Challenges in Uncertainty Quantification

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The NAFEMS Stochastics Working Group (SWG) has offered this exercise to the broader simulation community with the intent to grow individual capability while serving simulation practitioners with a new avenue for math-based design. The SWG has three focal areas, each with a roadmap for improvement: Technology, Education, and Publication. Our first Challenge Problem was designed to influence education collaboration with Academia, Government and Industry. There are 2 submissions "X" and "Y" which have met the entry requirements. The SWG has evaluated and compared the submissions with the intent to draw further discussion and practical research with the intent to enhance the use of Uncertainty Quantification by users of simulation-based design. The challenge problem was originally introduced at 2013 NAFEMS World Congress in Salzburg, Austria.

Challenge Problem

A typical electronic component or device in a subsystem may be represented by an equivalent resistive, inductive and capacitive (R-L-C) series circuit. The electric transients that occur within the subsystem are of interest. This particular challenge problem was chosen because the fundamental equations based on Kirchhoff's current and voltage laws are well known and R-L-C parameters are usually readily available to electrically characterize components or systems. This problem is also common among automotive and industrial application where simple devices are part of a much larger electrical architecture. The underlying physics and mathematical model in the form of ordinary differential equation (ODE) can be solved in a variety of software tools. Other analogies to such network include mass attached to a spring and damper or hydraulic pipe system with a dynamic pump and paddle wheel. A schematic of the R-L-C network for the device is shown in Figure 1.

The input signal to the device is a step voltage source (V) shown in the circle in Figure 1 while the output signal is the voltage across the capacitor. This capacitive voltage is sensitive to the R-L-C parameters. For this system of interest, the network parameters are assumed to be not known precisely. Uncertain estimates of R-L-C parameters were made available to the participants of this challenge. The goal is to evaluate the reliability of the device using two different criteria and quantify the value of the information provided regarding R-L-C parameters.

Requirements

The first functional requirement specifies a minimum voltage drop of 0.9 Volts across the capacitor element at a particular time, 10 milliseconds in this case. The second requirement states the capacitive voltage rise should occur within a specified duration, 8 milliseconds in this application. The voltage rise time is defined as the time from 0% to 90% of the input voltage. These two requirements can be mathematically represented as:

$$V_C(t = 0.01) \geq 0.9$$

$$t(V_C = 0.9) \leq 0.008$$

where V_C is the capacitive voltage and t is time.

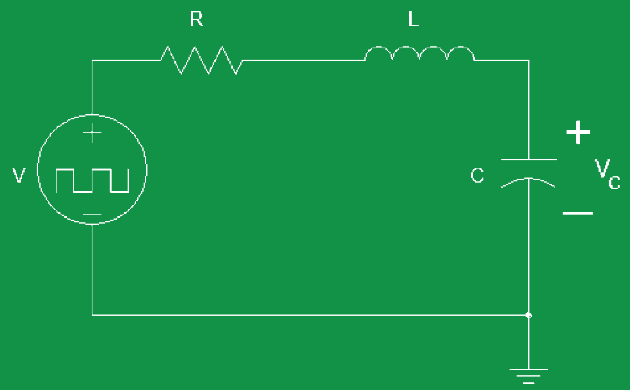

Figure 1: Equivalent R-L-C circuit model

Mathematical model

Equations representing this model are stated in the form of ordinary differential equations with zero initial conditions. For the sake of simplicity, the solution to the network was directly provided here. The system transfer function is defined as:

$$\frac{V_c}{V} = \frac{1/(LC)}{s^2 + (\frac{R}{L})s + \frac{1}{LC}}$$

Depending on the values of R, L and C, the system may be classified as underdamped, critically damped or over damped. The solution for each case may be obtained as:

Under damped ($\zeta < 1$):
$$V_c(\mathrm{t}) = \mathrm{V} + (A_1 \cos \omega t + A_2 \sin \omega t)e^{-\alpha t}$$
$$A_1 = -1 \quad A_2 = -\frac{\alpha}{\omega}$$

Critically damped ($\zeta = 1$):
$$V_c(\mathrm{t}) = \mathrm{V} + (A_1 + A_2 t)e^{-\alpha t}$$
$$A_1 = -1 \quad A_2 = -\alpha$$

Over damped ($\zeta > 1$):
$$V_c(\mathrm{t}) = \mathrm{V} + (A_1 e^{s_1 t} + A_2 e^{s_2 t})$$
$$A_1 = \frac{s_2}{s_1 - s_2} \quad A_2 = -\frac{s_1}{s_1 - s_2}$$

$$s_{1,2} = \frac{-R}{2L} \pm \sqrt{\left(\frac{R}{2L}\right)^2 - \frac{1}{LC}} \qquad \alpha = \frac{R}{2L} \qquad \omega = \frac{1}{\sqrt{LC}} \qquad \zeta = \frac{\alpha}{\omega}$$

Step voltage source V = 1.0 when t > 0. The coefficients A_1, A_2 in each case are solved from the initial conditions:

$$V_C(0) = 0 \qquad \frac{dV_C(0)}{dt} = 0$$

Parametric Characterization

Four cases of uncertainty estimates on the R-L-C parameters are presented in this challenge problem.

Case A: Intervals

R(Ω)	L(mH)	C (μF)
[40, 1000]	[1, 10]	[1, 10]

Case B: Multiple Intervals

Source	R(Ω)	L(mH)	C (μF)
1	[40, 1000]	[1, 10]	[1, 10]
2	[600, 1200]	[10, 100]	[1, 10]
3	[10, 1500]	[4, 8]	[0.5, 4]

Case C: Sampled Points

R(Ω)	L(mH)	C (μF)
{861, 87, 430, 798, 219, 152, 64, 361, 224, 614}	{4.1, 8.8, 4.0, 7.6, 0.7, 3.9, 7.1, 5.9, 8.2, 5.1}	{9.0, 5.2, 3.8, 4.9, 2.9, 8.3, 7.7, 5.8, 10.0, 0.7}

Case D: Incomplete Data

Source	R(Ω)	L(mH)	C (μF)
Interval	$[40, R_U]$	$[1, L_U]$	$[C_L, 10]$
Information	$R_U > 650$	$L_U > 6$	$C_L < 7$
Nominal	650	6	7

Challenge Problem Solutions

One team, from the UK's National Physical Laboratory, found that the main challenge was assigning appropriate probability distribution functions (PDFs) to the resistance, capacitance, and inductance. A key tool used in solving such problems is the principle of maximum entropy (PME), as recommended by the Guide to the Expression of Uncertainty in Measurement (GUM) and its supplements [1-3]. Applying this principle to cases A and D led to the team defining rectangular distributions to all variables in both cases. The variable limits and the ambiguous term "nominal" in case D complicated the optimization used when applying the PME to the problem. Case B required combining multiple sources of information through log-linear pooling which produces a single distribution expressed as a weighted geometric mean of the input distributions. This approach only works if there is a range of variable values common to all of the input distributions, which is not true for the inductance in case B. In order to obtain a valid distribution, the inductance range from source 2 was discounted. For Case C, the team assumed that these values are samples drawn randomly from an underlying univariate Gaussian distribution with unknown mean equal to the input quantity and unknown variance. This approach is underpinned by Bayes theorem. Once the input distributions had been obtained, random sampling and Latin hypercube sampling were used to obtain results for a range of sample sizes to look at how the results converged with increasing sample size for each case (Fig. 2) and the probability of failing to meet the requirements was evaluated for each model output.

The second team that participated in this challenge problem exercise used OpenCOSSAN software [4], which is a general purpose, flexible tool for numerical analysis, risk and uncertainty quantification. In the definition of the problem for Cases A and B, only bounds have been assigned for each uncertain quantity. According to the principle of maximum entropy, uniform distributions between the input bounds were assigned to the R, L and C parameters. Two distinct failure modes were considered when treating underdamped circuits and where the rise time or the voltage requirements are not satisfied. Monte Carlo simulation was used to compute the failure probability. A convergence study of the probability of failure with increasing number of samples was taken into account, leading to a trade-off between the simulation accuracy and execution time. In Case B, three distinct probabilities of failure were computed for three sources. These probabilities can be either kept as independent solutions or can be combined through assigning a weight to each source.

For Case C, it was assumed that the data points are the only possible values from a discrete pool. In this case the exact value of the probability of failure can be obtained by exploring all the possible combination and count the combinations that do not satisfy the requirements. However this approach can have numerical limitations as the input space grows and the number of combinations grows exponentially (curse of dimensionality). For Case D, the lower or upper bound for some of the variables are not defined. A parametric study was carried out by assigning different values to the bounds and exploring how the probability of failure evolved in function of the upper bound of R, L and the lower bound of C. Conclusions have been drawn on the importance of the different parameter over the probability of failure. Figure 3 shows the sample distribution of model response from discrete combinations of input parameters. The relative importance of R, L and C factors on voltage requirement can be observed in Figure 4.

Case	Probability of meeting voltage requirement	Probability of meeting time requirement
A	0.66	0.76
B	0.97	1.00
C	0.95	0.99
D	0.45	0.47

Table 1: Results of Submission #1

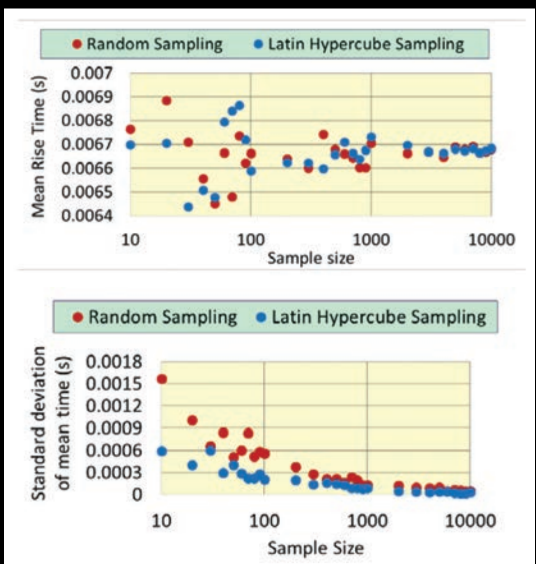

Figure 2: Convergence of Probabilities with Sample Size

Critical Review and Open Issues

The criteria for review, evaluation, and comparison of the challenge problem submissions was defined by the SWG based on what extent the given tasks were completed, technical significance of the solution in advancing the role of stochastics for robust design, general applicability of the proposed method, presentation and clarity of the assumptions.

Uncertainty propagation is carried out in both submissions for most cases using the Monte Carlo approach, both traditional and Latin Hypercube based sampling. These methods can easily be applied and generalized to other problems by non-specialists in stochastics. Both submissions report and discuss results for all 4 cases, although different approaches / assumptions were made for all but Case A. 'Value of

Case	Probability of NOT meeting voltage requirement	Probability of NOT meeting time requirement
A	0.268	0.364
B	{0.272, 0.512, 0.123}	{0.354, 0.67, 0.209}
C	0.15	0.23
D	1.0	0.104

Table 2: Results of Submission #2

information' or confidence level is not discussed in either paper but the focus was rather on convergence of solution based on sample size. As the traditional Monte Carlo sampling approach was taken by both, no advancement of methods or role of stochastics for robust design is promoted in the submissions. One drawback of direct Monte Carlo approach is its limited accuracy with not very high sample size to estimate probabilities far in the tail and more advanced methods might be required.

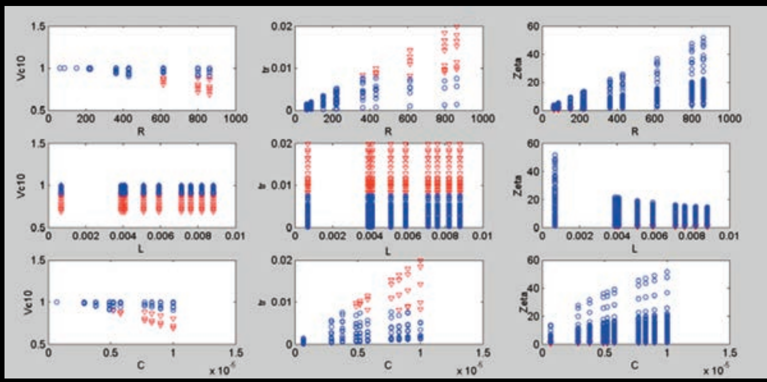

Figure 3: Various of Combinations of R, L, C

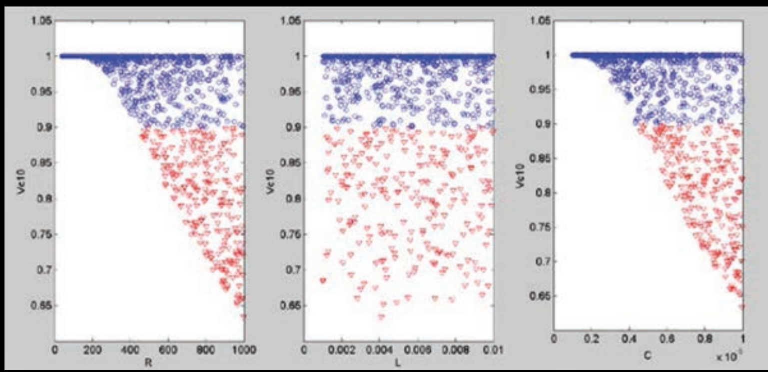

Figure 4: Effect of R, L and C on Voltage Requirement

Potential limitations exist based on approaches taken for Case B in both submissions. One submission may under estimate reliability based on use of overlapping range only for each parameter (not extreme ranges). The other submission presented separate results for each source of parameter intervals, but no recommendation on which results to use. When discrete input data is provided, one submission generated discrete output data while the other created a continuous distribution thus leading to different probability estimates. In case of missing data, different approaches were taken for characterizing input uncertainty. One submission assumed uniform distributions about the given nominal to fill in missing values, based on maximum entropy. The second submission assumed missing values to be m times the nominal, and tried several values to define the interval, but no discussion of which results to recommend is provided. A discussion of limitations was not provided in the submissions. An opportunity for further discussion exists in each case.

The agreement in approach and results for Case A provides a point of verification. With the other cases, different approaches are taken and several open issues for discussion can be raised:

- How can we quantify or even qualify the value of information obtained through uncertainty quantification approaches, especially when details are not clear or complete?
- How do we handle inconsistent information when describing sources of variation?
- How do we 'fit' distributions to limited data?

decisions based on these results. Stochastic Working Group will continue to learn from the challenge problem open items to develop a strategy for publications, education and industry outreach in the area of uncertainty quantification and propagation for large computational models.

References

[1] BIPM, IEC, IFCC, ILAC, ISO, IUPAC, IUPAP and OIML Guide to the expression of uncertainty in measurement (GUM:1995 with minor corrections) Bureau International des Poids et Mesures, JCGM 100, 2008.

[2] BIPM, IEC, IFCC, ILAC, ISO, IUPAC, IUPAP and OIML Evaluation of Measurement Data – Supplement 1 to the 'Guide to the Expression of Uncertainty in Measurement' – Propagation of distributions using a Monte Carlo method Bureau International des Poids et Mesures, JCGM 101, 2008.

[3] BIPM, IEC, IFCC, ILAC, ISO, IUPAC, IUPAP and OIML Evaluation of Measurement Data – Supplement 2 to the 'Guide to the Expression of Uncertainty in Measurement' – Extension to any number of output quantities Bureau International des Poids et Mesures, JCGM 101, 2011.

[4] Patelli, E., Broggi, M., de Angelis, M., Beer, M. "OpenCossan: An efficient open tool for dealing with epistemic and aleatory Uncertainties". Liverpool: Institute for Risk and Uncertainty, University of Liverpool.