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Propagating experimental UQ into simulations

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Contents

- Guide to Expression of Uncertainty in Measurement
- Simulations & sources of uncertainty
- Distributions
- Overall approach & details
- More information

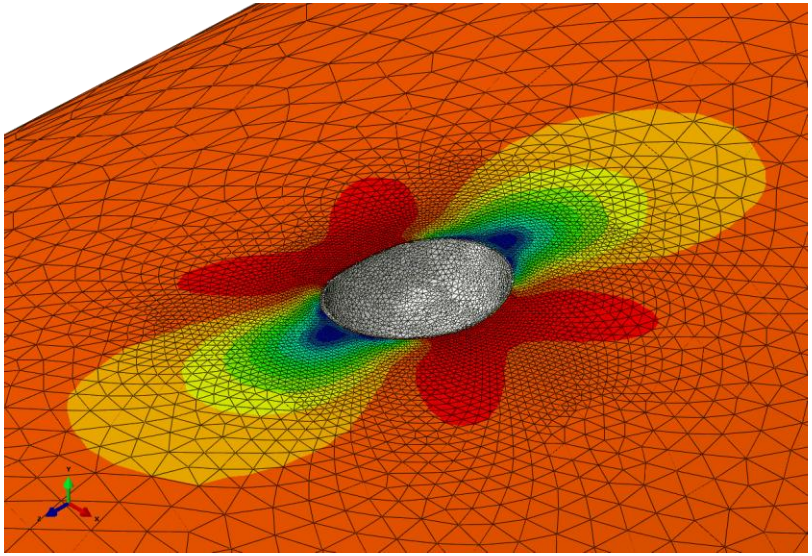
GUM recommendations

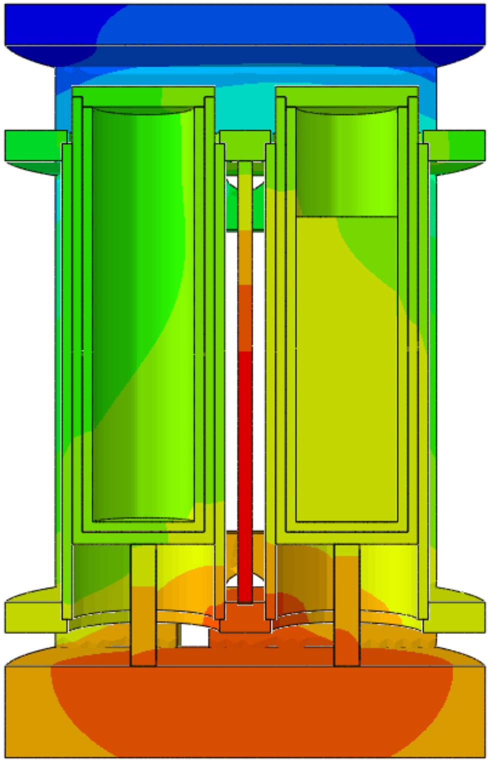
- Guide to the Expression of Uncertainty in Measurement
  - Current version uses analytical formulae, sensitivity coefficients etc.
  - Supplements discuss MC & sampling methods
  - http://www.bipm.org/en/publications/guides/gum.html
- Main steps:
  - Define inputs, outputs and model linking them;
  - Assign distributions to inputs;
  - Propagate input distributions through the model to give statistics of the output quantity.

- Define inputs, outputs and model linking them;

Simulation

- Starts from a question: clearly defined output
  - Location of result of interest may have associated uncertainty





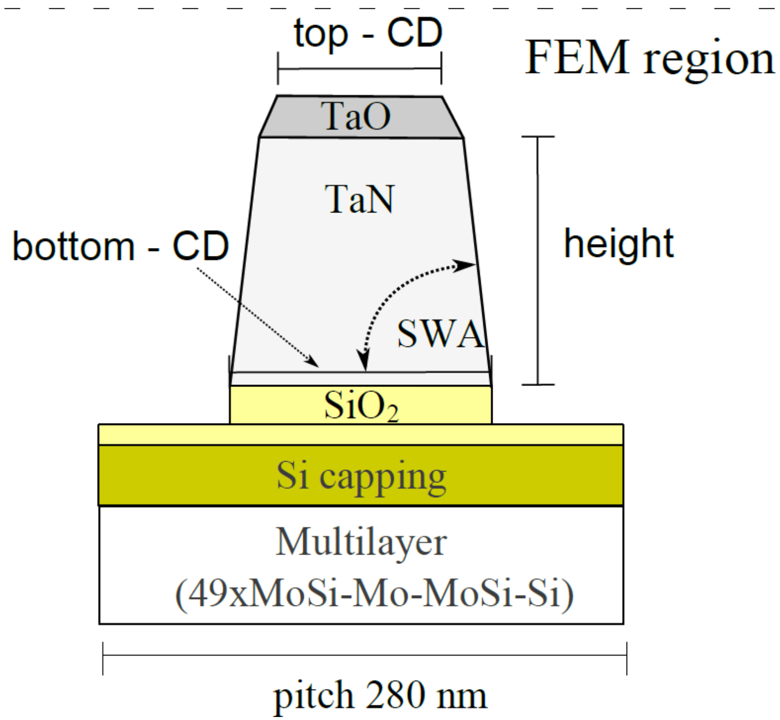
- Focus here is mostly on FE & related models

Simulation inputs

- Governing equations
  - Assume known: calibration/validation issue
- Solution method & software
  - Assume validated model of the problem exists
  - Mesh converged, time step stable, approximation of a high enough order, rounding errors negligible….
  - Ensure model is validated for any input parameters it might receive

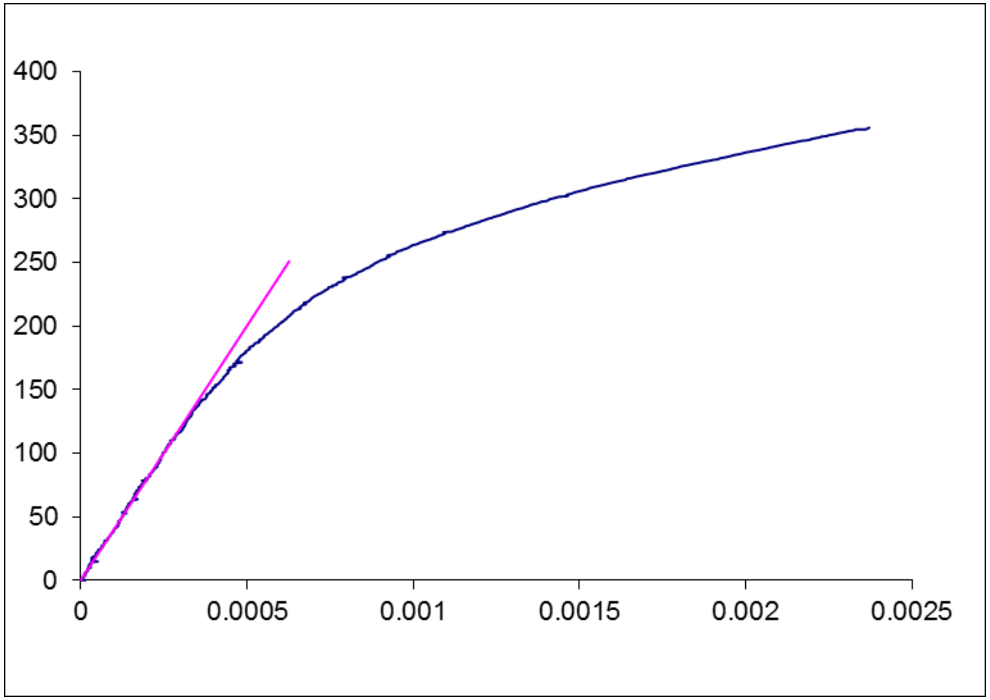
Simulation inputs

- Domain
  - Problem geometry: uncertain
  - Time period/frequency range: may be uncertain
    - Could be part of a boundary or loading condition
    - Could be a model output
    - Upper limit usually known for domain purposes



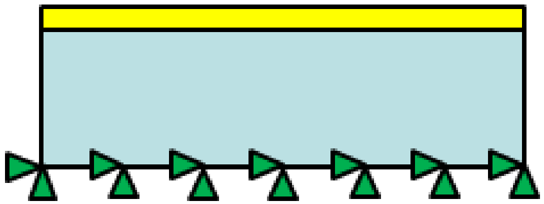
Simulation inputs

- Material properties
  - Parameters: uncertain
  - Underpinning material model: often not certainly known
    - Better addressed as a calibration/validation type problem
    - Can sometimes use cheap simple models as a correction to expensive ones (multifidelity approach)

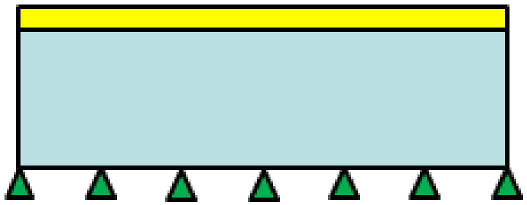


Simulation inputs

- Boundary & loading conditions: uncertain
  - point locations and values
  - bond/clamping quality
  - timings



Fully Clamped



In plane sliding

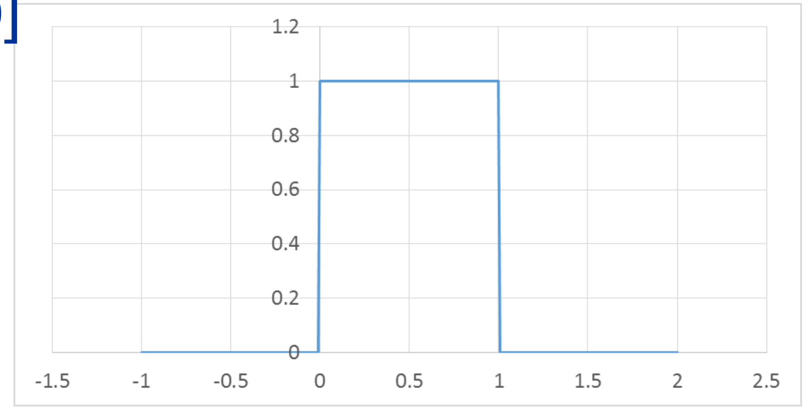
- Assign distributions to inputs

From information to distributions

- Use information to assign probability distributions to inputs
  - Measurements, expert opinion, physically reasonable bounds, previous model results, …
- GUM Supplement 1 section 6
  - “Such an assignment can be based on Bayes’ theorem or the principle of maximum entropy”
  - Choose a distribution consistent with the information that imposes minimal assumptions
  - Examples given for common information types

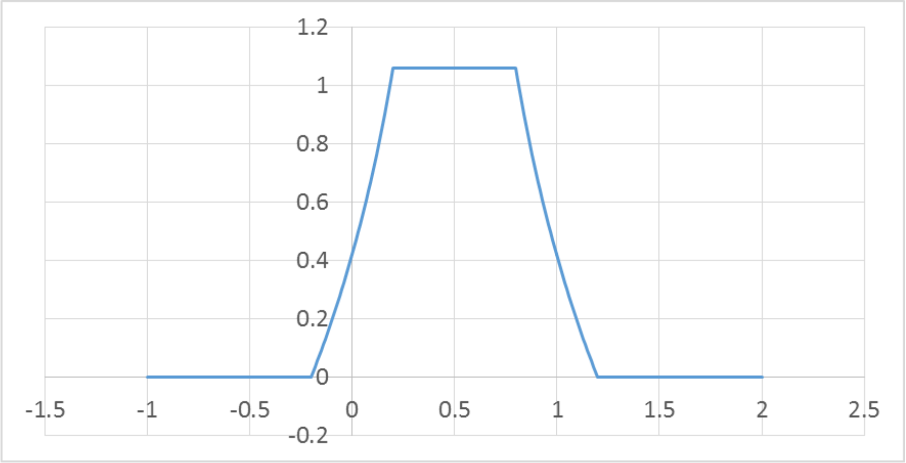
Common information types

- Lower & upper limits [a,b]



Uniform distribution
Mean (a+b)/2
Variance $(b-a)^2/12$

- Inexact lower and upper limits [A, B] in [a-d, a+d] [b-d, b+d]



Curvilinear trapezoid distribution
Mean (a+b)/2
Variance $(b-a)^2/12 + d^2/9$

Common information types

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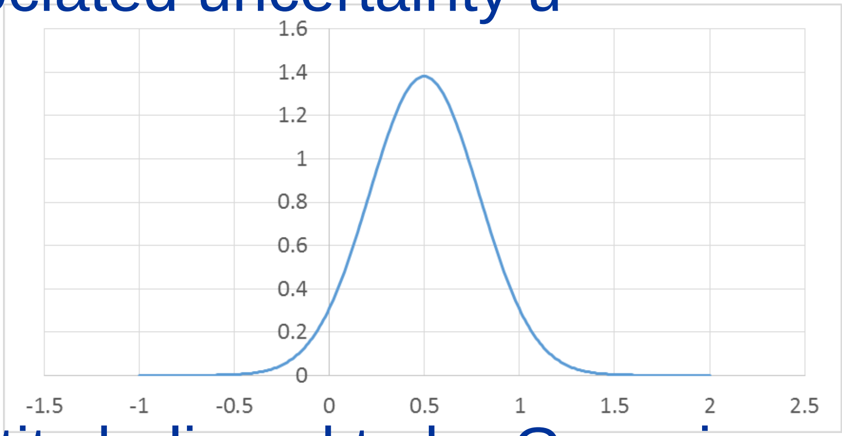
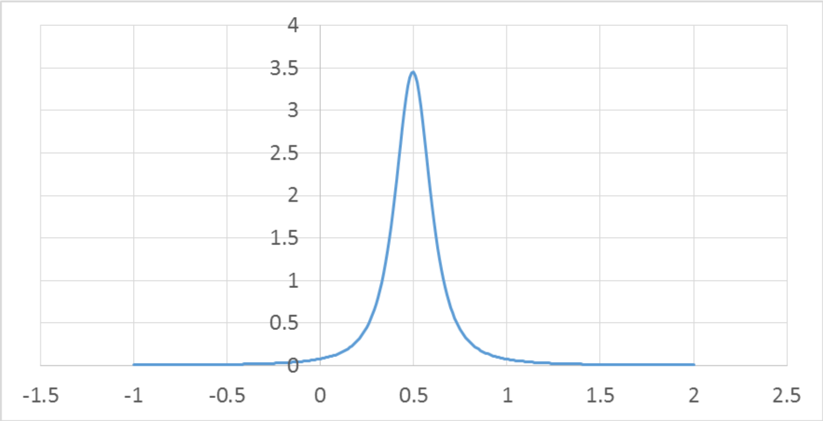
- Best estimate m & associated uncertainty u



Gaussian distribution
Mean m
Variance u^2

- n realisations of a quantity believed to be Gaussian



Student t distribution with
n-1 degrees of freedom
Mean m
Variance $s^2/n*[(n-1)/(n-3)]$

where s and m are sample mean & variance

Correlation

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- Requires assignation of a joint distribution
- Some uncertainty propagation methods cannot handle correlation between input variables
- Where possible, try to identify the cause of correlation & parameterise it directly
  - e.g. temperature dependent material properties: treat the temperature as random, not the properties as correlated
- Use random fields for spatially correlated variables
  - kriging, Gaussian process modelling

- Propagate input distributions through the model to give statistics of the output quantity.

Propagation

- Analytical formulae not ideal for FE type models

  Linearised: not OK for lots of models

  Need sensitivity coefficients: not good for black box software

- Monte Carlo not ideal for FE type models

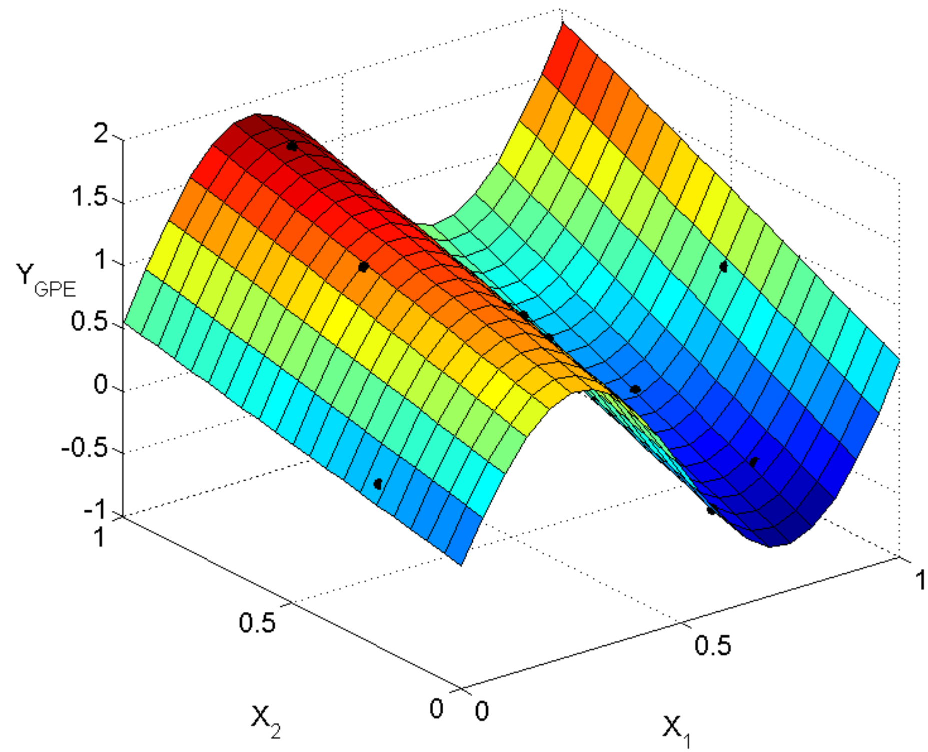
  Computational expense

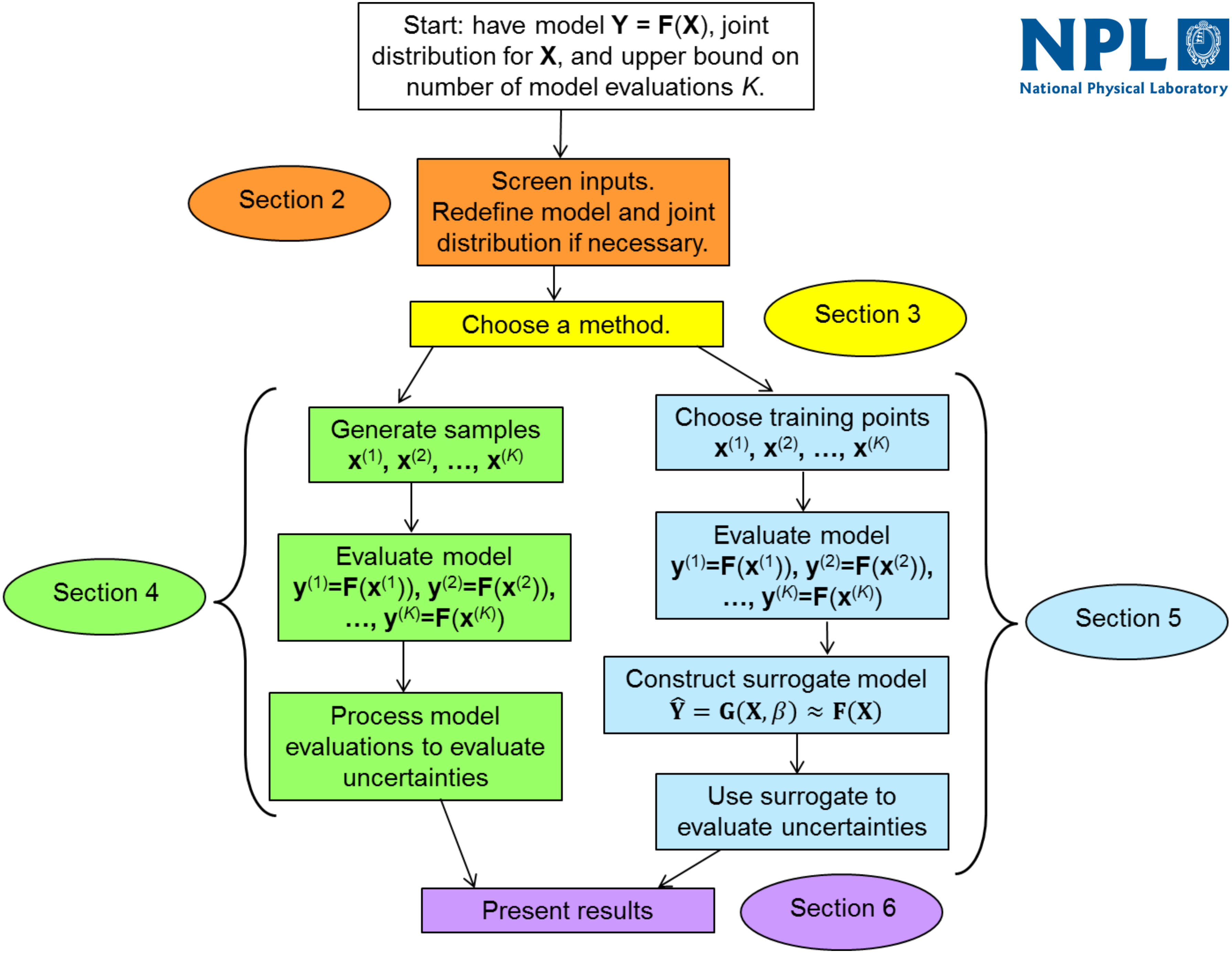
- Recent work looked at alternatives

  http://www.mathmet.org/publications/guides/index.php#expensive for problems where can't afford to do lots of model evaluations

Guide contents

- Multiple methods described
- Illustrated with a simple toy example
- Longer real world case study examples
  - thermophysical properties,
  - fluid flow,
  - scatterometry
- Written for general scientist audience
- Training slides based on the guide




Start: have model $\mathbf{Y} = \mathbf{F}(\mathbf{X})$, joint distribution for $\mathbf{X}$, and upper bound on number of model evaluations K.
Screen inputs. Redefine model and joint distribution if necessary.
Section 2
Choose a method.
Section 3
Generate samples $\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \ldots, \mathbf{x}^{(K)}$
Evaluate model $\mathbf{y}^{(1)}=\mathbf{F}(\mathbf{x}^{(1)}), \mathbf{y}^{(2)}=\mathbf{F}(\mathbf{x}^{(2)}), \ldots, \mathbf{y}^{(K)}=\mathbf{F}(\mathbf{x}^{(K)})$
Process model evaluations to evaluate uncertainties
Section 4
Choose training points $\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \ldots, \mathbf{x}^{(K)}$
Evaluate model $\mathbf{y}^{(1)}=\mathbf{F}(\mathbf{x}^{(1)}), \mathbf{y}^{(2)}=\mathbf{F}(\mathbf{x}^{(2)}), \ldots, \mathbf{y}^{(K)}=\mathbf{F}(\mathbf{x}^{(K)})$
Construct surrogate model $\hat{\mathbf{Y}} = \mathbf{G}(\mathbf{X}, \beta) \approx \mathbf{F}(\mathbf{X})$
Use surrogate to evaluate uncertainties
Section 5
Present results
Section 6

Input screening

Screen inputs. Redefine model and joint distribution if necessary.

- Design of experiments (DoE), Morris “One at a time” designs, Sobol’ indices
  - Define a set of values of the input quantities.
  - Evaluate the model using those input quantity values.
  - Process the results to get information about the sensitivity of the output quantities to the input quantities.
    - Identify any insignficant input quantities.
  - Redefine the model & distribution if necessary.

- Extra computational cost.
  - Can lead to better understanding of the model
  - Can reuse evaluations.

Why screen inputs?

- Can identify input quantities that are not important.
  - Some uncertainty evaluation methods work better for fewer input quantities.
  - Reduced model may run more quickly.
  - Sampling over a reduced input space may be more likely to be space filling.
- Understanding sensitivity can provide insight into underpinning physics.

Method choice

Choose a method.

- Can’t produce definitive advice that applies to all problems.
- Set of points to consider: depends on what is most important for your application.
- Advice on comparing methods in the guide.

- Methods are not necessarily mutually exclusive: may be able to use sampled points as training points for a surrogate model.

Points to consider

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- Number of input & output quantities
- Method complexity and software availability
- Prior knowledge of model and input quantities
- Nature of joint distribution of inputs
- Historical model evaluations & need for sample size flexibility

Smart sampling

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Generate samples
$\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \ldots, \mathbf{x}^{(K)}$

↓

Evaluate model
$\mathbf{y}^{(1)}=\mathbf{F}(\mathbf{x}^{(1)}), \mathbf{y}^{(2)}=\mathbf{F}(\mathbf{x}^{(2)}), \ldots, \mathbf{y}^{(K)}=\mathbf{F}(\mathbf{x}^{(K)})$

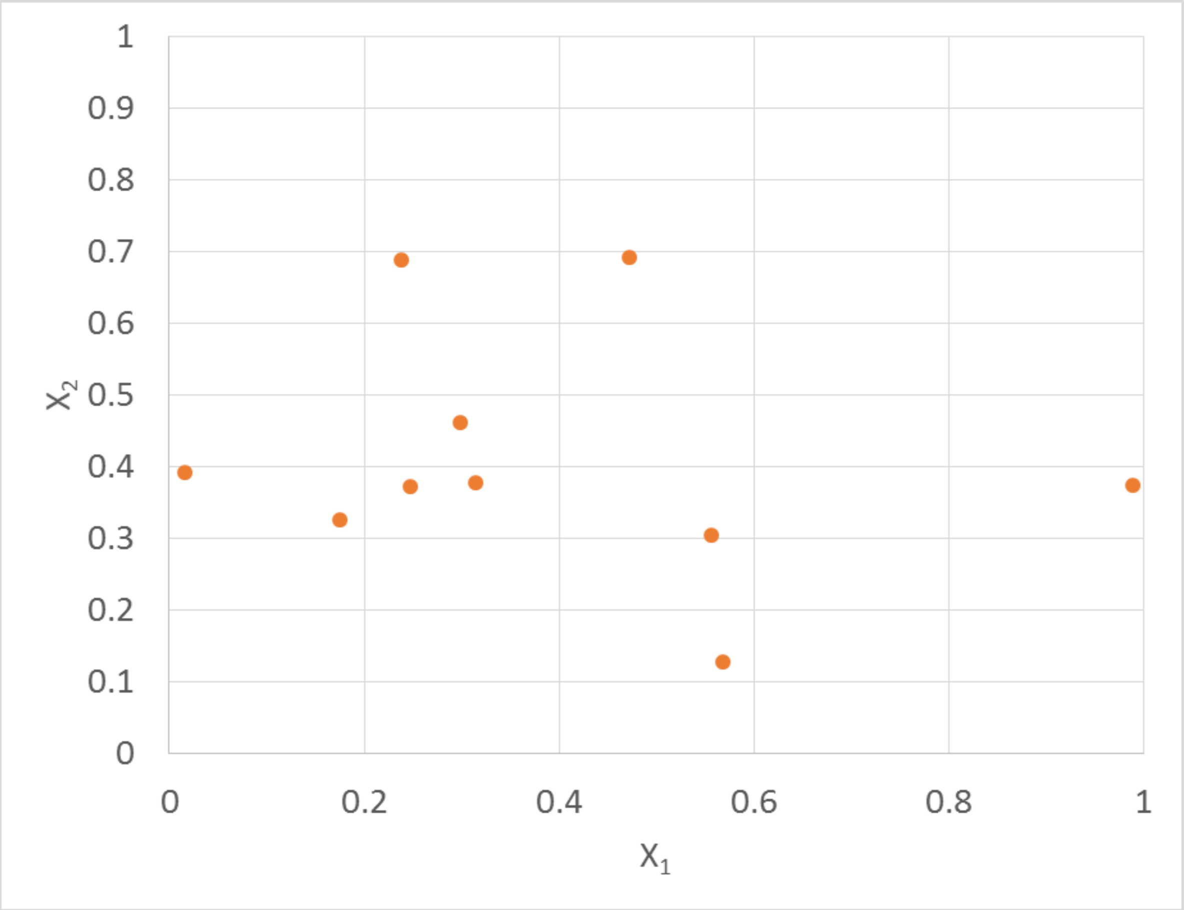
↓

Process model evaluations to evaluate uncertainties

- Methods for choosing input points more carefully
  - Importance sampling
  - Stratified sampling
  - Latin hypercube sampling

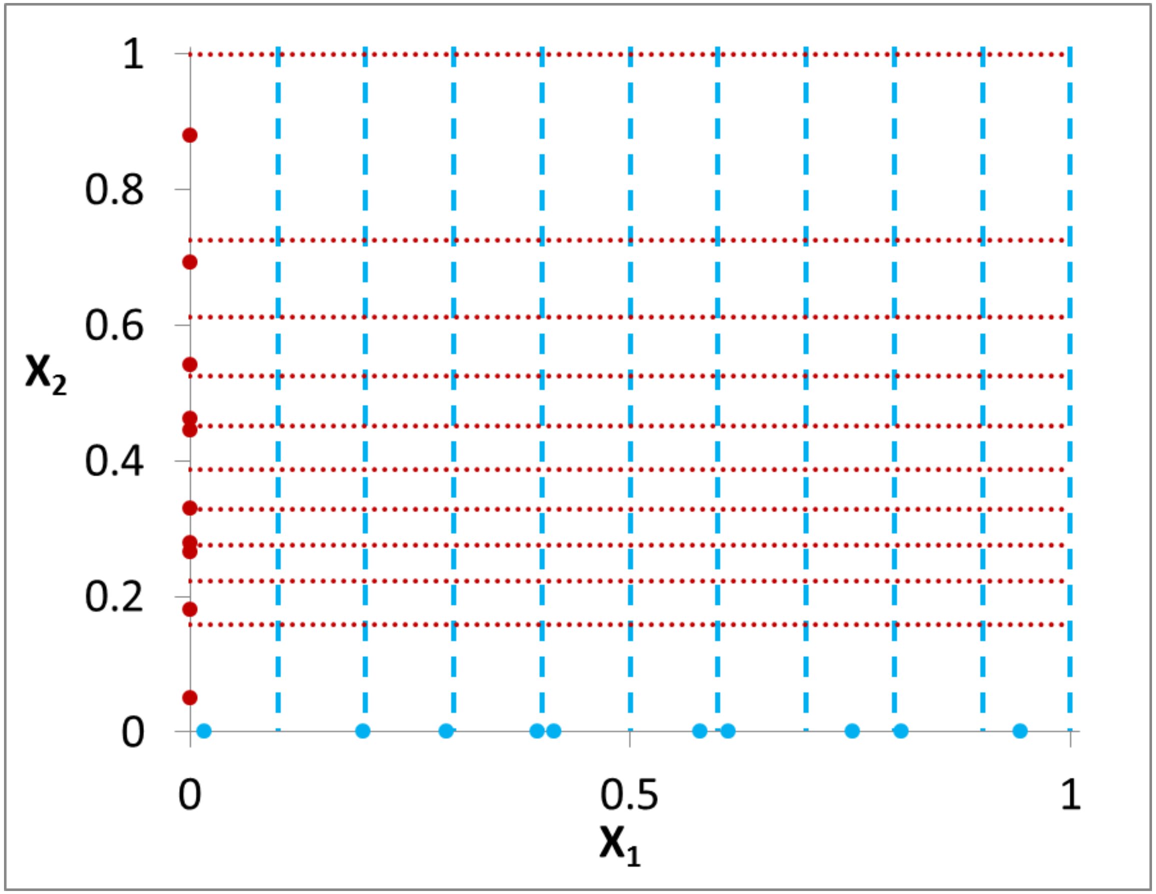
Problem with small Monte Carlo samples

X_1 uniformly distributed on [0, 1]
X_2 triangular on [0,1] with a mode of 0.25



- Doesn't span all of the sample space
- Large sample to sample variation

Latin hypercube sampling



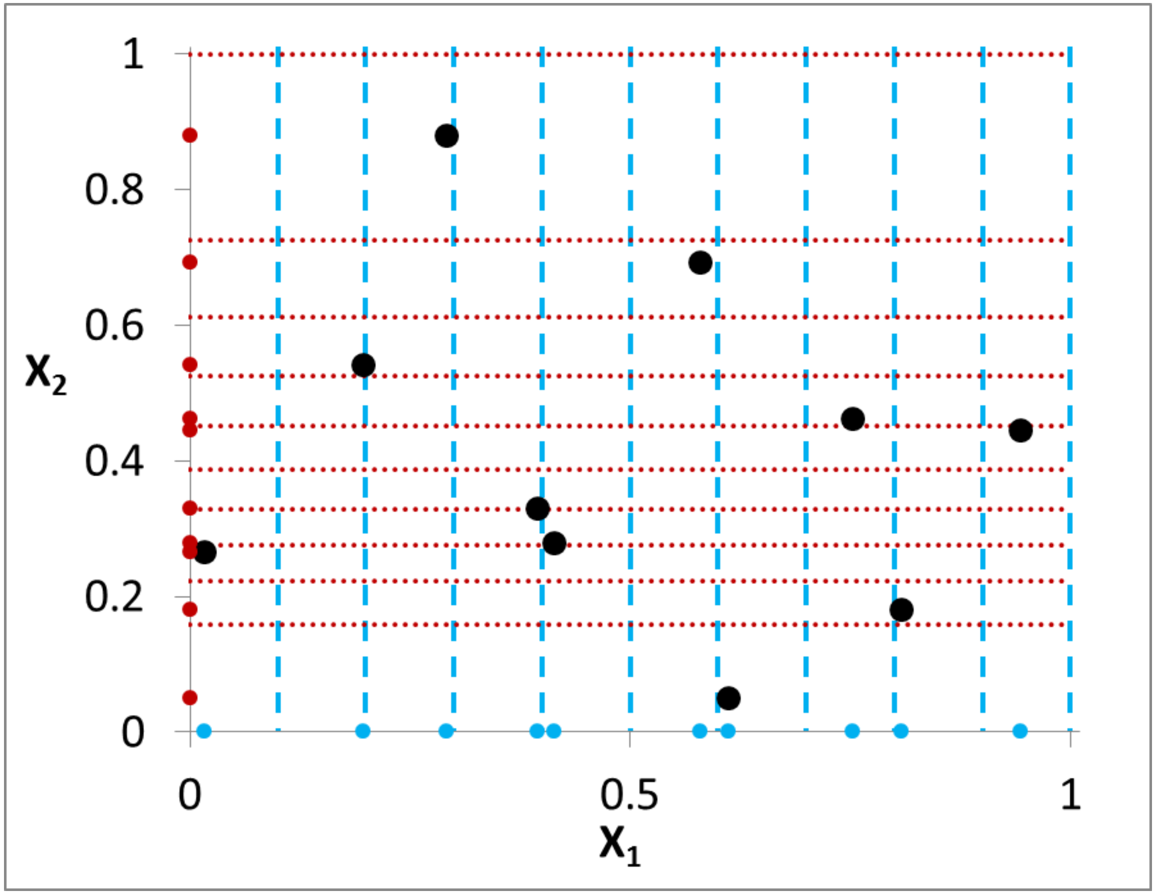
Divide each axis into n regions of equal probability.

Sample once within each region.

X_1 uniformly distributed on [0, 1]

X_2 triangular on [0,1] with a mode of 0.25

Latin hypercube sampling



Pair the points up randomly.

Can pair so as to be space filling via maximum distance criterion

Unbiassed estimates, lower sample to sample variation than MC

X_1 uniformly distributed on [0, 1]

X_2 triangular on [0,1] with a mode of 0.25

Surrogate models

Choose training points
$\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \ldots, \mathbf{x}^{(K)}$

↓

Evaluate model
$\mathbf{y}^{(1)}=\mathbf{F}(\mathbf{x}^{(1)}), \mathbf{y}^{(2)}=\mathbf{F}(\mathbf{x}^{(2)}), \ldots, \mathbf{y}^{(K)}=\mathbf{F}(\mathbf{x}^{(K)})$

↓

Construct surrogate model
$\hat{\mathbf{Y}} = \mathbf{G}(\mathbf{X}, \beta) \approx \mathbf{F}(\mathbf{X})$

↓

Use surrogate to evaluate uncertainties

- Approximate expensive model with cheaper one, evaluate uncertainties using cheap model
- Response surface methodology
- Gaussian process emulators
- Polynomial chaos

Training points?

- Can be regular grids
- Can be randomly chosen (Latin Hypercube)
- Can be between the two (Hammersley sequences)
- Space spanning is good
- Check sensitivity through the "leave one out" method
- Some modelling methods (Gaussian process modelling) supply an error estimate that can be used to guide "where next"

- All methods we tried performed well, but we may have looked at a nice problem

Polynomial chaos

- Has elements of sampling and elements of surrogate modelling.
- Idea is to
  - treat the model output quantities as random quantities directly,
  - approximate model output as an expansion of polynomials Ψ of random variables ξ,
    $$Y \approx \sum_{i=1}^{q} a_i \Psi_i(\boldsymbol{\xi})$$
  - evaluate expansion coefficients a_i from model evaluations at well-chosen points,
  - can derive statistics directly from these coefficients.

Comparison of methods

Good method has to be accurate and repeatable

Ten samples of size ten for all methods.
Reference values mean 0.66, std dev 0.57

	Mean of sample means	Std dev of sample means	Mean of sample Std devs	Std dev of sample Std devs
Random	0.58	0.22	0.51	0.05
Stratified	0.56	0.14	0.54	0.05
Latin hyp	0.65	0.03	0.58	0.05
Nearest	0.64	0.04	0.57	0.05
QRSM	0.68	0.07	0.66	0.26
Gauss proc	0.66	0.006	0.57	0.005

Conclusions

- Same steps as any other uncertainty propagation
  - Define inputs, outputs and model linking them;
  - Assign distributions to inputs;
  - Propagate input distributions through the model to give statistics of the output quantity.
- Smart sampling & surrogate models give more reliable answers from a small number of model runs than random sampling

Thanks

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