

An application of Graph Theory to MDAO problem formulation

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blah blah blah

Nomenclature

AAO	All-At-
MDAO	Multidisciplinary Design Analysis and Optimization
FPF	Fundamental Problem Formulation

I. Introduction

As the size and complexity of engineering systems grows the time and expense for setting up analysis models grows with them. Multidisciplinary Design Analysis and Optimization (MDAO) frameworks such as OpenMDAO[?] and ModelCenter have enabled a new level of analysis tool integration and paved the way for models of with more analysis tools and increasing numbers of multidisciplinary couplings. Such complex models present a distinct challenge proper implementation of any given solution strategy .

We propose the use of graph based problem formulation that generally describes a given problem, supports algorithmic manipulation to find beneficial solutions strategies, and enables automated implementation of those strategies inside an MDAO framework. In order to serve that purpose, the graph includes the following information:

- Discipline Analyses
- Discipline State Variables and Residuals
- Design Variables
- Constraints
- Objective or Objectives
- Coupling Constraints
- Parameters

Notably absent from the preceding list are any kind of solvers, optimizers, or other iterative solution finding tools. At it most basic, a problem formulation includes only information about what is being sought after in a given problem, or what the goals of a given problem are. It need not contain any information about solution paths or strategies to reach those goals.

We define a problem specification striped down to it's most essential parts to be the Fundamental Problem Formulation (FPF). By definition, the FPF for any given problem will be constant regardless of which MDAO framework, optimization architecture, optimization algorithm, or iterative solver is used to solve the problem.

The graph based syntax used in this work is based on the Design Structure Matrix (DSM). This provides several key features that make it useful for working with large scale MDAO problems. It provides a rigid

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structure that can be easily manipulated with a wide range of well establish graph-theory algorithms for the purposes of problem decomposition. It also provides a means for testing a given problem formulation to check if it is the FPF, and if not to reduce it to the FPF. Lastly, it lends itself well to interacting with MDAO frameworks.

II. Specific vs Fundamental Problem Formulation

For a simple, notional problem is given as follows:

$$\begin{aligned}
&\text{given } A : x, y \rightarrow m, z \\
&\quad B : x, z \rightarrow y^t \\
&\text{min. } f(m) \\
&\text{w.r.t. } x, y, z \\
&\text{s.t. } g(y^t, y) = 0
\end{aligned} \tag{1}$$

Where A and B represent analysis tools, f, g are the objective and constraint functions respectively. Equation 1 makes an inherent assumption about the solution strategy for the problem. Analysis A outputs z which is an input to B . Hence, A should be run before B with the y being iterated on to convergence with y^t . However, a different solution could be equally valid and still represent the same fundamental problem:

$$\begin{aligned}
&\text{given } B : x, z \rightarrow y \\
&\quad A : x, y \rightarrow m, z^t \\
&\text{min. } f(m) \\
&\text{w.r.t. } x, y, z \\
&\text{s.t. } g(z^t, z) = 0
\end{aligned} \tag{2}$$

Equation 2 differs only slightly from Eqn. 1. A is now dependent on the output of B , and z will be iterated on to satisfy g . Now the problem can be solved by running B first and then A . Since the formulations in Eqn. 1 and 2 both describe the same problem and neither can be the FPF. There must be a more fundamental description of the problem that is common between them. We present the FPF as follows:

$$\begin{aligned}
&\text{given } A : x, y \rightarrow m, z^t \\
&\quad B : x, z \rightarrow y^t \\
&\text{min. } f(m) \\
&\text{w.r.t. } x, y, z \\
&\text{s.t. } g1(z^t, z) = 0 \\
&\quad g2(y^t, y) = 0
\end{aligned} \tag{3}$$

The FPF in Eqn. 3 differs from both Eqn. 1 and Eqn. 2 because it has two constraints which both must be met. The presence of both of these constraints fully decouples the problem so that either A or B could be run first or both could be run simultaneously. By removing either constraint, and replacing it with a direct dependence between the two analyses you could regain the earlier two problem formulations.

III. Using DSM for Problem Formulation

As shown above, the mathematical language for specifying problem formulations is very general and can be used both for fundamental and specific problem formulations. Tedford and Martins used the above mathematical syntax to specify the FPF for a set of test problems and also to describe specific formulations for solving them with a number of optimization architectures.⁷ Their work demonstrates clearly how multiple specific problem formulations can all relate back to a common FPF.

The challenge with using this traditional mathematical syntax is that it is not easily manipulated or analyzed. A number of matrix based methods have been used successfully to translate the mathematical syntax into a more useful computational form. Steward's Design Structure Matrix (DSM) is a square adjacency matrix which captures the relationship between analysis tools where off diagonal elements of the matrix indicate coupling.[?] Since a DSM describes a square adjacency matrix, it can be represented in an equivalent directed graph where nodes represent analysis tools and edges represent information dependence between those tools. The ordering of elements in a DSM can be used to indicate execution order. For more complex problems, choosing the proper order to run analysis tools is a non-trivial task. Rogers et. al developed DeMAID to manipulate a DSM to find an ordering for analysis tools that reduces the cost of solving highly coupled systems.[?] This re-ordering yields multiple specific problem formulations which all solve the same FPF. In other words, manipulation of the DSM does not fundamentally alter the problem formulation, which makes DSM an excellent foundation for specifying the FPF itself. Traditional DSM only captures information about data dependency between analyses. Objective and constraint information is missing from the description of the problem.

An alternate matrix based syntax, called a Functional Dependency Table (FDT), was proposed by Michela and Papalambros. FDT represents the relationship between functions, including objectives and constraints, and specific variables that affect them.[?] Similar to DSM, FDT also describes an adjacency matrix of a graph. Unlike the DSM graph, however, the graph is undirected and nodes can represent analysis tools, objectives, or constraints. Edges between nodes represent a dependence on the same variable. Wagner and Papalambros made use of the FDT to solve a graph partitioning problem that yielded more efficient optimization problem decompositions.[?] While FDT succeeds at capturing the information about objectives and constraints, it neglects the data dependency captured by DSM. [TODO: There is more recent research to cite here. e.g. Allison's Work.]

[TODO: insert FDT of simple problem here]

Lamb and Martins included the variables, objectives, and constraint functions as nodes in an Extended DSM (XDSM) in order to capture a more complete description of solution strategies for MDAO problems.[?] By adding in those elements, they partially combined a traditional DSM with an FDT. This allows XDSM to represent data dependency between multiple analysis tools as well as between analysis tools and objective/constraint functions. With the additional information included in an XDSM Lu and Martins applied both ordering and partitioning algorithms on an MDAO test problem named the Scalable Problem.[?]

[TODO: insert XDSM for simple problem solved with MDF here]

Although XDSM captures part functional aspects of FDT, it leaves out the variables themselves. As a result, all variable information is aggregated so that for the problem from Eqn. 3 you can say that A depends on B or vice versa, but you can't identify which individual variables are interacting in the dependency cycle. Without the detailed variable information, you can't construct the compatibility constraints necessary to implement the problem. Additionally, XDSM requires the use of solver and optimizer blocks to represent the relationship between design variables and objectives/constraints. By introducing solver or optimizer blocks XDSM automatically provides some kind of solution strategy. Hence XDSM is too specific for use with a fundamental problem formulation.

By taking XDSM, removing the requirement for solver/optimizer nodes and adding in nodes for each variable we are able to fully describe the problem formulation for a general MDAO problem. In the following sections we describe the necessary syntax for specifying a problem formulation withing a DSM and show how to make use of the resulting graph to find the FPF from any given graph. For completeness we also present algorithms for converting between the general DSM and the more specific formulations discussed above.

IV. Graph Based Problem Formulation Syntax

IV.A. Formulation Graph Syntax

Rather than start with an adjacency, we chose to work directly with a directed cyclic graph to develop a syntax for the FPF. The following information must be provided to start:

- Analysis blocks: an analysis block represents any calculation, and each comes with
 - local inputs
 - local outputs

- execution properties: the properties associated with running the code, such as run time.
- Global parameters: these may serve as fixed inputs to the local inputs of analysis blocks
- Global outputs: these may represent
 - objectives
 - constraints
 - residuals: (not sure)

The graph representation of a data flow is cast to utilize the extensive library of algorithms in graph theory to analyze a directed weighted graph. Edge weights are used to represent the metrics associated with a data flow

- Run time: this metric is a property of an analysis block
- Fidelity: this metric is a property of an individual local output
- Expected Convergence

The key assumption is that identical variables are recognized as such. This serves as the basis for creating a data flow by connecting compatible input and output nodes with a directed edge. In order to represent the fact that execution of an analysis code does not depend on the number of outputs being used, it is represented as depicted in the following figure (not made yet).

This information immediately leads to the maximal connectivity graph, which is formed by placing a directed edge from each local output or global parameter to each matching local input or global output. Whenever multiple edges are connected to a single input a conflict occurs because only one may be used. Resolving these conflicts is one key challenge in creating a data flow.

IV.B. Solution Graph Syntax

What is the difference between a problem formulation and a problem solution method? Convert from a cyclic graph, to an acyclic graph

- cycles indicate convergence loops or design variable loops
- Problem can't be solved until all loops are *removed* by adding in solvers/optimizers
- *special* nodes for solvers and optimizers that *break* loops (from an algorithmic point of view)
- FPF represents the minimal amount of information necessary to define a problem
- Any solution path grows the graph complexity by adding edges and nodes (or possibly have an empty solution graph, which you build up as you remove edges from problem formulation graph?)

V. Example Problem

VI. Applications

VII. Conclusions

References