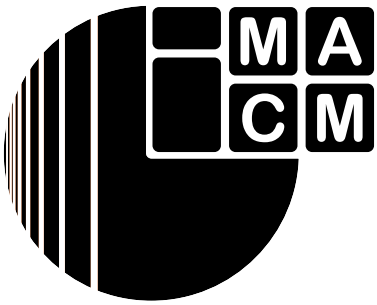

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Roland Pulch and Andreas Bartel and Sebastian Schöps

Abstract We consider coupled problems with uncertain parameters modelled as random variables. Due to the largely differing behaviour of subsystems in coupled problems, we introduce a strategy of adjusted grids defined in the parameter domain for resolving the stochastic model. This allows us to adapt quadrature grids to each subsystem. The communication between the different grids requires global approximations of coupling variables in the random space. Since implicit time integration methods are typically included, we investigate dynamic iteration schemes to realise this approach. Numerical results for a thermal-electric test circuit outline the feasibility of the method.

1 Introduction

In many applications, the simulation task addresses a coupled, multiphysical problem. Often the resulting models consist of differential algebraic equations together with partial differential equations, see [2]. Due to an inherent multirate or multiscale behaviour, a co-simulation of a coupled problem can be often efficient. Mathematically, this is also referred to as dynamic iteration, see [3]. Our application is in electrical engineering, where we consider a thermal-electric test circuit.

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Physical parameters of a coupled problem may exhibit uncertainties due to measurement errors, imperfections of an industrial production or other reasons. We quantify the uncertainties by random variables for the parameters and the solution becomes a random process. Statistics like the expected value and the variance can be computed by sampling methods or quadrature rules. Alternatively, a stochastic Galerkin method or stochastic collocation techniques can be used, see [4–6]. However, the Galerkin approach results in a much larger coupled system.

We investigate quadrature formulas in this paper. If the parts of the coupled problem show a different sensitivity with respect to the dependence on the random parameters, then the usage of quadrature on grids with different refinement levels becomes favourable. Thus we introduce different grids for the subsystems of a coupled problem. The application of this approach is straightforward in case of an explicit time integration scheme. To realise an implicit time integration, we apply a dynamic iteration to the overall problem, which decouples the subsystems to some extend. It follows that communications between the different parameter grids are required in discrete time points. Arbitrary global approximations of the solution on the random space are feasible for this communication. We use truncated expansions of the solution with respect to orthogonal basis polynomials depending on the random variables, i.e., a spectral approach appears in the probability space, see [6].

Finally, we test this strategy using a problem from [1], where an electric network is combined with thermal effects. Two different grids are applied for the two parts of the coupled problem. We test grids of several resolutions and based on a reference solution we qualitatively compare the achieved accuracies.

2 Problem Definition

We consider a time-dependent coupled problem consisting of two parts

$$\begin{aligned} \mathbf{F}_1\left(\mathbf{y}_1(t,\mathbf{p}),\mathbf{y}_2^{\mathrm{cpl}}(t,\mathbf{p}),t,\mathbf{p}\right) &= \mathbf{0}, \\ \mathbf{F}_2\left(\mathbf{y}_2(t,\mathbf{p}),\mathbf{y}_1^{\mathrm{cpl}}(t,\mathbf{p}),t,\mathbf{p}\right) &= \mathbf{0}, \end{aligned} \tag{1}$$

where parameters $\mathbf{p} \in \Pi \subseteq \mathbb{R}^Q$ are included. The operators $\mathbf{F}_1, \mathbf{F}_2$ represent ordinary differential equations (ODEs), differential algebraic equations (DAEs) or partial differential equations (PDEs) after a semidiscretisation in space. Hence time derivatives are involved in each part. The operators $\mathbf{F}_i$ comprise n_i equations and the solution of the system (1) is $\mathbf{y}_i : [t_0, t_{\mathrm{end}}] \times \Pi \to \mathbb{R}^{N_i}$ for $i = 1,2$, where initial values are given for all $\mathbf{p} \in \Pi$. The coupling variables are defined as $\mathbf{y}_i^{\mathrm{cpl}} := B_i \mathbf{y}_i$ with constant matrices $B_i \in \{0,1\}^{R_i \times N_i}$ such that the coupling variables include just a subset of $\mathbf{y}_i$ for each $i = 1,2$. Typically, it holds that $R_1 \ll N_1$ and $R_2 \ll N_2$, i.e., the coupling variables represent just a small portion of the solution. Furthermore, it is allowed that just one of two subsystems in (1) includes all the parameters. Generalisations to more than two subsystems are straightforward.

In many technical applications, implicit time integration schemes have to be applied, since either DAEs or stiff ODEs are involved. Due to a multirate behaviour, a co-simulation based on a dynamic iteration becomes efficient in some cases. Moreover, co-simulation is required if the equations of a subsystem in (1) are not available directly, i.e., just a software package is given including a numerical solver. We consider a dynamic iteration, where the total time span is split into windows with a first window $[t_0, t_{\mathrm{win}}]$. For a fixed $\mathbf{p} \in \Pi$, the iteration of Gauss-Seidel type for the coupled system (1) reads as

$$\begin{aligned} \mathbf{F}_1\left(\mathbf{y}_1^{(\nu+1)}(t,\mathbf{p}), \mathbf{y}_2^{\mathrm{cpl}\,(\nu)}(t,\mathbf{p}), t, \mathbf{p}\right) &= \mathbf{0}, \\ \mathbf{F}_2\left(\mathbf{y}_2^{(\nu+1)}(t,\mathbf{p}), \mathbf{y}_1^{\mathrm{cpl}\,(\nu+1)}(t,\mathbf{p}), t, \mathbf{p}\right) &= \mathbf{0}, \end{aligned} \qquad \text{for } \nu = 0,1,2,\ldots \tag{2}$$

using the starting values $\mathbf{y}_2^{(0)}(t,\mathbf{p}) \equiv \mathbf{y}_2(t_0,\mathbf{p})$. However, a numerical method outputs just the solutions $\mathbf{y}_1, \mathbf{y}_2$ on a discrete set of time points, which may also differ for the two subsystems. We assume that all coupling variables are interchanged in a few communication time points $\bar{t}_j$ with $t_0 \le \bar{t}_1 < \bar{t}_2 < \cdots < \bar{t}_J = t_{\mathrm{win}}$. Interpolation yields approximations of the coupling variables $\mathbf{y}_i^{\mathrm{cpl}}(t,\mathbf{p})$ for $t \in [t_0, t_{\mathrm{win}}]$ and $i = 1,2$.

Now we suppose that the parameters are not known exactly. To perform an uncertainty quantification, the parameters are modelled by random variables $\mathbf{p} : \Omega \to \Pi$ on some probability space $(\Omega, \mathscr{A}, \mu)$ with a joint density $\rho : \Pi \to \mathbb{R}$. Statistical information for a function $g : \Pi \to \mathbb{R}$ is obtained by probabilistic integrals

$$\mathrm{E}(g) := \int_\Omega g(\mathbf{p}(\omega))\, \mathrm{d}\mu(\omega) = \int_\Pi g(\mathbf{p})\, \rho(\mathbf{p})\, \mathrm{d}\mathbf{p} \tag{3}$$

provided that the integral exists. For example, probabilistic integration can be applied to the solution of (1) component-wise. Crucial information consists of the expected value and the standard deviation for the solution. Furthermore, higher moments and failure probabilities also represent integrals of the type (3). Our aim is to compute statistics of the solution $\mathbf{y}_1, \mathbf{y}_2$ for either the complete time interval or just at a final time.

A quadrature scheme or a sampling method yields an approximation of a probabilistic integral (3), see [6] and the references therein. We obtain a finite sum of the form $\mathrm{E}(g) \doteq w_1 g(\mathbf{p}^{(1)}) + \cdots + w_K g(\mathbf{p}^{(K)})$ with grid points $\mathbf{p}^{(1)}, \ldots, \mathbf{p}^{(K)} \in \Pi$ and weights $w_1, \ldots, w_K \in \mathbb{R}$. For $g = \tilde{g}(\mathbf{y}_1, \mathbf{y}_2)$ at some final time t_{end}, it follows that an initial value problem of the system (1) has to be resolved K times for the different realisations of the parameters.

3 Quadrature with Adjusted Grids

If the solutions of the subsystems in the coupled problem (1) behave differently with respect to the random parameters, then the application of different quadrature

formulas might become advantageous. For example, a higher variance within a subsystem often indicates that a higher accuracy of the quadrature is required. Thus we introduce two grids $\mathscr{G}_i := \{\mathbf{p}_i^{(1)}, \ldots, \mathbf{p}_i^{(K_i)}\}$ with $\mathbf{p}_i^{(k)} \in \Pi$ for $i = 1,2$ dedicated to the two parts of the coupled problem (1). In general, any grid is initiated by a quadrature scheme. The numbers of grid points K_1, K_2 may differ significantly. The subsystem for $\mathbf{F}_i$ together with its solution $\mathbf{y}_i$ is integrated in time on the grid $\mathscr{G}_i$ for each $i = 1,2$.

Following (2), we have to solve the problems

$$\begin{aligned} \mathbf{F}_1\left(\mathbf{y}_1^{(\nu+1)}(t,\mathbf{p}_1^{(k)}), \mathbf{y}_2^{\mathrm{cpl}\,(\nu)}(t,\mathbf{p}_1^{(k)}), t, \mathbf{p}_1^{(k)}\right) &= \mathbf{0} \qquad \text{for } k = 1,\ldots,K_1, \\ \mathbf{F}_2\left(\mathbf{y}_2^{(\nu+1)}(t,\mathbf{p}_2^{(k)}), \mathbf{y}_1^{\mathrm{cpl}\,(\nu+1)}(t,\mathbf{p}_2^{(k)}), t, \mathbf{p}_2^{(k)}\right) &= \mathbf{0} \qquad \text{for } k = 1,\ldots,K_2, \end{aligned} \tag{4}$$

in each step of the dynamic iteration. The first iteration step $\nu = 0$ in (4) for $\mathbf{F}_1$ can be computed directly using the globally defined initial values. The output is $\mathbf{y}_1^{(1)}(\bar{t}_j, \mathbf{p}_1^{(k)})$ for $k = 1,\ldots,K_1$ in the communication time points $\bar{t}_1, \ldots, \bar{t}_J$ introduced in Sect. 2. To this end, we need the coupling variables $\mathbf{y}_1^{\mathrm{cpl}(1)}(\bar{t}_j, \mathbf{p}_2^{(k)})$ for $k = 1,\ldots,K_2$ and $j = 1,\ldots,J$. Likewise, the output of $\mathbf{F}_2$ is the solution $\mathbf{y}_2^{(1)}(\bar{t}_j, \mathbf{p}_2^{(k)})$ for $k = 1,\ldots,K_2$ and thus has to be transformed into the coupling variables $\mathbf{y}_2^{\mathrm{cpl}(1)}(\bar{t}_j, \mathbf{p}_1^{(k)})$ for $k = 1,\ldots,K_1$, i.e., the evaluation on the other quadrature grid is crucial. This strategy repeats in each iteration step. Hence transitions between the two grids have to be defined for a fixed time point.

For the interchange of information between the two grids, we consider global approximations in the parameter space Π. An arbitrary global approximation method, which just requires the evaluations in the grid points, is feasible like an interpolation scheme, for example. Alternatively, we apply an approximation based on orthogonal basis polynomials with respect to the L^2-inner product of the probability space induced by the integral (3). Hence a truncated sum of the polynomial chaos expansion is used, see [6]. Let the time $\bar{t}$ be fixed. The global approximation reads as

$$\tilde{\mathbf{y}}_i^{\mathrm{cpl}}(\bar{t}, \mathbf{p}) := \sum_{m=0}^{M_i} \mathbf{u}_{i,m}(\bar{t}) \Phi_m(\mathbf{p}) \tag{5}$$

for $i = 1,2$ with known basis polynomials $\Phi_m : \Pi \to \mathbb{R}$ satisfying the orthonormality condition $\mathrm{E}(\Phi_m \Phi_n) = \delta_{mn}$. In general, all polynomials up to a certain degree are involved. The coefficient functions in (5) are determined approximately by

$$\mathbf{u}_{i,m}(\bar{t}) := \int_{\Pi} \mathbf{y}_i^{\mathrm{cpl}}(\bar{t}, \mathbf{p}) \Phi_m(\mathbf{p}) \rho(\mathbf{p}) \, \mathrm{d}\mathbf{p} \doteq \sum_{k=1}^{K_i} w_i^{(k)} \mathbf{y}_i^{\mathrm{cpl}}(\bar{t}, \mathbf{p}_i^{(k)}) \Phi_m(\mathbf{p}_i^{(k)}) \tag{6}$$

for $i = 1,2$, where the values $w_i^{(k)} \in \mathbb{R}$ represent the weights of quadrature formulas on the grids $\mathscr{G}_i$. Thus the sums (5) can be evaluated for an arbitrary $\mathbf{p} \in \Pi$. In particular, we obtain approximations of the coupling variables on each grid. Since the number of coupling variables is relatively low in comparison to the dimension of the

coupled problem, the computational effort for the global approximation is usually negligible compared to the time integration.

After the convergence of the dynamic iteration in a time window, the same approach is repeated in the next time window. Therein, initial values can be transformed between the two grids again by the above procedure. If the approximations have been computed at the final time t_{end}, then we reconstruct statistical data by quadrature formulas using the same grid points.

4 Simulation of a Test Example

To demonstrate the feasibility of the approach described in Sect. 3, we simulate a coupled problem introduced in [1], which consists of an electric part and a thermal part illustrated by Fig. 1. A resistor as well as a diode exhibit a voltage-current-relation depending on the temperature. The electric network is modelled by a nonlinear system of DAEs with dimension $N_1 = 3$. In the thermal part, the temperature of the resistor follows from a one-dimensional linear heat equation, where a semidiscretisation yields ODEs of dimension $N_2 = 20$. The diode receives a scalar temperature from the (right-hand) boundary of the PDE. More details can be found in [1].

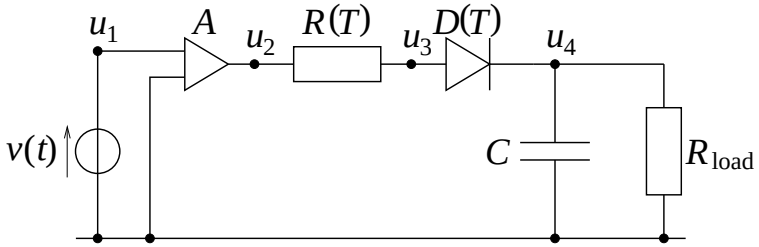

Fig. 1 Electric circuit with temperature-dependent resistor and diode.

The electric network is supplied by a sinusoidal input signal. We compute the numerical solution in the total time interval $[0\,\text{s}, 0.1\,\text{s}]$ and apply five time windows for the dynamic iteration (2). In our example, the solution of the electric part is more expensive than the thermal part, since smaller step sizes have to be used in time. The circuit part is solved first in this co-simulation. As communication time points, just the final times of each window are involved. The time integration of the subsystems is done by an implicit multistep method based on numerical differentiation formulas.

We introduce two random variables with independent uniform distributions. In the DAE part, the (temperature-independent) load resistance is a random parameter with variations of 10%. In the ODE part, the heat conduction coefficient becomes random with variations of 40%. Although the PDE and its ODE discretisation are

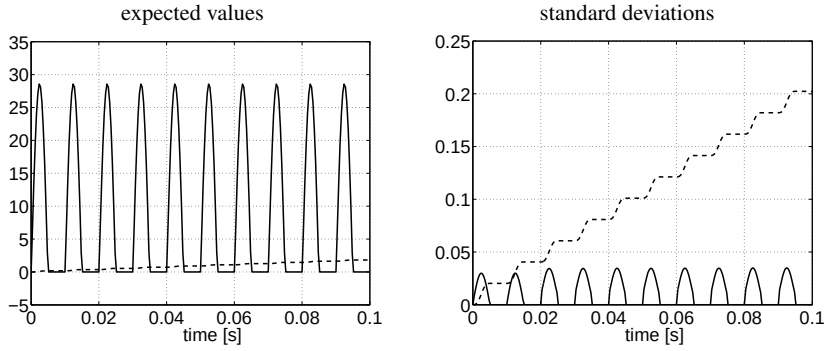

Fig. 2 Expected values as well as standard deviations for output voltage u_4 in unit [V] (solid line) and dissipated energy in unit [J] (dashed line) within circuit part.

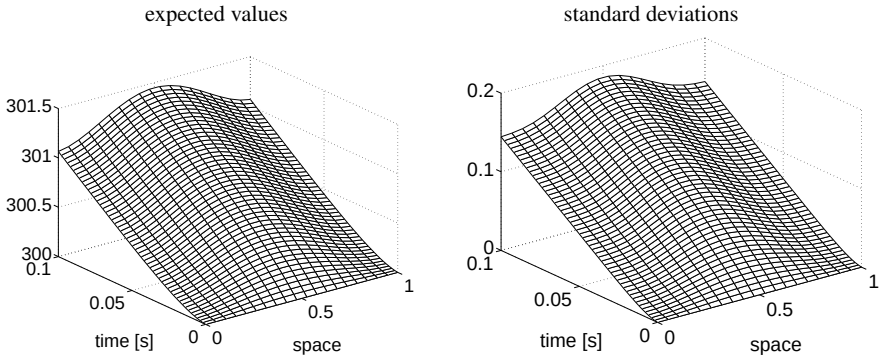

Fig. 3 Expected values as well as standard deviations for the resistor's temperature in unit [K] (spatial domain is standardised to $[0,1]$) within thermal part.

linear, the dependence of the solution on the parameters is nonlinear in each case. It follows that the parameter space represents a rectangle $\Pi \subset \mathbb{R}^2$.

As quadrature formulas, we employ the two-dimensional midpoint rule on grids of size $L_1 \times L_2$, i.e., L_1 nodes discretise the random resistance and L_2 nodes are dedicated to the random heat conduction. Two different quadrature formulas are considered, which gives a first grid $\mathscr{G}_1$ for the circuit part and a second grid $\mathscr{G}_2$ for the thermal part. In the communication between the grids, we use the global approximations defined by (5),(6), where all polynomials up to degree two are included ($M_1 + 1 = M_2 + 1 = 6$ basis functions).

To illustrate some statistics of the coupled problem, we compute the numerical solution for a combination of a first grid with size 8×6 and a second grid with size 6×8. Fig. 2 and Fig. 3 depict the first and second moment for the output of the circuit part and the thermal part, respectively, which result from the quadrature formulas associated to the two grids.

We also tried several other grid sizes for comparison. If two identical grids are chosen, then the evaluations of the coupling variables are available directly. Nev-

ertheless, we still perform the projections (6) and reconstructions (5) to investigate the accuracy. A reference solution is computed by the midpoint rule on a single grid with 40×40 nodes, where no transitions between different grids and thus no errors from global approximations occur. Table 1 demonstrates the comparison for the expected values as well as the standard deviations, where the maximum differences have been calculated for both all involved time points and all components of a subsystem.

Table 1 Maximum differences for statistics computed using different grids with respect to reference solution separately for circuit variables and temperature.

grid sizes		circuit variables		temperature	
first grid	second grid	expected value	st. deviation	expected value	st. deviation
10×10	10×10	4.6e-4	8.0e-3	6.2e-4	2.7e-3
5×5	10×10	1.3e-3	7.1e-3	1.9e-3	1.6e-2
5×5	5×5	4.9e-3	4.7e-2	1.1e-2	2.7e-2
8×6	6×8	1.3e-3	2.2e-2	2.7e-3	6.8e-3
8×4	4×8	2.8e-3	6.1e-2	8.3e-3	2.9e-2

5 Conclusions

We explained the need for coupled quadrature grids in uncertainty quantification and its algorithmic application within co-simulation. With a multiphysics example we showed the applicability and the prospect of the method.

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References

1. Bartel, A., Günther, M., Schulz, M.: Modeling and discretization of a thermal-electric test circuit. In: K. Antreich (eds.) Modeling, Simulation and Optimization of Integrated Circuits. ISNM Vol. 146, pp. 187–201. Birkhäuser (2003)
2. Bartel, A., Pulch, R.: A concept for classification of partial differential algebraic equations in nanoelectronics. In: L.L. Bonilla, M. Moscoso, G. Platero, J.M. Vega (eds.) Progress in Industrial Mathematics at ECMI 2006. Mathematics in Industry Vol. 12, pp. 506-511. Springer (2007)
3. Bartel, A., Brunk, M., Günther, M., Schöps, S.: Dynamic iteration for coupled problems of electric circuits and distributed devices. SIAM J. Sci. Comput. Vol. 35, No. 2, pp. B315–B335 (2013)
4. Chauvière, C., Hesthaven, J.S., Lurati, L.: Computational modeling of uncertainty in time-domain electromagnetics. SIAM J. Sci. Comput. Vol. 28, No. 2, pp. 751–775 (2006)
5. Pulch, R.: Stochastic collocation and stochastic Galerkin methods for linear differential algebraic equations. J. Comput. Appl. Math. Vol. 262, pp. 281–291 (2014)
6. Xiu, D.: Numerical Methods for Stochastic Computations: A Spectral Method Approach. Princeton University Press (2010)