MECA0010 – Reliability and stochastic modeling of engineered systems

Uncertainty quantification

Part 2 of 4 — Monte Carlo simulation

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Outline

Outline.

Context.

Example: Rolling a die.

LLN and CLT.

Monte Carlo simulation.

Example: Bending of a clamped beam.

Example: Metal forming.

References.

Model problem



Let x_1, x_2, \ldots, x_m be uncertain (e.g., imperfect knowledge at design time, imperfect manufacturing when compared to the design,...). Given a probabilistic characterization of the input variables x_1 , x_2, \ldots, x_m as a probability distribution, what is the probability distribution of the output variable y?

From the previous lecture: Functions of random variables

If the function g is an affine function of a single input variable (m = 1), y = g(x) = ax + b with a and b constants,

then, provided that the output variable is of the second order, we obtain for the mean \overline{y} :

$$\overline{y} = \int_{\mathbb{R}} y\rho_Y(y)dy = \int_{\mathbb{R}} (ax+b)\rho_X(x)dx = a\int_{\mathbb{R}} x\rho_X(x)dx + b\int_{\mathbb{R}} \rho_X(x)dx = a\overline{x} + b$$

and for the variance σ_Y^2 :

$$\sigma_Y^2 = \int_{\mathbb{R}} (y - \overline{y})^2 \rho_Y(y) dy = \int_{\mathbb{R}} \left(ax + b - (a\overline{x} + b) \right)^2 \rho_X(x) dx = a^2 \int_{\mathbb{R}} (x - \overline{x})^2 \rho_X(x) dx = a^2 \sigma_X^2.$$

We can readily generalize these expressions to affine functions of multiple input variables. In conclusion, for a transformation though an affine function, knowledge of the mean and variance of the input variables suffices to determine the mean and variance of the output variable.

From the previous lecture: Functions of random variables (continued)

If the function g is a general function of a single input variable (m = 1), where we mean by "general" that this function is not necessarily affine,

$$y = g(x),$$

then, provided that the output variable is of the second order, we obtain for the mean \overline{y} :

$$\overline{y} = \int_{\mathbb{R}} y P_Y(dy) = \int_{\mathbb{R}} g(x) P_X(dx), \text{ that is, if } P_X \text{ admits PDF } \rho_X, \ \overline{y} = \int_{\mathbb{R}} g(x) \rho_X(x) dx,$$

and for the variance σ_Y^2 :

$$\sigma_Y^2 = \int_{\mathbb{R}} (y - \overline{y})^2 P_Y(dy) = \int_{\mathbb{R}} (g(x) - \overline{y})^2 P_X(dx), \text{ that is, if } P_X \text{ admits PDF } \rho_X, \ \sigma_Y^2 = \int_{\mathbb{R}} (g(x) - \overline{y})^2 \rho_X(x) dx.$$

For a general function, we can no longer interchange the integral and this function. In conclusion, for a transformation though a general function, knowledge of the mean and variance of the input variables does not suffice to determine the mean and variance of the output variable! Knowledge of the probability distribution of the input variables and an integration method are required!

Characterization

- The objective of the characterization of uncertainties is to assign an appropriate probability distribution to the uncertain input variables.
- An appropriate probability distribution can be obtained by applying methods from mathematical statistics to the available information. In engineering, this available information typically consists not only of observed samples but also of applicable mechanical and physical laws.
 - Catalogs of probability distributions.
 - Principles of construction.
 - Methods for parameter estimation.
 - Methods for model selection.



Current ressearch allows to consider as uncertain not only scalar input variables but also geometries, fields of mechanical and physical properties, matrix-valued input variables, etc.

Characterization (continued)





Random geometry.

From: M. Arnst and R. Ghanem. Probabilistic electromechanical modeling of nanostructures with random geometry. *Journal of Computational and Theoretical Nanoscience*, 6:2256–2272, 2009.

Characterization (continued)





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Characterization (continued)





Random geometry.

From: M. Arnst and R. Ghanem. Probabilistic electromechanical modeling of nanostructures with random geometry. *Journal of Computational and Theoretical Nanoscience*, 6:2256–2272, 2009.

Characterization (continued)



Random fields.

From: M. Arnst. Inversion of probabilistic models of structures using measured transfer functions. Thèse de Doctorat, Ecole Centrale Paris, France, 2007.

Characterization (continued)



$$[K + i\omega D - \omega^2 M]\boldsymbol{u}(\omega) = \boldsymbol{f}(\omega).$$

Random matrices.

From: F. Nyssen, M. Arnst, and J.-C. Golinval. Experimental modal identification of mistuning in an academic bladed disk and comparison with the blades geometry variations. ASME Turbo Expo, 2015.

Characterization (continued)



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Deterministic quadrature

1D trapezoidal integration:

$$\int_{a}^{b} g(x)dx \approx \frac{h}{2} \sum_{k=1}^{n} \left(g(x_{k+1}) + g(x_{k}) \right).$$



2D trapezoidal integration:

$$\int_{a_1}^{b_1} \int_{a_2}^{b_2} g(x_1, x_2) dx_1 dx_2 \approx \frac{h_1}{2} \frac{h_2}{2} \sum_{k_1=1}^{n_1} \sum_{k_2=1}^{n_2} \dots$$



The computational cost grows exponentially with the number of input variables.

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Probabilistic quadrature quadrature

Monte Carlo simulation is a method for numerically approximating integrals of the form

$$\overline{y} = \int_{\mathbb{R}^m} g(x_1, x_2, \dots, x_m) \rho_{(X_1, X_2, \dots, X_m)}(x_1, x_2, \dots, x_m) dx_1 dx_2 \dots dx_m,$$

$$\sigma_Y^2 = \int_{\mathbb{R}^m} \left(g(x_1, x_2, \dots, x_m) - \overline{y} \right)^2 \rho_{(X_1, X_2, \dots, X_m)}(x_1, x_2, \dots, x_m) dx_1 dx_2 \dots dx_m,$$

Monte Carlo simulation is based on sampling. It is supported by theorems from probability theory, such as the law of large numbers and the central limit theorem.

One of the main advantages of Monte Carlo simulation is that its computational cost is independent of the number of input variables. Example: Rolling a die

Example: Rolling a die

Context:

- Random variable Z.
- Possible outcomes 1, 2, 3, 4, 5, and 6.
- Probability distribution such that $P(Z = 1) = P(Z = 2) = \ldots = P(Z = 6) = \frac{1}{6}$.
- Mean value $\overline{z} = 1 \times \frac{1}{6} + 2 \times \frac{1}{6} + \ldots + 6 \times \frac{1}{6} = \frac{21}{6} = 3.5.$

Partial sum of sequence of samples of random variable Z:

	1	2	3	4	5	6	7	8	9	10	
	4	3	1	1	5	4	4	1	4	6	
$\frac{1}{\nu}\sum_{\ell=1}^{\nu}z_{\ell}$	4.0	3.5	2.6	2.2	2.8	3.0	3.1	2.8	3.0	3.3	

• "Convergence" of the partial sum of a sequence of samples of a random variable?

To what?

$$\lim_{\nu \to +\infty} \frac{1}{\nu} \sum_{\ell=1}^{\nu} z_{\ell} = \overline{z}?$$



LLN and CLT

LLN and CLT

Convergence of sequence of random variables

Probability theory offers several ways in which a sequence of random variables can be considered to converge, namely, convergence almost surely, convergence in distribution, convergence in mean square, and convergence in probability, among other ways:

$$\bullet \quad \lim_{\ell \to \infty} \boldsymbol{Z}_{\ell} \stackrel{\text{a.s.}}{=} \boldsymbol{Z} \text{ if and only if } P\big(\lim_{\ell \to \infty} \boldsymbol{Z}_{\ell} = \boldsymbol{Z}\big) = 1.$$

•
$$\lim_{\ell \to \infty} \mathbf{Z}_{\ell} \stackrel{d}{=} \mathbf{Z}$$
 if and only if $\lim_{\ell \to \infty} P_{\mathbf{Z}_{\ell}} = P_{\mathbf{Z}}$.

•
$$\lim_{\ell \to \infty} Z_{\ell} \stackrel{\text{m.s.}}{=} Z$$
 if and only if $\lim_{\ell \to \infty} \int \|Z_{\ell} - Z\|^2 dP = 0$.

•
$$\lim_{\ell \to \infty} Z_{\ell} \stackrel{\text{prob}}{=} Z$$
 if and only if $\lim_{\ell \to \infty} P(\|Z_{\ell} = Z\| \ge \epsilon\}) = 0.$

These modes of convergence are related as follows:



Law of large numbers (LLN) and central limit theorem (CLT)

Law of large numbers (LLN): Let $\{Z_{\ell}\}_{\ell=1}^{+\infty}$ be a sequence of independent and identically distributed (i.i.d.) copies of a random variable Z with values in \mathbb{R} . If $\int |Z| dP < +\infty$, then the sequence $\{S_{\nu} = \frac{1}{\nu} \sum_{\ell=1}^{\nu} Z_{\ell}\}_{\nu=1}^{+\infty}$ converges almost surely to $\overline{z} = \int Z dP$, that is,

$$\lim_{\nu \to +\infty} \frac{1}{\nu} \sum_{\ell=1} Z_{\ell} \stackrel{\text{a.s.}}{=} \overline{z}$$

Central limit theorem (CLT): Let $\{Z_{\ell}\}_{\ell=1}^{+\infty}$ be a sequence of i.i.d. copies of a random variable Z with values in \mathbb{R} . If $\int |Z|^2 dP < +\infty$, then $\{\sqrt{\nu}(S_{\nu} - \overline{z}) = \sqrt{\nu} \left(\frac{1}{\nu} \sum_{\ell=1}^{\nu} Z_{\ell} - \overline{z}\right)\}_{\nu=1}^{+\infty}$ converges in distribution to a Gaussian r.v. with mean 0 and variance σ_Z^2 , that is,

$$\lim_{\nu \to +\infty} \sqrt{\nu} \left(\frac{1}{\nu} \sum_{\ell=1}^{\nu} Z_{\ell} - \overline{z} \right) \stackrel{\mathrm{d}}{=} N(0, \sigma_Z^2).$$

LLN and CLT

Law of large numbers (LLN) and central limit theorem (CLT) (continued)

Example: Rolling a die:

	1	2	3	4	5	6	7	8	9	10	
	4	3	1	1	5	4	4	1	4	6	
$\frac{1}{\nu}\sum_{\ell=1}^{\nu}z_{\ell}$	4.0	3.5	2.6	2.2	2.8	3.0	3.1	2.8	3.0	3.3	



Principle

To numerically approximate an integral of the form

$$\overline{y} = \int_{\mathbb{R}^m} g(x_1, x_2, \dots, x_m) \rho_{(X_1, X_2, \dots, X_m)}(x_1, x_2, \dots, x_m) dx_1 dx_2 \dots dx_m,$$

first, Monte Carlo simulation begins with simulating ν independent samples of (X_1, X_2, \dots, X_m) : $\{(x_1^{(\ell)}, x_2^{(\ell)}, \dots, x_m^{(\ell)}), 1 \le \ell \le \nu\};$

then, these independent samples of (X_1, X_2, \dots, X_m) are transformed through g, $y^{(\ell)} = g(x_1^{(\ell)}, x_2^{(\ell)}, \dots, x_m^{(\ell)}),$

to obtain the corresponding ν independent samples of Y: $\{y^{(\ell)}, 1 \leq \ell \leq \nu\};$

finally, the value taken by the integral is approximated as follows:

$$\overline{y} \approx \overline{y}^{\nu} = \frac{1}{\nu} \sum_{\ell=1}^{\nu} y^{(\ell)}.$$

Principle (continued)

By the LLN, provided that $\int_{\mathbb{R}^m} |g(x_1, x_2, \dots, x_m)| \rho_{(X_1, X_2, \dots, X_m)}(x_1, x_2, \dots, x_m) dx_1 dx_2 \dots dx_m < +\infty$, the approximation \overline{y}^{ν} will converge to \overline{y} as the number of samples is increased.

By the CLT, provided that $\int_{\mathbb{R}^m} (g(x_1, x_2, \dots, x_m))^2 \rho_{(X_1, X_2, \dots, X_m)}(x_1, x_2, \dots, x_m) dx_1 dx_2 \dots dx_m < +\infty$, the accuracy of the approximation \overline{y}^{ν} will improve with the square root $\sqrt{\nu}$ of the number of samples ν as this number of samples is increased.

This can readily be extended to the numerical approximation of σ_Y^2 .

Principle (continued)

- Monte Carlo simulation has the following advantages:
 - it is nonintrusive, that is, it requires only the repeated solution of g for different values assigned to its input variables; if the relationship g between the input variables and the output variable is implemented in a computational model, then this computational model need not be modified.
 - it is adapted to embarrassingly parallel computation.
 - convergence can be monitored during the computation.
 - the rate of convergence is independent of the number of input variables.
 - Note that Monte Carlo simulation can be improved using
 - advanced simulation procedures,
 - importance sampling,
 - multilevel approaches,

Sampling

- There exist many methods for numerically generating independent samples of a random variable:
 - Transformation methods.
 - Accept-reject methods.



- The principle of transformation methods is that the probability distribution of a random variable changes under a nonlinear transformation:
 - First, generation of an ensemble of independent samples of a uniform random variable,

 $\{\xi^{(1)},\ldots,\xi^{(\nu)}\};\$

then, transformation into an ensemble of independent samples of the given random variable,

$$\{x^{(1)} = f(\xi^{(1)}), \dots, x^{(\nu)} = f(\xi^{(\nu)})\}.$$

- It is not always easy to find an adequate transformation f.
- This extends to generating ensembles of independent samples of random vectors, random matrices, stochastic processes, etc.

Sampling (continued)

- Generating a "good" ensemble of i.i.d. samples of a uniform random variable requires advanced computational methods:
 - A deterministic, that is, repeatable, algorithm is generally used to generate a sequence of values that "appear" to be i.i.d. samples of a uniform random variable. This "appearance" can be rigorously defined with reference to various statistical tests.
 - Software for generating an ensemble of i.i.d. samples of a uniform random variable:
 - Matlab,
 - Intel MKL,
 - AMD GPUOpen,
 - **...**

The elementary rand functions provided by UNIX and C are not suitable for scientific computing.

Sampling (continued)

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- For example, there are several methods for transforming independent samples of a uniform random variable into independent samples of a random variable with a given probability distribution:
 - Box-Muller method,
 - isoprobability transform,

The Box-Muller method leads to independent samples from a Gaussian random variable:

• Generation of two sets of independent samples of a uniform r.v. with values in [0, 1]: $\{\xi^{(\ell)}, 1 \le \ell \le \nu\}$ and $\{\eta^{(\ell)}, 1 \le \ell \le \nu\}$.

Transformation into two sets of independent samples of zero-mean unit-variance Gaussian r.v.: $\{x^{(\ell)} = \sqrt{-2\log(\xi^{(\ell)})}\cos(2\pi\eta^{(\ell)}), \ 1 \le \ell \le \nu\},\$ $\{y^{(\ell)} = \sqrt{-2\log(\xi^{(\ell)})}\sin(2\pi\eta^{(\ell)}), \ 1 \le \ell \le \nu\}.$

Refer, for example, to [Robert and Casella, 2010] for the proof.

Sampling (continued)

Let Ξ be a uniform random variable with values in [0, 1]. Then, the cumulative distribution function is the nondecreasing function c_{Ξ} from [0, 1] into [0, 1] such that

$$c_{\Xi}(\xi) = P(\Xi \le \xi) = \xi.$$



Let X be a random variable with values in \mathbb{R} . Then, the cumulative distribution function is the nondecreasing function c_X from \mathbb{R} into [0,1] such that

$$c_X(x) = P(X \le x).$$





- Generators using the isoprobability transform proceed as follows:
 - Generation of a set of independent samples of a uniform r.v. Ξ with values in [0,1]:

$$\{\xi^{(\ell)}, \ 1 \le \ell \le \nu\}.$$

Transformation into a set of independent samples of a r.v. X with values in \mathbb{R} :

$$\{x^{(\ell)} = c_X^{-1}(\xi^{(\ell)}), \ 1 \le \ell \le \nu\}$$

• Proof: $P(c_X^{-1}(\Xi) \le x) = P(\Xi \le c_X(x)) = c_X(x).$

Example: Bending of a clamped beam

Example: Bending of a clamped beam

Context



Let y be uncertain (e.g., imperfect knowledge at design time, imperfect manufacturing when compared to the design,...). Given a probabilistic characterization of the Young's modulus in terms of a probability distribution P_Y , what are the mean \overline{u} and the variance σ_U^2 of the tip displacement?

Case of Young's modulus with Gaussian probability distribution

Let the Young's modulus be modeled as a Gaussian r.v. Y with mean \overline{y} and variance σ_Y^2 :

$$\rho_Y(y) = \frac{1}{\sqrt{2\pi\sigma_Y}} \exp\Big(-\frac{(y-\overline{y})^2}{2\sigma_Y^2}\Big).$$

Then one could consider applying Monte Carlo simulation as follows:

- first, generation of independent samples of the Gaussian r.v. $Y: \{y^{(1)}, y^{(2)}, \dots, y^{(\nu)}\};$
- subsequently, transformation through the model: $u^{(\ell)} = rac{p\ell^3}{3y^{(\ell)}j};$
- finally, estimation of the mean value of the tip displacement: $\overline{u} \approx \overline{u}^{\nu} = \frac{1}{\nu} \sum_{\ell=1}^{\nu} u^{(\ell)}$.

However, although some value for \overline{u}^{ν} would be obtained, it cannot be interpreted as an approximation of the mean of the tip displacement because this mean does not exist:

$$\int_{\mathbb{R}} \frac{p\ell^3}{3yj} \rho_Y(y) dy \quad \text{and} \int_{\mathbb{R}} \left(\frac{p\ell^3}{3yj}\right)^2 \rho_Y(y) dy \quad \text{do not exist if } \rho_Y \text{ is Gaussian PDF.}$$

Case of Young's modulus with gamma probability distribution

Let Y be modeled as a gamma r.v. with mean \overline{y} and dispersion level $\delta_Y = \sigma_Y/\overline{y}$: $\rho_Y(y) = \mathbb{1}_{\mathbb{R}^+_0}(k) \frac{1}{\overline{y}} \left(\frac{1}{\delta_Y^2}\right)^{\frac{1}{\delta_Y^2}} \frac{1}{\Gamma(\frac{1}{\delta_Y^2})} \left(\frac{y}{\overline{y}}\right)^{\frac{1}{\delta_Y^2} - 1} \exp\left(-\frac{y}{\delta_Y^2 \overline{y}}\right).$

We can run a Monte Carlo simulation as follows:

• first, generation of independent samples of the gamma r.v. $Y: \{y^{(1)}, y^{(2)}, \ldots, y^{(\nu)}\};$

- subsequently, transformation through the model: $u^{(\ell)} = \frac{p\ell^3}{3y^{(\ell)}j}$;
- finally, estimation of the mean value of the tip displacement: $\overline{u} \approx \overline{u}^{\nu} = \frac{1}{\nu} \sum_{\ell=1}^{\nu} u^{(\ell)}$.

If
$$\delta_Y \in [0, 1/\sqrt{2}]$$
, we can interpret \overline{u}^{ν} as an approximation of \overline{u} because
 $\int_{\mathbb{R}} \frac{p\ell^3}{3yj} \rho_Y(y) dy$ and $\int_{\mathbb{R}} \left(\frac{p\ell^3}{3yj}\right)^2 \rho_Y(y) dy$ exist if ρ_Y is a gamma PDF with $\delta_Y \in [0, 1/\sqrt{2}]$;

the LLN and the CLT ensure that \overline{u}^{ν} converges to \overline{u} and accuracy improves with increasing ν .

Example: Bending of a clamped beam

Case of Young's modulus with gamma probability distribution (continued)

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Simple Matlab implementation:
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```
p=1;
ell=1:
j=1;
ybar=1;
deltaY=0.1;
nu=10000;
xi=rand(nu,1);
y=gaminv(xi,1/deltaY^2,deltaY^2*ybar);
u=p*ell^3/3./y/j;
ubar=zeros(nu,1);
ubar(1)=u(1);
for k=2:nu
ubar(k)=(1/k)*(ubar(k-1)*(k-1)+u(k)):
end
figure; hold on;
fill([1:nu nu:-1:1],[ubar'+1.96*std(u)./sqrt([1:nu]) ...
ubar(end:-1:1)'-1.96*std(u)./sqrt([nu:-1:1])],[0.5 0.5 0.5]);
plot(ubar);
```

Example: Bending of a clamped beam

Case of Young's modulus with gamma probability distribution (continued)

Result provided by this simple Matlab implementation:





Manufacturing tolerances in metal forming

Raw materials variability:

• Material properties.

Process variability:

- Blank holder force.
- Initial dimensions.
- Friction.

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Modeling limitations:

- Constitutive model.
- FE discretization.

Input variables.



Product variability:

- Final dimensions.
- Springback.

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Prediction limitations:

• Numerical noise.

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Output variable.

Manufacturing tolerances in metal forming (continued)



Observed samples $(h_1^{\text{obs}}, s_1^{\text{obs}})$, $(h_2^{\text{obs}}, s_2^{\text{obs}})$, ..., $(h_n^{\text{obs}}, s_n^{\text{obs}})$.

h [MPa]	s [MPa]
1488	375
1485	403
1514	407
1500	377



 \blacksquare Mechanics and physics impose that h and s be positive.

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Uncertainty quantification – Lecture 2

Manufacturing tolerances in metal forming (continued)



Manufacturing tolerances in metal forming (continued)



Manufacturing tolerances in metal forming (continued)



Manufacturing tolerances in metal forming (continued)



Manufacturing tolerances in metal forming (continued)



Manufacturing tolerances in metal forming (continued)



Manufacturing tolerances in metal forming (continued)



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Manufacturing tolerances in metal forming (continued)



Manufacturing tolerances in metal forming (continued)



Manufacturing tolerances in metal forming (continued)



Manufacturing tolerances in metal forming (continued)



Manufacturing tolerances in metal forming (continued)



Manufacturing tolerances in metal forming (continued)



Manufacturing tolerances in metal forming (continued)



Manufacturing tolerances in metal forming (continued)

We estimate adequate values for the parameters of the bivariate gamma probability distribution by using the method of maximum likelihood as follows:

$$(\hat{\overline{h}}, \hat{\sigma}_{H}^{2}, \hat{\overline{s}}, \hat{\sigma}_{S}^{2}, \hat{\rho}) = \text{solution of} \max_{(\overline{h}, \sigma_{H}^{2}, \overline{s}, \sigma_{S}^{2}, \rho)} l(\overline{h}, \sigma_{H}^{2}, \overline{s}, \sigma_{S}^{2}, \rho),$$

where the likelihood of the parameters \overline{h} , σ_{H}^{2} , \overline{s} , σ_{S}^{2} , and ρ is given by

$$l(\overline{h}, \sigma_{H}^{2}, \overline{s}, \sigma_{S}^{2}, \rho) = \prod_{\ell=1}^{n} \rho_{(H,S)}(h_{\ell}^{\text{obs}}, s_{\ell}^{\text{obs}}; \overline{h}, \sigma_{H}^{2}, \overline{s}, \sigma_{S}^{2}, \rho).$$



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Manufacturing tolerances in metal forming (continued)

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Manufacturing tolerances in metal forming (continued)

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Manufacturing tolerances in metal forming (continued)

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Manufacturing tolerances in metal forming (continued)

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Manufacturing tolerances in metal forming (continued)

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Manufacturing tolerances in metal forming (continued)

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Manufacturing tolerances in metal forming (continued)

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Monte Carlo method:







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Manufacturing tolerances in metal forming (continued)

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Monte Carlo method:







Stochastic expansion method:





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Computationally inexpensive surrogate model

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Manufacturing tolerances in metal forming (continued)

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Monte Carlo method:







Stochastic expansion method:





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Computationally inexpensive surrogate model

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