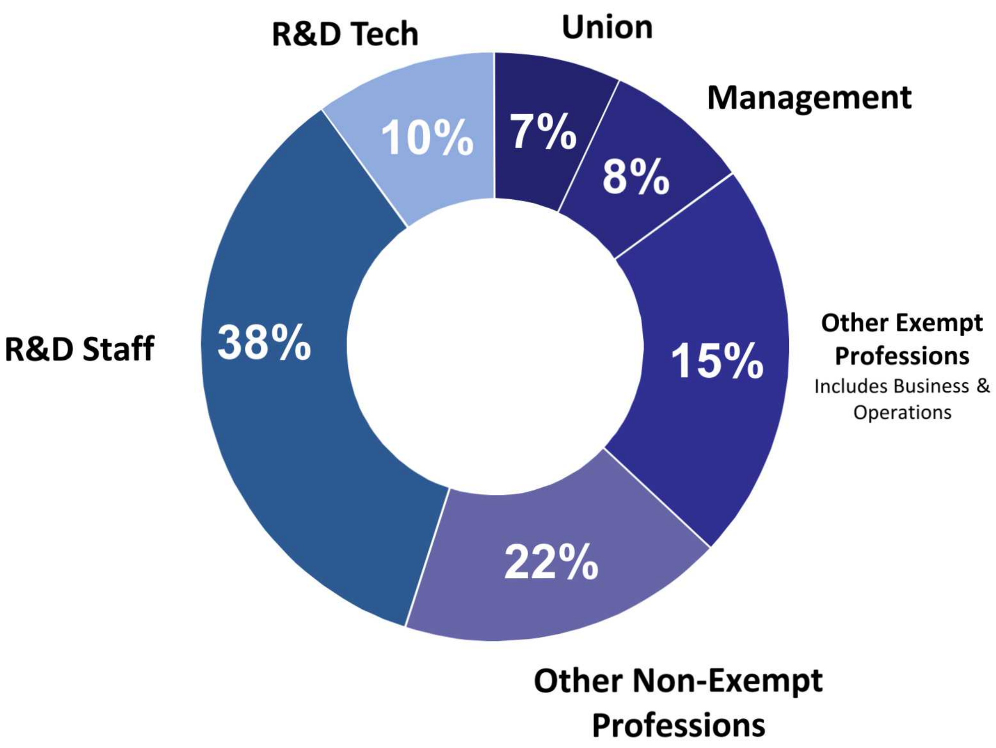


Our Workforce ~14,100 employees

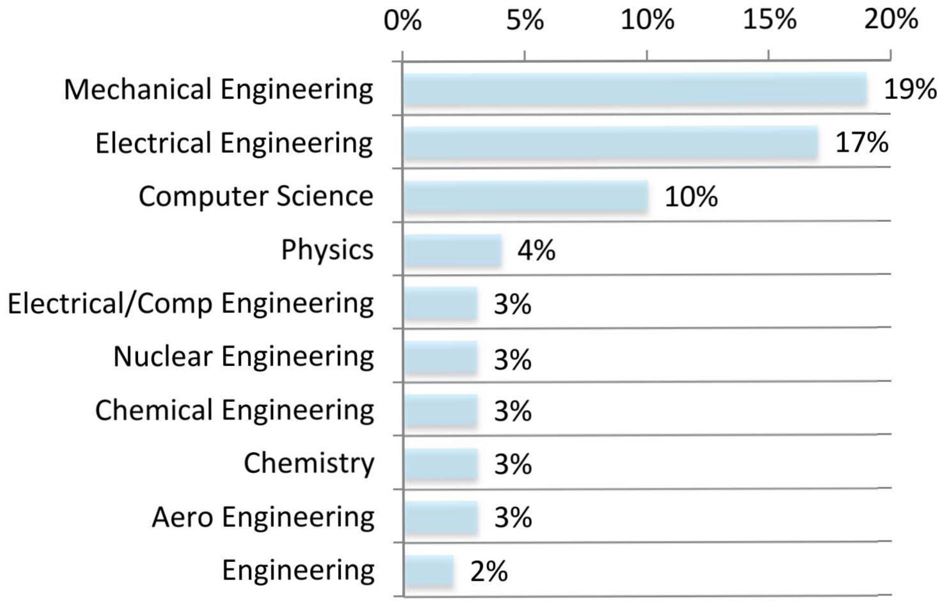
~12,300 Regular employees
~1,800 Temporary employees, students & postdoctoral appointees

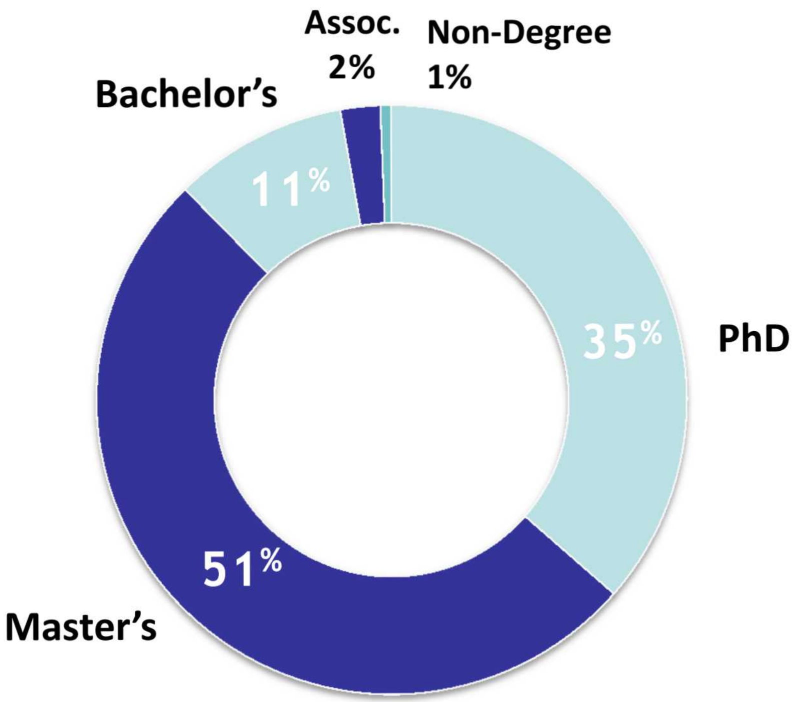
New Mexico Site: *(see breakout)*
Workforce: ~12,500
R&D employees: ~4,200
(R&D Staff & Technologists)

California Site: *(see breakout)*
Workforce : ~1,600
R&D employees: ~650
(R&D Staff & Technologists)



R&D by Discipline & Degree





Data as of July 2019

Top 10 job descriptions shown, Regular exempt non-management employees only

Internships

Encourages qualified students to develop interests in critical skills areas related to our mission, with the ultimate objective of developing our pipeline for our future. Available for Summer, Year Round and Co-op.

Eligibility Criteria

- Full-time enrollment status at an accredited school during the academic school year
- Undergraduate equivalent of 12 hours per semester
- Graduate equivalent of 9 hours per semester
- Must have a minimum cumulative GPA of 3.0 on a 4.0 scale for Technical, R&D, and Business interns; 2.5 on a 4.0 scale for Clerical and Labor interns
- Have U.S. citizenship for positions that require a security clearance or as stated in the job posting
- At least 16 years of age

Internships – Outreach and Networking Events

Summer Welcome Event

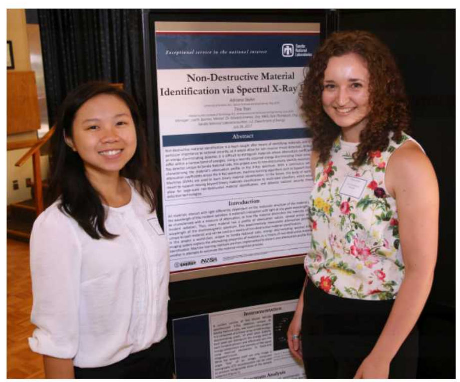
Intern Career Fair

Intern Symposium

Facility Tours

Speaker Forums

Professional Development Classes



Post-doc Opportunities

Key areas for post-docs at Sandia:

- Computer science/Computer Engineering
- Electrical Engineering
- Mechanical Engineering
- High-performance computing
- Microelectronics and microfluidics
- Nanotechnology
- Physics
- Chemistry/ Electro Chem
- Biosciences and biotechnology
- Radiation & electrical sciences
- Engineering sciences
- Pulsed power sciences
- Materials science & engineering

Eligibility Criteria

- A recent PhD (conferred 5 years prior to employment) or the ability to complete all PhD requirements before hire date.

Fellowship Opportunities

Sandia provides postdoctoral fellows with professional development opportunities and prepares fellows to conduct independent, groundbreaking research.

Postdoctoral Fellowships

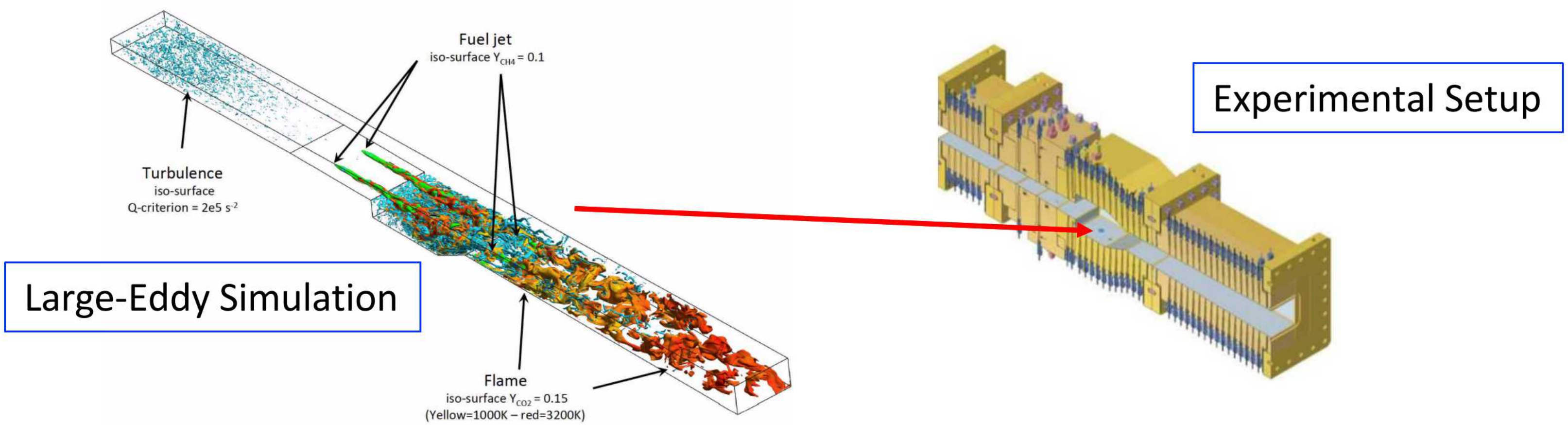
- Harry S. Truman Fellowship
- Jill Hruby Fellowship
- John Von Neumann

**Sign up for Automated Job Notifications!*

Motivation and Context

- Scramjet Engine
  - *optimize design under uncertainty*
- Energy Exascale Earth System Model – Land Component
  - *model parameterization and optimal sensor placement*
- Analysis workflows

Scramjet Engine – Design Optimization



Sponsored by DARPA (EQUiPS program)

Engine Configuration: NASA Langley Hypersonic International Flight Research and Experimentation (HIFiRE) direct connect rig (HDCR)

Partners:

Challenges

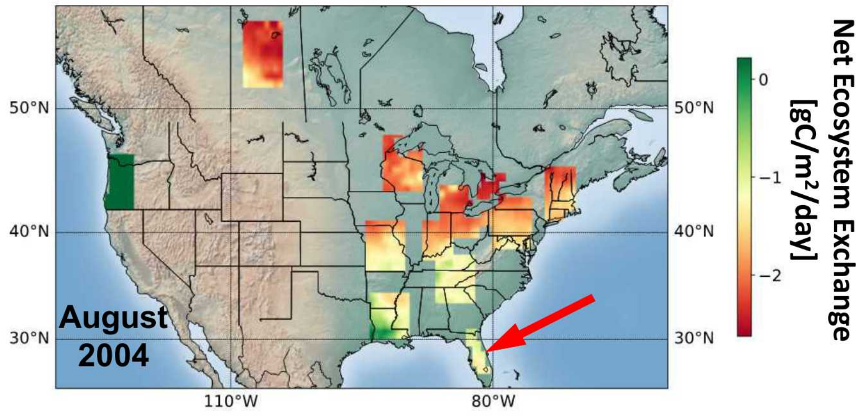
Computational Expense – o(10^4-10^5) CPU hours/model evaluation

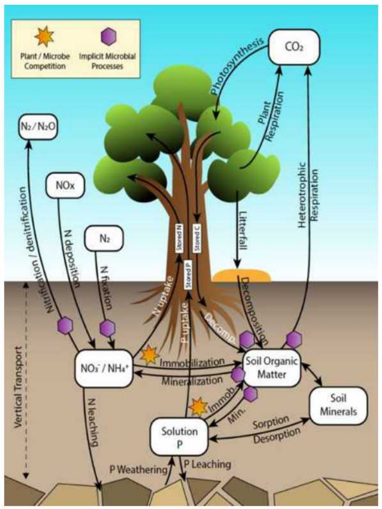
- large range of scales (spatial/temporal) needed to capture the entire geometry

Large number of parameters, both discrete - o(50) - and distributed

E3SM Land Model – Optimal Sensor Placement

Sample E3SM simulations to help decide on future experimental sites





Schematic of biogeophysical processes in E3SM – Land Model

Sponsored by DOE BER/ASCR

Understanding physical processes is critical to understand the climate feedbacks and their sensitivity to uncertainties in parameters and model structure

Partners: Sandia National Laboratories, Oak Ridge National Laboratory, Massachusetts Institute of Technology

Challenges

Nonlinear input/output dependencies

Large number of input parameters (10s-100s);

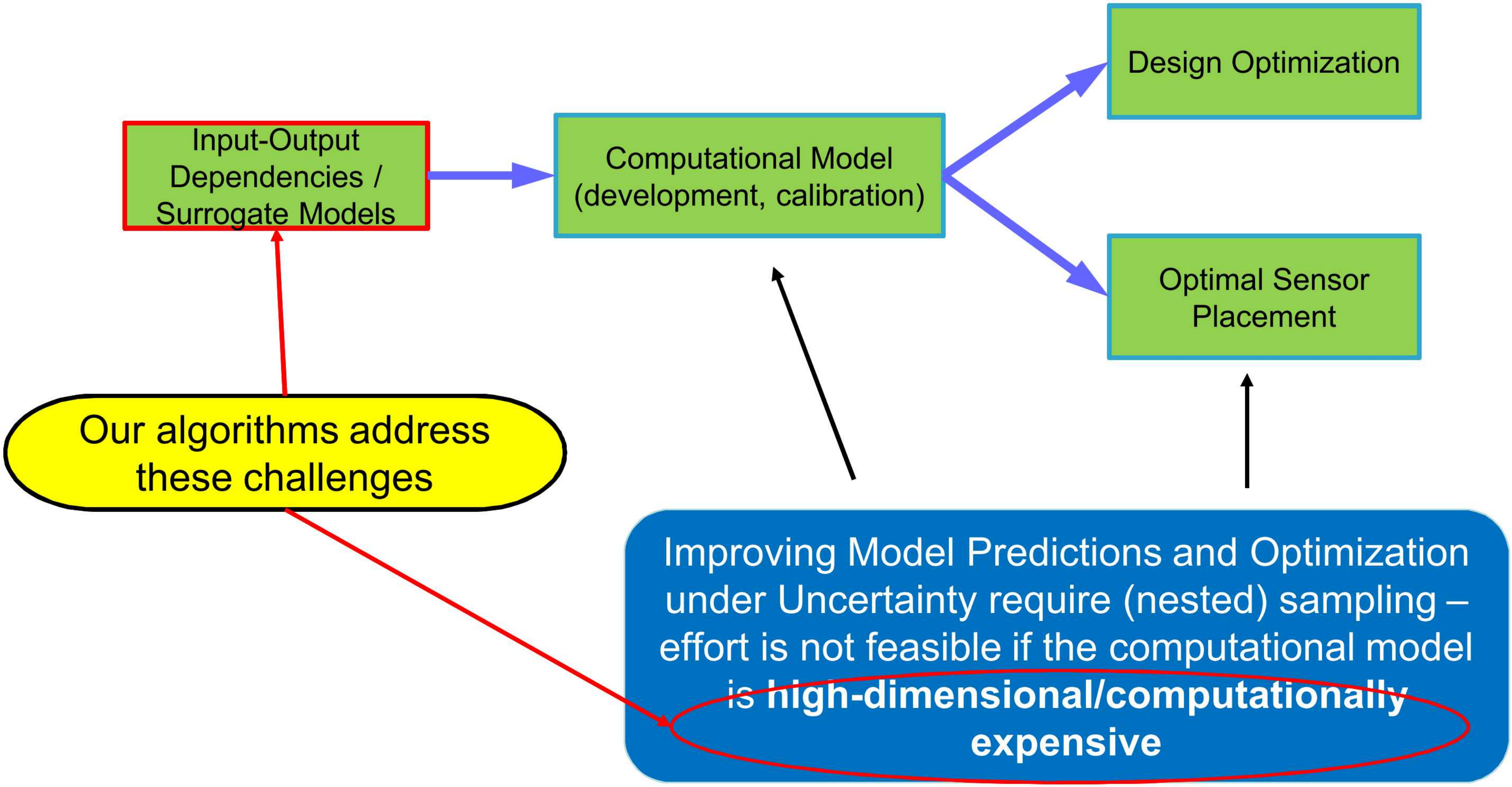
Land cells with different parameterizations

Computational Expense: o(10^4) CPU hours/land cell

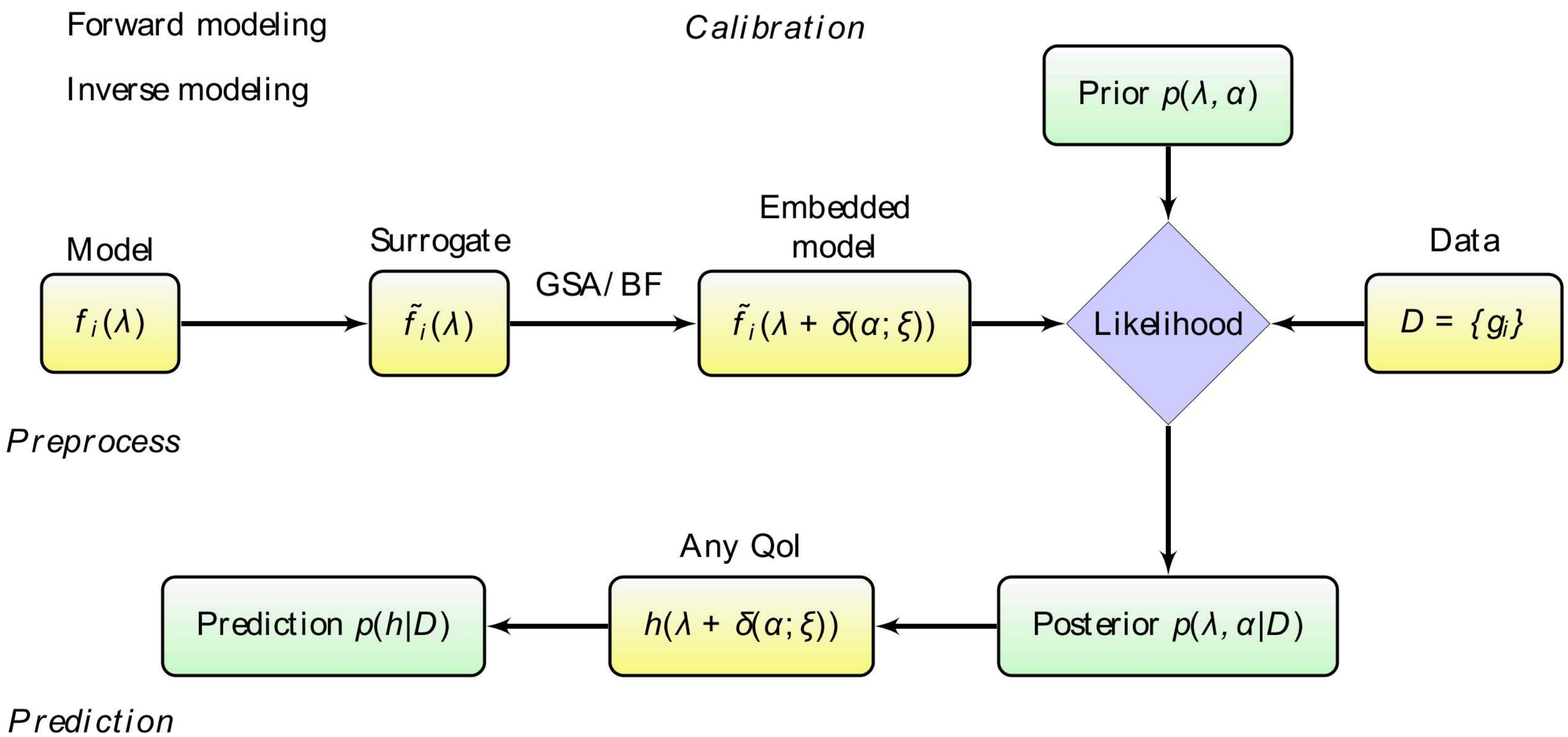
FASTMATH

Work synchronized with FASTMath Institute

Advanced UQ+ML Algorithms are Required To Enhance Modeling Efforts



UQ Analysis Workflows



Inverse & Forward UQ

- **Dimensionality reduction**
- (Noisy) Data Assimilation
- Model validation and comparison
- Confidence assessment

- Optimal design
- Decision support

High Dimensionality is a Major Challenge in UQ

- High dimensionality is the result of
  - Large number of uncertain parameters/inputs
  - Large number of degrees of freedom in random field inputs

- Model Calibration and Forward UQ efforts are in general challenged in this context
  - (Quasi) Monte Carlo methods are slow to converge
  - Spectral techniques (e.g. Polynomial Chaos) typically require an unfeasible number of model evaluations for very high dimensional systems
    - output quantities of interest (QoI) need to be relatively ***smooth***

- In most engineering systems only a small number of inputs are important for subsets of QoIs
  - Explore techniques for global sensitivity analysis (GSA) to identify important model inputs
  - Employ algorithms to detect low-dimensional behavior in the input-output space

Multiple Algorithms to Exploit Structure in High-Dimensional Models and Reduce Computational Cost

Sandia National Laboratories

Supervised Learning Algorithms

- Polynomial Chaos Expansions via Sparse Regression
- Low-rank Functional Tensor Train Models
- Neural Network Models

Unsupervised Learning Algorithms

- Low-dimensional Manifolds: Discovery and Sampling

Scramjet RAPTOR

E3SM E^3SM Energy Exascale Earth System Model

DAKOTA Explore and predict with confidence.

UQTk

Design Algorithms Adapted to Specific Challenges

Various surrogate types explored

UQ

ML

- **Polynomial chaos (PC):**
  - Misnomer: nothing to do with chaos as in dynamical systems
  - Essentially a polynomial fit/regression to the black-box model
  - Extremely convenient for uncertainty propagation, moment estimation, global sensitivity analysis
    - e.g., PC surrogate allows extraction of sensitivity indices ‘for free’
  - Can deal with highly non-linear models, but certain level of smoothness is assumed

- **Low-rank tensor representations:**
  - Nature is low-rank: only subset of inputs act together at the same time
  - More flexible than PC, but harder to construct

- **Neural networks:**
  - Can deal with non-smooth behaviors
  - Cons: much harder to train, even harder to interpret

Robust and Adaptive Sparse Regression to Discover Sparsity in Model Inputs

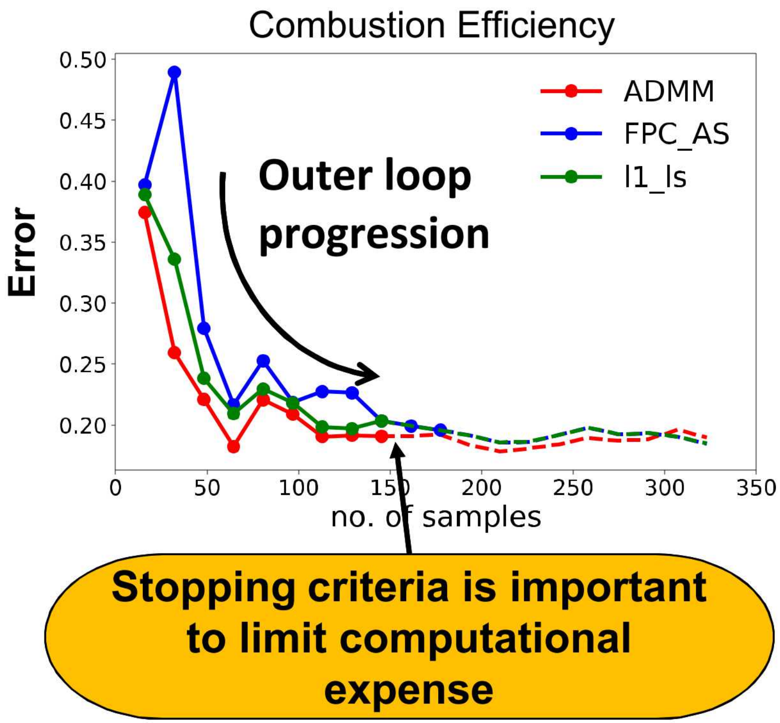
- Focus on Polynomial Chaos Expansions (PCEs) to express input-output dependencies
  - large number of coefficients and expensive model -> **system is underdetermined**
  - Compressive sensing seeks sparse solutions, discover the set of coefficients for terms that explain the available data
- Existing sparse PCE regression techniques (U. Colorado Boulder, SNL groups) *are challenged when fitting data with large noise* & the right number of samples required discover the model structure is not known a-priori for realistic computational models

Our new approach *mitigates overfitting & determines the required no. of model evaluations adaptively* through cross-validation and a strategy to guide stop-sampling decision

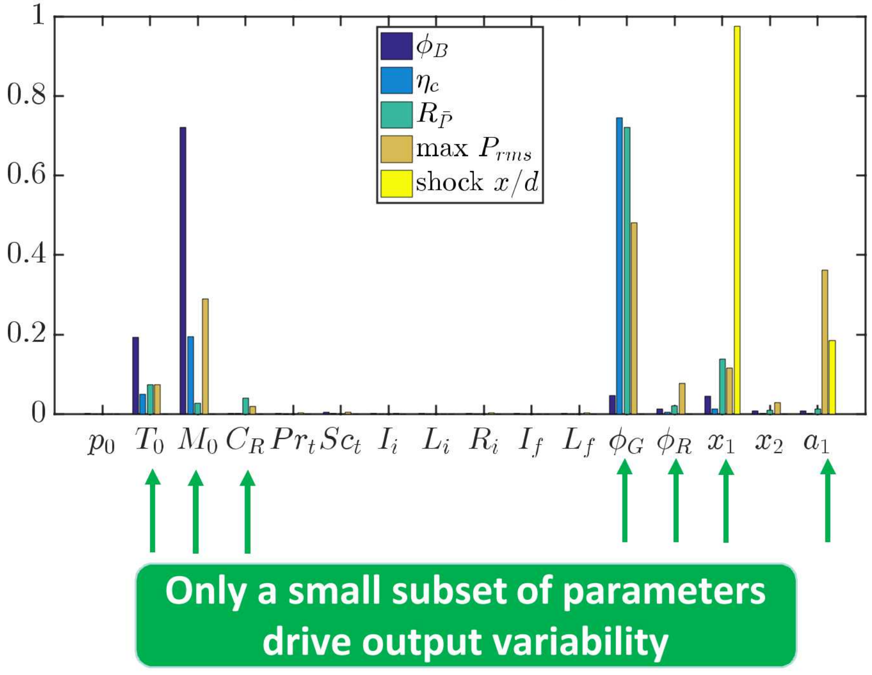
- use just enough samples to construct the surrogate model!

Use Sparse Regression for Sensitivity Analysis to Enable Design Optimization

- Novel combination of algorithms for sparse regression for Polynomial Chaos Expansions
  - **Inner loop** for data fitting
  - **Outer loop** employing filters to decide if no. of samples is sufficient



o(10^2-10^3) reduction in computational expense



Huan, Safta, et al, SIAM/ASA JUQ (2018)

Huan, Safta, et al, AIAA Journal (2018)

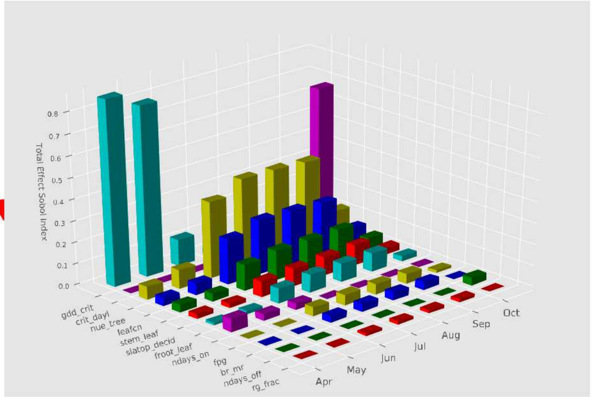
Sparse and Low-Rank Surrogates

- Exploit model structure to reveal sparse low-rank interactions between model components and associated parameters
  - Surrogate model accuracy 4-8%; improvement of by a factor of 2 over classical surrogate model approaches

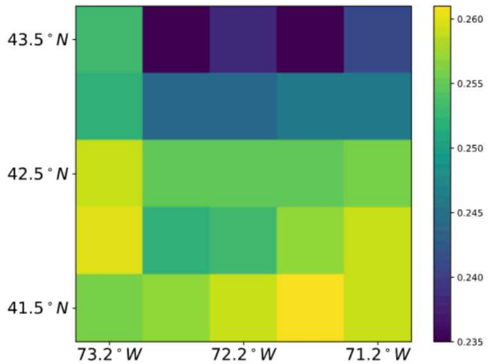
$$f(x_1, x_2, \ldots x_d) = \sum_{i_0=1}^{r_0} \sum_{i_1=1}^{r_1} \cdots \sum_{i_d=1}^{r_d} f_1^{(i_0 i_1)}(x_1) f_2^{(i_1 i_2)}(x_2) \cdots f_d^{(i_{d-1} i_d)}(x_d)$$

- Explore parametric functional tensor train representations to augment the low-rank models over the Land Model inputs with spatio-temporal dependencies (Joint work with FASTMath)

Total Effect Sobol Indices at US-Ha1

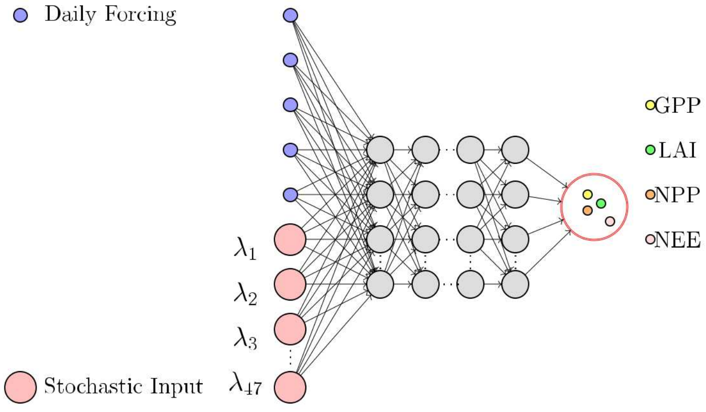


LEAFCN Sobol Index near US-Ha1

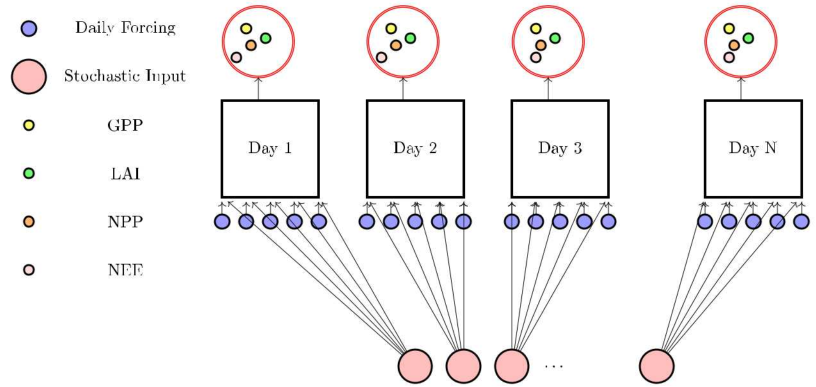


Neural Network Surrogates Allow More Flexibility

Multilayer Perceptron (MLP)

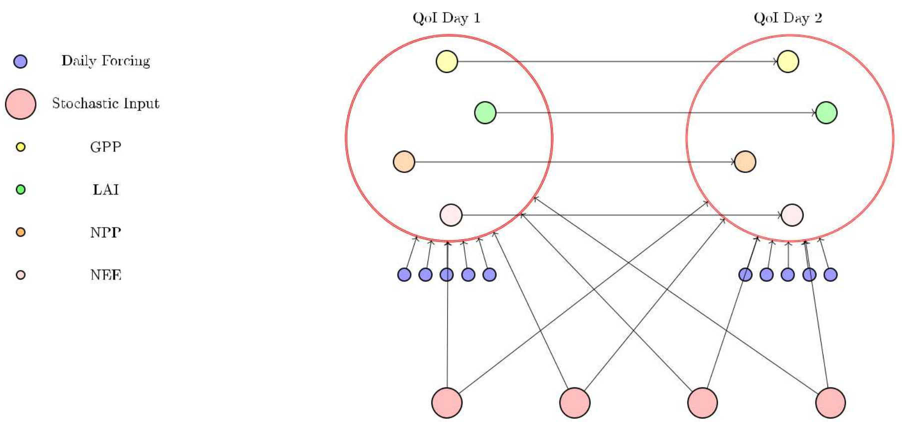


Recurrent Neural Network (RNN)

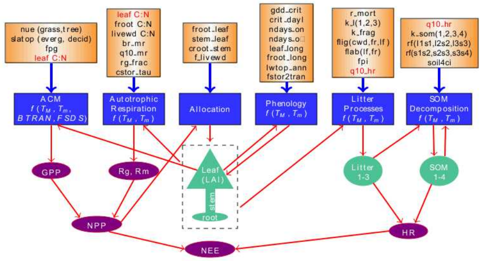


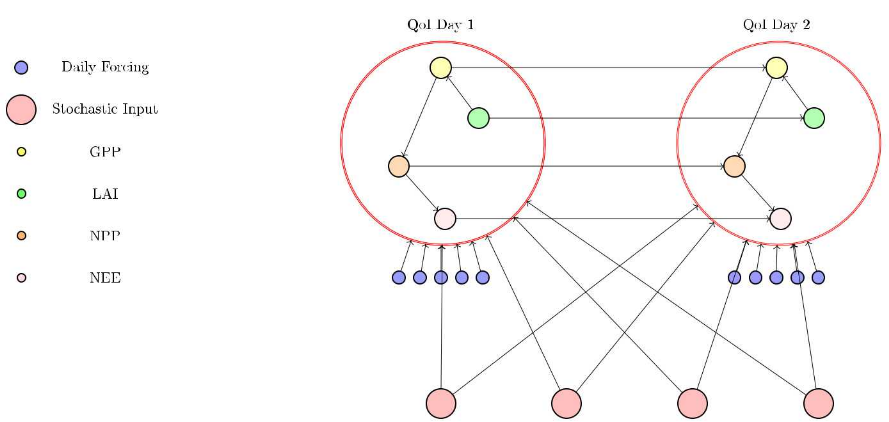
We have created specialized RNN architecture knowing the connections between processes

Vanilla long short-term memory (LSTM) network

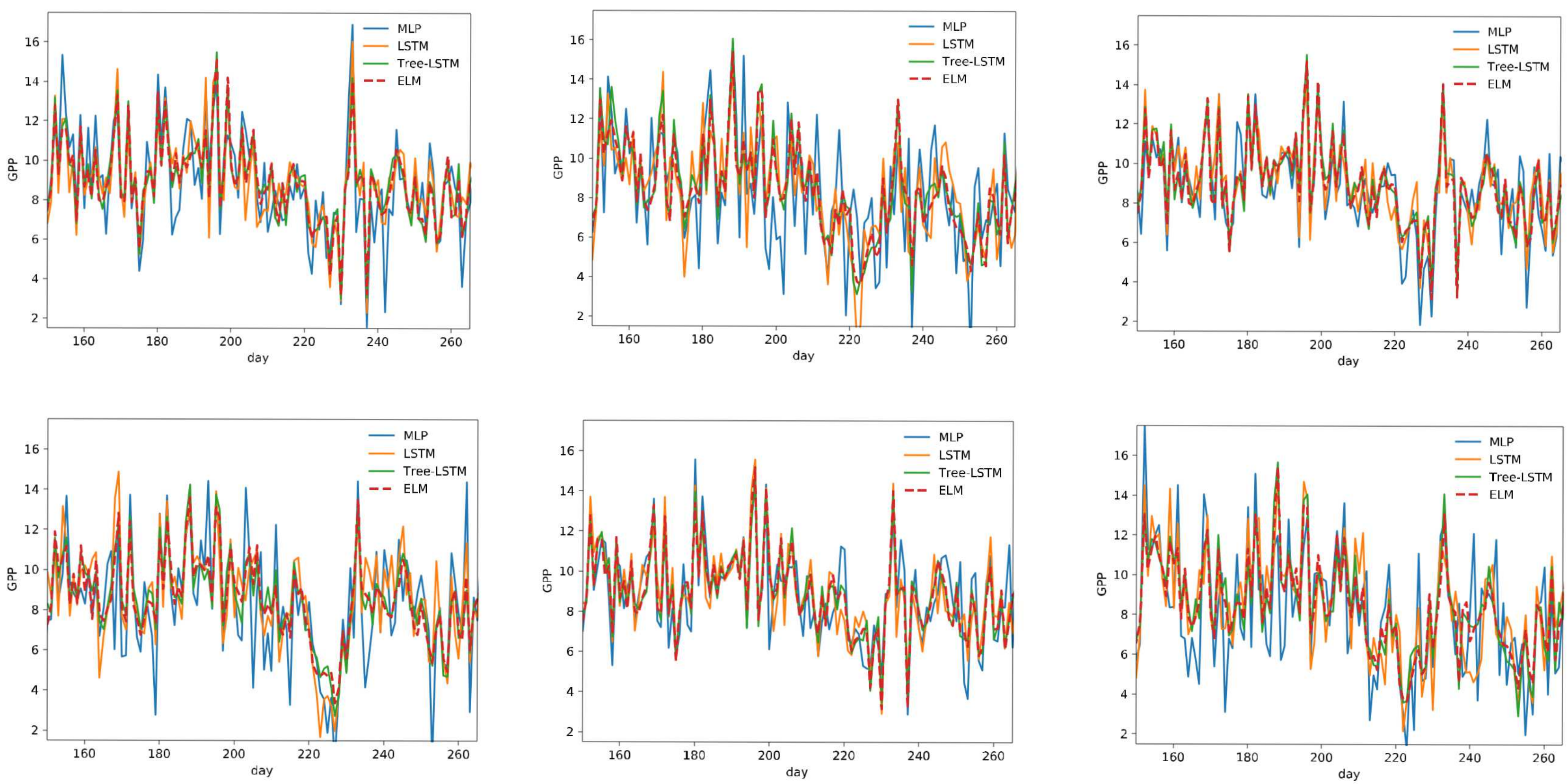


Physics-informed LSTM

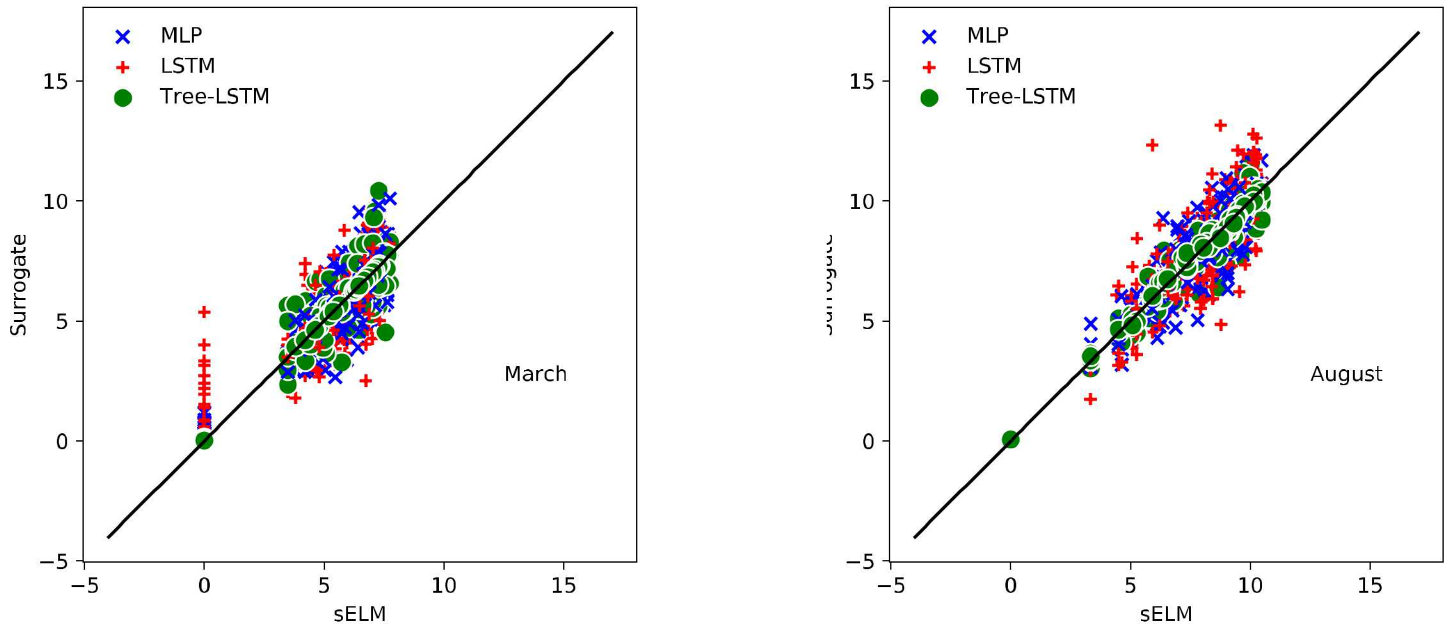




Physics-informed RNN architecture captures daily dynamics well with a fraction of the cost



Physics-informed RNN architecture captures daily dynamics well with a fraction of the cost



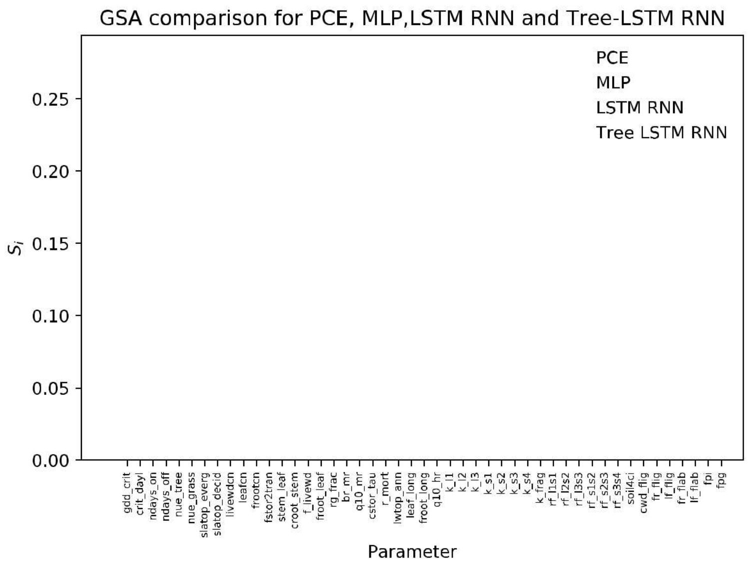
Physics-informed RNN architecture captures daily dynamics well with a fraction of the cost

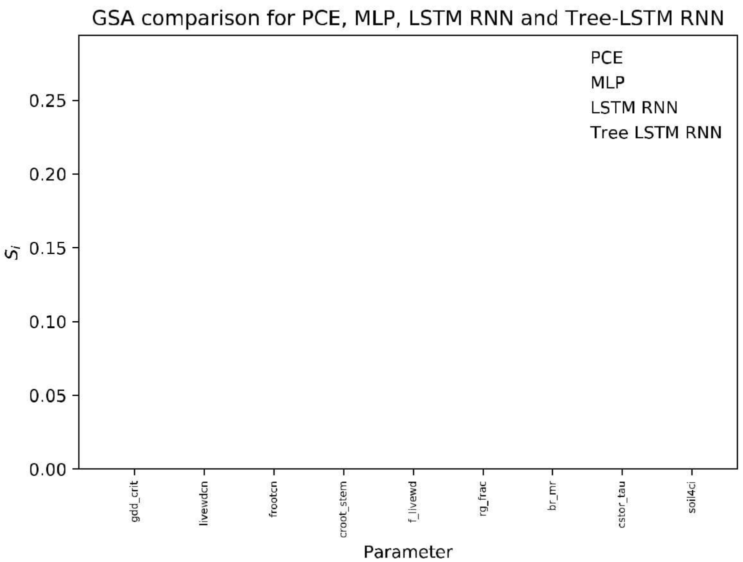
Price to pay?

Compared to PC…

a) GSA is not “free”, and requires extensive sampling of the ML surrogates.
*Not a big deal if the limiting factor is the ELM expense

b) Does not come with uncertainties





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Scramjet RAPTOR

E3SM E3SM Energy Exascale Earth System Model

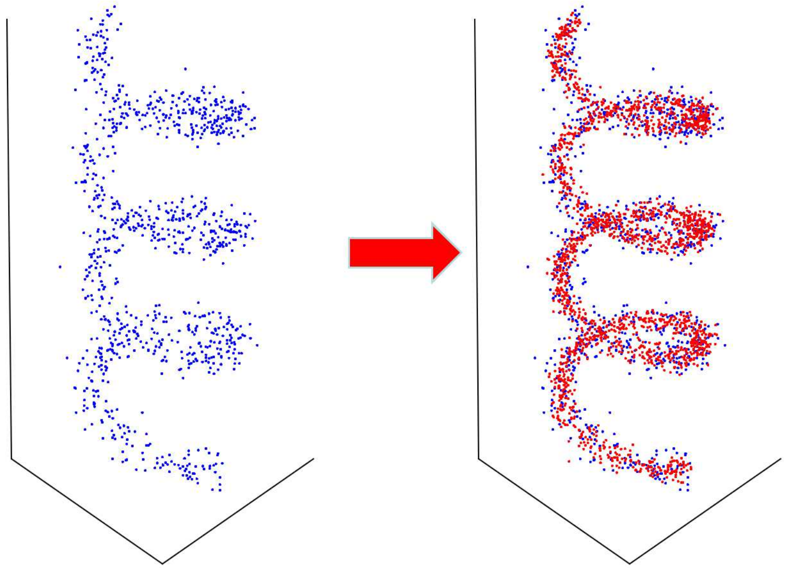
DAKOTA Explore and predict with confidence.

UQTk

Design Algorithms Adapted to Specific Challenges

Exploit Intrinsic Structure in the Input-Output Space

- Use a set of samples (input-output state space) to delineate a manifold ***M***
  - Employ diffusion maps and stochastic differential equations that discover low-dimensional structures embedded in the state space
  - The manifold ***M*** provides an algebraic basis to generate synthetic samples that are statistically consistent with the training data
    - **The computational cost for these samples is negligible compared to the cost of the original computational model**



Novel set of algorithms that combine Markov Chain sampling with Diffusion Maps

↓

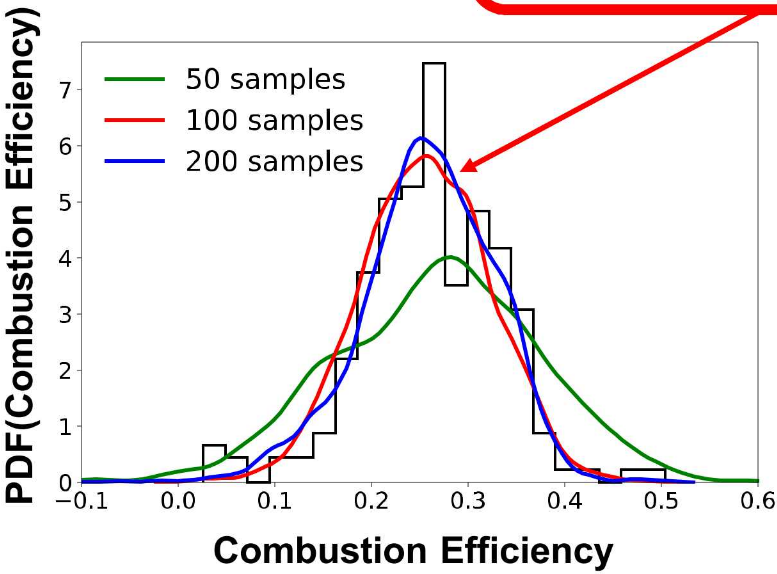
Benefits from increased dimensionality in the output space – when outputs are correlated

Soize, Ghanem, Safta, et al, submitted to J. of Comp. Phys. (2018)

Computationally Cheap Model Samples from Low-Dimensional Manifolds

- ***Manifold construction is adaptive – testing for statistical convergence as samples are added to the training database***
  - 2D "LES" cost: 10k CPU hours/run; 3D LES cost: 200k CPU hours/run
  - 11 input parameters, 5 design parameters, 5 quantities of interest

100 runs are sufficient to construct a diffusion manifold for the Scramjet Model



Sample on the Manifold

Computationally Cheap Model Samples Making Design Optimization Studies Feasible!

Soize, Ghanem, Safta, et al, submitted to AIAA Journal (2018)

Outcome

- Developed new algorithms aimed at removing bottlenecks in engineering design workflows:
  - Sparse Regression & Low-dimensional Manifolds techniques reduced the computational expense by 2-3 orders of magnitude for the Scramjet LES model **making design optimization feasible!**
  - Neural Network Models tackled non-linearities in the E3SM-Land Model with increased accuracy compared to previous algorithms – allowed **accurate selection of parameters that are important to the model!**
- Revealed new information on interactions between E3SM-Land Model components
  - Resulted in improved coupling between land model processes
- Algorithms implemented (or in progress) in Dakota & UQTk.

DAKOTA Explore and predict with confidence.

UQTk

Work supported by DARPA & DOE (SciDAC & BER/ASCR)

For more information

- References
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  - "Global Sensitivity Analysis and Estimation of Model Error, Toward Uncertainty Quantification in Scramjet Computations," Huan, **Safta**, et al, AIAA Journal (*2018*): doi.org/10.2514/1.J056278
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  - "Enhancing Model Predictability for a ScramJet Using Probabilistic Learning on Manifolds," Soize, Ghanem, **Safta**, et al, , submitted to AIAA Journal (*2018*)
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- Other selected references:
  - "Uncertainty quantification in LES of channel flow," **Safta** et al, International Journal for Numerical Methods in Fluids (*2017*), doi:. 10.1002/fld.4272
  - "Efficient Uncertainty Quantification in Stochastic Economic Dispatch," **Safta** et al, IEEE Transactions on Power Systems (*2017*), doi: 10.1109/TPWRS.2016.2615334
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