Review of Formulations for Structural and Mechanical System Optimization

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Abstract.

Alternative formulations for optimization and simulation of structural and mechanical systems, and other related fields are reviewed. The material is divided roughly into two parts. Part 1 focuses on the developments in structural and mechanical systems including configuration and topology optimization. Here the formulations are classified into three broad categories: (i) The conventional formulation where only the structural design variables are treated as optimization variables, (ii) simultaneous analysis and design (SAND) formulations where design and some of the state variables are treated as optimization variables, and (iii) a displacement based two-phase approach where the displacements are treated as unknowns in the outer loop and the design variables as the unknowns in the inner loop. Part 2 covers more general formulations that are applicable to diverse fields, such as economics, optimal control, multidisciplinary problems and other engineering disciplines. In these fields, SAND-type formulations have been called mathematical programs with equilibrium constraints (MPEC), and partial differential equations (PDE) constrained optimization problems. These formulations are viewed as generalization of the SAND formulations developed in the structural optimization field. Based on the review, it is concluded that the basic ideas of the formulations presented in diverse fields can be integrated to conduct further research and develop alternative formulations

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and solution procedures for practical engineering applications. The paper lists 187 references on the subject.

Keywords: nested analysis and design (NAND) optimization, simultaneous analysis and design (SAND) optimization, mathematical programs with equilibrium constraints (MPEC), PDE-constrained optimization

Major Abbreviations

DB:	Displacement Based Two-Phase Formulation
FEM:	Finite Element Method
KKT:	Karush-Kuhn-Tucker
LP:	Linear Programming
MDO:	Multidisciplinary Design Optimization
MPEC:	Mathematical Programs with Equilibrium Constraints
NAND:	Nested Analysis and Design (conventional formulation)
NLP:	Nonlinear Programming
ODE:	Ordinary Differential Equations
PDE:	Partial Differential Equations
SAND:	Simultaneous Analysis and Design
SDP:	Semidefinite Programming
SLP:	Sequential Linear Programming
SQP:	Sequential Quadratic Programming
rSQP	Reduced SQP method

1. Introduction

Since 1960s, various formulations for optimization of problems in many diverse fields, such as structural, chemical, industrial and mechanical engineering, economics, optimal control and others have been developed and discussed in the literature. These formulations are reviewed with the objective of possible cross fertilization of ideas that can lead to better approaches for optimization of complex systems.

In the structural optimization literature, three basically different formulations for optimum design have been presented. The first one is called the *conventional formulation* where only the structural design variables are treated as the optimization variables. This is also called the *nested analysis and design* (NAND) approach. The second set of formulations is known as the *simultaneous analysis and design* (SAND) approach. In these formulations, some of the state variables, such as the displacements, are also treated as optimization variables in addition to the traditional design variables. The governing equilibrium equations are treated as equality constraints. The third formulation is known as the displacement based two-phase approach where the displacements are treated as optimization variables in the outer loop and the design variables as the unknowns in the inner loop.

Parallel developments of SAND-type optimization formulations and their solutions strategies have also taken place in other fields since 1970s. A general class of formulations known as *mathematical programs with equilibrium constraints*, or in short MPECs, has been developed and studied. The word “equilibrium” in MPEC refers to the variational equalities or inequalities that model the equilibrium phenomenon in engineering and other applications. Another class of formulations that has been presented and analyzed recently is known as the *partial differential equations* (PDE)-constrained optimization. In these formulations, the equilibrium equations are expressed in a continuum form, the PDEs. In addition to these literatures, SAND-type approaches have been used to solve optimal control problems. We shall present an overview of these literatures.

Thus, the objective of this paper is to review various formulations for optimization and simulation of structural and mechanical systems, and other related fields. The literature on this topic has grown substantially in recent years. To cover the material properly, the paper is divided roughly into two parts. Part 1 consisting of Sections 2 to 7 focuses on the developments in structural optimization including configuration and topology optimization. Part 2 consisting of Sections 8 to 11 covers developments on the subject in other diverse fields, such as economics, other engineering disciplines, optimal control, and multidisciplinary design optimization. Section 2 presents an overview of the entire literature. Section 3 describes the conventional formulation and Section 4 covers simultaneous analysis and design (SAND) formulations. Literature on linear and nonlinear problems is covered, and optimization algorithms that have been used for SAND formulations are discussed. Section 5 describes the displacement based two-phase formulation for structural optimization. Section 6 presents a comparative evaluation of the three formulations, the conventional, SAND, and the displacement based two-phase. Section 7 covers the literature on configuration and topology optimization of structures. Section 8 describes the PDE-constrained optimization formulation where the equilibrium equations are kept in the continuum form. Section 9 covers the formulation of mathematical programs with equilibrium constraints (MPEC). Section 10 covers the literature on optimal control problems, and Section 11 covers the literature on multidisciplinary design optimization. Finally, some concluding remarks are given in Section 12.

2. Overview of literature

Various formulations that have been used to solve different optimization problems can be classified into two broad categories: (i) conventional formulation (also called nested analysis and design, NAND) where only the design variables are treated as the independent optimization variables, and (ii) formulations where the state variables and the design variables for the system are simultaneously treated as independent optimization variables, and the governing analysis equations are treated as equality constraints. We present more details of these formulations later in the paper; here we present an overview of the literature on the subject.

In the structural optimization literature, the simultaneous analysis and design (SAND) formulation is a major class of alternative formulations that has been discussed since 1960s. Besides the design variables, the SAND formulations also include some of the state variables as optimization variables. Some earliest attempts to include state variables in the structural optimization problem were by Schmit and Fox (1965). The basic idea was to transform an inequality constrained minimization problem in the design variable space into an unconstrained problem in a space of mixed design and state variables. Fuchs (1982, 1983) presented explicit optimum design methods (SAND) for linear elastic trusses. Explicit expressions for the objective function and the constraints could be obtained. A SAND formulation based on an element-by-element preconditioned conjugate gradient technique was proposed by Haftka (1985), and Haftka and Kamat (1989). It was concluded that the simultaneous approach was competitive with the conventional nested approach, and that it was more efficient for large-scale problems. Shin *et al*. (1988) considered the simultaneous analysis and design approach to solve the problem with eigenvalue constraints. Ringertz (1989) formulated the minimum weight design of structures with geometrically nonlinear behavior in two different ways. All the equilibrium equations or a few of them were treated as constraints. Both design variables and displacements were treated as optimization variables. Ringertz (1992) also presented methods for the optimal design of nonlinear shell structures. The matrix sparsity in the constraint Jacobian was exploited because of the large number of variables. Kirsch and Rozvany (1994) presented several alternative but equivalent formulations for structural optimization problems. These included design variable space (conventional), SAND, optimality criteria (OC), and some simplified SAND formulations. Other methods, such as the augmented Lagrangian method, have also been used with SAND formulations (Larsson and Rönnqvist 1995). The SAND formulation proposed by Orozco and Ghattas (1991, 1997) was solved by a reduced SQP method. Geometrically nonlinear behavior of the structure was included in the formulation and sparsity of problem functions was exploited in the calculations.

In recent years, various SAND formulations have been successfully applied to the configuration and topology design of structures (Bendsøe 1995; Bendsøe and Sigmund 2003). It is well-known that a crucial step for success of the SAND formulations is the solution of very large scale optimization problems. Therefore considerable focus has been put on the development of new algorithms to solve large scale optimization problems (Ringertz 1995; Ben-Tal and Roth 1996; Ben-Tal and Zibulevsky 1997; Orozco and Ghattas 1997; Jarre *et al.* 1998; Maar and Schulz 2000; Herskovits *et al.* 2001; Hoppe *et al.* 2002; and others).

Another alternative approach of optimum structural design is the so-called displacement based two-phase procedure. In a paper by Missoum and Gürdal (2002), the two-phase optimization procedure of McKeown (1977, 1989, 1998) was presented and applied to optimize trusses. The formulation solved the problem in two phases, the inner and outer problems. In the inner problem, the cost was minimized subject to satisfaction of the equilibrium equations. The displacement field was specified and the design variables were the independent variables. In the outer problem, the displacements were determined to minimize the cost function subject to the stress and displacement constraints. That work has also been extended to nonlinear problems

(Missoum *et al*. 2002a,b).

Optimality criteria (OC) methods have also been classified as a kind of alternative formulation by some researchers (Kirsch and Rozvany 1994), because the solution space includes both the design variables and the Lagrange multipliers. Starting from the Karush-Kuhn-Tucker (KKT) conditions, iterative update relations are derived for the variables. The optimality conditions are treated as additional constraints, and satisfied at the optimal point (Khot *et al.* 1979). Such procedures are not reviewed in the current paper.

It turns out that the SAND-type formulations have also been discussed in other fields since 1970s. These are known as mathematical programs with equilibrium constraints, or in short MPECs. An MPEC is an optimization problem having primary constraints that are expressed as a parametric variational inequality or a complementarity system. The MPECs can also be viewed as a generalization of the so-called bilevel programs, also known as mathematical programs with optimization constraints. The basic idea of MPEC was introduced in the operations research literature in the early 1970s by Bracken and McGill (1973, 1974a,b,c). These ideas can also be traced back the economic problem of Stackelberg game (Stackelberg 1952). The MPEC has evolved as a major research field in recent years and has been put on a firm mathematical foundation (Lou *et al.* 1996; Outrata *et al.* 1998). The MPEC formulation covers many diverse applications, such as economics, chemical engineering, and many more. As a particular example, structural analysis and design problems in unilateral frictional contact have been discussed with the MPEC formulation (Hilding *et al.* 1999).

Other developments of optimization formulations and their solutions strategies have also taken place recently. These are known as partial differential equations (PDE) constrained optimization problems (Biegler *et al.* 2003). Most simulation problems in engineering fields involve solutions of partial differential equations. Therefore, following the SAND concept, the simulation variables can also be treated as optimization variables and the PDEs as equality constraints. Many times the PDEs are obtained as a result of some variational principle to model an equilibrium phenomenon. Therefore, PDE-constrained optimization can be viewed as a special case of the MPEC.

3. Conventional formulation

The most common approach for structural optimization has been the one where only the design variables are treated as optimization variables. All other response quantities, such as displacements, stresses, strains and internal forces are treated as implicit functions of the design variables. In this section, some technical details of the conventional NAND approach for optimization of structural and mechanical systems are presented. This is done by considering a linear analysis problem (small displacements and linearly elastic material model) in the discretized form. The approach can also be described for nonlinear analysis, using a continuum form of the analysis equations that is more general because it is not tied to any particular discretization (Arora 1995; Haug *et al.* 1986). However, this will not be done here to keep the presentation of the basic ideas clearer and straightforward.

3.1 **Formulation**

To describe the current approach, let us define the following notation:

$\mathbf{b}$ = a k-dimensional vector of design variables that describes design of the system.

$\mathbf{z}$ = an n-dimensional vector of generalized displacements.

For linear small displacement analysis, the governing equilibrium equation for the system is discretized as follows:

$$\mathbf{K}(\mathbf{b})\mathbf{z} = \mathbf{F}(\mathbf{b}) \tag{1}$$

where

$\mathbf{K}(\mathbf{b})$ = is a nonsingular $n \times n$ stiffness matrix that depends on the design of the system

$\mathbf{F}(\mathbf{b})$ = an n dimensional vector of equivalent external loads applied at the nodes of the discretized model for the system.

For a given design $\mathbf{b}$ and boundary conditions, (1) is assembled using contributions from each finite element, and solved for the state variable vector $\mathbf{z}$. Using the vector $\mathbf{z}$, strains and stresses at all points of the structure can be evaluated. (1) has been implemented into many computer programs to analyse various structural systems. These programs are now widely used in practice. It is important to note that when the system is nonlinear (large displacements, elastoplastic material), (1) becomes nonlinear because $\mathbf{K}(\mathbf{b})$ and $\mathbf{F}(\mathbf{b})$ start to depend on the state variables $\mathbf{z}$ for the system. This complicates the solution process for (1) because it requires incremental and iterative procedures, such as the Newton-Raphson approach.

The optimal design problem is defined as follows:

Find the design variable vector $\mathbf{b}$ to minimize a cost function,

$$f = f(\mathbf{b},\mathbf{z}) \tag{2}$$

subject to the inequality constraints

$$\mathbf{g}(\mathbf{b},\mathbf{z}) \leq \mathbf{0} \tag{3}$$

Equality constraints if present in the formulation can be treated quite routinely. Note that in the above formulation, variables $\mathbf{b}$ and $\mathbf{z}$ are not independent, they are related by the equilibrium condition in (1). It is obvious that design variables $\mathbf{b}$ can be treated as independent optimization variables, while $\mathbf{z}$ as dependent variables. Therefore, it is natural to set up a nested analysis and optimization process, using an analysis code, to calculate $\mathbf{z}$ using given $\mathbf{b}$. This is the central idea of the conventional formulation; i.e., to treat $\mathbf{b}$ as the only optimization variable and treat $\mathbf{z}$

as a function of $\mathbf{b}$, $\mathbf{z}=\mathbf{z}(\mathbf{b})$. In the MPEC literature, this procedure is called the *implicit programming* approach. Since the displacement based FEM is a powerful analysis method and readily available, the conventional formulation has been the usual approach to solve optimization problems. Another reason for the popularity of the conventional formulation is that the widely-used approximate resizing rules can be obtained based on optimality criteria (Haftka 1985). Other analysis methods are also available for the conventional formulation of optimal design, such as the force method (Sedaghati and Esmailzadeh 2003), boundary element method or meshfree method (Kim *et al.* 2003). Equation (1) therefore needs to be consistent with the corresponding analysis method. Structural analysis techniques based on conjugate gradient minimization of the energy functional have also been used for design optimization (Barthelemy *et al.* 1991).

3.2 **Gradient evaluation**

Numerical values for $\mathbf{z}$ can be obtained from the state equation (1) once $\mathbf{b}$ is specified. However, an explicit functional form for $\mathbf{z}$ in terms of $\mathbf{b}$ cannot be obtained. In other words, $\mathbf{z}$ cannot be eliminated from the optimization problem by substitution. In the gradient based optimization process, derivatives of the cost function $f(\mathbf{b},\mathbf{z})$ and the constraint functions $\mathbf{g}(\mathbf{b},\mathbf{z})$ with respect to $\mathbf{b}$ are needed. The explicit expressions for these derivatives in terms of $\mathbf{b}$ cannot be obtained, since $\mathbf{z}$ is an implicit function of $\mathbf{b}$. Therefore, usually the finite difference methods have been used to calculate the gradients since they are easy to implement and explicit expressions for the cost and constraint functions are not needed. However, the finite difference methods have accuracy problems, i.e., the so-called “step-size” dilemma (Haftka and Gürdal 1992). Another drawback is that they are slow because they require a repeated solution of the state equation (1).

To derive analytical expressions for gradients of the functions, implicit differentiation procedures need to be used, which is called *design sensitivity analysis*. To explain this process, the calculation of derivatives of one of the functions, say $f(\mathbf{b},\mathbf{z})$, is briefly explained. Other functions can be treated similarly. Taking total derivative of $f(\mathbf{b},\mathbf{z})$ with respect to $\mathbf{b}$, we get

$$\left.\frac{df(\mathbf{b},\mathbf{z}(\mathbf{b}))}{d\mathbf{b}}\right|_{k\times 1} = \left.\frac{\partial f(\mathbf{b},\mathbf{z})}{\partial \mathbf{b}}\right|_{k\times 1} + \left.\frac{d\mathbf{z}(\mathbf{b})}{d\mathbf{b}}\right|_{k\times n} \left.\frac{\partial f(\mathbf{b},\mathbf{z})}{\partial \mathbf{z}}\right|_{n\times 1} \tag{4}$$

Calculation of the partial derivatives of $f(\mathbf{b},\mathbf{z})$ with respect to $\mathbf{b}$ and $\mathbf{z}$ presents no particular difficulty because explicit dependence of the function on $\mathbf{b}$ and $\mathbf{z}$ is known. However, calculation of $\frac{d\mathbf{z}}{d\mathbf{b}}$ in (4) needs further analysis and explanation. To calculate this $k \times n$ matrix, we take a total derivative of the state equation (1) with respect to the design variables $\mathbf{b}$ and rearrange the resulting equation to obtain:

$$\mathbf{KZ} = \mathbf{S} \tag{5}$$

where

$$\mathbf{Z}\big|_{n\times k} = \frac{d\mathbf{z}(\mathbf{b})^T}{d\mathbf{b}}\;; \quad \mathbf{S}\big|_{n\times k} = \frac{\partial}{\partial \mathbf{b}}(\mathbf{F}(\mathbf{b}) - \mathbf{K}(\mathbf{b})\mathbf{z})^T \tag{6}$$

Equation (5) looks deceptively simple and similar to the state equation (1). However, its solution variable $\mathbf{Z}$ is not a vector but a matrix of dimension $n \times k$. The right side $\mathbf{S}$ is also a matrix of the same dimension. Once the right side has been calculated, (5) can be solved using the same process that was used for solving (1). The decomposed matrix $\mathbf{K}$ needs to be saved for re-use with (5), requiring certain amount of data manipulation and storage. If iterative methods are used to solve the state equation (1), then the decomposed $\mathbf{K}$ is not available. Then (5) must also be solved using the iterative solution process which can be more time consuming compared to the foregoing procedure where the decomposed $\mathbf{K}$ is available.

The calculation of the matrix $\mathbf{S}$ in (6) requires partial differentiation of the equilibrium equation for each finite element with respect to the design variables $\mathbf{b}$ and then assembly of the matrix $\mathbf{S}$ using these data. This process requires additional programming to extend the analysis code in order to implement the design sensitivity analysis. In addition, if new finite elements are added or the current ones are updated, the code for the design sensitivity analysis needs to be modified accordingly. Further, implementation of design sensitivity analysis for nonlinear and multi-physics problems becomes more complex and computationally more expensive because $\mathbf{K}$ and $\mathbf{F}$ depend on the state of the system as well. This is one of the stumbling blocks for engineering applications of optimization.

The above procedure for design sensitivity analysis is called the *direct differentiation method*. There is an alternate approach of design sensitivity analysis called the *adjoint variable method*. To derive that method, (5) is substituted into (4) as $\mathbf{Z} = \mathbf{K}^{-1}\mathbf{S}$, and an adjoint problem is defined with adjoint load as $\partial f / \partial \mathbf{z}$. The adjoint displacement vector is substituted into (4) to obtain an expression for the design gradient. Under certain circumstances, this method is more efficient than the direct differentiation method. However, the method is even more difficult to implement into analysis codes, especially for nonlinear and transient dynamic problems. Substantial literature is available that describes theoretical as well as implementation aspects of the design sensitivity analysis approaches (Haug *et al.* 1986; Arora 1995; and many other references).

Conventional optimization formulations and solution methods for structural and mechanical systems can be difficult to use for design of practical structural and mechanical systems due to the following two main reasons: (i) Many practical applications are complex requiring interaction between several disciplines; i.e., require the use of different analysis software that are discipline-specific. Since they are independent programs, it is difficult to integrate them into the conventional design optimization formulations and algorithms. (ii) The conventional formulation requires design sensitivity analysis which is difficult to implement and maintain with existing analysis software.

To alleviate some of the difficulties noted above, several different research avenues have been explored in the literature. First, efficient structural reanalysis methods for analyzing a modified structure have been developed (Kirsch 2000, 2002; Kirsch and Papalambros 2001; Kirsch *et al.* 2002, 2004). These methods can be useful for efficient analysis of updated designs and for calculation of the design derivatives during the optimization process. Second, various methods to develop approximate models, the so-called meta-models, such as the response surface approximations, have been proposed and evaluated for optimization of complex structural and mechanical systems (Myers and Montgomery 2002; Krishnamurthy 2003). Third, some alternative formulations have also been proposed and evaluated for optimization of structural and mechanical systems since early 1960s. We will focus on review of the literature on this third way of solving the problem and discuss their advantages and disadvantages.

4. Simultaneous analysis and design (SAND)

In this approach, the state and design variables are treated simultaneously as optimization variables. The equilibrium equation becomes an equality constraint in terms of the variables. SAND basically formulates the optimization problem in a mixed space of design and state variables, to imbed the analysis equations in one single optimization problem; therefore no explicit structural analysis or design sensitivity analysis is needed. Note that there are in fact a lot of interesting formulations derived from SAND, especially in shape and topology optimization of structures, which are presented in Section 7. The SAND formulation in the current section follows the most common way of presentation in the literature.

4.1 **Formulation**

In the SAND approach, the formulation of the problem is modified by treating the state and design variables $\mathbf{z}$ and $\mathbf{b}$ as independent optimization variables. To describe the approach, let us define a composite vector of optimization variables as

$$\mathbf{x} = \begin{bmatrix} \mathbf{b} \\ \mathbf{z} \end{bmatrix} \tag{7}$$

Note that if the structure is subjected to multiple loading conditions, the vector $\mathbf{x}$ will include multiple $\mathbf{z}$ vectors, one for each loading condition. In terms of the vector $\mathbf{x}$, the optimization problem is now defined as follows:

Find $\mathbf{x}$ to minimize the cost function

$$f = f(\mathbf{x}) \tag{8}$$

subject to the constraints

$$\mathbf{h}(\mathbf{x}) = \mathbf{K}(\mathbf{b})\mathbf{z} - \mathbf{F}(\mathbf{b}) = \mathbf{0} \tag{9}$$

$$\mathbf{g}(\mathbf{x}) \leq \mathbf{0} \tag{10}$$

Although linear FEM based analysis equation (9) is considered here, the concept of SAND is quite broad, other analysis methods can be used. Various state variables can be included as optimization variables (Fuchs 1982; Kirsch and Rozvany 1994; Achtziger 1996, 1999a,b, 2000; Tin-Loi 1999a, 2000; and others). The governing equations for general nonlinear or eigensolution problems can be used as equality constraints similar to (9). Note that SAND formulations based on the force method and mixed analysis methods have also been presented (Kirsch 1981, 1993; Kirsch and Rozvany 1994).

4.2 **Gradient evaluation**

The alternate formulation in (8) to (10) looks like a standard optimization problem. In the optimization process, partial derivatives of the functions with respect to $\mathbf{x}$ are needed; i.e., with respect to $\mathbf{b}$ and $\mathbf{z}$. Partial derivatives of f and $\mathbf{g}$ with respect to $\mathbf{b}$ and $\mathbf{z}$ can be easily calculated as noted before. Partial derivative of $\mathbf{h}$ with respect to $\mathbf{z}$ gives the stiffness matrix $\mathbf{K}$ and the partial derivative of $\mathbf{h}$ with respect to $\mathbf{b}$ gives the matrix $\mathbf{S}$ defined in (6). However, $\frac{d\mathbf{z}}{d\mathbf{b}}$ is not needed and no system of equations needs to be solved in the numerical solution process.

Note that the SAND formulation does not require $\mathbf{h}(\mathbf{x}) = \mathbf{0}$ be satisfied exactly at each iteration of the optimization process, i.e., the equilibrium equation need not be satisfied at every iteration, which can be advantageous for nonlinear problems. It needs to be satisfied only at the final solution point. This actually implies that the vector $\mathbf{h}(\mathbf{x}) = \mathbf{0}$ never needs to be solved for $\mathbf{z}$ because $\mathbf{z}$ is treated as an independent variable. The element level equilibrium equations can be used in the solution process. Thus the alternate formulation is ideally suited for implementation on a parallel computer where each finite element can be assigned to one processor. All processors can be used to generate the element level quantities and thus speed-up the optimization process considerably (Haftka 1985; Haftka and Kamat 1989).

Also as noted before, the equilibrium equation (9) may not be the displacement based FEM equation, even though it is the most commonly used one. Most work in the literature has used displacements as optimization variables. However, similar to the conventional formulation, the force method or the mixed method can also be combined with the SAND formulations. The SAND can also be combined with the optimality criteria methods (Kirsch and Rozvany 1994). More recent analysis model - cellular automata (CA) has been imbedded into SAND formulations as equality constraints (Canyurt and Hajela 2004). Besides displacements, other state quantities, such as forces and stresses can also be used as optimization variables (Fuchs 1982; Kirsch and Rozvany 1994; Muralidhar *et al.* 1996; Muralidhar and Rao 1997; Achtziger 1999a,b; Tin-Loi 1999a, 2000; Stope and Svanberg 2003; Wang and Arora 2004).

4.3 **Literature for linear problems**

In the paper by Saka (1980a), a method was presented for the optimum shape design of trusses. The method obtained the optimum locations of the joints, employing the concept of a ground structure. In the formulation, the displacements of the joints were treated as optimization variables in addition to member areas and joint coordinates. For the solution of the nonlinear design problem, linear approximation scheme was adopted. The proposed design procedure did not require the structural analysis equations to be solved during the iterative process. Saka proposed an alternate formulation for minimum weight design of rigid frames, subject to both stress and displacement constraints (Saka 1980b). Optimization variables included not only the areas of the members, but also the displacements of joints. Displacement method was used in the formulation. Element stiffness equations were imposed as equality constraints. The nonlinear optimization problem was transformed to a linear programming problem and the Simplex method was used to solve the problem after the move limits were specified. The author pointed out that the numbers of iterations to search the optimum solutions were smaller compared to the conventional formulation.

Fuchs presented an explicit optimum design method for linear elastic trusses of given geometry and material properties (Fuchs 1982, 1983). Three techniques were presented, according to the three classical analysis methods – force, displacement and hybrid (or mixed) methods. The formulation was in a mixed space of design and state variables. Explicit expressions for the objective function and the constraints in terms of the variables could be obtained. The structures were optimized using sequential unconstrained minimization techniques (SUMT) with a conjugate directions algorithm. In the case of a single loading condition without variables linking, the proposed method was very efficient. In other cases for variable linking and multiple load cases, efficiency of the method depended on the specific problem.

The penalty function method was used to solve the simultaneous analysis and design problem by Haftka (1985). The preconditioned conjugate gradient method and the Newton method were used to minimize the penalty function. The element-by-element formulation and a pre-conditioner were used to treat the equilibrium equation in the penalty function. A 72-bar truss subjected to stress constraints and a wing box structure subjected to nonlinear collapse constraints were optimized. SAND formulation showed substantial computational savings compared to the conventional nested approach.

Ringertz (1986) presented a branch and bound algorithm for topology design of truss structures, subject to stress and displacement constraints. The central idea was to use a ground structure to select a minimum weight truss. A sequence of sub-trusses called candidate trusses were generated and analyzed. Both cross-sectional areas and displacements were treated as independent variables; therefore it was possible for member cross-sectional areas to reach zero. Several criteria were used to discard non-optimal configurations rapidly. Three different optimization methods, including sequential quadratic programming (SQP) were used to solve the nonlinear problem. SQP generally solved the problems quite rapidly.

Bendsøe *et al.* (1991), and Ben-Tal and Bendsøe (1993) proposed two alternate approaches for topology design of trusses for maximum stiffness with a prescribed volume. The ground structure was used, and the problem was formulated in terms of cross-sectional areas and nodal displacements. The optimization problem could be solved by a SAND approach. Alternatively, this large, nonconvex formulation was transformed to an equivalent, unconstrained and convex problem in terms of nodal displacements only. This new formulation was mathematically proved to be equivalent to the original problem, and solved by a non-smooth, steepest descent algorithm. In both the methods, explicit solution of the equilibrium equations and the assembly of the global stiffness matrix were avoided. It was noted that this algorithm was attractive computationally.

Topology optimization of trusses for minimum weight using the SAND formulation was presented by Sankaranarayanan *et al.* (1994). The ground structure approach was used, and the design considered stress and displacement constraints. An extended interior penalty function formulation of SAND was compared with an augmented Lagrangian formulation. The SAND formulation was also compared with the minimum compliance formulation. Several example problems of truss topology design were solved. The augmented Lagrangian approach worked better than the penalty function approach. It was also concluded that the minimum compliance method might not get the true optimal design.

Kirsch and Rozvany (1994) focused on presentation of several alternate but equivalent formulations for the structural optimization problem. The formulations discussed were different with respect to the independent variables, the analysis methods and the form of resulting constraints. The analysis methods included the displacement, force and the mixed methods. The problem formulations considered included design variable space formulation, SAND formulation, and some formulations based on optimality criteria. Details of the formulations were discussed for truss type structures. Some simplified SAND formulations that could be solved using linear programming were also described. Note that the SAND formulations based on the force method were also presented in the monographs by Kirsch (1981, 1993). The basic idea was to treat the redundant forces as optimization variables in addition to the design variables, and the compatibility conditions are treated as equality constraints. This has advantages in some cases, such as when the number of redundant forces is small. However, sometimes it is tedious to identify a determinate system for complex structures.

Other optimization methods were employed in the SAND formulations of truss design, such as the augmented Lagrangian (AL) method with duality (Larsson and Rönnqvist 1995). The displacements and design variables were optimized simultaneously. The formulation was based on linear objective function, stress constraints and explicit bounds on the variables. Two techniques were used for the Lagrangian subproblems. Numerical experiments were performed for different values of the penalty parameter and the rate at which it was increased. It was concluded that the SAND approach using the AL was promising for further research.

A SAND approach based on cellular automata (CA) and cellular genetic algorithm (CGA) for analysis and optimization was presented by Canyurt and Hajela (2004). The structural analysis model was based on CA – a relatively new alternative computational model (Kita and Toyoda 2000; Hajela and Kim 2001; Abdalla and Gürdal 2004). The optimization was performed by the CGA. Therefore, the analysis and optimization evolved simultaneously in a unified cellular computational framework. Three SAND formulations were developed and compared. It was concluded that SAND formulations were far more efficient than the conventional formulation. The SAND formulation with CA based analysis was even more efficient than that combined with the FEM analysis. The approach was applied to discrete structural systems for sizing and shape design. Parallelization potential for the CGA based SAND was noted as another advantage of the approach.

4.4 Literature for nonlinear problems

A major difference between SAND and the conventional approaches is that the implicit dependence between the analysis and design variables becomes explicit. In the conventional formulation, nonlinear analysis equations must be solved for any design update. However, the SAND approach does not require repeated solution of the nonlinear analysis equations, since they need to be satisfied only at the optimal solution. The equations of equilibrium in (9) become nonlinear that are treated as equality constraints. Therefore, SAND has additional advantages for nonlinear problems. For such problems, (9) can be written as

$$\mathbf{h}(\mathbf{x}) = \mathbf{P}(\mathbf{b},\mathbf{z}) - \mathbf{F}(\mathbf{b}) = \mathbf{0} \tag{11}$$

where **P**(**b**,**z**) is the internal force vector. The evaluation of $\mathbf{h}$ in (11) is quite straightforward, as no matrix decomposition is needed. Suppose $\mathbf{F}$ is not a function of $\mathbf{z}$, then the derivatives of (11) are given as

$$\frac{\partial \mathbf{h}(\mathbf{x})}{\partial \mathbf{b}} = \frac{\partial \mathbf{P}(\mathbf{b},\mathbf{z})}{\partial \mathbf{b}} - \frac{\partial \mathbf{F}(\mathbf{b})}{\partial \mathbf{b}} \tag{12}$$

$$\frac{\partial \mathbf{h}(\mathbf{x})}{\partial \mathbf{z}} = \frac{\partial \mathbf{P}(\mathbf{b},\mathbf{z})}{\partial \mathbf{z}} = \mathbf{K}_T(\mathbf{b},\mathbf{z}) \tag{13}$$

where $\mathbf{K}_T(\mathbf{b},\mathbf{z})$ is the tangent stiffness matrix, and $\frac{\partial \mathbf{P}(\mathbf{b},\mathbf{z})}{\partial \mathbf{b}}$ in (12) can be calculated in an element-by-element manner. If the equilibrium equation in (11) is derived from the minimum potential energy, the tangent stiffness matrix in (12) can also be obtained as Hessian of the strain energy U as $\nabla^T \nabla U(\mathbf{x})$ (Ringertz 1992, 1995).

Schmit and Fox (1965, 1966) included state variables in the structural optimization problem that was called “an integrated approach to structural synthesis”. The material nonlinearity was considered in the stress-strain relationship. The basic idea was to transfer an inequality constrained minimization problem in design variable space, into an unconstrained problem in a space of mixed design and state variables. The penalty function technique and a steepest-descent type procedure were used. The cross-sectional areas, stresses of bar elements, free nodal displacements and the position of the attachment point were treated as variables, and the equilibrium equations were taken as equality constraints. The results in the papers indicated that the integrated approach offered the prospect of making substantial improvements in the efficiency of the structural synthesis process, particularly when linearization of the structural analysis problem was inappropriate.

Smaoui and Schmit (1988) presented an integrated approach to the minimum weight design of geometrically nonlinear static truss structures with geometric imperfections. The design considered constraints on displacements, stresses, local buckling and cross sectional areas. The independent variables included design and response quantities simultaneously. The FEM equilibrium equations were treated as equality constraints. A generalized reduced gradient (GRG) algorithm was used to solve the integrated problem. It was also concluded that the simultaneous formulation could detect elastic instabilities efficiently.

Simultaneous and nested approaches were compared for three truss optimization problems in Haftka and Kamat (1989). Geometrically nonlinear analysis of the truss structure was included in the formulation. The SAND formulation was solved using the penalty method and the projected Lagrangian method. The nested formulation was solved either by the projected Lagrangian method or the GRG method. For the penalty method, an element-by-element conjugate gradient approach with a pre-conditioner was used. It was concluded that the simultaneous approach was competitive with the conventional nested approach, and that it was more efficient for large-scale problems.

Ringertz (1989) formulated the minimum weight design of structures with geometrically nonlinear behavior in two different ways. In the first one, the design variables and displacements were treated together as independent variables. All the equilibrium equations were treated as constraints. In the second one, the displacements were transformed such that only a few of the equilibrium equations needed to be treated as constraints. The design variables and only the transformed displacements were treated as independent variables. The optimization problems associated with both formulations were solved using an SQP method. It turned out that the first formulation led to a larger problem; however, the functions and gradients were relatively easy to evaluate.

Ringertz (1992) presented a method for the optimal design of geometrically nonlinear shell structures subject to conservative external loads. Shell thicknesses and cross-sectional dimensions of beam stiffeners were used as design variables. The nonlinear optimization problem was solved using a Newton barrier method. In a later paper, an algorithm for optimal design of nonlinear stiffened shell structures was presented (Ringertz 1995). The algorithm used numerical optimization techniques and the nonlinear finite element analysis to find a minimum weight structure subjected to equilibrium, stability and displacement constraints. An SQP method was used to solve the resulting nonlinear optimization problem. System stability constraints were considered in the formulation. Matrix sparsity in the Jacobian of constraints was exploited for numerical efficiency.

The truss optimization problem was formulated as a SAND problem by Orozco and Ghattas (1991, 1997). Geometrically nonlinear behavior of the structure was included in the formulation. A reduced SQP method was presented to solve the problem. In that approach, a QP subproblem was defined in the entire optimization variable space for the search direction. Then it was desired to utilize the structure of the problem functions so that the existing finite element analysis programs might be utilized. Orthogonal or coordinate basis decomposition of the Jacobian of the equality constraints was performed. Using the decomposition, the search direction determination QP subproblem was obtained only in terms of the reduced variables (i.e., same as the number design variables). It was concluded that the reduced SAND formulation required fewer structural analyses but the same amount of storage as NAND. SAND formulation was large but sparse. To make it tractable, sparse matrix approaches must be used (Orozco and Ghattas 1991).

Tin-Loi (2000) discussed optimum shakedown design of discretized elastoplastic structures subjected to variable repeated loads and residual displacement constraints. The problem was formulated according to the classical lower bound theorem of shakedown, considering appropriate constraints on deflections from existing bounding results. The resulting SAND formulation was directly solved as an NLP by using an available modelling system.

4.5 **Optimization techniques for SAND**

The SAND formulations have been solved successfully by various methods in the literature. New solution techniques have been developed in recent years. SUMT based on the penalty function techniques were used by Schmit and Fox (1965), Fuchs (1983), Haftka (1985), Haftka and Kamat (1989), and Ringertz (1992). Augmented Lagrangian methods were considered by Sankaranarayanan *et al.* (1994), and Larsson and Rönnqvist (1995). Saka (1980a,b) and Achtziger (1999a,b) used the sequential linear programming (SLP) approach. A generalized reduced gradient (GRG) algorithm was used to solve the integrated problem by Smaoui and Schmit (1988), and Tin-Loi (1999a,b, 2000). Haftka and Kamat (1989), and Orozco and Ghattas (1991) used the projected Lagrangian algorithm. Various SQP methods were used by Ringertz (1986, 1989, 1995), Orozco and Ghattas (1991, 1997), Schulz and Bock (1997), Dreyer *et al.* (2000), Stolpe and Svanberg (2003), Schulz (2004), and Wang and Arora (2004). Ben-Tal and Nemirovski (1993), Ben-Tal and Roth (1996), Jarre *et al.* (1998), Maar and Schulz (2000), Herskovits *et al.* (2001), Hoppe *et al.* (2002), Herskovits (2004), and Hoppe and Petrova (2004) used newly-developed interior point algorithms to solve SAND formulations. Multigrid methods combined with SQP or interior point method have been successfully applied to SAND formulations by Dreyer *et al.* (2000), and Maar and Schulz (2000). A genetic algorithm has also been recently applied to SAND formulation (Canyurt and Hajela 2004).

5. Displacement based two-phase formulation

5.1 Formulation

The displacement based approach was introduced by McKeown (1977) for optimization of composite structures. Although there are variations in the method used by different researchers, the central ideas are the same: the design problem is divided into a two-level optimization problem, where only the design variables are treated as optimization variables in the inner problem, and only the displacements are treated as variables in the outer problem.

The inner optimization problem is defined as follows: for given displacements $\mathbf{z}$, find the design variable vector $\mathbf{b}$ to minimize a cost function,

$$f = f(\mathbf{b}) \tag{14}$$

subject to the side constraints on $\mathbf{b}$, as well as the governing equilibrium constraints:

$$\mathbf{h}(\mathbf{b}) = \mathbf{K}(\mathbf{b})\mathbf{z} - \mathbf{F}(\mathbf{b}) = \mathbf{0} \tag{15}$$

The solution of the inner problem in (14) and (15) provides only a temporary optimal solution corresponding to the given displacement field $\mathbf{z}$. In order to find the true optimal solution for the original problem, the displacements $\mathbf{z}$ need to be treated as optimization variables and updated. Thus the outer problem is to find the displacement vector $\mathbf{z}$ to minimize the cost function in (14) (expressed in terms of $\mathbf{z}$) :

$$f = f(\mathbf{z}) \tag{16}$$

subject to the constraints

$$\mathbf{g}(\mathbf{z}) \leq \mathbf{0} \tag{17}$$

Constraints in (17) may include stress or displacement requirements. Nonlinear analyses can be similarly considered if the governing equilibrium equation in (15) is replaced by the corresponding nonlinear equation.

5.2 **Gradient evaluation**

Equation (15) is much like (9) in the SAND formulation, except that the state variable $\mathbf{z}$ is known. In the numerical solution process, partial derivative of $\mathbf{h}$ with respect to $\mathbf{z}$, and $\frac{d\mathbf{z}}{d\mathbf{b}}$ are not needed; therefore, no sensitivity analyses or solutions of the equilibrium equations are needed. Note also that in the displacement based formulation, $\mathbf{h}(\mathbf{b}) = \mathbf{0}$ is not required to be satisfied exactly at each iteration of the solution process for the inner problem; it needs to be satisfied only at the final solution of the inner problem.

For the outer problem where $\mathbf{z}$ is treated as the optimization variable, derivative of f in (16) with respect to $\mathbf{z}$ is needed. However, an explicit expression for f in terms of $\mathbf{z}$ is not known. Therefore an implicit differentiation procedure must be used. Using such a procedure an explicit expression for derivative of (16) with respect to the displacements can be obtained (McKeown 1989; Missoum and Gürdal 2002).

5.3 **Literature overview**

The displacement based method was introduced for optimal design of multilaminar, fiber-reinforced continua (McKeown 1977). The structures of maximum stiffness were considered. It was shown that the proposed algorithm based on the functional LP, was convenient to solve the nonlinear mixed-integer programming problem. In a later paper, the author analyzed his two-phase algorithm and applied it to optimize trusses (McKeown 1989). The outer problem was solved using either sequential linear programming (SLP) or another NLP algorithm. The displacement field for the structure was specified for the inner problem. The inner problem is similar to the ones in Wang *et al.* (1984), and Ringertz (1985). McKeown (1998) expanded the two-phase optimization procedure to geometry and layout design of trusses. Instead of using a complex ground structure, the author considered growing least-volume trusses, starting from the simplest possible layout. The outer problem included only the displacements and position variables, while the inner problem included the cross-sectional areas of the bars. That approach for the optimal-layout problem was shown to be well suited to deflection-space methods of solution, which allowed the geometry and layout to be optimized simultaneously. General features of the proposed method were discussed and it was concluded that the method could greatly reduce the problem size and was feasible for practical applications.

Wang *et al.* (1984) also presented a two-stage LP procedure for the minimum weight design of trusses. In the first stage, the so-called behavior stage, the joint displacements were chosen as the basic variables and their optimum values were found by using an optimality criterion method - the maximum total strain energy criterion using LP. In the second stage, the structural stage, the design variables, i.e., the cross-sectional were chosen as variables and the minimum weight design was obtained, using again the LP. The authors pointed out that the method could avoid the need for repeated iterations and structural reanalyses. It was effective for the minimum weight design of trusses-type structures with stress, displacement and geometric constraints.

Striz and Sobieszczanski-Sobieski (1996) proposed a displacement based multilevel approach for structural optimization. In the system level, the unbalanced loads in the global equilibrium equations were minimized subject to displacement constraints. The optimization variables were the coefficients of the assumed global displacement functions. In the subsystem level, structural weight was minimized subject to the stress constraints. The sizing variables were treated as independent variables. The method was in fact a two-phase method. Since the subsystems level optimizations were independent of each other, they could be performed in parallel (Plunkett *et al.* 2001). In a recent paper by Subramaniyam *et al.* (2004), the system level FE analysis and optimization was parallelized as well by using the domain decomposition and the super-element formulation. Several large-scale trusses were optimized using a dense SQP solver.

In a paper by Missoum and Gürdal (2002), the two-phase optimization procedure of McKeown (1977, 1989) was presented and applied to optimum design of static and dynamic trusses. In the inner loop, the problem was shown to be linear, and so LP was used to solve the problem. In the outer loop, the sequential linear programming (SLP) algorithm was used. Since the weight was an implicit function of the displacements, a procedure was presented to calculate derivatives of the weight with respect to the displacements. Two truss examples were optimized to show that the procedure was more efficient than the conventional approach.

Gu *et al.* (2002) extended the displacement based optimization approach to design trusses with nonlinear material behavior. Path independent material models were used. It was noted that some times the inner problem could be infeasible because there might not be a structure that could satisfy the specified displacement field. Therefore slack variables were added to the equilibrium equation to define a relaxed problem that had feasible solutions. Several truss problems were solved with linear and nonlinear (elastic-perfectly-plastic, elaso-plastic with hardening) behavior to demonstrate the methodology and compare the solutions wherever they were available. The displacement variables were normalized using the minimum and maximum allowable values.

Geometric and material nonlinearities were included in the formulation by Missoum *et al.* (2002a). It was shown that the displacement based approach was quite efficient compared to the conventional NAND approach. Missoum *et al.* (2002b) also extended their work to the optimization of geometrically nonlinear frames. If the cross sectional areas and the second moment of the areas were taken as unknown variables, the inner problem turned out to be an LP problem even for nonlinear equilibrium equations. Two dimensional frame examples were solved and it was shown that the displacement based approach could obtain similar results as the conventional NAND approach. However, the displacement based approach required much more computational time, indicating that there were some convergence difficulties.

6. Comparison of conventional, SAND and displacement based formulations

Table 1 lists the sizes of all the three formulations discussed earlier. The following symbols are used: k = dimension of design variables vector $\mathbf{b}$; n = dimension of state variables (e.g., displacement) vector $\mathbf{z}$; m = number of inequality constraints in $\mathbf{g} \le \mathbf{0}$ (e.g., stress constraints, excluding bounds on variables). Assume that there are $2k$ bound constraints on the design variable vector $\mathbf{b}$, and $2n$ bound constraints on the state variable vector $\mathbf{z}$. For the displacement based formulation, the numbers in the brackets are for the inner problem, and outside the brackets are for the outer problem. When the slack variables are introduced, the numbers of variables and constraints may change in the displacement based formulation. Table 2 lists the comparison of the three formulations - the conventional, SAND and displacement based. Advantages and disadvantages of each formulation are discussed.

In both the alternative formulations, displacements are chosen as optimization variables by most researchers, and the analysis equations are treated as equality constraints. The inclusion of displacements as variables simplifies the constraint expressions and computer implementations.

The reason is that they lead to a simpler form for the constraints which the optimization algorithm can treat more efficiently. Also the alternative formulations avoid repeated analysis of the structure; therefore, they are more efficient. This will also be the case for nonlinear structures where the conventional formulations need to solve the equilibrium equations at each iteration, which is expensive.

Table 1 Number of variables and constraints for different formulations

	Conventional Formulation	SAND Formulation	Displacement Based Formulation
No. of Variables	k	$k+n$	n [k or $k+2n^*$]
No. of Equality Constraints	0	n	0 [n]
No. of Inequality Constraints	$m+2n$	m	m [0]
No. of Simple Bounds	$2k$	$2k+2n$	$2n$ [$2k$ or $2k+2n^*$]

*When slack variables are considered.

In the SAND formulations, the optimization problem is very large because there are more variables in a single optimization process. It can easily exceed the capacity of current optimization codes and computers. However, SAND formulations simplify the forms of constraints and their Jacobians, which are advantageous for numerical algorithms and implementations. The displacement based formulation basically decomposes the original problem to two smaller subproblems, which can be solved more efficiently. However the application of the displacement based formulation is not as straightforward as the SAND formulation. The decomposition to some extent complicates the problem, and some aspects of it are still not fully understood (Missoum *et al.* 2002b). The cost function in terms of the state variables is not defined everywhere in the displacement space, which may make the outer problem non-differentiable. Another difficulty is that the inner problem may have no solution. Therefore, slack variables need to be introduced to relax the equilibrium equations. Beside these, variable and constraint scaling are needed in both the formulations to reduce numerical difficulties, since they include variables and constraints of different orders of magnitude.

7. Configuration and topology design

Many interesting formulations for configuration and topology design optimization have been presented in the literature. These include the ground structure approach for discrete element structures and a more general continuum topology optimization formulation. Mijar *et al*. (1998) have used a continuum topology optimization approach to design bracing systems for framed structures. The literature on the subject of topology optimization is vast and many good

Table 2 Advantages and disadvantages of three formulations

Formulation	Advantages	Disadvantages
Conventional	1. Least number of optimization variables. 2. Equilibrium equation is satisfied at each iteration. 3. Intermediate solutions may be usable.	1. Equilibrium equation must be solved at each iteration, which can be expensive. 2. Constraints are implicit functions of the variables; their evaluation requires analysis. 3. Design sensitivity analysis must be performed. 4. Implementation is tedious. 5. Dense Jacobian and Hessian matrices; difficult to treat large-scale problems
SAND	1. Formulations are explicit in terms of variables. 2. Equilibrium equation is not solved at each iteration. 3. Many constraints become linear in variables. 4. Jacobians and Hessian are sparse. 5. Design sensitivity analysis is not needed. 6. Implementation is relatively straightforward. 7. Multi-physics problems are easier to optimize. 8. Lagrange multipliers for more constraints become available which may give further insights for practical applications.	1. Numbers of variables and constraints are large. 2. Intermediate solutions may not be usable. 3. Optimization algorithms for large-scale problems must be used. 4. For efficiency, advantage of sparsity of the Jacobians and Hessians must be utilized. 5. Optimization variables need to be normalized.
Displacement Based	1. Two smaller sub-problems are solved. 2. Equilibrium equation is not solved at each iteration. 3. The inner problem is linear or quadratic. 4. Design sensitivity analysis is not needed.	1. The outer problem may be non-differentiable. 2. The inner problem may have no solution. 3. Displacement variables need to be normalized.

references are available that describe various formulations and solution algorithms (Bendsøe and Kikuchi 1988; Bendsøe and Mota Soares 1993; Jog et al. 1994; Ohsaki 1995; Rozvany *et al.* 1995; Bendsøe 1995; Swan and Kosaka 1997a,b; Eschenauer and Olhoff 2001; Bendsøe and

Sigmund 2003; and others). In this paper, we will focus on describing only some recent work related to the SAND formulation and the corresponding computational algorithms for topology optimization. It turns out that the SAND formulation is an important foundation for these design problems. A typical approach for topology optimization is to minimize the external work (compliance), where design variables together with the displacements are the optimization variables (Beckers and Fleury 1997). These problems are not convex when the equilibrium equations are included in the formulation. However, they may be reformulated as convex problems in different ways. Bendsøe *et al.* (1994), Bendsøe (1995), and Bendsøe and Sigmund (2003) reviewed different formulations for minimizing the compliance for the truss geometry and topology design. They noted that the compliance could be expressed in a number of equivalent potential or complementary energy formulations using the member forces, displacements and bar areas. Using the duality principles and non-smooth analysis it was shown how displacement-only and stress-only formulations could be obtained. The equilibrium equations were part of these formulations even though they might be in the dual problem or other simplified forms. Topology optimization has also been re-formulated into some alternative formulations, such as semidefinate programming (SDP) (Ben-Tal and Nemirovski 1997; Kočvara *et al.* 2000; Ben-Tal *et al.* 2000; Kočvara 2002), and linear programming (LP) problems (Achtziger *et al.* 1992; Muralidhar and Rao 1997). Some detailed SAND formulations and references to the convex re-formulations mentioned above can be found in the monographs by Bendsøe and Mota Soares (1993), Bendsøe (1995), and Bendsøe and Sigmund (2003).

The most common way to formulate a structural topology optimization is the *minimization of compliance*, defined as:

$$\frac{1}{2}\mathbf{F}^T\mathbf{z} \tag{18}$$

subjected to the state equations (1), and the constraints on the total volume and each element volume:

$$\sum \mathbf{v} = V_{total} \tag{19}$$

$$\mathbf{v}^L \leq \mathbf{v} \leq \mathbf{v}^U \tag{20}$$

where $\mathbf{F}$ and $\mathbf{z}$ are the same as defined in (1). $\mathbf{v}$ is the vector of element volumes and $\mathbf{v}^L$ and $\mathbf{v}^U$ are the corresponding lower and upper bounds. V_{total} is the total given volume of the structure. Although the problem of minimization of compliance can be solved by the SAND approach (Bendsøe *et al.* 1991; Ben-Tal and Bendsøe 1993), direct minimization of the weight for truss topology design by the SAND approach is also possible. This was studied by Ringertz (1986), Sankaranarayanan *et al.* (1994), Achtziger (1996, 1999a,b), Petersson (2001), Stolpe and Svanberg (2003a,b), and many others. Oberndorfer *et al.* (1996) discussed the advantages and disadvantages of these two formulations. They showed that for the condition where the allowable stresses for tension and compression members of trusses were identical, the two formulations became equivalent.

The beauty of the SAND and displacement based formulations for topology design is that both cross-sectional areas and displacements are treated as independent variables; therefore it is possible for member cross-sectional areas to reach zero value without causing singularity or non-differentiability. If the ground structure method is used in topology design, there are a very large number of cross-sectional areas and a relatively small number of displacement variables; therefore, the SAND formulation has an advantage, since the size of the problem is not increased substantially. The use of various SAND formulations for configuration and topology design can be found in Saka (1980a), Ringertz (1986), Bendsøe *et al.* (1991), Achtziger *et al.* (1992), Grossmann *et al.* (1992), Bendsøe and Mota Soares (1993), Ben-Tal and Bendsøe (1993), Bendsøe *et al.* (1994), Sankaranarayanan *et al.* (1994), Bendsøe (1995), Muralidhar *et al.* (1996), Ben-Tal and Roth (1996), Ben-Tal and Zibulevsky (1997), Muralidhar and Rao (1997), Jarre *et al.* (1998), Hilding *et al.* (1999), Achtziger (1999a,b, 2000), Kočvara *et al.* (2000), Ben-Tal *et al.* (2000), Maar and Schulz (2000), Petersson (1999, 2001), Hoppe *et al.* (2002), Stope and Svanberg (2003a,b, 2004), and Bendsøe and Sigmund (2003). Displacement based two-phase approaches for configuration and topology design have also been used by Wang *et al.* (1984), McKeown (1989, 1998), Gu *et al.* (2002), and Missoum and Gürdal (2002).

Achtziger (1996, 1999a,b, 2000) studied truss topology optimization using SAND formulations, with the nodal displacements or the internal forces treated also as optimization variables. Truss topology optimization including different bar properties for tension and compression members was presented by Achtziger (1996). It was found that the bar properties had a large influence on the optimal design. In later papers (Achtziger 1999a,b), optimal truss topology design subject to stress, slenderness, and local buckling constraints was studied. It was proved that the inclusion of slenderness constraints could guarantee a solution, which could not be done otherwise with the inclusion of only the classical equilibrium, stress, and local buckling constraints. After eliminating the discontinuity of constraints and applying a linearization concept, the final formulation was solved using the SLP method. Achtziger (2000) discussed the same design problem by a technique that minimizes a continuous function on a finite set of continuous constraints. A method was proposed to approximate the original problem by a standard NLP problem that depended on a parameter. It was proved that each solution to the approximating problem was a solution to the original one, provided that the parameter was large enough.

Muralidhar and Rao (1997) presented new models for optimal truss topology design for limit states based on a unified elastic/plastic analysis. Several equivalent formulations to maximize the load-carrying capacity were presented for a prescribed volume subject to complementary energy and stresses constraints. The original convex but high-dimensional nonlinearly constrained formulation was transferred to several simpler but nonsmooth equivalent models, using the duality principles. These simpler design models greatly reduced the problem size, since they did not contain element volumes as variables. Furthermore, the strictly plastic and elastic limit design models were reduced to LP problems, and were shown to be equivalent to the widely studied model for minimum compliance topology design of elastic trusses.

Ben-Tal and Roth (1996) described a path-following interior point algorithm, which employed a truncated logarithmic barrier function for large-scale constrained convex programming and min-max problems. Ben-Tal and Zibulevsky (1997) later studied nonquadratic augmented Lagrangians for which the penalty parameters were functions of the multipliers for solving convex programs. More importantly, a new type of penalty/barrier function was introduced and used to construct an efficient algorithm. The algorithms were applied to large-scale convex quadratically constrained truss topology models transformed from the original minimization of the compliance model. Jarre *et al.* (1998) studied optimal truss topology design problem using the same formulation; however, they used a primal-dual predictor-corrector interior-point method, which showed efficiency for large-scale problems.

Kočvara (1997) presented a bilevel programming approach for topology optimization of trusses to minimize compliance with displacement constraints. The upper-level problem was to minimize the gap between the actual and prescribed displacements. The lower level problem was to minimize the compliance to find the stiffest structure satisfying the displacement constraints.

At the lower level a standard truss topology problem was formulated in a way to be solved by the efficient interior point algorithms. The overall bilevel problem was solved by the so-called implicit programming approach, which was nonsmooth. In the implicit programming approach, the state variables were implicitly eliminated from the problem.

Petersson (1999) studied some convergence results in perimeter-controlled topology optimization of elastic continuum structures. The approach was claimed to be attractive, because it could predict “black-white” topologies without the use of homogenization techniques. It showed that a new perimeter which measured lengths of structural edges after projection onto the coordinate axes was appropriate to approximate the intended original problem. Petersson (2001) also studied the continuity of the design-to-state mappings for stress-constrained minimum weight design of trusses with variable topology. The goal was to investigate continuity of the changes of the forces and nodal displacements present in equilibrium equations with respect to modification of the cross-sectional areas. In these papers, the simultaneous and nested formulations were discussed in parallel.

Kočvara *et al.* (2000) and Ben-Tal *et al.* (2000) presented solutions of the free material design problem via semidefinite programming (SDP). In the first paper, the so-called cascading - an approach to robust material optimization, was developed. The design variables were the material properties at each point of the structure. In the second paper, multiple loading cases with contact conditions were considered. The stiffest structure with respect to one or more given loads was designed where both the distribution of the material and the material properties could vary freely. After some transformation steps and a suitable discretization, the problem was transferred to a formulation for which the solution was shown to exist. The resulting large-scale SDP problems were solved by an interior point method.

Maar and Schulz (2000) developed a new simultaneous interior point multigrid method for topology optimization based on homogenization. The linear-quadratic subproblems in the interior point method were solved efficiently by the multigrid methods. As discussed by the authors, the application of multigrid methods to structural optimization problems enhanced the state of the art of this important research area. In another paper, Dreyer *et al.* (2000) combined a multigrid solution technique in the framework of SQP to solve topology optimization problems. The focus was on two formulations: one was the simultaneous multigrid method for solution of the QP subproblems, and the other was a reduced SQP with multigrid solution of the linearized mode equation. The multigrid methods for saddle-point problems were also discussed.

Hoppe *et al.* (2002) presented a primal-dual Newton-type interior-point method for topology optimization of a conductive electromagnetic medium with a fixed geometry and bound constraints for the conductivity. The objective was to minimize the energy dissipation, and the elliptic differential equation for the electric potential was treated as an equality constraint. The PDE-constrained problem was discretized by finite-elements and formulated as a SAND problem. A condensed primal-dual system was obtained from the KKT optimality conditions and was solved by transforming iterations to determine the search directions. In a later paper by Hoppe and Petrova (2004), the same interior point algorithm was applied to the optimal shape design of microstructured materials based on homogenization and adaptivity. The paper focused on the shape optimization of new biomorphic microcellular silicon carbide ceramics produced from natural wood by biotemplating. The best combination of materials and shapes in order to achieve the optimal pre-specified performance of the composite material was pursued.

Kočvara (2002) studied the modelling and solution of the truss design problem with global stability constraints. The stability constraint was based on the linear buckling formulation. The problem was formulated as a nonconvex SDP problem and solved by an interior point algorithm. Although the general problem could be formulated as a SAND problem, the final solution technique was not based on SAND.

Stolpe and Svanberg (2003a) presented a simultaneous formulation for stress-constrained truss topology optimization. The element forces were also treated as optimization variables besides sizing variables and nodal displacements in the SAND formulation. A general-purpose optimization method and code were used. They discussed that the method might find also “singular optima” without using perturbation techniques. In a later paper, (Stolpe and Svanberg 2004), a stress-constrained truss-topology and material-selection problem that could be solved by linear programming was presented. The cost of the structure was minimized subject to stress constraints under a single load condition. They concluded that the global optimum could be obtained, and the optimal design always contained at the most two different materials.

Schulz (2004) studied efficient simultaneous solution approaches for practical large optimization problems that include PDE-models. The two applications included a parameter identification problem of Bingham flow and topology design in electro-magnetics. Reduced SQP methods and simultaneous QP iterations were discussed. It was concluded that the algorithms had considerably less overall computational complexity in comparison to a black-box approach.

The SAND formulation is also a key component when formulating structural design problems with integer design variables. Grossmann *et al.* (1992) studied some mixed-integer linear programming (MILP) re-formulations for some nonlinear discrete design optimization problems. It turned out that the MILP model could be solved to yield a global optimum solution. One application considered was topology design of trusses. Bollapragada *et al.* (2001) presented a logic-based branch-and-cut method for truss design problems. The proposed method was able to solve substantially larger problems than MILP, even though the nonlinearities disappeared in the mixed integer model. Stolpe and Svanberg (2003b) presented topology optimization of discretized continuum structures as linear mixed 0-1 programs. It was shown that a large class of nonlinear 0-1 topology optimization problems could equivalently be modelled as linear mixed 0-1 programs. These included the common minimum weight design problems subject to stress and displacement constraints. It was shown that the global optimum solutions could be obtained.

8. PDE-constrained optimization

Recently, a general class of formulations known as PDE (partial differential equations)-constrained optimization has been presented and discussed. In this formulation, the equilibrium equations are kept in the continuum form instead of the discretized form given in (1). Use of the continuum form offers flexibility in terms of the range of applications of optimization to many different fields including multidisciplinary applications. Also, many PDE solution algorithms and solvers, including the finite element method, can be used to perform optimization of complex systems. The design or the control variables may also be described in the distributed parameter form and discretized for numerical calculations. In the PDE-constrained optimization literature, the term “decision variables” is used to represent design or control variables, or both of them. Problems of optimal design, optimal control, and parameter estimation of systems from many diverse application areas can be formulated in this way.

It is clear that the PDE-constrained optimization formulation is a generalization of the discretized optimization formulations discussed in the previous sections. Therefore it is important to note that the conventional NAND and the SAND approaches discussed previously are applicable directly to the PDE-constrained optimization formulations. Thus all the advantages and disadvantages discussed previously for NAND and SAND approaches apply to this formulation as well.

A recent workshop, the *First Sandia Workshop on Large-Scale PDE-Constrained Optimization*, was held to focus on the issues related to this topic. The basic idea was to bring researchers in the fields of PDE and optimization together to foster greater synergy and collaboration between these communities. The proceeding of this workshop is an excellent source of references that describe the state-of-the-art on this subject (Biegler *et al.* 2003). The major topics discussed at the workshop included: large-scale computational fluid dynamics (CFD) applications, multifidelity models and inexactness of simulations, sensitivities for PDE-based optimization, NLP algorithms and inequality constraints, time-dependent problems, and software frameworks for PDE-constrained optimization. Several papers on these topics are included in the proceedings. Seven challenging issues needing further research and collaboration between the PDE and optimization communities were identified. We present a brief overview of these interesting research problems in the following paragraphs.

8.1 Problem size in PDE-constrained optimization

When the optimization problem, formulated in terms of continuous state and decision variables, is discretized, it can easily lead to millions of variables and equations. For some industrial applications, simulations are nearing gigascale dimensions and terascale memory requirements. The number of decision variables can vary from just a few to the same order as the number of state variables; e.g., problems of topology design of structures, and optimal control of dynamic systems. Solution of such large scale optimization problems requires robust and efficient methods. Such algorithms have also been under development based on the Newton method to solve KKT optimality conditions for the problems, leading to sequential quadratic programming (SQP) algorithms. A variation of SQP is the reduced space algorithm, called rSQP, as discussed previously in Section 4.4. In addition, algorithms based the interior point concept have been developed for large scale problems. Some of these programs are known as SNOPT, SOCS, KNITRO, and LOQO (Biegler *et al*. 2003).

8.2 Integration of NLP and PDE-solvers

For practical applications of optimization, a major challenge is to somehow integrate an existing well tested PDE solver with an NLP algorithm. Four types of such integrations are presented and discussed. These integrations depend heavily on the simulation procedures used in the PDE solvers. Therefore, before discussing the integration approaches, an overview of the simulation procedures is given.

All simulation procedures are based on some discretization of the state variables and the use of Newton-type algorithms to solve nonlinear system of equations. The basic idea of the simulation algorithms is to derive the residual in the state equations to zero. The residual can be interpreted as the error in the solution estimate from the true discretized solution. For a linear system, the residual vector $\mathbf{r}$ is defined using (1) as $\mathbf{r}(\mathbf{z}) = \mathbf{Kz} - \mathbf{F}$. Note that for linear systems the residual $\mathbf{r}(\mathbf{z})$ is a linear function of the state variables $\mathbf{z}$; however, in general it is a nonlinear function of $\mathbf{z}$. To derive the residual to zero during the iterative solution process, Jacobian of the residual is needed. This Jacobian is the matrix $\mathbf{K}$ for the above residual equation which is a constant matrix. However, for nonlinear problems, the Jacobian changes at every iteration of the iterative solution process, as seen in (13), which can require massive computational effort. Therefore many PDE solvers evaluate only an approximate Jacobian while still guaranteeing global convergence to the solution. In addition, many PDE solvers use an iterative procedure to solve the linear system of equations which does not require an explicit exact or approximate

Jacobian; only a matrix-vector product is needed. All these procedure have implications in terms of integration of NLP and PDE solvers for optimization of systems. This is discussed further in the following paragraphs.

The first approach of integrating a PDE solver with an NLP solver is based on the NAND formulation where only the decision variables are treated as optimization variables. Here, the PDE solver can be used easily as a black box if finite difference gradient evaluation is used. Only a small number of decision variables can be treated since the PDE solver must be called repeatedly to simulate the system for a change in each decision variable. This finite difference gradient evaluation may also have accuracy problems. If analytical gradients must be evaluated, then the integration of NLP and PDE solvers becomes more involved requiring additional programming. In the structural optimization literature, this procedure has been demonstrated for many classes of problems using direct and adjoint variable methods of design sensit6ivity analysis (Arora 1995; and many other references).

The second approach is based on the SAND idea where state and decision variables are treated simultaneously as optimization variables. This approach requires at least the Jacobians of the constraint functions and the residual of state equations which is usually not a part of the PDE solver output. Therefore these matrices need to be generated outside the PDE solver, which requires additional programming. The problem, however, is quite sparse and good sparse NLP solvers must be used to solve the optimization problem. The problem of implementation of the SAND approach with the existing finite element analysis programs for structural optimization has been recently studied (Wang and Arora 2004).

The other two possible intermediate implementations between NAND and SAND are related to the rSQP approach explained earlier in Section 4.4. In these approaches, the state variable portion of the search direction vector is eliminated from the search direction determination subproblem by the use of the PDE solver. The direct differentiation or the adjoint approach can be used here. Thus a reduced QP subproblem is obtained to determine the search direction. The advantage of these approaches compared to the NAND approach is that the equilibrium equation need not be solved or satisfied at each iteration. The disadvantages are that the right hand side of the linear system must be formed and the PDE solver must be called to solve the linear system with many different right hand sides. This is equivalent to one iteration of the Newton method to solve nonlinear system of equations. The process becomes complicated for nonlinear and time dependent problems, especially when the adjoint method is used. In any case, these approaches are improvements over the NAND approach. More details of these approaches can be found in Orozco and Ghattas (1997) and Biegler *et al*. (2003).

8.3 Physics-based globalizations and inexact solution

For nonlinear and poorly conditioned problems a number of strategies are used to achieve convergence of the PDE solver. These are called PDE physics-based globalization: mesh sequencing, continuation methods on nonlinear parameters, low fidelity precursor models that provide good initial points for discretized PDEs, and approximate Jacobians that are known to enlarge the region of attraction of the Newton method. Also, the large-scale PDE solvers are often inexact because they are iterative. Many times a reduction in the residual by several orders of magnitudes is acceptable; i.e., an inexact solution is adequate. The challenge here is to integrate these globalizations and inexactness into the NLP algorithms.

8.4 Approximate Jacobians

One of the sources of inexactness in PDE solvers is that they do not construct the exact Jacobians of the PDE residuals. In terms of the structural and mechanical simulation problems, this means that they do not construct the exact stiffness matrices during the solution process. For convergence and numerical performance of the algorithms, exact Jacobians are not needed. However, exact PDE Jacobian is needed to compute gradient of the Lagrangian for search direction calculation and termination of the algorithm. Also many modern Krylov-based PDE solvers approximate the matrix-vector products directly through directional differencing of the residual. Use of approximate Jacobians has implications for PDE-based optimization strategies and algorithms. Exact Jacobians are essential for the SAND approach but not necessary for the NAND. Approximate Jacobians also affect the two intermediate rSQP methods in different ways. The direct rSQP approach can use the same matrix-free approach to evaluate the reduced gradients in the decision variable space. However, for the adjoint rSQP approach which is needed for problems with a large number of decision variables, the matrix-free approach cannot be used without the ability to evaluate matrix-vector products with the transpose of the Jacobian. Therefore exact Jacobians are need here.

8.5 Implicitly-defined and nonsmooth PDE residuals

For many complex problems, the PDE residual is only implicitly defined, e.g., use of moving meshes to treat dynamic interfaces, multiscale models, complex constitutive models, contact problems, and plasticity yield conditions. Some of these problems involve internal computations that are not apparent in the PDE residuals. Additional difficulty is that the residual may not smoothly depend on the state variables. In some cases, the nonsmoothness is inherent in the problem formulation. In other cases, the nonsmoothness is introduced into the residual calculation due to the use of advanced computational devices, e.g., due to adaptive meshing, time stepping or moving mesh schemes. In some cases, the nonsmoothness can be mitigated through reformulation of the problem, e.g., some contact analysis problems. In other cases, fixed meshes or fixed order methods may need to be used.

8.6 Treatment of inequalities

Most optimal design or control problems have bounds on decision and state variables, called the pointwise constraints. When these variables are discretized, the bounds on them lead to a large number of inequality constraints. In the SAND approach, the evaluation of gradients of these constraints is relatively straightforward. However, with the NAND approach, linear systems need to be solved with both direct and adjoint methods of sensitivity analysis. If interior point methods are used, all the constraints are collapsed into a barrier function; therefore gradient of only one function is needed. In cases where this is applicable, the adjoint method of sensitivity analysis may be used for efficiency of calculations.

8.7 Time-dependent problems

All the computational issues discussed for the steady-state PDE optimization are valid and amplified for the dynamic PDE optimization. For such problems, the numbers of decision and state variables become a definite issue. For SAND methods, the entire history of the state variables must be stored which can pose challenge for the storage and manipulation of large amount of data. For NAND type of approaches, the number of decision variables determines whether to use the direct or the adjoint method of sensitivity analysis. Accuracy of the gradients also becomes an issue.

9. Mathematical programs with equilibrium constraints (MPEC)

Mathematical programming with equilibrium constraints (MPEC) is a general class of optimization problems in which some of the constraints are defined by a parametric variational inequality or the so-called complementarity system (Lou *et al.* 1996). The variational equality or inequality constraints model the equilibrium requirements. The MPEC formulation is an extension of the so-called *bilevel programs*, also known as the *mathematical programs with optimization constraints*. The complementarity system of equations mentioned above is a result of the optimality conditions for the optimization constraints. It turns out that the SAND formulations discussed in the literature on structural and mechanical system optimization can be viewed as a special case of the MPEC.

The general MPEC is a nonconvex and nondifferentiable optimization problem which is computationally difficult to solve (Lou *et al.* 1996). Various formulations of MPEC have been studied by Lou *et al.* (1996), Outrata *et al.* (1998), and others. Existence of optimal solutions has been discussed. Exact penalty functions for the complementarity system have been employed to obtain the first order optimality conditions for the MPEC. Numerical algorithms for solving MPEC problems have also been presented. Examples of MPEC problems discussed in the monograph by Lou *et al.* (1996) are: the Bracken-McGill bilevel programs, Stackelberg game, misclassification minimization, motion planning of robot hands, residual minimization of complementarity systems, the parametric feasibility problem, the continuous network design problem, origin-destination demand adjustment problem, a discrete transit planning problem, a facility location and production problem, optimal design problem in mechanical structures, and optimal prestress of cracked structures. Ferris and Pang (1997) have provided a detailed review of engineering and economic applications of complementarity problems. They have presented an extensive documentation of applications of finite-dimensional nonlinear complementarity problems in engineering and equilibrium modelling.

In engineering applications, the MPEC problems can be formulated in a continuum form where a variational principle governs the equilibrium state of the system, such as the principle of minimum potential energy or Hamilton's principle. An advantage of the continuum formulation is that the solution procedure is not tied to any particular numerical approach. Thus it offers more flexibility for numerical solution of the problem. However, to keep the presentation of the basic ideas clearer, we stay with the discretized models of the system. To present and discuss an MPEC problem, consider an elastic body that comes into contact with a rigid smooth object. The problem is to design the body such that an objective function is minimized subject to equilibrium and other requirements, such as non-penetration of bodies, stress and displacement constraints. Using the notations used earlier, the problem is defined as follows:

$$\underset{\mathbf{b}}{\text{minimize}}\ f(\mathbf{b},\mathbf{z}) \tag{21}$$

subject to

$$\underset{\mathbf{z}}{\text{minimize}}\, V(\mathbf{b},\mathbf{z}) \tag{22}$$

$$\mathbf{g}(\mathbf{b},\mathbf{z}) \le \mathbf{0} \tag{23}$$

and

$$\mathbf{c}(\mathbf{b}) \le \mathbf{0} \tag{24}$$

In the outer problem, $f(\mathbf{b},\mathbf{z})$ is the overall objective function to be minimized over the design variables **b**. In the inner problem, the total potential energy function $V(\mathbf{b},\mathbf{z})$ is minimized over the state variable **z**. Some of the constraints in Eq. (23) may be imposed in the inner optimization problem while others may be imposed in the outer problem. For example, contact and non-penetration constraints may be imposed while solving the inner problem while the stress and displacement constraints may be imposed in the outer problem. Also some of these constraints may be equalities. The constraints in Eq. (24) that depend only on the design variables are imposed in the outer problem. The foregoing formulation is an instance of the bilevel optimization problems.

With the assumption of linearly elastic behavior under small displacements, the total potential energy function is given as

$$V(\mathbf{b},\mathbf{z}) = \tfrac{1}{2}\mathbf{z}^T\mathbf{K}(\mathbf{b})\mathbf{z} - \mathbf{z}^T\mathbf{F}(\mathbf{b}) \tag{25}$$

where **K**(**b**) is the structural stiffness matrix, and **F**(**b**) is the equivalent external force vector. Many times the constraints in Eq. (23) can be written as linear function of **z** as

$$\mathbf{g}(\mathbf{b},\mathbf{z}) = \mathbf{A}(\mathbf{b})\mathbf{z} - \mathbf{z}_0 \le \mathbf{0} \tag{26}$$

where **A**(**b**) is a matrix of appropriate dimension and $\mathbf{z}_0$ is a specified vector. Now, writing the KKT optimality conditions for the inner problem, Eqs. (22) and (23) in the formulation can be replaced by the following conditions:

$$\mathbf{K}(\mathbf{b})\mathbf{z} - \mathbf{F}(\mathbf{b}) + \mathbf{A}(\mathbf{b})^T\mathbf{p} = \mathbf{0} \tag{27}$$

$$\mathbf{p} \ge \mathbf{0}\,; \quad \mathbf{g}(\mathbf{b},\mathbf{z}) = \mathbf{A}(\mathbf{b})\mathbf{z} - \mathbf{z}_0 \le \mathbf{0}\,; \quad \mathbf{p}^T\mathbf{g}(\mathbf{b},\mathbf{z}) = 0 \tag{28}$$

where **p** is the Lagrange multiplier vector for the constraints in Eq. (26). **p** is interpreted as the forces required to impose the constraints; e.g., if the constraints in Eq. (26) represent the non-penetration contact conditions then **p** represents the vector of contact forces. For the frictionless contact case, it represents the normal contact forces between the deformable body and the rigid object. The conditions in Eq. (28) represent the complementarity problem.

Hilding *et al.* (1999) presented a detailed review of optimization of structures in unilateral mechanical contact. Emphasis was put on linear elastic structures in frictionless contact. In particular, for optimization problems where an energy objective was used, a unified framework was presented in the continuum as well as the discretized forms. Papers related to friction problems, optimal design involving variational inequalities, and pure sensitivity analysis were also briefly discussed. They explained that, in general, structural optimization problems involving contact could not be treated by classical smooth optimization theory; instead, modern fields such as non-smooth optimization and MPECs needed to be used.

Various formulations and algorithms for contact analysis problems have also been studied by Mijar and Arora (2000a,b). Variational equality and inequality formulations were studied for frictionless and frictional contact problems. Simple example problems were solved to study behavior of the numerical algorithms. Solutions with some algorithms were shown to be dependent on the penalty parameter value and the load step size. Although the contact analysis problems can be formulated and solved using standard optimization algorithms, they can also be formulated using MPEC formulation. Such formulations are nondifferentiable and generlized Newton method must be used to solve them (Mijar and Arora 2000b). Recently, Mijar and Arora (2004a,b) have also presented an augmented Lagrangian algorithm for frictional contact problems where the solution does not depend on the user-specified penalty parameter or the load step size.

Ferris and Tin-Loi (1998, 1999) presented an NLP approach for the identification of elastic limits and hardening moduli using the displacement information. They also discussed a minimum weight elastoplastic problem involving displacement and complementarity constraints. The research dealt with discretized structures, holonomic plasticity (reversible and path-independent), and constraints on displacements. They investigated numerically the application of two simple algorithms, both based on use of the general purpose NLP codes. One was a parametric method, and the other was a penalty method.

Tin-Loi (1999a) proposed a method for the minimum weight design of path-independent plastic structures. An MPEC formulation with member areas, stresses, nodal displacements, and plastic multipliers as optimization variables was developed for trusses. After applying a smoothing scheme, the problem was transferred to a standard NLP and solved by a generalized reduced gradient method. Tin-Loi (1999b) also presented the numerical solution of a class of unilateral contact structural optimization problems. The weight of a structure was minimized subject to frictionless unilateral contact conditions and constraints on the magnitudes of contact forces, displacements, stresses and cross-sectional areas. The problem was formulated as an MPEC. The non-smooth problem was solved using two standard NLP algorithms: a penalty method, and a smoothing method.

Pang and Tin-Loi (2001) presented a penalty interior point algorithm for a parameter identification problem in elastoplasticity. Identification of the yield limits and hardening moduli from the knowledge of the displacement response of the structure under a given set of proportional loads was studied. Under the assumptions of piecewise linear holonomic plasticity and a suitably discretized structure, the inverse problem could be formulated as an MPEC. A penalty interior point algorithm (PIPA) was proposed for solving the identification problem.

Ferris and Tin-Loi (2001) formulated the limit analysis of frictional block assemblies as an MPEC. The computation of collapse loads of discrete rigid block systems, characterized by frictional and tensionless contact interfaces, was formulated and solved by introducing appropriate relaxation of the complementarity conditions.

Tin-Loi and Que (2001, 2002a,b) and Que and Tin-Loi (2002a,b) studied NLP approaches for an inverse problem in quasi-brittle fracture and they evaluated the cohesive fracture parameters from a wedge splitting test. This was an indirect parameter identification of cohesive crack properties. Based on the availability of load-deflection data, obtained from such standard tests as the three-point bending and wedge splitting, the parameter identification problem was formulated as an MPEC. A number of numerical algorithms that were based on the standard NLP formulation and evolutionary search techniques were investigated. Computational results, using the actual experimental data, were presented to compare the proposed schemes.

Evgrafov and Patriksson (2003) studied stochastic structural topology optimization based on discretization and penalty function approach. Unilateral constraints were considered. The resulting non-smooth stochastic optimization problem was an instance of stochastic MPEC, or stochastic bilevel programs. A solution scheme based on approximating the topology optimization problem by a sequence of sizing optimization problems, and approximating the probability measure was proposed.

Although many researchers have aimed to simply transform an MPEC into a standard NLP problem and solve it by various parametric, smoothing, relaxation or penalty methods, substantial attention has also been devoted to further understanding and development of theories and efficient algorithms to solve MPECs. A *penalty interior point algorithm* (PIPA), an *implicit programming algorithm* and a *piecewise* SQP were presented by Lou *et al.* (1996). Patriksson and Wynter (1999) studied stochastic MPECs. Some basic parallel iterative algorithms for discretely distributed stochastic MPEC were discussed. Scholtes and Stöhr (1999) studied theoretical and computational aspects of an exact penalization approach to MPECs. A globally convergent trust region method was developed. Complementarity constraint qualifications and simplified B-stationarity conditions (Bouligand first-order optimality conditions) for MPECs were studied by Pang and Fukushima (1999). With the aid of some novel complementarity constraint qualifications, some simplified primal-dual characterizations of a B-stationary point were derived. Andreani and Martinez (2001) proved that stationary points of the sum of squares of the constraints were feasible points for the MPEC under reasonable sufficiency conditions.

They showed the reasons for the NLP algorithms to be successful when applied to the MPECs. Wan (2002) presented some further investigation on feasibility conditions of MPECs. It was demonstrated that these feasibility conditions were also sufficient for quadratic programming subproblems arising from the penalty interior point algorithm (PIPA) and the smooth SQP algorithm for solving MPECs. Birbil *et al.* (2004) presented an entropic regularization approach for the MPECs. A new smoothing approach based on entropic regularization was proposed. A three-dimensional null-space approach for the MPECs with steps related to nonlinear inequality constraints, the complementarity conditions and the objective function was proposed by Nie (2004).

10. Optimal control

The SAND-type approaches have also been used to solve open-loop optimal control problems for trajectory design in aerospace engineering (Enright and Conway 1991; Schulz *et al.* 1998; Betts 2000), robotic or human motion planning (Kaplan and Heegaard 2001, 2002; Lo *et al.* 2002; Bottasso and Croce 2004), and chemical or biotechnological process engineering (Cuthrell and Biegler 1986; Biegler 1988, 1998; von Schwerin *et al.* 2000; Riascos and Pinto 2004). These problems involve the solution of differential algebraic equations (DAEs), or just differential equations (DEs). The standard optimal control problem is to find the control history $\mathbf{u}(t)$ that minimizes the performance index in the time interval $[t_0, t_f]$, as (Hull 2003):

$$f = \phi(t_f, \mathbf{y}_f) + \int_{t_0}^{t_f} L(t, \mathbf{y}, \mathbf{u}) dt \tag{29}$$

subject to the system dynamics equations

$$\dot{\mathbf{y}} = \ell(t, \mathbf{y}, \mathbf{u}) \tag{30}$$

and the prescribed initial conditions

$$t_0 = t_{0_s}; \quad \mathbf{y}_0 = \mathbf{y}_{0_s} \tag{31}$$

and the prescribed final conditions

$$\varphi(t_f, \mathbf{y}_f) = \mathbf{0} \tag{32}$$

The basic idea of the SAND approach is to discretize the system of first order differential equations (30), and define a finite dimensional approximations or parametric representation for the state and control variables. The discretized state equations are treated as equality constraints in the optimization process, converting the optimal control problem into an NLP problem, which is solved numerically. Several viable approaches are available. If the design variables together with the state variables and control variables are all treated as optimization variables, the approach is called the *direct collocation/transcription* method. If the control variables are eliminated from the system (i.e., only the design variables and the state variables are treated as optimization variables), it is called the *differential inclusion* method (Hull 1997; Hull 2003). Another possibility is the so-called *multiple shooting* technique (Betts and Huffman 1991; Leineweber *et al.* 2003).

Different discretization techniques for the state equations have been studied in the literature. In general there are two classes of methods to transfer the DAEs or DEs to an algebraic system of equations. One is to use some polynomial interpolation between the time grid points, and the other is to use a series expansion in terms of orthogonal polynomials, such as Legendre or Chebyshev polynomials (Vlassenbroeck 1988; Fahroo and Ross 2002). For the former case, the most common ways are the trapezoidal or Simpson's quadrature schemes based on piecewise quadratic or cubic polynomials (Hargraves and Paris 1987; Betts 1990; Enright and Conway 1991, 1992; von Stryk and Bulirsch 1992). Explicit or implicit Runge-Kutta methods were used to discretize the state equations by Albuquerque and Biegler (1997), Biehn *et al.* (2000), and

Betts *et al.* (2000, 2002a,b). Higher degree polynomials for direct collocation were studied by Herman and Conway (1995), and Hu *et al.* (2002). If very smooth trajectory is required, B-spline curves can also be used to parameterize the dynamic equations (Neuman and Sen 1973; Lo *et al.* 2002). Seywald (1994), Coverstone-Carroll and Williams (1994), and Kumar and Seywald (1996a,b) discussed a technique to eliminate the controls while solving optimal control problems via direct methods. Conway and Larson (1998) presented a comparison of collocation and differential inclusion methods in direct trajectory optimization.

Different optimization algorithms have been used for direct collocation or multiple shooting, among which the SQP and interior point algorithm are the popular choices. Hargraves and Paris (1987), Tanartkit and Biegler (1996), Schulz and Bock (1997), von Schwerin *et al.* (2000), Betts (2000), Cervantes and Biegler (2000), and Itle *et al.* (2004) used SQP. The interior point algorithm was employed by Cervantes *et al.* (2000, 2002). Since the resulting NLP is large and sparse, sparse NLP were extensively discussed (Betts and Huffman 1992, 1993, 1999; Cervantes and Biegler 1998; Cervantes *et al.* 2002). Parallel computation was considered by Betts and Huffman (1991). A detailed survey of the numerical methods for simultaneous optimization and control can also be found in Betts (1998).

11. Multidisciplinary design optimization (MDO)

The SAND formulation is also called the *infeasible path* (IP) approach for aerodynamic design that was pioneered by Rizk (1983). Later, more research was done for this problem (Frank and Shubin 1992; Shubin 1995; Orozco and Ghattas 1992, 1996). Other applications of SAND formulation can be found in heat transfer; e.g., Hrymak *et al.* (1985) presented optimization of extended heat transfer surfaces.

The SAND formulation has also been demonstrated in many multidisciplinary design optimization (MDO) papers and has been called the *all-at-once* (AAO) formulation (Haftka *et al.* 1992; Cramer *et al.* 1994; Shubin 1995; Balling and Sobieszczanski-Sobieski 1996; Balling and Wilkinson 1997). Haftka *et al.* (1992) discussed the interdisciplinary optimization of engineering systems from the standpoint of the computational alternatives available to the designers. Optimization of the system could be formulated in several ways, i.e., NAND or SAND formulations. Cramer *et al.* (1994) presented three MDO formulations, namely multidisciplinary feasible (MDF), AAO, and individual discipline feasible (IDF) formulations. In AAO formulation, the optimization problems were very large and residuals were evaluated in all disciplines. No existing analysis codes were necessary. Though AAO was computationally least expensive, it required a higher degree of software integration. Balling and Wilkinson (1997) studied available multidisciplinary design optimization approaches on common test problems. It turned out that the AAO formulation showed the most efficiency among all the approaches for the test problems. Detailed reviews of various MDO formulations can be found in the literature (Balling and Sobieszczanski-Sobieski 1996).

12. Concluding remarks

Alternative formulations for optimization of structural and mechanical systems, including configuration and topology design, are reviewed. Features of various formulations are discussed and their advantages and disadvantages are delineated. These include simultaneous analysis and design (SAND), displacement based two-phase approach, mathematical programs with equilibrium constraints (MPEC), and partial differential equations (PDE) constrained formulations. If design variables and some state variables are combined together in a single and large optimization problem, then the SAND formulation is obtained. In the displacement based formulation, two separate optimization problems are defined and solved in a sequence: the inner problem where the displacements are kept fixed and the design variables are updated, and the outer problem where the design is kept fixed and the displacements are updated.

MPEC is a more general formulation where the equilibrium constraints are defined by variational equalities or inequalities, such as the one for the contact analysis problem. In addition, the formulation has complementarity system of equations that make the problem nondifferentiable. MPEC can also be considered as a special case of the so-called bilevel optimization problems where some of the constraints involve optimization. It is noted that the equilibrium equation (1) is obtained as a necessary condition for minimization of the total potential energy of the structure. Thus the SAND formulation can also be considered as a special case of the MPEC. This formulation has been studied recently and mathematical foundations for its solution have been presented. First and second order optimality conditions for the formulation have been developed and computational algorithms for its numerical solution have been presented and demonstrated. Some MPEC problems can be reformulated and solved by the standard NLP algorithms.

Another recent formulation is the PDE-constrained optimization of systems. This formulation is similar to the SAND approach except that the equilibrium equations are written as PDEs; i.e., in the distributed parameter form. The formulation offers more flexibility for numerical calculations because any discretization scheme can be used to solve the PDEs.

In addition to the foregoing literature, SAND-type formulations for the optimal control problem and multidisciplinary optimization problems are briefly reviewed.

Based on this review of the literature, the current status and future opportunities for research on alternative formulations for optimization of structural and mechanical systems are as follows:

1. Most of the formulations in the structural optimization literature have been discussed

for truss structures; they need to be extended to other complex structures.

2. Most of the formulations have focused on use of the displacement based FEM. Other analysis methods need to be considered, such as the force methods, mixed methods, meshless methods, boundary element methods, and others.
3. Implementation aspects with the existing analysis programs have not been adequately discussed; this important aspect needs to be addressed (Wang and Arora 2004).
4. Sparse matrix approaches must be used to solve the problem with the SAND formulation since the optimization problem is large but sparsely populated.
5. Parallel processing must be considered to solve very large-scale problems.
6. Transformation of the solution variables needs to be considered, since various variables can be of different orders of magnitude.

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