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Stochastic Multidisciplinary Analysis with High-Dimensional Coupling

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This paper presents a novel approach for efficient uncertainty quantification and propagation in multidisciplinary analysis with a large number of coupling variables. The proposed methodology has three elements: Bayesian network, copula-based sampling, and principal component analysis. The Bayesian network represents the joint distribution of multiple variables through marginal distributions and conditional probabilities, and it updates the distributions based on new data. This paper uses this concept to develop a novel approach for probabilistic multidisciplinary analysis, that is, inference of distributions of the coupling variables by enforcing the interdisciplinary compatibility condition (which is treated similar to data for updating). The Bayesian network is built using only a few iterations of the coupled multidisciplinary analysis, without iterating until convergence. A copula-based sampling technique is employed for efficient sampling from the joint and conditional distributions. Further savings are achieved through dimension reduction using principal component analysis. A mathematical example and an aeroelastic analysis of an aircraft wing are used to demonstrate the proposed probabilistic multidisciplinary analysis methodology.

Nomenclature

C	=	copula function
C_r^n	=	n-dimensional Gaussian copula
D_{KL}	=	Kullback–Leiber divergence
e	=	evidence
f	=	probability density function
G	=	one iteration of the feedback coupled system
g	=	disciplinary output
H	=	joint CDF function
h_l	=	lower bound of the integral
h_u	=	upper bound of the integral
i	=	index of iteration number
L	=	likelihood
m	=	number of function evaluations
N	=	normal distribution
n	=	number of dimensions
P	=	probability
U	=	set of variables in Bayesian network
u, v	=	coupling variables
X	=	random variables
x	=	model input
y	=	model output
δ	=	integration window size
ε	=	difference between outputs from two iterations
θ	=	model parameter
$\boldsymbol{\mu}$	=	mean vector
π	=	parent node in Bayesian network
ρ_s	=	Spearman's rank correlation
Σ	=	covariance matrix
σ	=	standard deviation
τ	=	Kendall's rank correlation
Φ	=	standardized univariate normal distribution
Φ_R	=	standardized multivariate normal distribution with correlation matrix R

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I. Introduction

MANY engineering system analyses are composed of multiple disciplinary analyses that are governed by different physics. Interaction between individual disciplines is typically modeled by exchanging physical quantities between individual analyses (e.g., displacements and pressures exchanged between fluid and structural analyses, to model fluid–structure interaction). In many problems, computational models are available for individual disciplinary analyses, but not for coupled system analysis; even if the latter exists, the computational cost of the coupled analysis is usually quite high, therefore, research in multidisciplinary analysis (MDA) and multidisciplinary design optimization (MDO) seeks to alleviate the computational expense while maintaining interdisciplinary compatibility.

The coupling between two disciplines can be divided into two categories depending on the direction of information flow: 1) feed-forward, or unidirectional coupling, and 2) feedback, or bidirectional coupling. Problems such as fluid–structure interaction (FSI), thermal–structure interaction, and fluid–structure–combustion–thermal interaction usually require feedback analysis. A common example of FSI is the aeroelastic analysis of an aircraft wing shown in Fig. 1. Finite element analysis (FEA) of the structure calculates the nodal displacements, which are transferred to the computational fluid dynamics (CFD) analysis of the fluid; the CFD analysis calculates the nodal pressures, which are then transferred back to the structural analysis. The coupled relationship between the analyses are demonstrated in Fig. 2. The FEA and CFD analyses are repeated until the nodal pressures and nodal displacements converge (i.e., the interdisciplinary compatibility condition is satisfied). Such aeroelastic analysis is an essential component of aerospace vehicle design [1].

Three approaches have been pursued for such feedback-coupled MDA [2]: 1) the field elimination method, which reduces one or more disciplinary analyses by integral transforms or model reduction techniques, and treats the remaining fields through a simultaneous time-stepping scheme; 2) the monolithic method, which regards the coupled analyses as a monolithic entity and solves it using a single solver; and 3) the partitioned method, which solves the individual analyses separately with different solvers. Commonly used field elimination treatments include proper orthogonal decomposition (POD) and Krylov subspace methods [3,4]. A model-constrained adaptive sampling methodology has been developed to improve the fidelity of the reduced-order model [5]. Each approach has its own difficulties: Field elimination is restricted to linear problems that allow direct decoupling and may lead to numerical difficulties. The

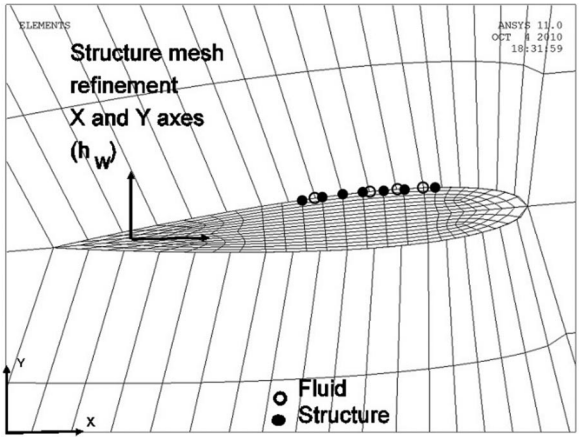


Fig. 1 NACA0012 airfoil structural and fluid meshes.

monolithic method maintains the conservation properties at the interface and is commonly used to solve time-dependent problems; its solution accuracy, however, is tightly associated with the time step, and it may be computationally expensive [6]. Partitioned methods such as the fixed-point-iteration (FPI) approach (iterative analysis until coupling variables converge) and the staggered solution approach [2,7] usually require a considerable amount of computational effort.

When high-fidelity models are used for each individual disciplinary analysis of the MDA, all the aforementioned approaches are potentially expensive, even for deterministic analysis. In the presence of uncertainty sources, the disciplinary analyses need to be executed repeatedly, thus MDA under uncertainty can become computationally unaffordable. Therefore, the central motivation of this paper is to reduce the computational burden of the multidisciplinary analysis under uncertainty. When high-fidelity models are used for individual disciplinary analyses, typically a large number of coupling variables are present, such as the nodal pressures and displacements in the preceding aeroelasticity example. Existing methods for MDA under uncertainty (such as SOFPI and LAMDA described below) become unaffordable in the presence of high-dimensional coupling. Therefore, this paper proposes a framework for efficient MDA under uncertainty by exploiting the concept of Bayesian networks, which is found to be effective for high-dimensional problems.

A simple approach to extend the deterministic MDA to nondeterministic MDA is by conducting Monte Carlo sampling outside fixed-point iteration (called SOFPI in [8]). This method could be computationally expensive if high-fidelity disciplinary analyses are used. Therefore, a considerable amount of attention has been devoted to finding efficient alternatives for MDA under uncertainty.

In the context of MDO under uncertainty, Kokkolaras et al. [9] developed an advanced mean value method, which was extended by Liu et al. [10] by using moment matching and considering the first two moments. Gu et al. [11] proposed a worst-case uncertainty propagation method using derivative-based sensitivities. Li and Azarm [12] developed a multi-objective collaborative robust optimization approach that considers interval uncertainty and both continuous and discrete design variables for multidisciplinary problems. Jiang et al. [13] proposed a spatial-random-process approach for both aleatory and epistemic uncertainty propagation in low-dimensional multidisciplinary analysis.

Several studies have particularly focused on uncertainty propagation in the context of reliability analysis for multidisciplinary systems. Du and Chen [14] included the disciplinary constraints in the most probable point (MPP) estimation for reliability analysis. Mahadevan and Smith [15] developed a multiconstraint first-order reliability method (FORM) for MPP estimation. Nonprobabilistic approaches such as fuzzy sets theory [16,17] and evidence theory [18] have also been studied. Sankararaman and Mahadevan [8] proposed a likelihood-based approach for MDA. This methodology estimates the probability density function (PDF) of the coupling variables by calculating the probability of satisfying interdisciplinary compatibility. The method obtains a theoretically exact solution while preserving the functional dependence between the coupling variables. Although the formulation of LAMDA is exact, approximation was introduced in the implementation through the use of FORM to compute the PDFs of the coupling variables [8]. Liang et al. [19] extended the LAMDA method to include model uncertainty by using an auxiliary variable approach.

The focus of this paper is on uncertainty propagation in high-dimensional coupled analysis. High-dimensional coupling refers to a large number of coupling variables between individual disciplines. The coupling variables in the same direction could be correlated with each other. The uncertainty quantification of coupling variables therefore becomes the estimation of their joint distribution. A general formula to compute the joint probability for more than two variables based on first-order approximation was provided by Hohenbichler and Rackwitz [20], and its accuracy was improved by Gollwitzer and Rackwitz [21] using asymptotic analysis. Because this approach is based on a first-order approximation, the accuracy of the solution is highly affected by the nonlinearity of the problem.

Consider the example of aeroelasticity analysis, where nodal pressures and nodal displacements exchanged by CFD and FEA are both vectors of large size. The computational effort for even a first-order approximation increases dramatically with the dimension, whereas the solution accuracy drops even faster. Furthermore, most of the nonintrusive simulation models are computationally expensive, hence the function evaluations demanded by the LAMDA method is quite prohibitive. Therefore, a Bayesian network-based approach is adopted in the paper to overcome these challenges, to evaluate the aforementioned joint PDF using only samples of input, output, and coupling variables, as opposed to the LAMDA method, which requires multiple evaluations of the MDA computational model.

A Bayesian network (BN) is essentially the representation of a multivariate distribution through a directed acyclic graph that represents variables with nodes and their dependence relationships with edges. Within mechanical systems, it has been used for system reliability assessment [22], model validation under uncertainty [23], diagnosis [24], and uncertainty quantification [25]. The Bayesian network is capable of incorporating a large number of variables and exhibits strong capability for uncertainty integration from multiple aleatory and epistemic sources [26,27]. A Bayesian network can be created using multivariate samples to describe the statistical dependence among the variables and can be updated using available data. In this paper, the satisfaction of the interdisciplinary compatibility is shown to be mathematically similar to updating with observed data, and thus the joint PDF of the coupling variables can be computed using the Bayesian updating process.

The estimation of the posterior distribution requires an appropriate sampling technique. Common algorithms such as Markov chain Monte Carlo sampling [28] and expectation–maximization [29] are computationally prohibitive for large size problems. To overcome this challenge, a copula-based sampling technique is introduced in this paper to efficiently generate samples from the Bayesian network. A copula is a function that relates the joint cumulative distribution function (CDF) of multiple variables to their marginal CDFs and their correlations [30,31]. The copula has been used to obtain the joint CDF in many fields, such as actuarial science and statistics [31], and in investigating reliability analysis and reliability-based design optimization for correlated [32] and non-Gaussian [33] input random variables. Bayesian network and Gaussian copula have also been exploited for multi-objective optimization, where both the input–output relations and the output dependencies are preserved [34]. Given interdisciplinary compatibility, the copula is conditionally sampled [26] to estimate the conditional joint distribution of all the variables.

Copulas can be categorized into parametric and nonparametric (or empirical) copulas. A multivariate Gaussian copula is explained in this paper for the sake of illustration and due to its efficiency in sampling conditional PDFs. The covariance matrix needs to be calculated given samples of all variables. In the aeroelasticity problem, the coupling variables in each direction (e.g., pressure, displacement) are correlated to each other. This issue leads to difficulty in the numerical implementation because the quantities at neighboring nodes are highly correlated, causing singularity in the

covariance matrix of the copula. Therefore, a principal component analysis (PCA) [35] is adopted to capture the dominant variance in the data and reduce the dimensionality, and the Bayesian network is built in the principal component space. Note that both PCA and Gaussian copula are the additional techniques we use to improve the efficiency in implementing the basic idea of the Bayesian network. Applying dimension reduction techniques in MDO has been commonly used [4]. The essential idea is to reduce the dimensions of the input and output variables for individual disciplinary analysis using POD (the same with PCA). Then, a surrogate model with the reduced inputs and outputs (reduced-order model) is used to substitute the original expensive analysis to perform FPI. In contrast, this paper avoids using surrogate models and FPI, which is the essential idea and fundamental difference with the existing research.

The contributions of this paper can be summarized as follows:

1) Develop a Bayesian network approach for stochastic MDA.

2) Use copula-based sampling for efficient construction of the joint PDF of coupling variables that satisfy interdisciplinary compatibility.

3) Use principal component analysis to reduce the dimension of the Bayesian network.

The proposed approach consisting of the preceding three contributions is referred to as Bayesian network and copula-based multidisciplinary analysis (BNC-MDA) in this paper. The proposed method is compared against LAMDA using a mathematical MDA problem first, and is then used to illustrate aircraft wing aeroelastic analysis under uncertainty. The rest of the paper is organized as follows. Section II introduces the basic LAMDA approach and discusses its difficulty in high-dimensional coupled MDA. Section III develops the proposed BNC-MDA methodology. Two numerical examples (a mathematical example and an aeroelastic problem) are presented in Sec. IV to demonstrate the proposed methodology. Section V provides concluding remarks.

II. Likelihood Approach for MDA Under Uncertainty

This section briefly reviews the LAMDA approach [8] and analyzes its shortcomings in the application to problems with a large number of coupling variables.

A. Feedback-Coupled Analysis

Consider the MDA model shown in Fig. 3 with two coupled analyses, where u_{12} and u_{21} are the input variables for "analysis 1" and "analysis 2," respectively, whereas x_s is shared by both, and u_{12} and u_{21} are coupling variables. In FPI, the individual analyses are repeated until u_{12} and u_{21} converge to satisfy the interdisciplinary compatibility.

Figure 4 describes the information flow in a single iteration of the coupled analysis, which is denoted by a function G. The input of G (i.e., u_{12}) is the output of analysis 1 in the previous iteration, whereas the output of G (i.e., U_{12}) is used as the input of analysis 2 in the following iteration. Interdisciplinary compatibility is satisfied when $u_{12} = U_{12}$. In stochastic MDA, a major concern is to quantitatively estimate the probability distribution of the coupling variable values given the interdisciplinary compatibility condition.

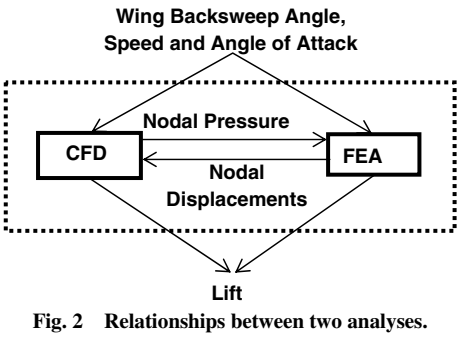


Fig. 2 Relationships between two analyses.

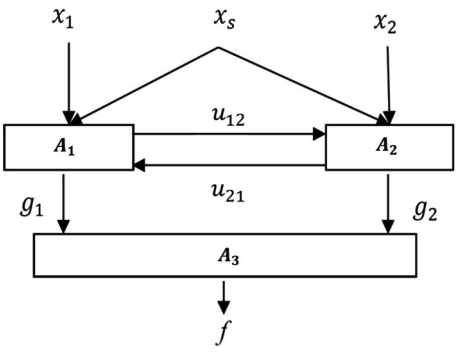


Fig. 3 Two-disciplinary coupled analysis.

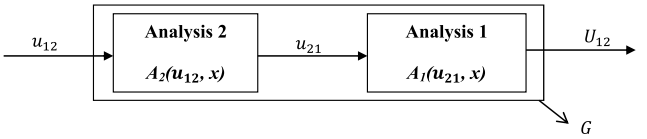


Fig. 4 One iteration of the coupled analysis.

B. LAMDA Approach

The LAMDA approach replaces the bidirectional coupling with unidirectional coupling, that is, only the coupling in one direction is removed. Therefore, the dependence between the coupling variables of the two directions is still preserved.

In Fig. 4, the probability of satisfying interdisciplinary compatibility for a given value of u_{12} [i.e., $P(U_{12} = u_{12}|u_{12})$] is simply proportional to the likelihood of u_{12}, that is,

$$L(u_{12}) \propto P(U_{12} = u_{12}|u_{12}) \tag{1}$$

For a given instance of u_{12}, the output U_{12} is stochastic because of the uncertainty in input variable X; therefore, the output uncertainty is represented by the conditional PDF $f_{U_{12}}(U_{12}|u_{12})$. For a continuous PDF, the probability of U_{12} equaling a particular value is zero. Therefore, an infinitesimal window is applied around u_{12} (i.e., $[u_{12} - \delta/2, u_{12} + \delta/2]$, and the probability is approximated by integrating the conditional PDF through the window

$$P(U_{12} = u_{12}|u_{12}) \cong \int_{u_{12}-\frac{\delta}{2}}^{u_{12}+\frac{\delta}{2}} f_{U_{12}}(U_{12}|u_{12})\,\mathrm{d}U_{12} \tag{2}$$

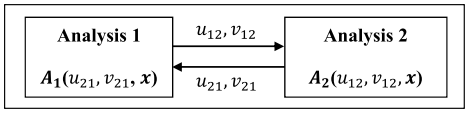
The likelihood $L(u_{12})$ is proportional to this probability, as shown in Eq. (1). The PDF of the converged coupling variable u_{12} can be then calculated as

$$f(u_{12}) = \frac{L(u_{12})}{\int L(u_{12})\,\mathrm{d}u_{12}} \tag{3}$$

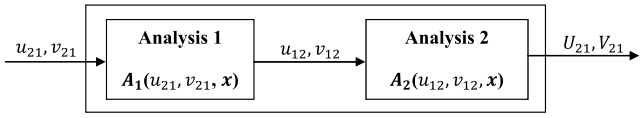
A recursive adaptive version of Simpson's quadrature [36] is used in [8] to evaluate the integral in Eq. (3). The likelihood functions are evaluated at a few values of u_{12} and the entire PDF is constructed by interpolation. The same method can be used to calculate the PDF of u_{21} in the opposite direction.

C. Issue with High-Dimensional Coupling

In high-dimensional coupled problems where the coupling quantities are large in number, each individual discipline accepts and yields a large number of coupling variables as inputs and outputs, respectively (e.g., displacements and pressures at a large number of nodes in coupled FEA/CFD analyses). In this case, the joint distribution of the coupling variables needs to be evaluated. Consider a problem with two coupling variables in each direction, as shown in Fig. 5a. A single iteration is shown in Fig. 5b. To estimate the joint



a) Coupled analysis with two coupling variables in each direction



b) One iteration of the coupled analysis

Fig. 5 Two-dimensional coupled analysis and one iteration representation. a) Coupled analysis with two coupling variables in each direction; b) One iteration of the coupled analysis.

distribution of U_{21} and V_{21} under interdisciplinary compatibility, suppose a first-order approximation of the bivariate joint distribution is adopted [37].

The coupling variables from analysis 2 to analysis 1 are denoted by u_{21} and v_{21}. To evaluate the joint PDF value at an instantiation of (u_{21}, v_{21}, the FORM analysis needs to be conducted to compute four joint CDFs F_1 at $u_{21} + \delta_1, v_{21} + \delta_2, F_2$ at $(u_{21} + \delta_1, v_{21} - \delta_2), F_3$ at $(u_{21} - \delta_1, v_{21} + \delta_2)$, and F_4 at $u_{21} - \delta_1, v_{21} - \delta_2$. Then finite difference can be used to obtain the joint PDF value at (u_{21}, v_{21}):

$$f(u_{21}, v_{21}) = \frac{F_1 - F_2 - F_3 + F_4}{4\delta_1\delta_2} \tag{4}$$

As the number of coupling variables increases, the number of function evaluations required by the preceding finite difference procedure becomes very large. For example, consider two disciplinary analyses coupled by n variables in each direction. If 10 integration points are taken for each variable, 10^n points will need to be evaluated in the n dimensional hypercube. At least $2n + 1$ FORM analyses need to be executed at each point for the finite difference analysis. Assuming m function evaluations are required for each FORM analysis to converge (on average), the total number of function evaluations is $10^n \times (2n + 1) \times m$. As n increases, the number of function evaluations will become enormous, resulting in prohibitive computational effort. In addition, because FORM is a first-order approximation, the nonlinearity of the function G may also affect the accuracy, and the approximation may get worse as the dimension becomes higher. Consequently, the problems that can be solved by the original LAMDA approach (implemented using FORM and finite difference) are confined to low-dimensional coupling where the functions are inexpensive to evaluate and not highly nonlinear. Therefore, Sec. III develops a Bayesian network-based approach to implement the LAMDA concept to high-dimensional problems.

III. Proposed Methodology: Bayesian Network and Copula-Based Sampling

The Bayesian network approach is investigated in this section, together with a copula-based sampling technique, to overcome the challenges of high-dimensional coupling discussed earlier. Given samples of coupling variables yielded by individual disciplinary analyses in two consecutive iterations, a Bayesian network is constructed to represent the joint distribution of these coupling variables. Next, a copula-based sampling technique is used to generate samples of the coupling variables that satisfy interdisciplinary compatibility. Compared with SOFPI and LAMDA, the proposed BNC-MDA approach is found to provide excellent balance between efficiency and accuracy.

A. Bayesian Network for Coupling Variables Distribution

A BN is a probabilistic graphical model that represents a multivariate joint distribution (nodes) through univariate distributions and conditional probabilities (edges). A common usage of the Bayesian network is to infer the posterior distribution of the nodes given observed data (evidence). The posterior probability of event U given evidence e could be evaluated using Bayes' theorem as

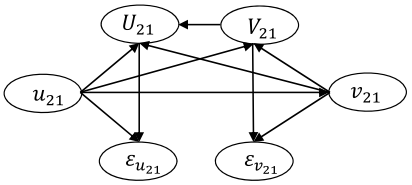


Fig. 6 Bayesian network connecting coupling variables in two successive iterations.

$$P(U|e) = \frac{P(U, e)}{P(e)} = \frac{P(U, e)}{\Sigma_U P(U, e)} \tag{5}$$

In a coupled analysis, the uncertainty regarding the coupling variables in MDA can be represented by their probability distributions conditioned on interdisciplinary compatibility. The Bayesian network for the two-discipline analysis of Fig. 5, regarding two coupling variables in one direction, is shown in Fig. 6. In this network, u_{21} and v_{21} represent the coupling variable values generated from the i^{th} iteration, whereas U_{21} and V_{21} are the corresponding values from the $((i + 1)$th iteration. The differences of the corresponding variable values between the two iterations are represented by $\varepsilon_{u_{21}}, \varepsilon_{v_{21}}$, that is,

$$\varepsilon_{u_{21}} = U_{21} - u_{21}, \qquad \varepsilon_{v_{21}} = V_{21} - v_{21} \tag{6}$$

Because of the input uncertainty, the coupling variables and the difference terms are all stochastic quantities. The Bayesian network can be trained using samples of these variables, generated by first generating samples of input variables x and executing the ith and the $(i + 1)$th iterations of the coupled analysis. Note that the x variables are not included in the BN, because our interest is in connecting the coupling variables in two consecutive iterations for the same x. The evidence e, which is interdisciplinary compatibility being satisfied, can be represented as $[\varepsilon_{u_{21}}, \varepsilon_{v_{21}}] = [0, 0]$. Therefore, the joint PDF of U_{21}, V_{21}, u_{21} and v_{21} given the compatibility condition, is

$$\begin{aligned} &f_{U_{21},V_{21},u_{21},v_{21}}(U_{21}, V_{21}, u_{21}, v_{21}|U_{21} = u_{21}, V_{21} = v_{21}) \\ &\quad = f_{U_{21},V_{21},u_{21},v_{21}}(U_{21}, V_{21}, u_{21}, v_{21}|\varepsilon_{u_{21}} = 0, \varepsilon_{v_{21}} = 0) \end{aligned} \tag{7}$$

This formulation could be easily extended to coupled analyses with higher dimensions. The accuracy of the Bayesian network depends on the number of training samples. In the Bayesian network in Fig. 6, the samples of the coupling variables used to construct the Bayesian network are obtained from two consecutive iterations of the original coupled analysis. Because a full convergence analysis is not required, collecting a large number of samples of the coupling variables becomes more realistic for high-fidelity models.

To evaluate the joint posterior distribution in Eq. (7), a proper sampling technique is required. Markov chain Monte Carlo sampling is frequently used in Bayesian updating [38], however, this technique is usually time consuming. Therefore, a copula-based sampling technique is employed here to estimate the joint PDF in an efficient manner.

B. Copula-Based Sampling

Copulas in statistics describe functions that "join together" one-dimensional distributions to form multivariate distributions. Consider n random variables $X_1, \ldots, X_n$ with continuous CDFs $F_1(x_1), \ldots, F_n(x_n)$. A copula function related to $X_1, \ldots, X_n$ is defined as

$$C(u_1, \ldots, u_n) = P[F_1(X_1) \le u_1, \ldots, F_n(X_n) \le u_n] \tag{8}$$

The copula C is thus the joint CDF of the marginal CDFs. The copula contains the dependence information between the variables and can also be written as

$$C(u_1, \ldots, u_n) = P[X_1 \le F_1^{-1}(u_1) \ldots, X_n \le F_n^{-1}(u_n)] \quad (9)$$

Equation (9) shows how a copula can be used in the Monte Carlo technique: One can directly sample the joint CDF values u_i from a copula and take the inverse of the marginal CDFs to retrieve the samples of the corresponding X_i. The uniqueness of the copula is ensured by Sklar's Theorem [30].

Multiple choices for copula type are available. In the context of stochastic MDA, the copula should be able to perform conditional sampling from Eq. (7) so as to evaluate the joint distribution of the coupling variables that satisfy interdisciplinary compatibility. The Gaussian copula has an analytical solution for conditional sampling; therefore, it is very fast and is explored next.

When building a multivariate Gaussian copula based on samples of the variables, a transformation of the variable values from marginal distributions to an equivalent normal space before sampling from the copula, and an inverse transformation after sampling from the copula, are required. Converting the sample-based empirical marginal distributions to equivalent normal space requires a monotonic transformation of the original samples. The linear correlation of the samples will not be preserved after this transformation. Rank correlation coefficients such as Kendall's τ or Spearman's ρ_s are invariants under monotonic transformation of the marginal distribution and therefore maintain the correlation between the random variables when transformation is applied for copula sampling. In this paper, Spearman's ρ_s is adopted as a replacement of Pearson's ρ to estimate the correlation coefficient matrix for Gaussian copula. (Note that the Gaussian copula is a less restrictive assumption than a multivariate normal assumption because it allows the marginal distributions to be any type.)

The Gaussian copula has limitations such as lack of tail dependence. Therefore, we first verify the Gaussian copula assumption by generating samples from the Gaussian copula 100 times and comparing against the training data. If the determinant of the normal rank correlation matrix of the training data falls within the 90% bounds of the determinant obtained from the Gaussian copula, then the Gaussian copula assumption is assumed to be valid [39].

However, if the Gaussian copula assumption cannot be verified to be adequate, then a non-Gaussian copula should be adopted. Several options such as Gumbel, Clayton, and Frank copulas are available in the literature; however, these are only able to characterize the dependence between two variables. If one of these bivariate copulas is chosen, then a vine-based strategy [39] may need to be implemented for multivariate sampling. Another copula that can address more than two variables is the Student's t copula. The aeroelastic wing example in Sec. IV.B implements both the Gaussian and t copulas and compares their performance.

If other copulas are chosen, the sampling efficiency of the stochastic analysis will be downgraded. However, the overall computational effort in stochastic MDA is mostly dominated by the physics analysis and in generating the samples to train the BN. Compared with this, the effort in sampling is negligible with or without the Gaussian copula assumption. The key element in the proposed methodology is constructing the BN of the coupling variables using samples of only a few consecutive iterations of the coupled MDA. Other elements such as copula and PCA (discussed next) are minor compared with this.

C. Dimension Reduction of the Bayesian Network

The technique of BNC-MDA could be used for both the forward problem (i.e., uncertainty propagation) and the inverse problem (i.e., Bayesian inference). The size of the Bayesian network for a high-dimensional problem increases as the number of variables increases. For example, in the aeroelastic problem shown in Fig. 1 (and later discussed in Sec. IV.B), the FEA mesh has 258 nodes. Each node has one nodal pressure and three nodal displacements (along each coordinate). Therefore, it leads to a coupled system with 258 nodal pressures as coupling variables in one direction and 774 nodal displacements as coupling variables in the other. Using the proposed decoupled approach, we can simplify the problem by only looking at the direction with fewer coupling variables. Nevertheless, it still requires us to build a BN similar to Fig. 6, but with 258 nodes each for the nodal pressure at the i^{th} iteration, the $(i+1)^{\text{th}}$ iteration, and the difference between them (thus 774 nodes in one BN). This will cause a tremendous amount of work constructing the network. Meanwhile, the nodal pressures in adjacent nodes are highly correlated with each other. This may lead to a singular covariance matrix affecting the sampling.

Therefore, PCA is adopted in this paper for the purpose of reducing the dimensionality of the BN. PCA, also known as Karhunen–Loeve expansion or proper orthogonal decomposition [35], depending on the field of application, maps correlated variables to an uncorrelated space using an orthogonal transformation. The resulting uncorrelated variables are referred to as principal components (PCs). Each principal component is a linear combination of the original variables; all the principal components are orthogonal to each other, hence no redundant information is stored. The number of principal components is as large as the original set of variables, but the first few principal components may capture a large fraction of the total variance of the original data if the original variables have strong correlation. Therefore, use of PCA helps to reduce the number of variables (i.e., first few principal components) while including most of the variance in the problem.

In the context of high-dimensional coupled MDA, coupling variables in each direction constitute a vector. Considering one iteration of the coupled analysis as shown in Fig. 7, assume that the input coupling variable u_{21} is a vector consisting of N components, and so is the output U_{21}. Considering the variability in input x, if we draw M random samples of x, then each component of the vectors u_{21} and U_{21} has the corresponding M samples.

The M pairs of u_{21} and U_{21} are first merged into a single $2M \times N$ matrix: the first M rows as samples of input u_{21} and last M rows as samples of output U_{21}, and each column representing one component of the vector u_{21} (and the corresponding component of U_{21}). We denote this $2M \times N$ data matrix by X. The singular value decomposition is denoted as $X = U\Sigma V^T$, where Σ is a $2M \times N$ rectangular diagonal matrix with $\sqrt{(\lambda_i)}$, $i = 1, \ldots, N$, at the first N diagonal entries and zeros at the rest. V is the $N \times N$ matrix of the eigenvectors of $X^T X$ and U is a $2M \times 2M$ matrix of vectors, each of which is calculated as $u_i = 1/\sqrt{(\lambda_i)}\, X v_i$

$$Y^T = X^T U = V\Sigma^T U^T U = V\Sigma^T \quad (10)$$

where each row of Y is a linear transformation of the corresponding row in X. That is

$$X = UY \quad (11)$$

If W denotes the first l rows of U, and Z denotes the first l columns of Y, then approximation of X by $\tilde{X}$ is achieved as

$$\tilde{X} = WZ \quad (12)$$

The selected number of principal components (PCs) is l. The number of PCs required is determined by the amount of variance captured. Note that the matrix Z consists of two parts: the top M rows are the principal components for input u_{21} (i.e., $\text{PC}^i_{u_{21}}$, $i = 1, \ldots, l$), whereas the bottom M rows are the principal components for output U_{21} (i.e., $\text{PC}^i_{U_{21}}$, $i = 1, \ldots, l$). After PCA, the differences between the corresponding principal components of u_{21} and U_{21} are calculated as

$$\varepsilon^i_{\text{PC}} = \text{PC}^i_{u_{21}} - \text{PC}^i_{U_{21}} \quad (13)$$

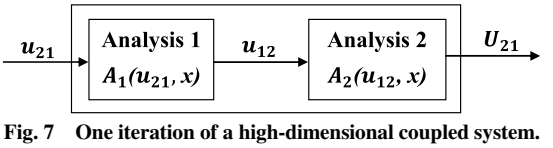


Fig. 7 One iteration of a high-dimensional coupled system.

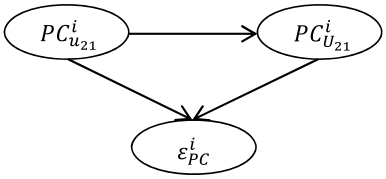


Fig. 8 Bayesian network using the *i*th principal component.

and a Bayesian network is built with the quantities in Eq. (13). The resulting Bayesian network has $3l$ nodes. A simplifying approximation is also possible, by assuming the uncorrelated nodes to be separated (no edges). In that case, the full Bayesian network is decomposed into l smaller Bayesian networks with three nodes each. The smaller Bayesian network for the ith principal component is shown in Fig. 8.

Once the network is built, impose $\varepsilon^i_{\mathrm{PC}} = 0$ and update the distribution of $\mathrm{PC}^i_{u_{21}}$. Before PCA, there was one BN for the entire problem containing all the correlated coupling variables in one direction. After applying PCA, we have a few principal components that are uncorrelated. As a result, we have a smaller BN with all the principal components in one network, or if the preceding approximation is invoked, a few separate BNs for the principal components, each with only three nodes, as shown in Fig. 8. Thus, in the example in Sec. IV.B, if 10 or 20 principal components are used to implement the proposed methodology, the monolithic BN with 774 nodes is either reduced to a smaller size BN with 30 or 60 nodes, or based on the preceding approximation, decomposed into 10 or 20 independent BNs, each with only three nodes. Therefore, by using PCA, we can reduce a large BN in two ways and drastically improve the efficiency in solving high-dimensional problems. The updated samples of the first few principal components are converted to the original correlated space using Eq. (12) to get the joint distribution of the coupling variables under the interdisciplinary compatibility condition.

Note that PCA is applied in this paper in a manner different from previous applications of PCA in the context of MDA. In previous applications, PCA is used to identify the principal components among the inputs and outputs, and then a reduced-order model is built in terms of the principal components [4]. However, in this paper, we use PCA only to reduce the dimension of the Bayesian network; the training samples for the Bayesian network are generated from the analysis of the full model, not a reduced-order model.

In summary, the proposed BNC-MDA methodology has four elements: 1) A Bayesian network is built using the samples of the coupling variables from two consecutive iterations. 2) The distributions of the coupling variables are estimated using a Bayesian network by enforcing the interdisciplinary compatibility condition, in a manner similar to updating the Bayesian network with observed data. 3) A copula-based sampling technique is adopted for efficient sampling from the joint distribution. 4) Principal component analysis is used to reduce the dimension of the Bayesian network for further efficiency of the BNC-MDA methodology. Note that the coupled multidisciplinary analysis (only a few iterations) is only required in the first element and dominates the computational effort. The effort in the other three elements is negligible compared with that for the first element, as will be demonstrated later in the aeroelasticity example. The more iterations the coupled physics analysis requires for convergence, and the longer each individual disciplinary analysis takes, the more time will be saved by using BNC-MDA.

It is also worth noting that the proposed BNC-MDA framework is a sample-based methodology. This method includes two stages of sampling processes: 1) generating samples as training points for the Bayesian network, and 2) after the BN is built, samples are generated conditioned on the compatibility condition; this is a separate step from step 1. The input distributions come into play in the first stage, while generating training points for the BN. The input distributions can be correlated or uncorrelated; the training samples should be generated accordingly. It is significant to realize that generating samples of the input variables is the step before constructing the Bayesian network.

IV. Numerical Examples

In this section, a mathematical problem with two coupling variables in each direction is first presented to compare the previous methods (SOFPI, LAMDA) and the proposed BNC-MDA method. A multidisciplinary aeroelastic analysis of an aircraft wing is then used to demonstrate the effectiveness of the proposed approach to higher-dimensional problems.

A. Mathematical MDA Problem

The numerical example in [8] is modified to include two coupling variables in each coupling direction. This is an extension of the problem discussed in Du and Chen [40], and later in [15] where only two analyses were considered. The functional relationships are shown in Fig. 9. The input variables $x = [x_1, x_2, x_3, x_4, x_5]$ are assumed to be normally distributed: $N(1, 1)$ and independent of each other. The independent and normal input assumption does not affect the proposed BNC-MDA methodology. If some of the input variables are correlated, we need to jointly sample these variables, then propagate them through one iteration of the coupled analysis to calculate the corresponding coupling variable values. However, the Bayesian network is only built after the training samples are generated. These training samples could be generated in a correlated or independent manner, depending on the problem data.

In Fig. 9, the coupling variables are u_{12}, v_{12} from analysis 1to "Analysis 2," and u_{21}, v_{21} in the opposite direction. For the purpose of illustration, only the joint distribution of u_{21} and v_{21} is estimated and the joint distribution of u_{12} and v_{12} can be calculated using the same method. In this example, we focus on calculating the PDFs of the coupling variables and do not calculate any further system output.

Once the joint distribution of the coupling variables in one direction is obtained, one can propagate Monte Carlo samples of this joint distribution through one iteration of the feedback-coupled analysis, as shown in Fig. 5b, to obtain the corresponding samples of g_1, g_2, and f. Then these samples can be used to construct the joint distribution of g_1, g_2, and f. The dependence relations among g_1, g_2, f, and the coupling variables are preserved, because the connection between the two disciplinary analyses are not completely severed.

Three different approaches (i.e., SOFPI, LAMDA, and BNC-MDA) are implemented to solve this problem. To execute the SOFPI method, 10,000 samples of inputs are generated, which requires 107,421 function evaluations in total. A two-dimensional kernel density estimation technique is adopted to build the joint distribution. The resultant joint distribution of the coupling variables is used as the benchmark solution.

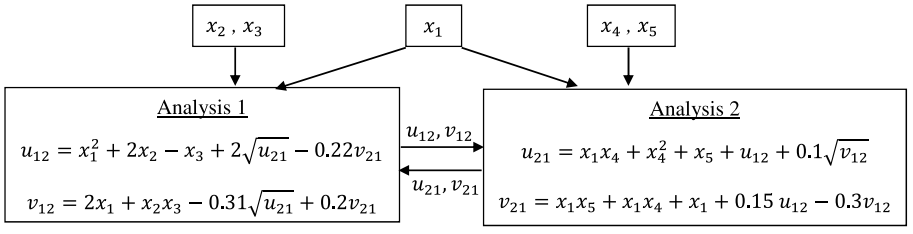


Fig. 9 Mathematical example of two-discipline coupled analysis.

Table 1 Comparison of computational cost

Approach	No. of input samples	Integration values for $u_{21} \setminus v_{21}$	Total no. of function evaluations
SOFPI	10,000	N\A[a]	107,421
LAMDA	N\A	8:0.5:15 \ 0:0.25:3.5	14,619
BNC-MDA	1,000	N\A	2,000

[a]Where N/A represents not applicable.

Table 2 Results using SOFPI, LAMDA, and BNC-MDA

	U_{21}		V_{21}		
	μ	σ	μ	σ	$\rho_{U_{21}V_{21}}$
SOFPI	11.65	0.69	1.6	0.16	0.24
LAMDA	11.48	0.67	2.02	0.17	0.52
BNC-MDA	11.59	0.69	1.59	0.15	0.24

In the LAMDA method, 10 integration values are chosen in Eq. (2) for each coupling variable. Therefore, a total of 100 likelihood values need to be evaluated, and an overall 14,619 function evaluations are required. A cubic spline interpolation is then exploited to construct the entire joint distribution.

In the BNC-MDA method, 1000 samples of the input and output of the function in Fig. 5b are generated. The training points for building the Bayesian network are generated by samples of the input variables x_1 to x_5 and coupling variables u_{21}, v_{21} to run through one iteration of the coupled analysis to calculate U_{21}, V_{21}. Samples of the outputs after the first and second iterations of the coupled MDA are collected; the number of function evaluations is twice the number of the samples, which in this case is 2000. The computational cost of the three approaches is summarized in Table 1. The outputs from the two iterations together with their differences are used to construct the Bayesian network shown in Fig. 6. Note that PCA is not used within BNC-MDA in this example, because there are only two coupling variables in each direction. The results using the three approaches are listed in Table 2, and the marginal distributions are compared in Fig. 10.

It can be concluded from Table 2 and Fig. 10 that the proposed BNC-MDA method is able to capture the probability distribution of V_{21} and the value of the and the value of the $\rho_{U_{21}V_{21}}$ better than the original LAMDA, even though the mean and standard deviation of the marginal distribution of U_{21} calculated by LAMDA and BNC-MDA are both quite close to the benchmark solution. The Kullback–Leiber (K-L) divergence [41] is estimated for the marginal distributions of U_{21} for further comparison of accuracy.

The K-L divergence of distribution q from distribution p denoted by $D_{\mathrm{KL}}(p||q)$, is a measure of the information lost when p is approximated by q. A smaller value of the K-L divergence indicates a greater similarity between the two distributions. For continuous distributions p and q, the K-L divergence is defined as

$$D_{\mathrm{KL}}(p||q) = \int_{-\infty}^{+\infty} p(x) \ln \left[\frac{p(x)}{q(x)}\right] \mathrm{d}x \tag{14}$$

In practice, the PDFs are evaluated numerically, and the K-L [41] divergence is calculated as

$$D_{\mathrm{KL}}(p||q) = \Sigma_{i=1}^{n} \ln \left[\frac{p(x_i)}{q(x_i)}\right] p(x_i) \tag{15}$$

where p and q represent the PDF values at x_i, and n is the number of points at which the PDFs are evaluated; in this paper, $n = 1000$. The K-L divergence is only defined if areas of p and q each sums to one, and $p(x_i) > 0$ and $q(x_i) > 0$ simultaneously. The K-L divergence value with respect to SOFPI is 0.033 for LAMDA and 0.016 for BNC-MDA; thus, the BNC-MDA method results in a better approximation to the benchmark solution than the LAMDA approach (also confirmed by Fig. 10).

This mathematical example demonstrates the advantage of the proposed BNC-MDA method for bivariate coupling in each direction. The method achieves an accurate result, while requiring much fewer function evaluations compared with both SOFPI and LAMDA. The next example illustrates the benefits of BNC-MDA in the case of high-dimensional coupling.

B. MDA for Aircraft Wing

In this section, a three-dimensional aeroelastic analysis of an aircraft wing is used to illustrate the proposed BNC-MDA method. A cantilevered wing with a NACA 0012 airfoil is adopted [42]. We use ANSYS to perform the fluid–structure interaction analysis of the wing. The fluid and structure meshes are shown in Fig. 11.

This problem consists of hundreds of coupling quantities in each direction. In this case, the computational effort of LAMDA, even if combined with PCA (LAMDA+PCA), will still be very high, whereas the accuracy will be worsened (due to the use of finite difference and the construction of a joint probability distribution with a sparse grid of integration points and using FORM). The total number of function evaluations in the LAMDA method assuming 10 integration values for each coupling variable is $10^n \times (2n+1) \times m$ (n: number of coupling variables; m, average number of function evaluations for each FORM analysis). If n is too large and only 20 principal components are used, the "LAMDA + PCA" approach still needs $10^{20} \times 21 \times m$ function evaluations, which is an enormous amount of computing effort. Therefore, the LAMDA + PCA approach is not affordable and not pursued here. BNC-MDA, which requires much fewer training samples of the input and coupling variables (and not fully convergent analysis) to construct the Bayesian network, is very efficient in solving the problem; its accuracy will be compared with the SOFPI approach next.

This example is run with two different mesh sizes (258 nodes and 1218 nodes) next. The backsweep angle (BW) is chosen to be the input variable with natural variability and is assumed to be normally distributed as $N(0.4, 0.04)$ without loss of generality. To perform the coupled FSI analysis, 110 realizations of the backsweep angle are

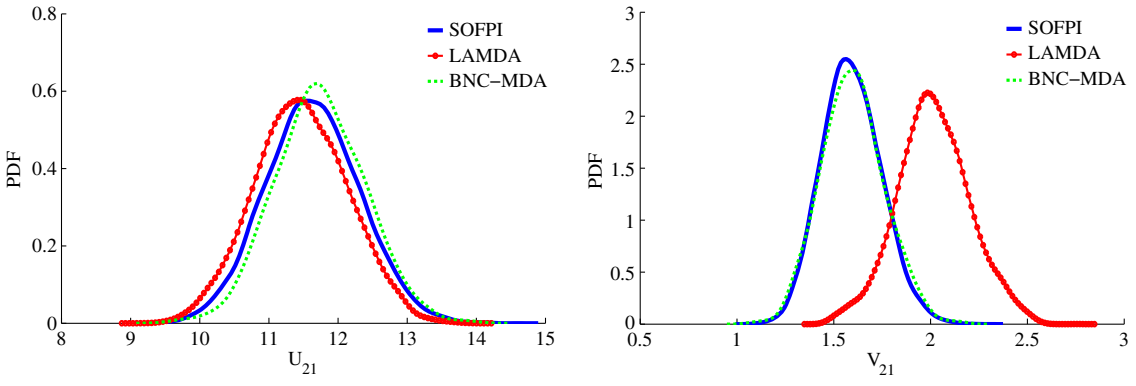
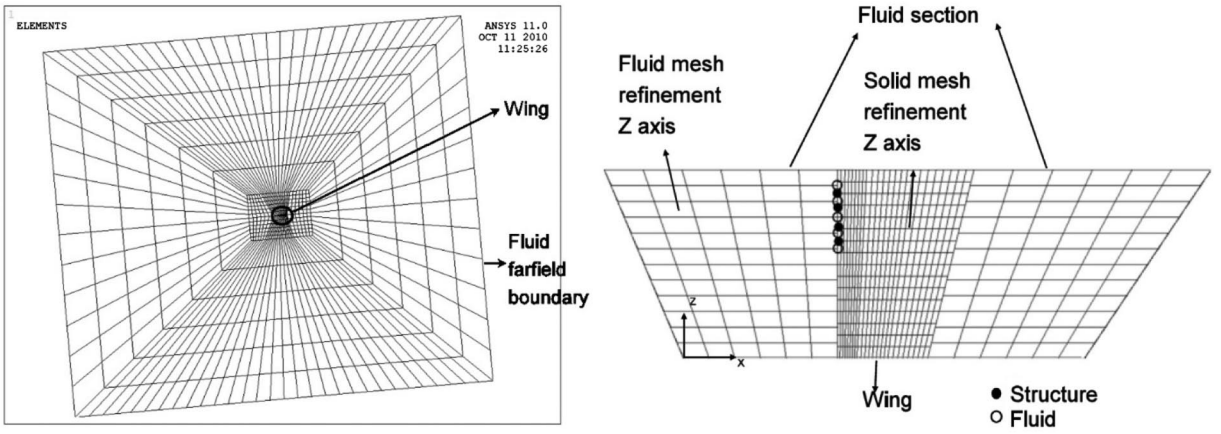


Fig. 10 Marginal PDFs of coupling variables.



a) Overall view b) Fluid and structure meshes

Fig. 11 Fluid and structure meshes and refinement parameters.

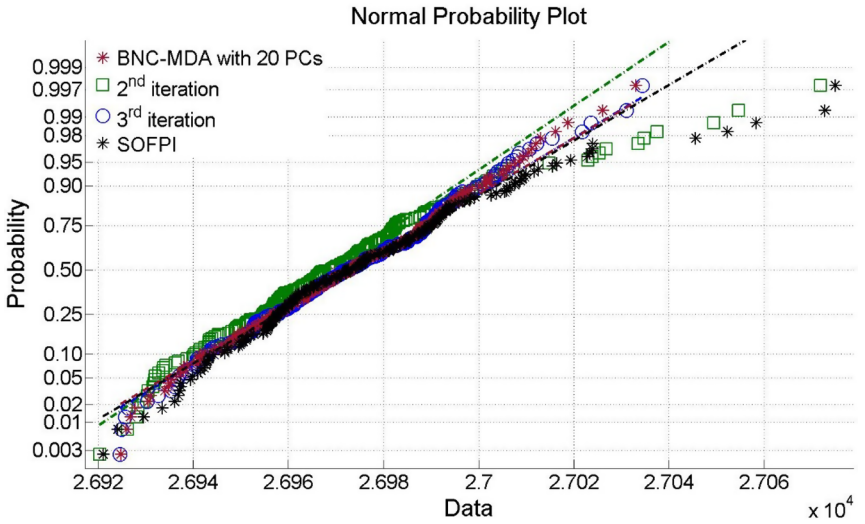


Fig. 12 Normal probability plot of pressure from four cases at node 1.

sampled. The values of nodal pressure oscillate drastically in the first and second iterations; typically a large bias between the PDFs of the coupling variables will occur, and the resulting difference term ε will be either all positive or all negative. If the empirical CDF of ε for the copula is computed using all positive (or all negative) values, the conditional sampling will need an extrapolation to calculate the conditional joint distribution given $\varepsilon = 0$. This will significantly decrease the accuracy the proposed approach. To balance the solution accuracy and the computational efficiency, the FSI analysis is terminated after three iterations, and the Bayesian network is built with the nodal pressure results of the second and third iterations.

Six cases are discussed here: 1) BNC-MDA method using first 10 principal components, 2) BNC-MDA method using 15 principal components, 3) BNC-MDA method using 20 principal components, 4) BNC-MDA method using 30 principal components, 5) output collected after two iterations, and 6) output collected after three iterations. For cases 1–4, 5000 samples are generated using the BN to estimate the coupling variable distributions. The result of SOFPI is used as the benchmark solution.

Figure 12 shows the normal probability plot of cases 3, 5, and 6, as well as the benchmark solution (SOFPI) at node 1. Cases 3 and 6 are closer to the SOFPI distribution compared with case 5. For an n-variable distribution, the K-L divergences for all marginal distributions are computed, and an average value is estimated using Eq. (16):

$$\text{Average } D_{\text{KL}} = \frac{\sqrt{\Sigma_{i=1}^{n}[D_{\text{KL}}^{i}(p||q)]^2}}{n} \tag{16}$$

where D_{KL}^{i} denotes the K-L divergence of the marginal distribution for the ith node, and n is the total number of the nodes. For the sake of comparison, the Student's t copula is also used to implement the BNC-MDA approach. Table 3 summarizes the average K-L divergences for all six cases, using both Gaussian and t copulas.

The following observations are made:

1) The results using the Gaussian and t copulas are similar for this problem.

2) For cases 1–4, as the number of used principal components increases, the K-L divergence becomes smaller and converges after 20 PCs. As more principal components are taken, more variance of the original data is captured, and the results are refined; however, for this example, 20 PCs are seen to be sufficient.

3) Case 6 approaches the converged results better than case 5. As the iteration number (of the physics analysis) increases, the stability of the solution is enhanced, and the differences between the results from consecutive iterations will become smaller. Also, the third iteration of FPI achieves similar accuracy as the BNC-MDA result in the wing problem; therefore, very few further iterations of FPI are needed for convergence. The proposed BNC-MDA approach saves the computational effort by reducing the total number of iterations in the feedback-coupled analysis. Therefore, the more iterations the FPI analysis requires for convergence, and the longer each individual disciplinary analysis takes, the more time will be saved by using BNC-MDA.

4) In the implementation of BNC-MDA in this example, the large BN is broken into several separated small BNs for sampling, as in Fig. 8. This is an approximation because "uncorrelated" does not

Table 3 Kullback–Leiber divergence for different scenarios (258 nodes)

	BNC-MDA				FSI	
	10 PCs	15 PCs	20 PCs	30 PCs	Second iteration	Third iteration
Average D_{KL}^{Gauss}	0.25	0.19	0.16	0.16	0.21	0.18
Average $D_{KL}^{'}$	0.24	0.21	0.20	0.19		

imply "independent." To verify the accuracy of this approximation, we have also considered an unseparated network with 20 principal components connected to each other as shown in Fig. 13. Each node in the network represents a random variable. The 40 nodes on the top left and top right denote the principal components of the nodal pressure after the second and third iterations, respectively. The bottom 20 nodes, each connected to two nodes, represent the differences between the corresponding values. This unseparated BN is costly to build, and requires care in connecting the nodes correctly because it is particular to each problem, whereas the separated network is generic and only consists of three-node networks as in Fig. 8. Thus, the separated network, although approximate, is easy to implement for high-dimensional problems, but its accuracy needs to be verified. The average D_{KL} is computed between the results of the unseparated network and the independent network, and is found to be 0.063, which indicates very similar solutions given by both methods. Therefore, the approximation of individual separated BNs improves the efficiency of the BNC-MDA methodology for this example without too much sacrifice of the accuracy.

5) To demonstrate the scalability of the proposed BNC-MDA approach, the same aeroelasticity problem is considered with a finer mesh of 1218 nodes. Thus, the number of coupling variables in each direction is increased to 1218 (nodal pressures) and 3654 (nodal displacements). The same 110 realizations of the input variables (as in the coarse mesh model) are used to perform both BNC-MDA and fixed-point iteration for this scaled-up problem. The FPI for the finer mesh model takes an average of six iterations and 750 s for convergence corresponding to each single realization of the input variables. Disciplinary analysis results (i.e., CFD and FEA) after the third and fourth iterations are recorded and used to implement the proposed BNC-MDA methodology. It takes the desktop PC about 550 s to complete a four-iteration analysis for each realization of the input variable. The computational costs of FPI and BNC-MDA, just for the coupled physics analysis, are compared in Table 4. It can be concluded from Table 4 that the computational savings with BNC-MDA improves with the size of the problem. The main reason for the savings in computational effort is that the coupled physics analysis is not run untilfull convergence; only a few iterations are used to build the Bayesian network (three iterations for the coarse mesh case, and four iterations for the fine mesh case). The CPU time reported in Table 4 also includes the time to build the model for each sample of input realization, which actually takes up 50% of the computational effort for a fully converged analysis. That is, for the 258-node model, it takes about 1 min to build the model and one more minute to converge in about six iterations. Thus, the BNC-MDA approach takes 1.5 min (on average) per sample, compared with 2 min per sample for SOFPI. In terms of function evaluations, the savings is 50% in this problem. The savings would be more impressive if the fixed-point iteration took many more iterations to converge. So the computational savings is problem dependent. In the earlier mathematical example (Sec. IV.A), BNC-MDA needed only 2000 function evaluations compared with 107,421 by SOFPI, thus giving a 98% savings in computational effort.

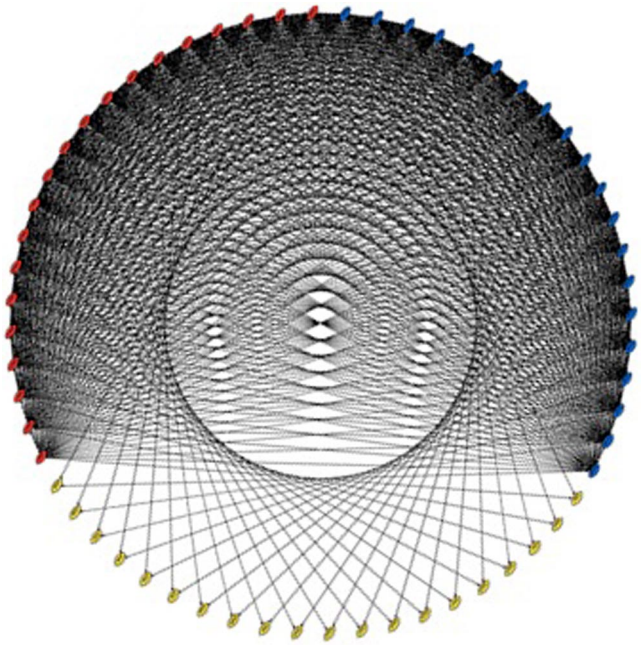


Fig. 13 Unseparated Bayesian network with 20 principal components.

Table 4 Computational effort comparison between FPI and BNC-MDA

No. of nodes	FPI, s	BNC-MDA, s	Time saved, s
258	14,300	9,350	4,950
1,218	82,500	60,500	22,000

Table 5 Time required for sampling (seconds) by BNC-MDA with different numbers of principal components

No. of Nodes	10 PCs	15 PCs	20 PCs	30 PCs
258	12.77	18.90	26.52	37.89
1218	11.29	16.58	21.95	32.38

6) The number of principal components only comes into the picture in sampling the Bayesian network, after generating training samples from the coupled physics analysis. The time required for sampling by BNC-MDA with different numbers of principal components is shown in Table 5. It is seen that, for the same number of principal components, there is no significant difference in the sampling effort between the coarser and finer physics models, because the Bayesian network has the same dimension between the two cases for the same number of principal components. The number of principal components will affect the accuracy of the result, but the effect on computational cost is insignificant compared with the cost of the physics (FSI) analysis. This is because the principal components only affect the dimension of the Bayesian network.

7) A very important observation is the comparison of computational effort between Tables 4 and 5. Table 5 shows that the computational effort in building the Bayesian network and subsequent sampling is negligible compared with the physics analysis effort shown in Table 4.

V. Conclusions

This paper proposed a new approach for uncertainty propagation through high-dimensional coupled multidisciplinary analysis. The Bayesian network technique is exploited for this purpose and the joint probability distribution of the coupling variables given interdisciplinary compatibility is computed using conditional sampling of the Bayesian network. A copula-based sampling technique, which is not

restrained by the type of marginal distributions of the variables, is introduced for efficient sampling of the BN. The joint probability distribution of the coupling variables is estimated using conditional sampling with the copula. Principal component analysis is adopted to decrease the dimensionality of the Bayesian network. A mathematical MDA example and an aeroelastic wing analysis example demonstrate the efficiency and accuracy of BNC-MDA.

The accuracy of the BNC-MDA result depends on the number of training samples used to construct the BN, and could be further enhanced by generating more input samples. Note that each sample only requires a few iterations of the coupled physics analysis instead of a fully converged solution as in FPI. Thus, the proposed BNC-MDA approach is promising for high-dimensional problems. Future research needs to investigate the performance of this approach for very high-dimensional problems and its incorporation within design optimization under uncertainty for high-dimensional multidisciplinary problems.

Appendix: Gaussian Copula Sampling

Consider the Bayesian network shown in Fig. 6. Six random variables are presented in the network, including $U_{21}, V_{21}, u_{21}, v_{21}, \varepsilon_{u_{21}}$, and $\varepsilon_{v_{21}}$. Let P represent the marginal CDFs of the random variables, such that $P_{U_{21}} = F_{U_{21}}(U_{21}), P_{V_{21}} = F_{V_{21}}(V_{21}), \ldots, P_{\varepsilon_{v21}} = F_{\varepsilon_{v21}}(\varepsilon_{v21})$. Note that P can be any type of valid unidimensional CDF. Let R be a symmetric, positive definite correlation matrix, such that

$$\mathrm{diag}(R) = (1, 1, \ldots, 1)^T \tag{A1}$$

Let Φ_R be the standardized multivariate normal distribution with correlation matrix R. The multivariate Gaussian copula of the six random variables is defined as

$$C_R(P) = \Phi_R[\Phi^{-1}(P_{U_{21}}) \cdots \Phi^{-1}(P_{\varepsilon_{v_{21}}})] \tag{A2}$$

where Φ^{-1} is the inverse of the standard univariate normal distribution function Φ. The density of the Gaussian copula is given by

$$C_R(u) = \frac{1}{\sqrt{\det(R)}} \exp\left[-\frac{1}{2} \begin{pmatrix} \Phi^{-1}(P_{U_{21}}) \\ \vdots \\ \Phi^{-1}(P_{\varepsilon_{v_{21}}}) \end{pmatrix} \cdot (R^{-1} - 1) \cdot \begin{pmatrix} \Phi^{-1}(P_{U_{21}}) \\ \vdots \\ \Phi^{-1}(P_{\varepsilon_{v_{21}}}) \end{pmatrix} \right] \tag{A3}$$

To conditionally generate samples from the Gaussian copula, the linear correlation matrix for the equivalent normal distribution of $U_{21}, V_{21}, \ldots, \varepsilon_{v21}$ is first calculated based on the rank correlation coefficient (Spearman's ρ_s). The equivalent normal corresponding to $\varepsilon_{u_{21}} = 0$ and $\varepsilon_{v_{21}} = 0$ are obtained by $\varepsilon'_{U_{21}}(0) = \Phi^{-1}[F_{\varepsilon_{u2j}}(0)]$, $\varepsilon'_{V_{21}}(0) = \Phi^{-1}[F_{\varepsilon_{v_{21}}}(0)]$. The mean vector and covariance matrix for the four-dimensional (dimension $= 6 - 2$) conditional joint normal distribution can be calculated as follows.

Let μ and Σ denote the mean vector and covariance matrix of the random variables in the equivalent normal space $[U'_{21}, V'_{21}, u'_{21}, v'_{21}, \varepsilon'_{u_{21}}, \varepsilon'_{v_{21}}]$; $\boldsymbol{\mu}$ is a vector of zeros with six entries, and Σ can be evaluated from the correlation matrix R. If μ and Σ are partitioned as

$$\mu = \begin{bmatrix} \mu_{U'_{21}} \\ \mu_{V'_{21}} \\ \mu_{u'_{21}} \\ \mu_{v'_{21}} \\ \mu_{\varepsilon'_{u21}} \\ \mu_{\varepsilon'_{v21}} \end{bmatrix}$$

$$\Sigma = \begin{bmatrix} 1 & \Sigma_{U'_{21}V'_{21}} & \Sigma_{U'_{21}u'_{21}} & \Sigma_{U'_{21}v'_{21}} & \Sigma_{U'_{21}\varepsilon'_{u_{21}}} & \Sigma_{U'_{21}\varepsilon'_{v_{21}}} \\ \Sigma_{V'_{21}U'_{21}} & 1 & \Sigma_{V'_{21}u'_{21}} & \Sigma_{V'_{21}v'_{21}} & \Sigma_{V'_{21}\varepsilon'_{u_{21}}} & \Sigma_{V'_{21}\varepsilon'_{v_{21}}} \\ \Sigma_{u'_{21}U'_{21}} & \Sigma_{u'_{21}V'_{21}} & 1 & \Sigma_{u'_{21}v'_{21}} & \Sigma_{u'_{21}\varepsilon'_{u_{21}}} & \Sigma_{u'_{21}\varepsilon'_{v_{21}}} \\ \Sigma_{v'_{21}U'_{21}} & \Sigma_{v'_{21}V'_{21}} & \Sigma_{v'_{21}u'_{21}} & 1 & \Sigma_{v'_{21}\varepsilon'_{u_{21}}} & \Sigma_{v'_{21}\varepsilon'_{v_{21}}} \\ \Sigma_{\varepsilon'_{u21}U'_{21}} & \Sigma_{\varepsilon'_{u21}V'_{21}} & \Sigma_{\varepsilon'_{u21}u'_{21}} & \Sigma_{\varepsilon'_{u21}v'_{21}} & 1 & \Sigma_{\varepsilon'_{u21}\varepsilon'_{v21}} \\ \Sigma_{\varepsilon'_{v21}U'_{21}} & \Sigma_{\varepsilon'_{v21}V'_{21}} & \Sigma_{\varepsilon'_{v21}u'_{21}} & \Sigma_{\varepsilon'_{v21}v'_{21}} & \Sigma_{\varepsilon'_{v21}v'_{21}} & 1 \end{bmatrix}$$

then the conditional joint distribution of $U'_{21}, V'_{21}, u'_{21}, v'_{21}$ given $\varepsilon'_{u_{21}} = \varepsilon'_{u_{21}}(0), \varepsilon'_{v_{21}} = \varepsilon'_{v_{21}}(0)$ is denoted as $f[U'_{21}, V'_{21}, u'_{21}, v'_{21} | \varepsilon'_{u_{21}} = \varepsilon'_{u_{21}}(0), \varepsilon'_{v_{21}} = \varepsilon'_{v_{21}}(0)) \sim N(\tilde{\mu}, \tilde{\Sigma})]$, where the conditioned mean vector $\tilde{\mu}$ and covariance matrix $\tilde{\Sigma}$ are

$$\tilde{\mu} = \mu_C + \Sigma_{C\varepsilon}\Sigma_{\varepsilon\varepsilon}^{-1}(\varepsilon - \mu_\varepsilon) \tag{A4}$$

$$\tilde{\Sigma} = \Sigma_{CC} - \Sigma_{C\varepsilon}\Sigma_{\varepsilon\varepsilon}^{-1}\Sigma_{\varepsilon C} \tag{A5}$$

Eqs. (A4) and (A5) can be used as the parameters of the Gaussian copula, samples of which are generated and adopted to estimate the probability distribution of the converged coupling variables.

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