

ASC Predictive Science - V&V and UQ



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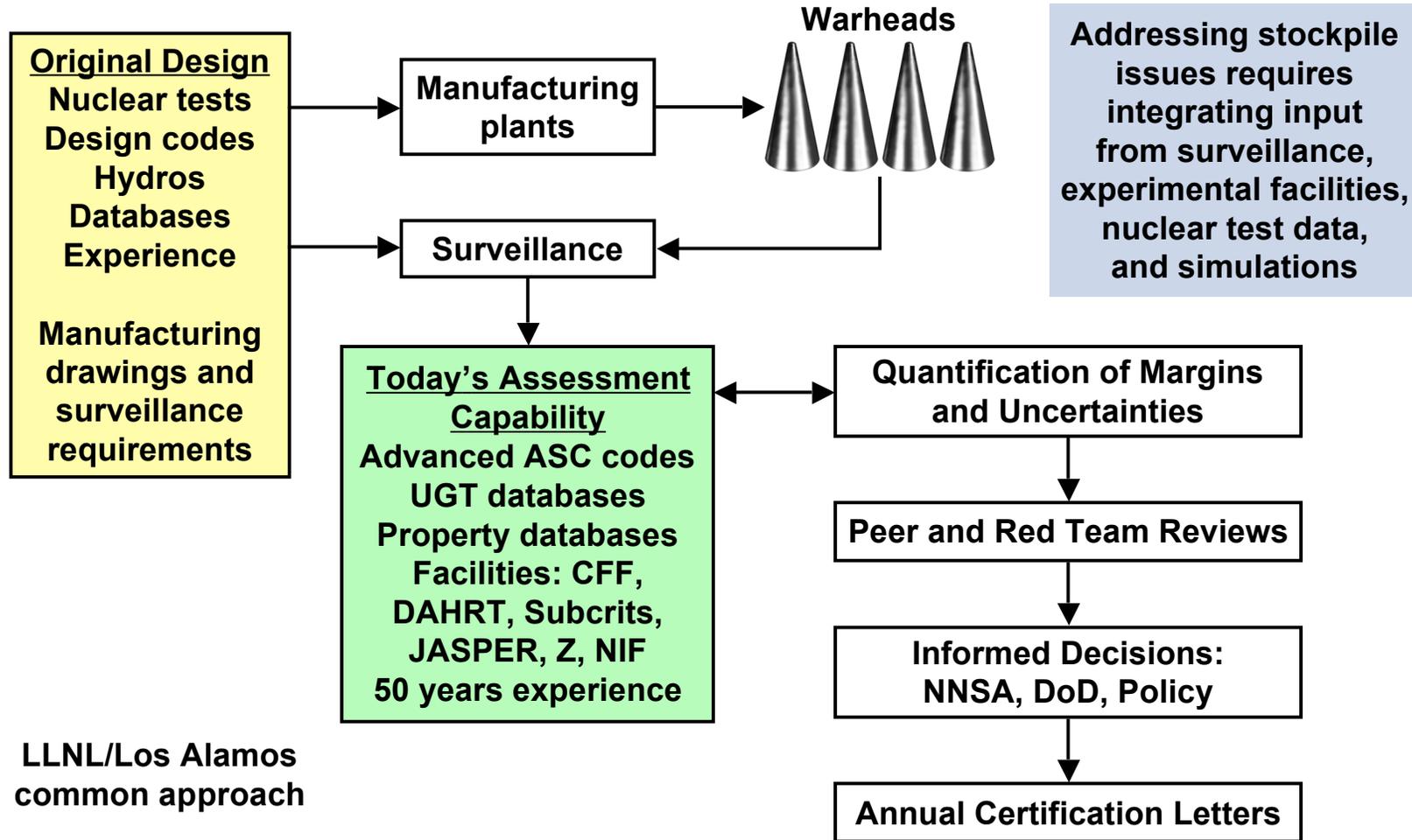
LLNL Perspective of Broad Goals for PSAAP Program



- **Position students to be able to make effective use of multi-petaflop machines for both capability and capacity calculations in their careers**
- **Understand the importance of the V&V process for establishing the credibility of the basis for high value or high consequence decisions**
- **Develop efficient methods to explore the usefulness of millions of calculations to determine sensitivities and options in design space**
- **Explore the techniques for data mining of these massive sets of calculations**
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Credibility of simulations will have a key role in addressing the major problems facing us today

Predictive Science is being developed in NNSA to replace full scale experimental testing

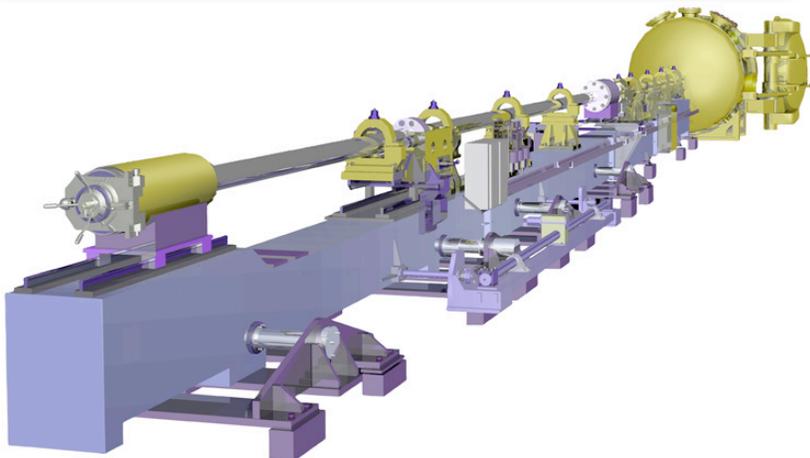


LLNL/Los Alamos common approach

Assessments of warhead performance “at target” involves both reliability and QMU



- **Standard industrial reliability techniques are applied to the myriad components of the weapon system to determine the probability that the system will arrive at target and fire the device**



- **The performance of the device is assessed based on fundamental physics data taken from experimental measurements**

The V&V Program supports QMU and the ASC roadmap to predictive capability



- **Apply Software Quality Engineering as an integral component of increasing the confidence in ASC codes**
- **Identify and assess adjustable code parameters with PDFs provided by ASC and Science Campaigns**
- **Apply sensitivity analysis to guide resource investments**
- **Develop methodologies to quantify uncertainties (competing methods will be fostered) and use them to assess weapon performance**
- **Assure these methodologies meet the criteria for numerical convergence**

**V&V will provide the discipline and the structure
for the UQ in QMU**

V&V is an essential part of the ASC product cycle, and an important interface to Science Campaigns



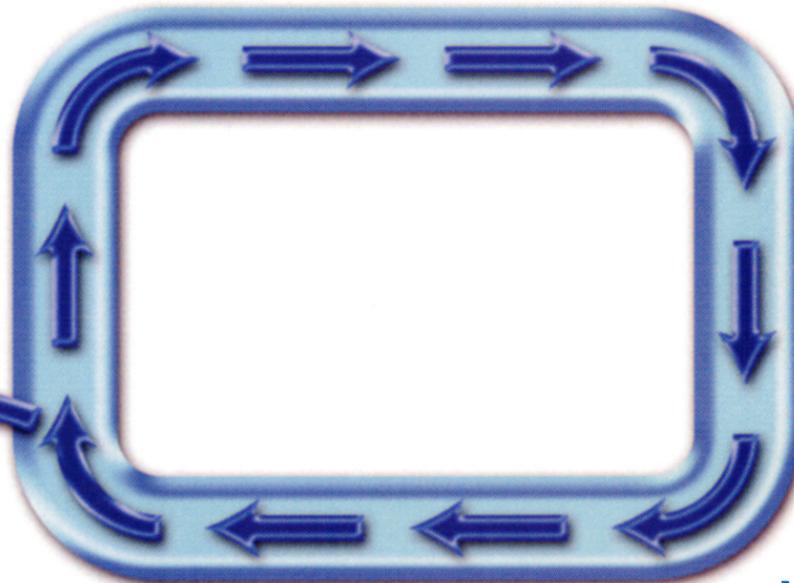
New Capability (new models)

Focused Experiments

Literature search
Technical assessment

Software Quality Assurance SQA (SQA)

Version release
Regression testing
Change control
Code coverage
Code A' = Code A



UQ for QMU

Assessment of code
Physics and numerics
Code A' = Code A
Method A = Method B

Validation Tests

Comparison with experiments
Integral test problems
Regression testing
Code coverage

Verification Tests

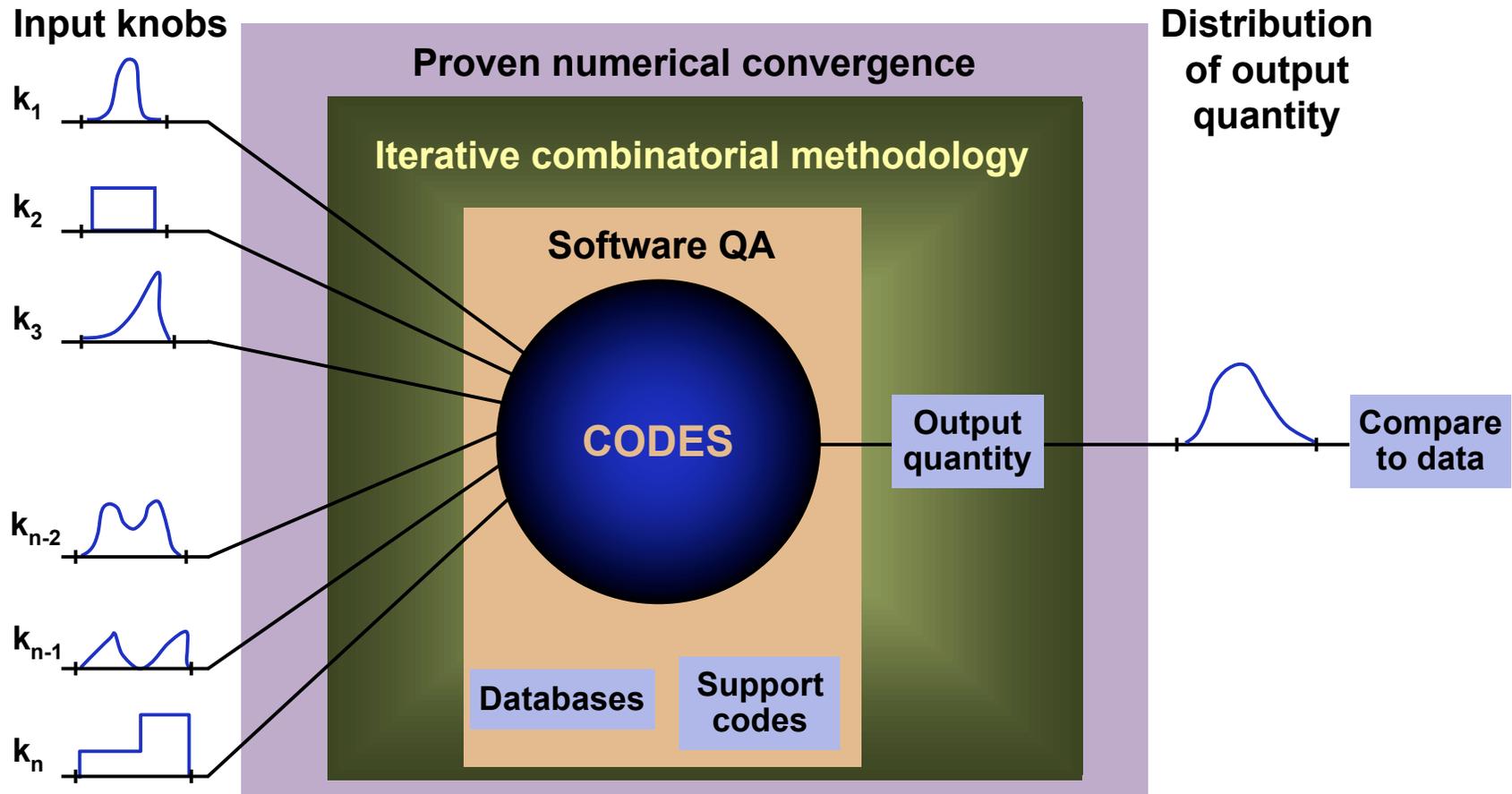
Analytical test problems
Numerical convergence
Code coverage
Regression testing
Code A' = Code A

Necessary (and probably sufficient) conditions for achieving predictive capability



- Codes with assured software quality
- Problems run with demonstrated numerical convergence
- Complete identification of all parameters that can be “adjusted”
(free parameters)
- Development of distribution functions for the “free parameters”
- An iterative combinatorial methodology that samples the hyperspace of free parameters and uses the code as an “operator” to project a quantity of interest
- Capacity computing sufficiently large to accommodate all of the above in 3D
- Program to elucidate underlying physical phenomena via experiment, theory, and simulation (new model development)
- An ability to explain the anomalies in the experimental database (develop new model or theory)

We will quantify probability distributions in key adjustable code parameters and their impact on weapon performance



The codes have hundreds of adjustable parameters; sensitivity analysis will down-select the important ones; UQ techniques can create the final output distributions

We know where the current “free parameters” are—they are in the current codes



- **If a designer can input a parameter change into the deck that changes an output, then that parameter is a free parameter**
- **Numerical parameters (e.g., mesh size, rezoning settings, mesh “stiffeners”, etc.) can play in the game, but can be “studied” to convergence**
- **All free parameters have a distribution function (point values or ranges with shapes, means, moments, etc.)**
- **The multiple free parameters and their distributions form a hyperspace of inputs and the code (as operator) projects that hyperspace onto an axis of interest**
- **Must assure that the models are accurate otherwise the parameter variations represent Sensitivity Quantification not Uncertainty Quantification**

In most cases, the physics of our devices will not exhibit chaotic behavior (barring obvious errors in Monte Carlo statistics)

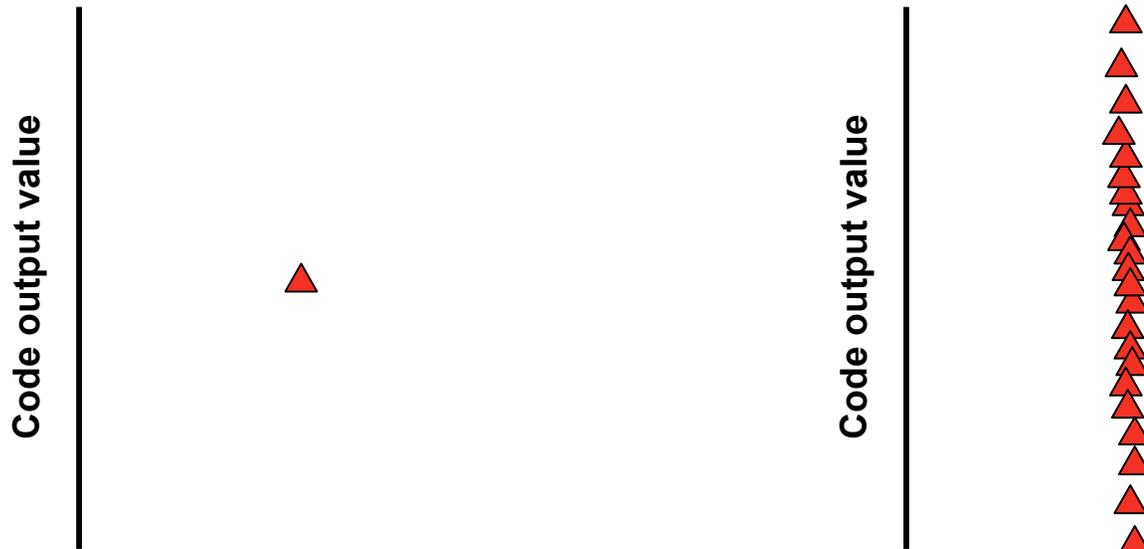
Complex computational simulations generally consist of aleatory and epistemic input variables



- **Aleatory (Latin “*alea*”—throwing of dice)**
- **Epistemic (Greek “*Episteme*”—knowledge)**
- **An aleatory input distribution must be sampled based on a probabilistic outcome and is random (the dice must be rolled at each input step)**
- **An epistemic distribution is based on scientific assumptions regarding the range of the variable and its distribution**
- **Input parameters for the physics package are purely epistemic (currently)**

This makes the interval of the input variable the most important thing to know when beginning the iterative combinatorial methodology

Error bars should not be applied to single calculations, but uncertainties can be assessed for an ensemble of calculations for a model

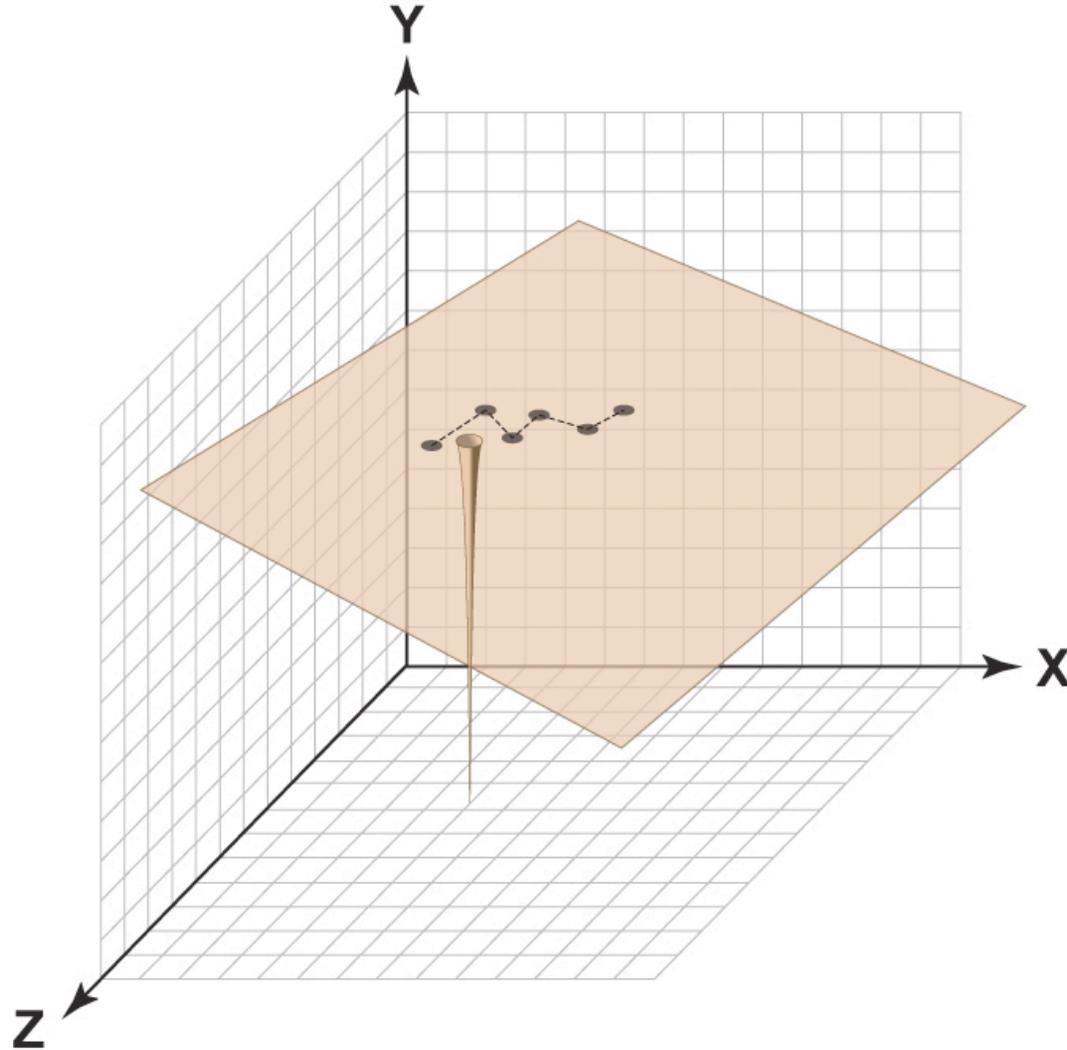


The “error” associated with one computer simulation is essentially the round-off error of the computer hardware

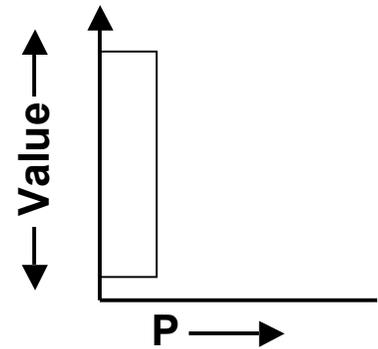
An ensemble of calculations where the input parameters span the available space define the uncertainty associated with a particular model

Is the distribution of the ensemble uncertainty meaningful?

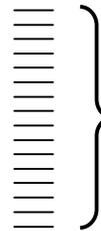
The potential interactions among free parameters produce non-linearities that could prove disastrous to performance



We would like to robustly locate the singularities in our hyperspace of variables



Epistemic variable



Number of sample points = M

Number of free parameters = N

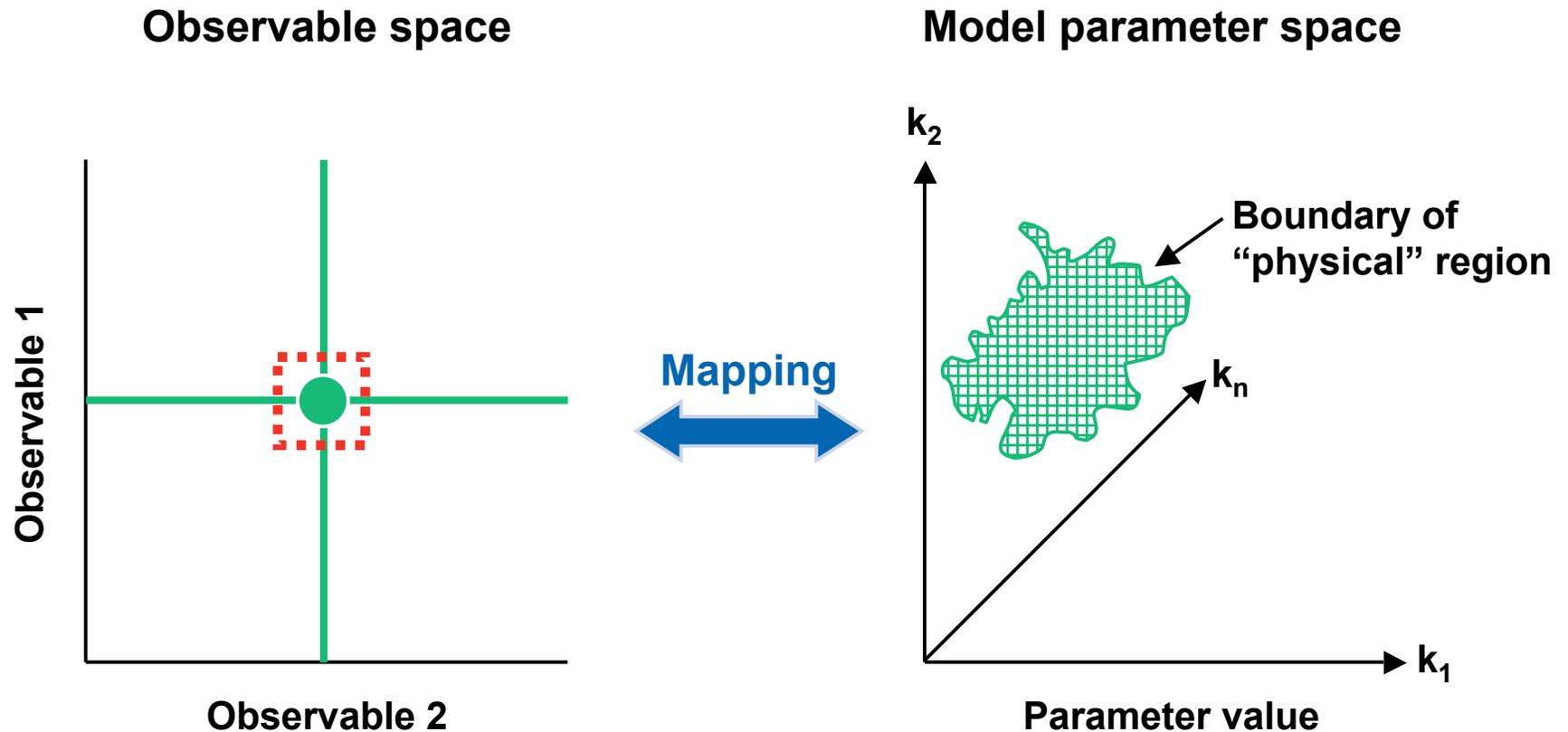
The Curse of Dimensionality

Total number of samples required = $(M)^N$

3 samples	2 parameters	$(3)^2$
10 samples	10 parameters	$(10)^{10}$
100 samples	600 parameters	$(10)^{1200}$

Each sample represents a computation in 1D, 2D, or 3D with numerical convergence

Since calibrated models are used, a single experimental point maps to a volume in the model parameter space



We may be able to use this technique to extract the allowed and forbidden regions of multi-parameter models

What does predictive capability (sufficiently numerically converged) and in 3D mean for capacity machines?



- 3D design calculations probably require fine zones
- A full device 3D numerical convergence study cannot be run today on purple (100 teraflops)
- A full model set (50–100 data points) in 3D (fully converged) with fine zoning to do parameter surveys will require 10 petaflops of capacity to leave room for others
- Full vetting of the adjustable parameters to match data using stochastic bootstrapping (or MOAT, MC, LHS, etc.) and sampling all of the distribution functions could consume 10–100 petaflops of capacity



We can use sensitivity analysis to cut down on the number of sample free parameters

There are unique “capabilities” that a “capacity” machine can provide to the program



- There is nothing wrong with performing sensitivity analysis in 1D or 2D on one processor
- A good 1-D run can be accomplished in 30 minutes
- A 120,000 processor machine can run one billion calculations in 6 months
- This does not solve the “Curse of Dimensionality” (M^N), but it helps us narrow the playing field

Our greatest hope is that we can get our models sufficiently refined so that we live in “flatland”

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Technical Challenges for PSAAP Program

- **New hardware architectures that we may or may not like**
- **Processor scaling limitations (capability runs)**
- **Capacity runs (How much is enough?)**
- **Curse of Dimensionality**
- **Data mining methods and tools**
- **Utilization of laboratory machines**

**The duration of this program implies that we must
be flexible and responsive**



PSAAP Center interactions with labs

- **Availability of laboratory computers**
- **Peer reviews and exchanges**
- **Invited technical seminars**
- **Personnel exchanges as needed**
- **Invitations to scheduled events in ASC**
- **General discussions of NNSA problems and issues in V&V**
- **Sharing of V&V and UQ methods among the centers**

**This can only succeed if people are self motivated
to interact and stretch their comfort zone**