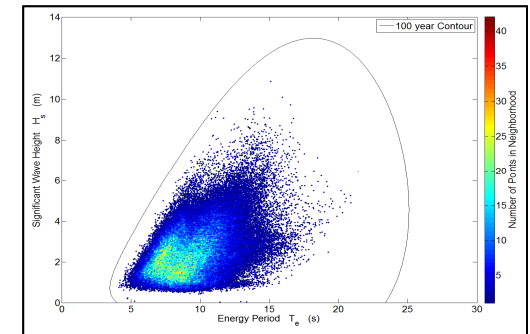
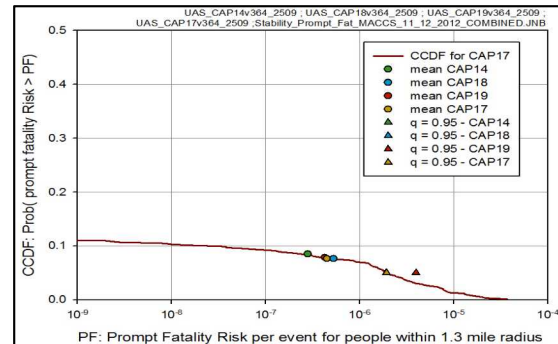
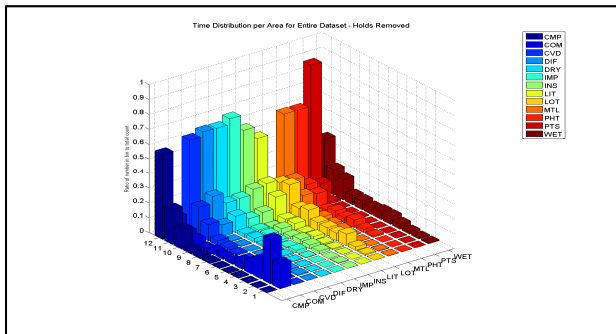


Exceptional service in the national interest



On the Application of Mathematics to Complex Problems

C. Sallaberry - 6224

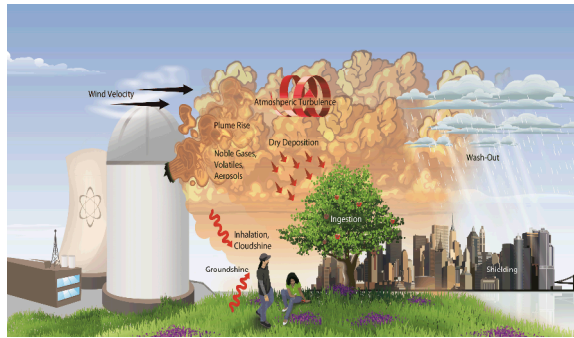
Dealing with complex systems

Always a team effort

- Complex systems require a large spectrum of skills going from theoretical physics/chemistry/geology ... to mathematics and programming.
- All of the work presented would not have been successfully completed without the effort of others within and outside of Sandia.
- Main Collaborators at Sandia are Aubrey Eckert-Gallup, Jon Helton, Rémi Dingreville and Dusty Brooks.
- This is what makes complex systems so interesting. They always offer the opportunity **to learn, teach and meet new people.**
- And the beauty of mathematics is that it can be used in many different fields of study.

Example of applications (1/3)

- Large spectrum of problem



Reactor Consequence Analysis



Radwaste Storage and Transportation



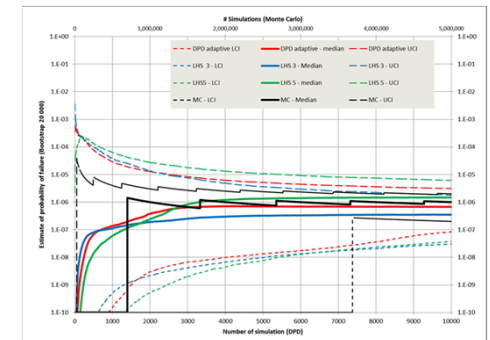
Wave Energy Converter



Wafer Fabrication



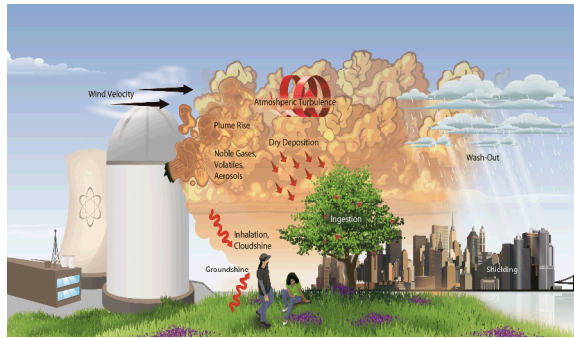
Weapon's Safety



Research and Development

Example of applications (2/3)

- Each requiring different skills ...



Sensitivity and uncertainty analysis



Uncertainty characterization



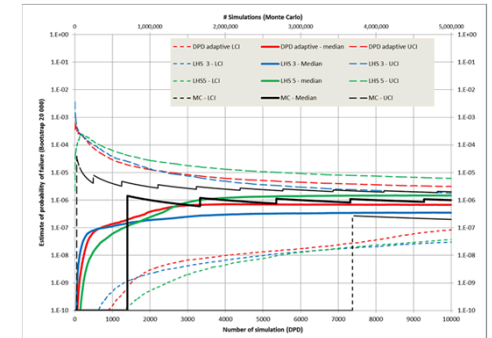
Extreme events prediction



Production optimization



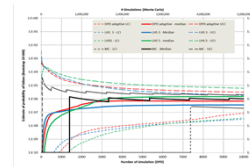
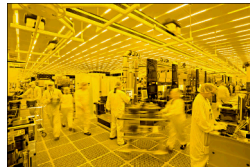
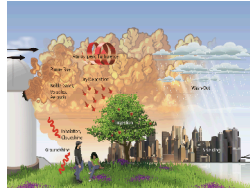
Numerical modelling



Developing new
ideas/concepts

Example of applications (3/3)

- But with the same global strategy



Use a “top-down” approach

- Look at global system at high level.
- Decompose into smaller tasks (that can be correlated).
- Analyze each task by itself and with respect to its parents/linked tasks.
- Consider range of solutions/alternatives.
- Select and implement the best strategy.

Always keep
ultimate goal in
mind

Mathematical skills presented

- Uncertainty and Sensitivity Analysis beyond simple linear regression (SOARCA-UA).
- Numerical estimation of probability of success/failure on a competing system (weak link/strong link for PLOAS).
- Estimation of extreme events (WEC).
- Uncertainty Quantification (UQ-UFD).
- Optimization of production lines (Wafer-Fab).
- Optimization of error and uncertainty reduction for complex systems (LDRD).

SOARCA-UA — Presentation of the problem

- SOARCA stands for State Of the Art Reactor Consequence Analysis.
- UA stands for Uncertainty Analysis.
- Two codes developed at Sandia:
 - MELCOR (<http://melcor.sandia.gov/>) analyzing severe accidents in nuclear power plant.
 - MACCS (MELCOR Accident Consequence Code Systems (<http://energy.gov/ehss/maccs2>) estimating the consequence of an accident to the population.
- Codes have been used to estimate consequences from Fukushima Daiichi accident.
- Purpose is to take uncertainty into account in SOARCA analyses.
- First analysis performed on Peach Bottom power plant (SAND REPORT SAND2012-10702P).
- Second analysis on Surry reactor (expected completion by mid 2015).

What was/is the request?

Propagate uncertainty and analyze the consequences. Provide unambiguous and defensible approach.

SOARCA-UA — Uncertainty characterization and propagation

- Selection of important inputs (relative to their contribution to overall uncertainty).
- Develop rigorous techniques to assess uncertainty and provide ^{ACEG4} **associated documentation**.
- Propagate uncertainty within the system via Monte Carlo method.
- Check for **statistical stability** : Monte Carlo is a numerical method and accuracy of the technique needs to be tested.

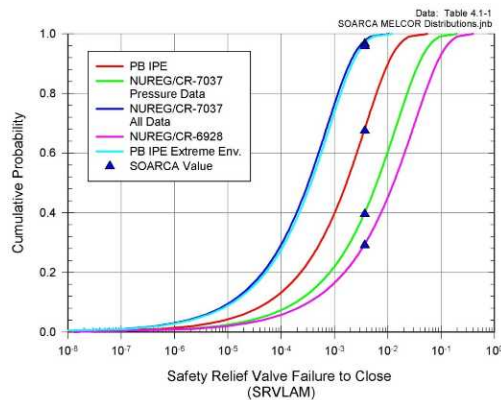
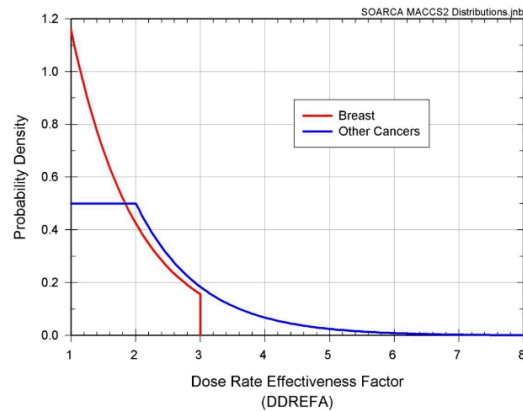
Slide 8

ACEG4

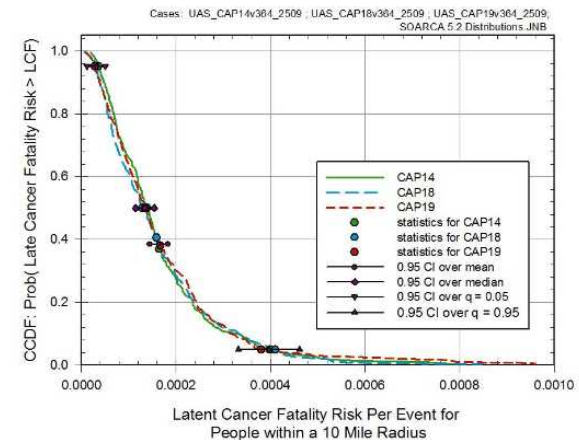
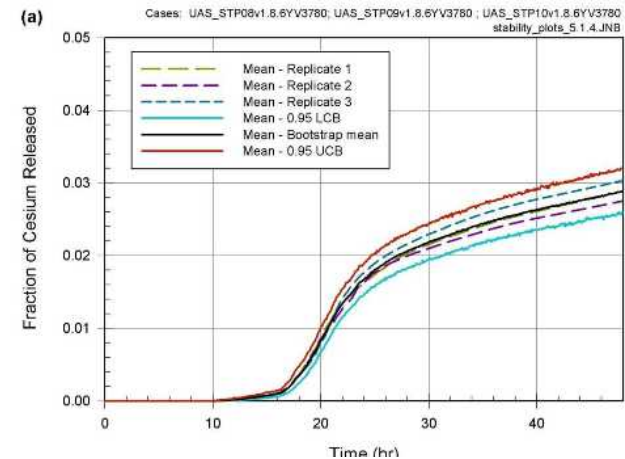
Added provide

Eckert-Gallup, Aubrey C, 2/13/2015

SOARCA-UA — Results of uncertainty propagation and stability analysis



Estimation of input uncertainty



Representation of output uncertainty with confidence intervals

(1/2)

- Going beyond traditional stepwise regression. Limitations of such regression are linearity (or monotonicity) assumption and additive model (no conjoint influence).
- Three other techniques considered: quadratic regression, recursive partitioning (tree regression), MARS (splines).
- **Why consider several regressions?** Each regression has its own set of assumptions that may be violated for some studied relations. Further, the more flexible the regression technique, the more likely it is to over-fit (i.e. finding a relation where there is none).
- In conclusion, we prefer to rely on a strategy that tests potential relations in different ways and cross-validate.
- All strong relations are checked visually (and qualitatively) using scatterplot representations.

SOARCA-UA – Sensitivity analysis techniques (2/2)

Table 6.1-5 Regression analyses over time when the fraction reaches 0.001 of the iodine inventory released over the first 48 Hours

	Rank Regression			Quadratic			Recursive Partitioning			MARS		
Final R ²	0.42			0.67			0.87			0.68		
Input	R ² inc.	R ² cont.	SRRC	S _i	T _i	p-val	S _i	T _i	p-val	S _i	T _i	p-val
BATTDUR	0.32	0.32	0.52	0.32	0.41	0.00	0.30	0.43	0.00	0.39	0.43	0
SRVOAFRAC	0.40	0.08	0.29	0.13	0.27	0.00	0.20	0.46	0.00	0.22	0.36	0
FFC	0.41	0.01	0.13	0.00	0.03	0.23	0.01	0.04	0.02	0.00	0.00	0.55
RRDOOR	0.42	0.00	0.13	0.00	0.20	0.00	0.00	0.00	1.00	---	---	---
CHEMFORM	0.42	0.00	0.04	0.01	0.00	1.00	---	---	---	0.00	0.00	1
SRVFAILT	0.42	0.00	-0.06	0.01	0.00	1.00	0.00	0.00	1.00	0.00	0.03	0.11
FL904A	0.42	0.00	-0.05	0.02	0.05	0.05	0.00	0.00	0.54	0.05	0.02	0.17
SRVLAM	0.42	0.00	0.04	0.12	0.39	0.00	0.21	0.41	0.00	0.18	0.39	0
SC1141_2	---	---	---	0.04	0.09	0.00	0.03	0.03	0.07	0.00	0.00	1
DGASKET	---	---	---	0.01	0.08	0.01	0.00	0.00	1.00	---	---	---
H2IGNC	---	---	---	0.02	0.02	0.28	0.00	0.02	0.23	0.00	0.01	0.4
RHONOM	---	---	---	0.00	0.02	0.29	0.00	0.09	0.00	---	---	---
SC1131_2	---	---	---	0.02	0.02	0.35	0.00	0.03	0.05	0.01	0.00	1
SLCRFRAC	---	---	---	0.00	0.00	1.00	---	---	---	0.01	0.06	0
RRIDFRAC	---	---	---	0.00	0.00	1.00	0.00	0.00	1.00	0.01	0.00	1
RRODFRAC	---	---	---	---	---	---	0.03	0.00	0.61	0.00	0.00	1
EBOLT	---	---	---	---	---	---	0.04	0.00	1.00	---	---	---
DHEADSOL	---	---	---	---	---	---	---	---	---	0.00	0.06	0
RDSTC	---	---	---	---	---	---	---	---	---	0.01	0.00	0.4

Example of influence not captured by simple stepwise regression

CPLOAS – Description of the problem

- **Problem:** Determine Probability of Loss Assured Safety (PLOAS) for weak link (WL)-strong link (SL) systems
- **Characteristics of problem:**
 - Multiple WLs and SLs.
 - Time-dependent link properties and failure values.
 - Possible random variability (i.e., aleatory uncertainty) in link properties and failure values (e.g., temperature, pressure, ...).
 - Possible state of knowledge (i.e., epistemic) uncertainty in link properties and failure values.
 - Link properties and possibly failure values determined by complex mechanistic calculations.
- **Definitions of PLOAS to be considered:**
 - Failure of **all** SLs before failure of **any** WL
 - Failure of **any** SL before failure of **any** WL
 - Failure of **all** SLs before failure of **all** WLs

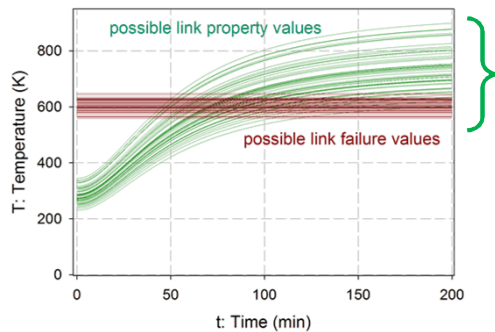
What was/is the request?

Develop methodology and code to determine PLOAS for preceding problem characterized and PLOAS definition

Example from SAND2012-8248

CPLOAS — Results (aleatory uncertainty)

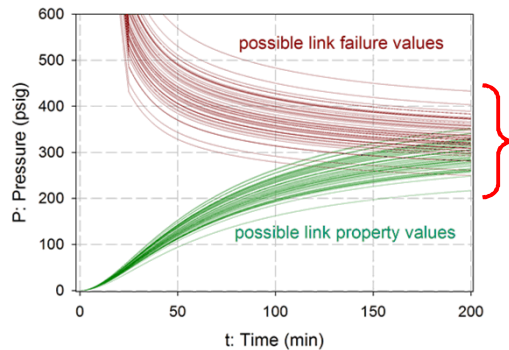
Weak Link



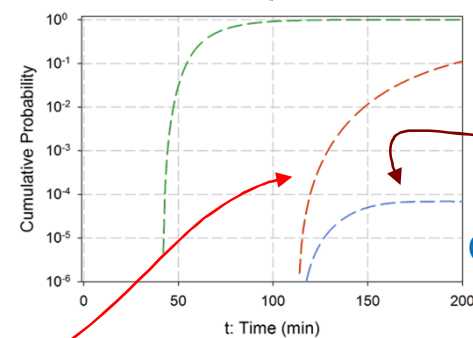
Link Failure corresponds to a property value curve crossing a Failure value curve.

CDF for WL failure

Strong Link



CDF for SL failure



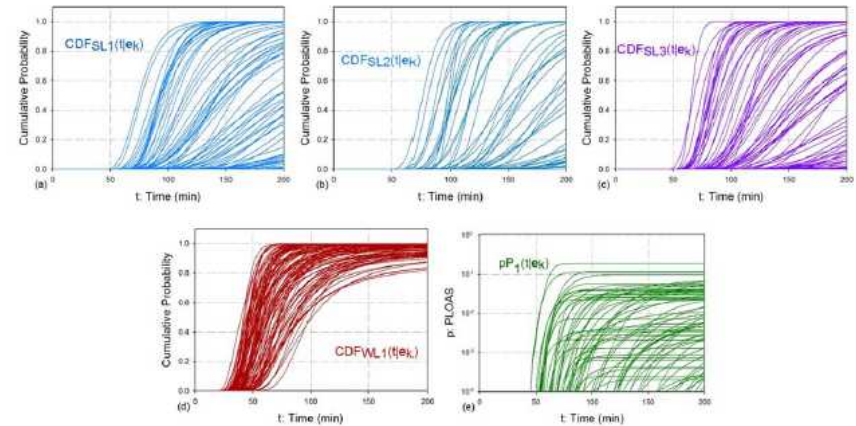
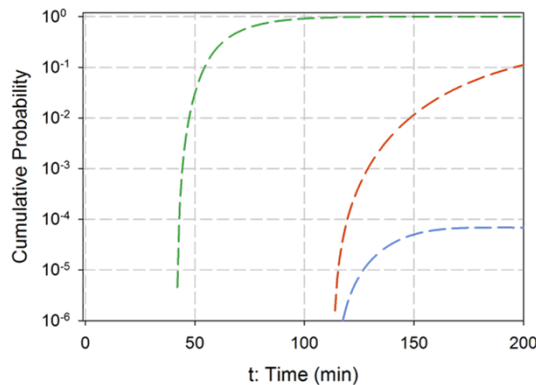
CDFs for link Failure combine to produce CDF for PLOAS.

CDF for PLOAS

The uncertainty here is due to randomness (variation from component to component for instance).

CPLOAS — Results (epistemic uncertainty)

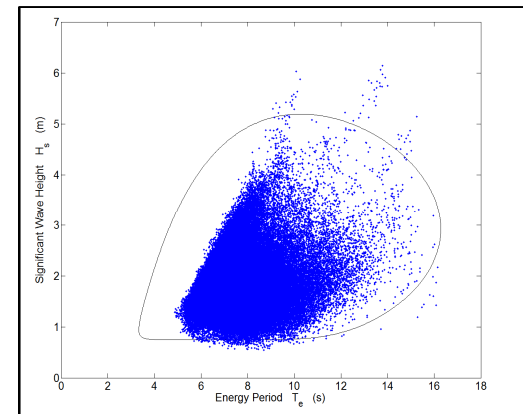
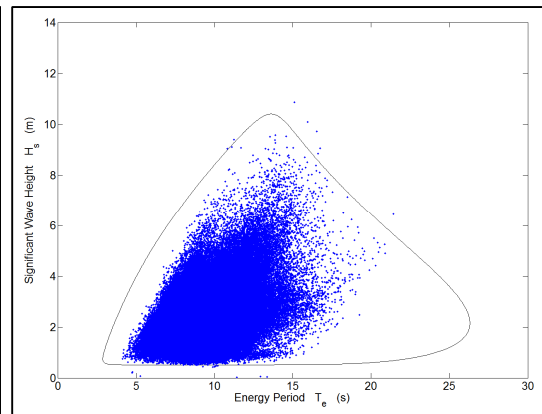
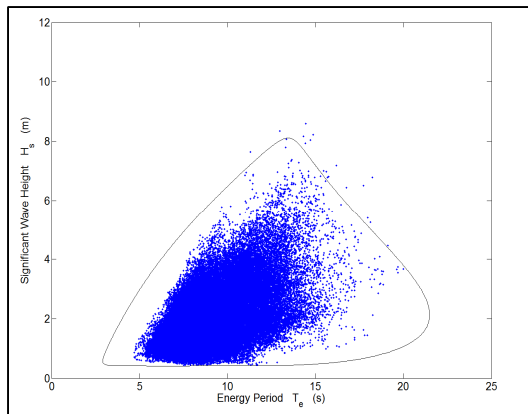
- We introduce uncertainty due to lack of knowledge.
- Each single curve becomes a distribution of curves.
- This “lack of knowledge” uncertainty could (in theory) be reduced with more work.



Example from SAND2012-8248

Wave Energy Converter - Introduction

- **Problem Studied:** Sea states need to be studied in order to estimate their (positive and negative) effects on potential wave energy converters.
- **Characteristics of problem:**
 - Sea states are characterized by wave height and energy period.
 - Method to generate contour using inverse FORM developed by Winterstein et al. in 1993, still the reference used in standard design practice up to present.
 - However, method is not accurate for extreme events: data points collected on a 10 year period fall outside of the 100-year contour generated using this traditional method

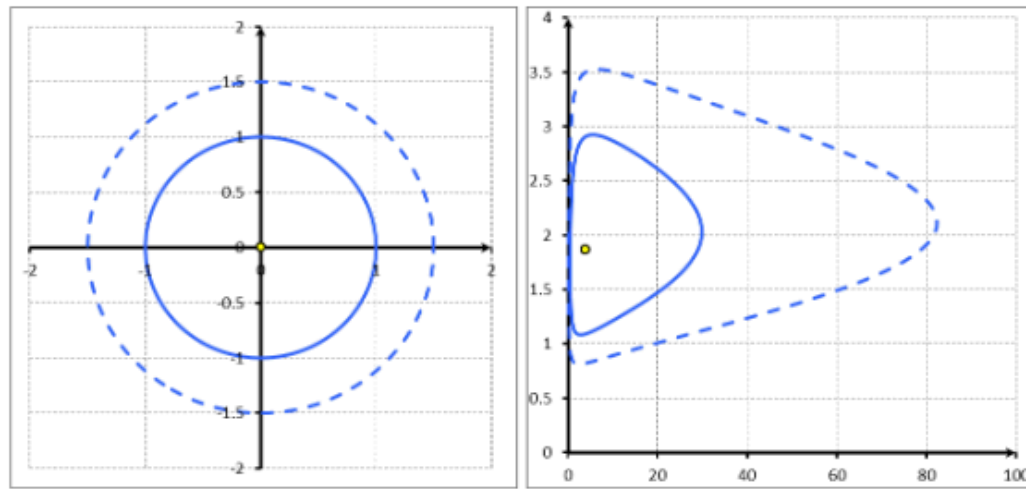


What was/is the request?

Improve the methodology used in order to better represent extreme sea states

WEC — Inverse FORM approach

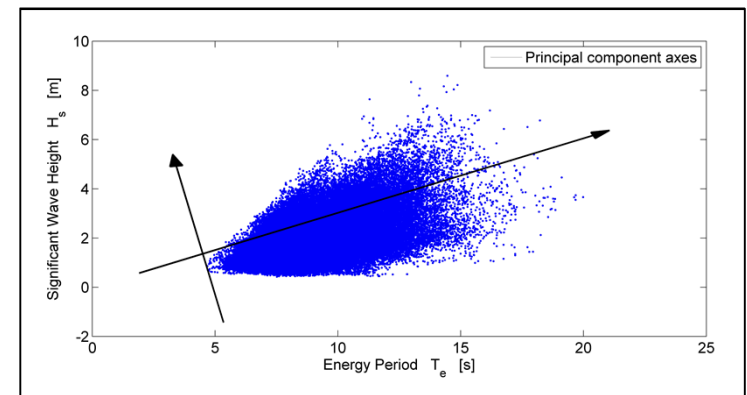
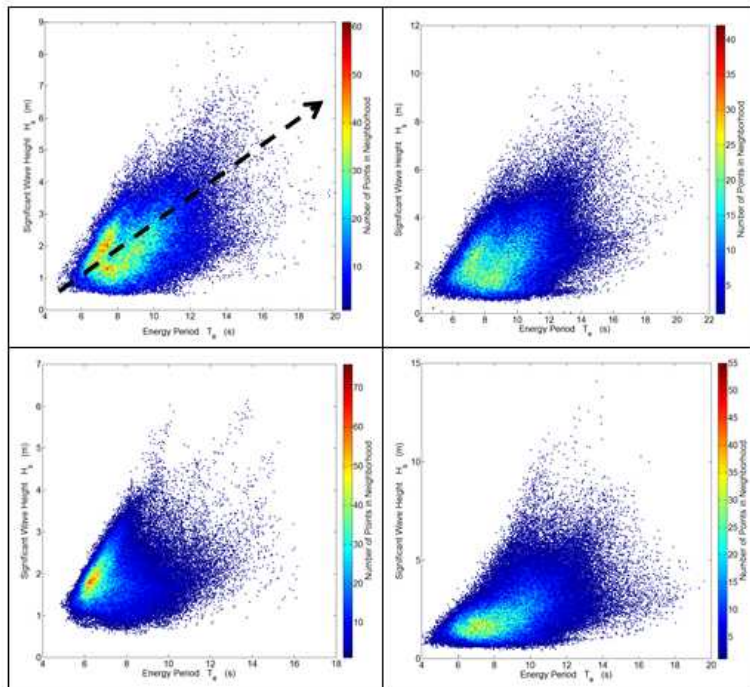
- FORM (First order reliability method) consists in moving into a standardized normal space characterizing uncertainty to estimate likelihood to be beyond a threshold value.
- I-FORM (Inverse FORM) start from the standardized normalized space and reserve the operation to estimate a probability contour.



Example from SAND2014-17550

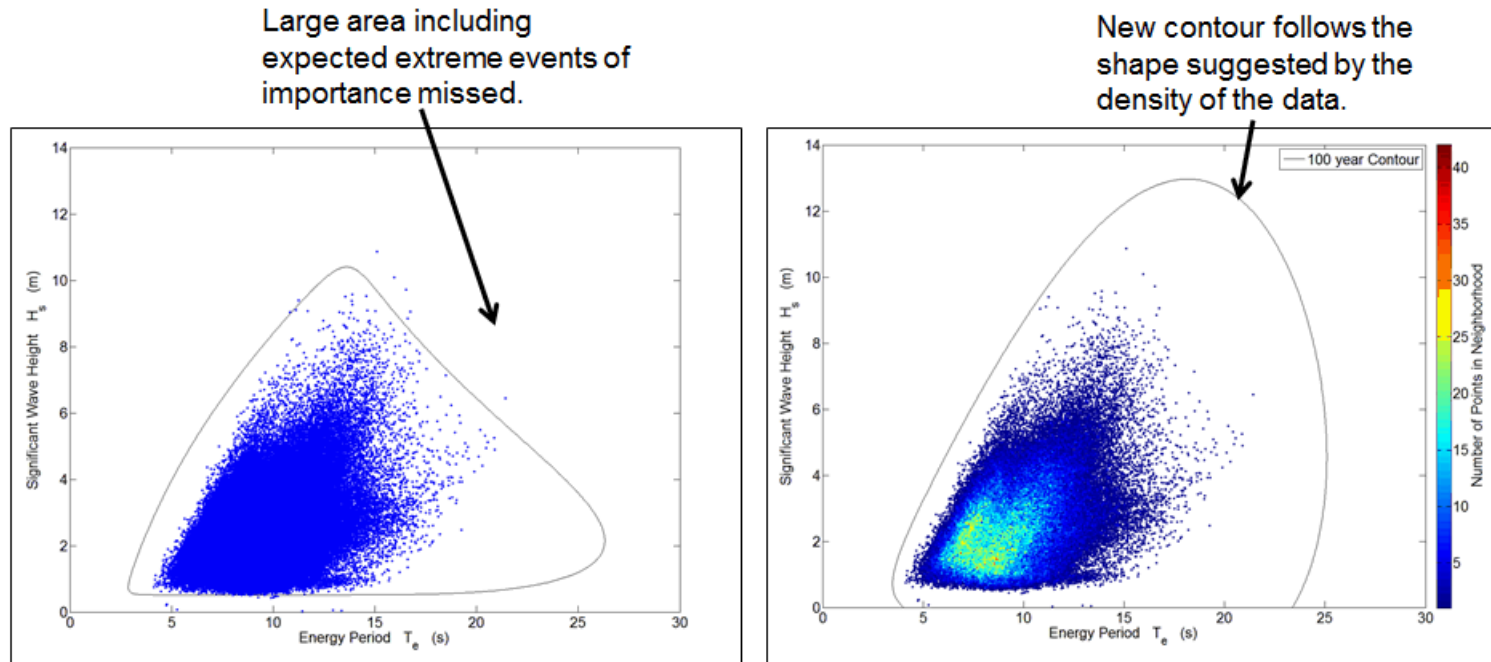
WEC — Principal components

- Problem of initial methodology is that it considers that effect of significant wave height and energy period are not dependent. Density of data extracted shows it is not the case.



Principal components redefine the referential such that data projections are uncorrelated and sorted with decreasing variance (i.e. largest variance first)

WEC — Results



Environmental contour created using the original methodology (left) and the new methodology (right)

- Journal article sent to Ocean Engineering.
- Our expectation is that this approach will define a new international standard.

UQ-UFD — Description of the problem

- **Problem:**

- DOE has been interested in identifying and ranking the gaps (i.e., lack of knowledge) with respect to degradation mechanisms that may affect radioactive waste during storage and transportation.
- Several analyses have been done but they are mostly qualitative and only supported by expert elicitation.

- **Approach:**

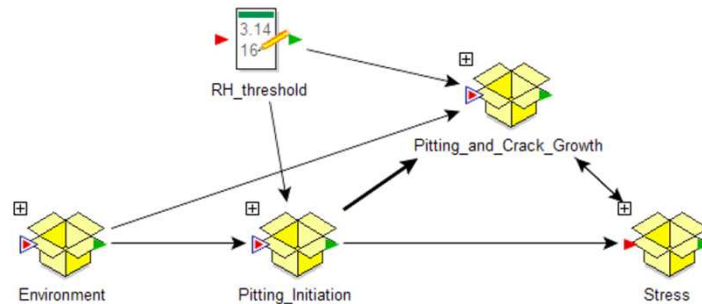
- Use of existing documentation describing the degradation mechanisms and rely on this knowledge to build a more quantitative approach.
- Select an example (Stress Corrosion Cracking due to Weather conditions) to demonstrate feasibility of the approach.

What was/is the request?

Develop methodology allowing the representation of uncertainty in a more quantitative way and that leads to ranking of importance for the “gaps” (i.e. uncertainties related to the system).

UQ-UFD — Development of corrosion model

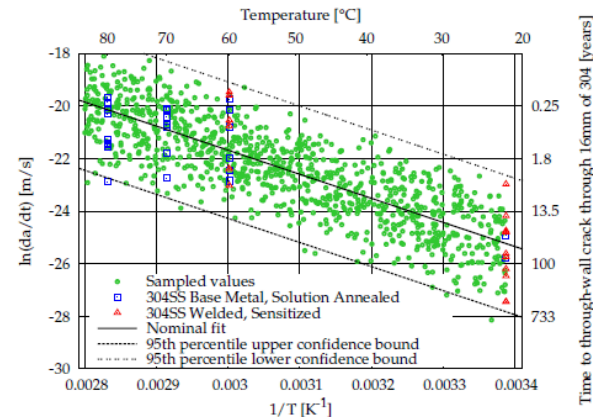
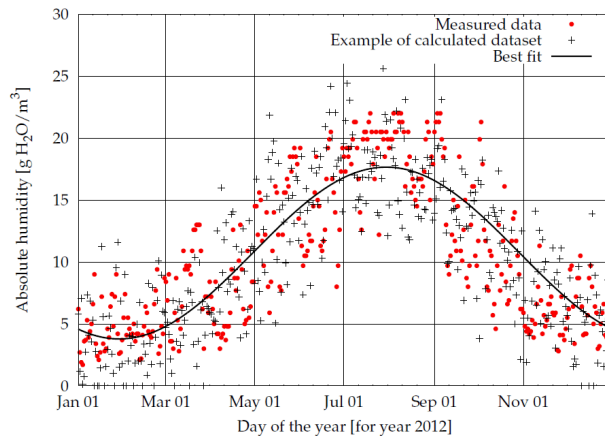
- Development of a corrosion model including environmental variables, pitting initiation and growth, pitting to crack transition and crack growth.



- Simulation of daily activity for a period of 100 years and study evolution of crack growth as well as ranking of major contributing factors (with respect to their uncertainty).

UQ-UFD – Uncertainty representation and conclusions

Uncertainty based on **observations and experiments**. More quantitative and defensible than expert elicitation only.



Evaluation of the input parameters having the biggest impact on the time in storage before the first through wall crack occurs are (i) crack growth rate at 80°C , (ii) crack growth rate at fixed reference conditions (amplitude-factor), (iii) location of the second weld, and (iv) crack growth exponent; with the top two input parameters leading to 60-80% of the variance. These are areas identified for additional data needs to improve uncertainty.

WAFER-FAB — Scope of the problem

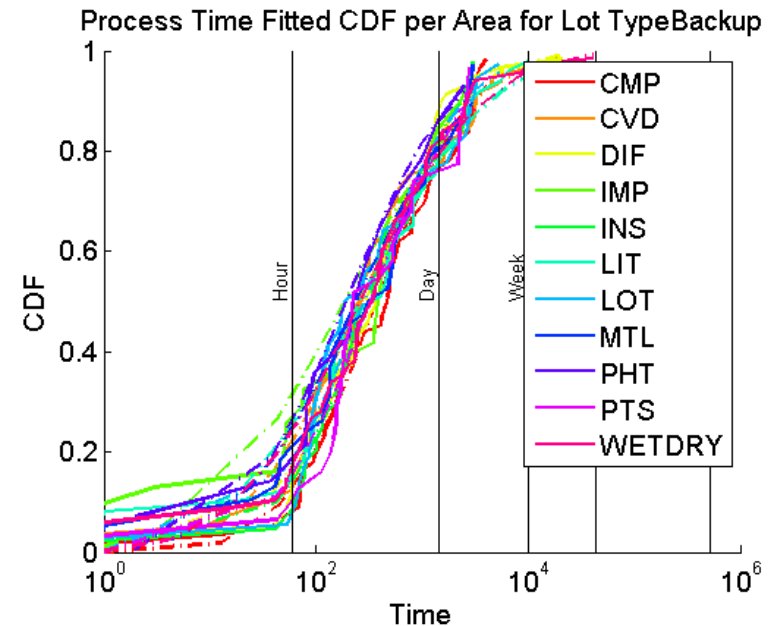
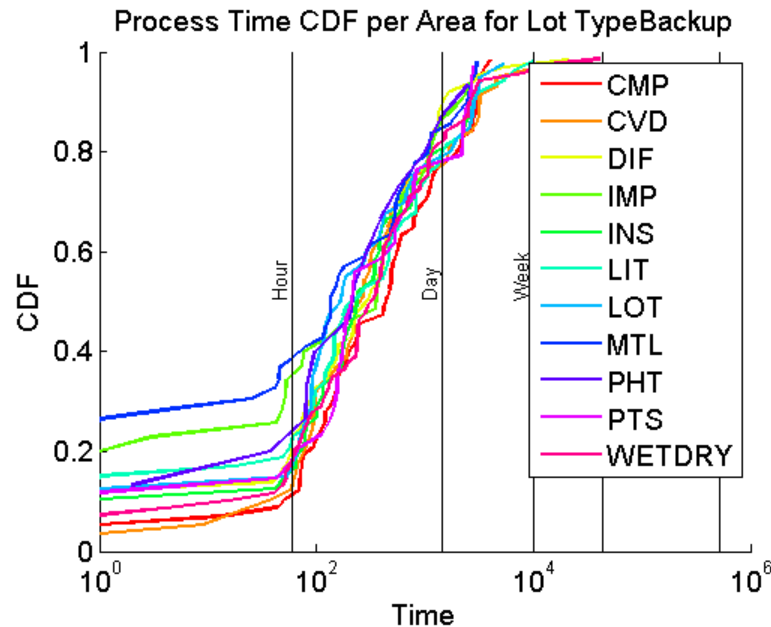
- Wafer fabrication involves many steps in a specific order, typically found in factory work.
- However, the steps may change from lot type to lot type, duration changes from one lot to another of the same type and research and development introduces a lot of variability.
- It is nonetheless important to estimate as accurately the quantity of work and required personnel to meet schedule demands.

What was/is the request?

- What would be the required number of staff (based on area of expertise) to fulfill all requests within the appropriate schedule for a given year?
- Is it possible to characterize a system that is strongly perturbed by research and development projects, whose process time are really varying?
- What are the consequences of adding “priority” and “hot” wafer lots within a pre-defined process ?

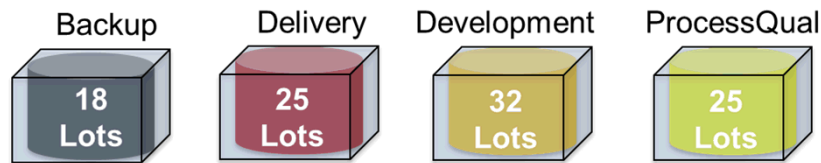
WAFER-FAB — Data description and fitting

- Data has been “cleaned” from noisy perturbation, then fit to appropriate probability distributions.

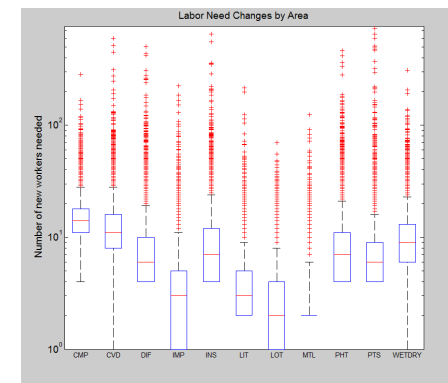
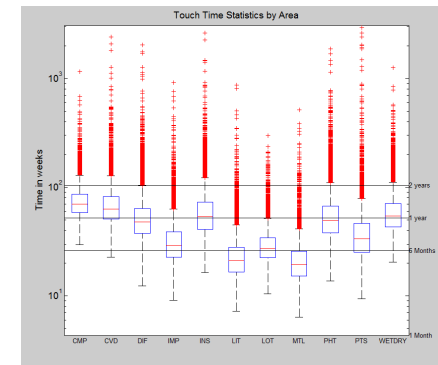


WAFER-FAB — Regression model for prediction

- A regression model has been built to represent possible futures, summarized as box-plots and confidence intervals.
- This helps the decision maker to assess the amount of staff required.



Available Weeks for Work: 4
Percentile Bounds for Estimates: 10% and 90%



Research and Development-

Description

- All of the previous projects require one major aspect: being able to think about each problem (small or large) from different angles.
- The best way for that is to work as a team of people from different background and skills.
- **But also** it means that at the individual basis one should spend some time to stay on top of his/her field of expertise and expand his/her knowledge as much as possible.
- **Therefore** spending a small percentage of time to learn and develop new techniques is a crucial component of success in solving complex systems in the long run.

Error and uncertainty – Example of R&D project

- The output of interest and derived conclusions in complex systems are almost always affected by numerical accuracy of the method used. They arise from both the accuracy of the numerical models and the accuracy of the technique used to represent uncertainty (Monte Carlo for instance).
- These two aspects are sometimes considered separately but never altogether. However, they both influence the answer and potentially the conclusion.
- Considering both in the same framework and then being able to optimize the quality of the solution by working on the weakest of the two accuracies will lead to a more robust and defensible analysis and increase confidence for the decision maker.

Conclusion

- Continuous development of mathematical abilities based on strong background knowledge is a key for success.
- Ability to work with team members from many fields of expertise enhances the quality of deliverables for each project.
- Informative dialogue with colleagues and customers helps to integrate many levels of background knowledge.
- Personal integration of empirical mathematical skills and computer programming and optimization generates highly functional products for many different applications.
- Combination of these abilities establishes the skills needed to adaptively conquer the analysis of complex systems in any field.

References

■ SOARCA-UA:

- Sandia National Laboratories ***State-of-the-Art Reactor Consequence Analyses Project. Uncertainty Analysis of the Unmitigated Long-Term Station Blackout of the Peach Bottom Atomic Power Station.*** NUREG/CR-7155 - SAND2012-10702P

■ PLOAS:

- Helton JC, Pilch M, Sallaberry CJ. **Probability of Loss of Assured Safety in Systems with Multiple Time-Dependent Failure Modes: Representations with Aleatory and Epistemic Uncertainty.** *Reliability Engineering and System Safety* 2014; 124: 171-200.
- Sallaberry CJ, Helton JC. **CPLOAS_2 User Manual.** SAND2012-9305. Albuquerque, NM: Sandia National Laboratories; 2013.
- Groth KM. **CPLOAS_2 V2.10 Verification Report.** SAND2014-16321. Albuquerque, NM: Sandia National Laboratories; 2014.

■ WEC:

- Eckert-Gallup AC, Sallaberry CJ, Dallman A.R. Neary V.S. **Modified Inverse First Order Reliability Method (I-FORM) for predicting Extreme Sea States** - SAND2014-17550. Albuquerque, NM: Sandia National Laboratories; 2014.