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Dynamically Reconfigurable Approach to Multidisciplinary Problems

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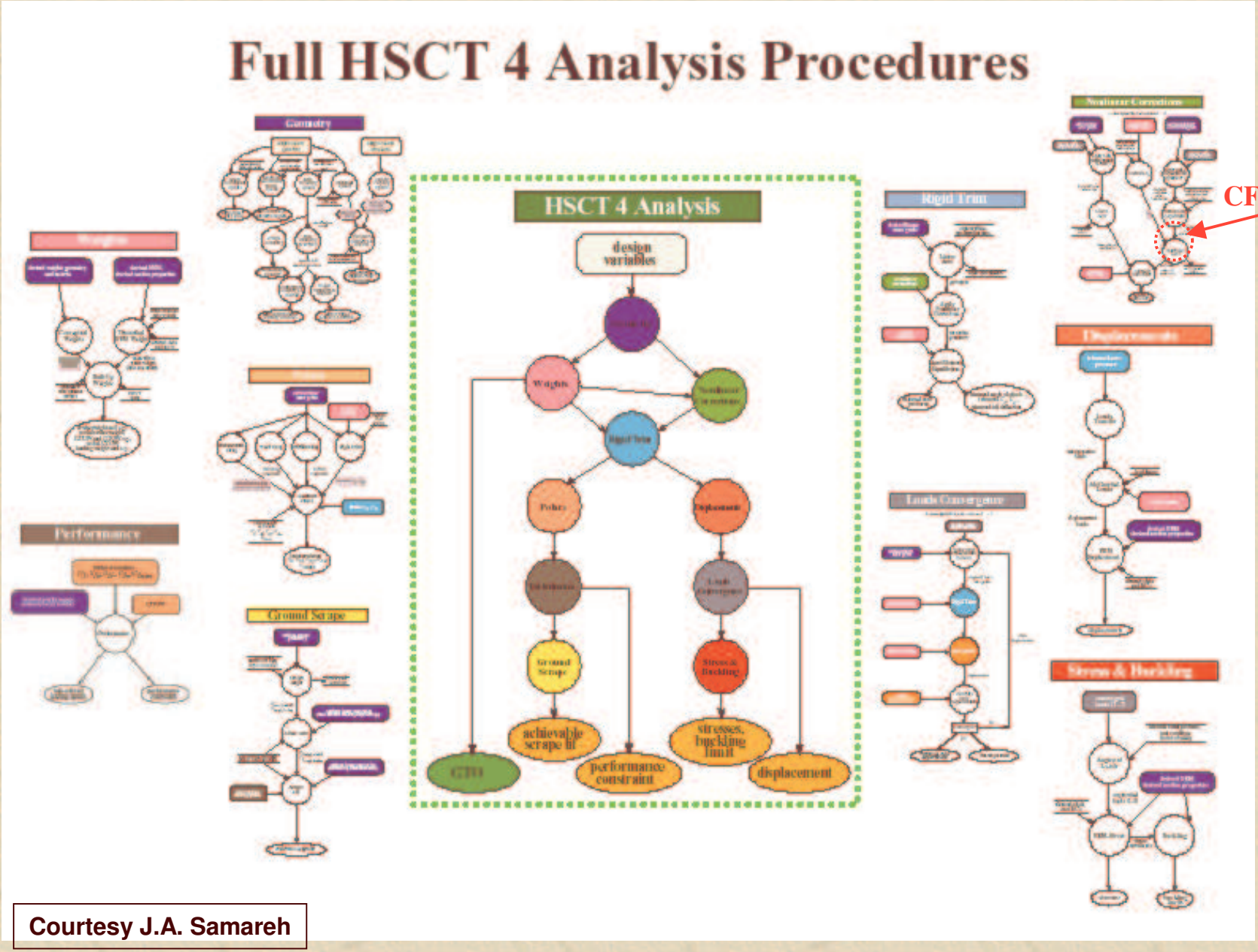
Example: a multidisciplinary analysis (MDA)



Courtesy J.A. Samareh

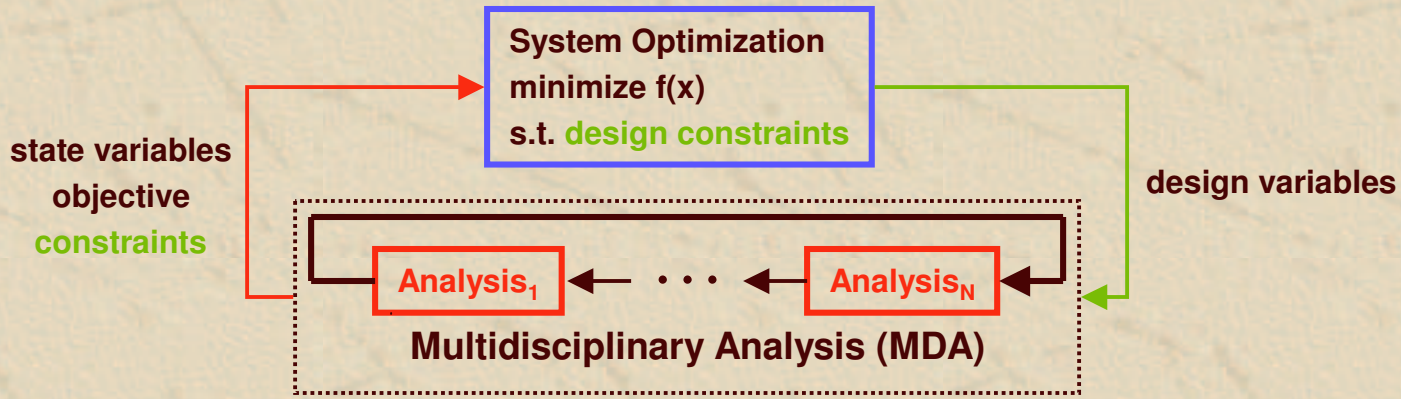
What is reconfigurability?

- Computational component-based approach to MDO problem synthesis that allows for straightforward transformation among problem formulations within optimization algorithms
- Assumption: MDO-based NLP $\subsetneq$ design problem
- Outline
  - Effect of problem formulation on tractability
  - Origins of reconfigurability
  - Illustration for 3 formulations and barrier-SQP
  - Long-term plans

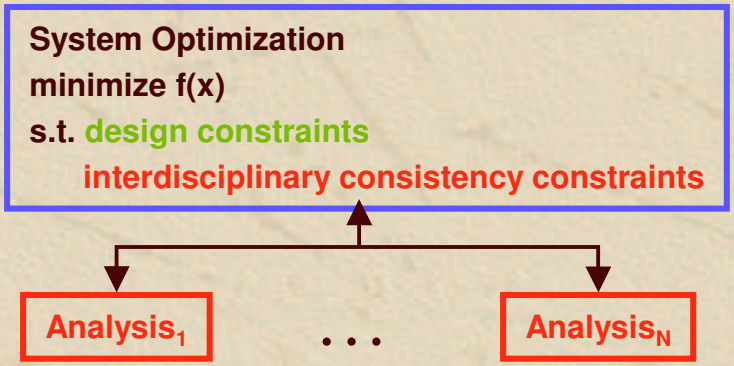
Influence of formulation on performance

Example: HPCCP formulation study, Alexandrov & Kodiyalam, AIAA 1998-4884

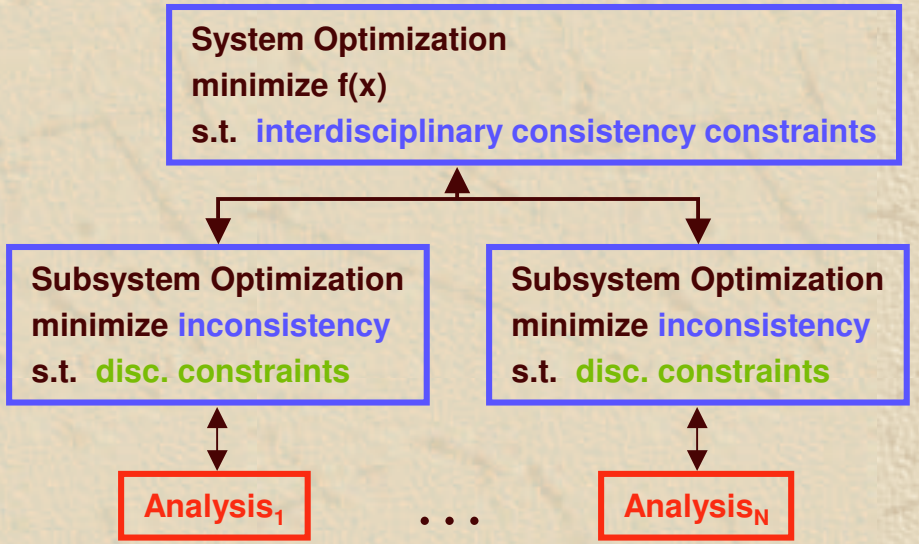
Fully Integrated Optimization (FIO)



Distributed Analysis Optimization (DAO)



Collaborative Optimization



Influence of formulation on performance, cont.

- Test problems from MDO Test Suite (small, simple)
- Several performance metrics
- Dramatic differences in performance
  - Computational and analytical studies (see paper for refs.): analytical features of formulations, e.g., the degree of disciplinary autonomy, directly affects the ability of numerical algorithms to solve the problem reliably and efficiently

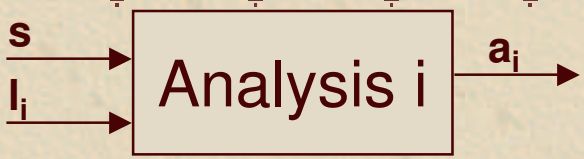
Problem / Method	1	2	3	4	5	6	7
FIO	610	220	610	81	3234	5024	8730
DAO	9530	8976	382	N/A	544	932	N/A
CO	15626	19872	1785	2102	837	40125	691058

Representative # analyses

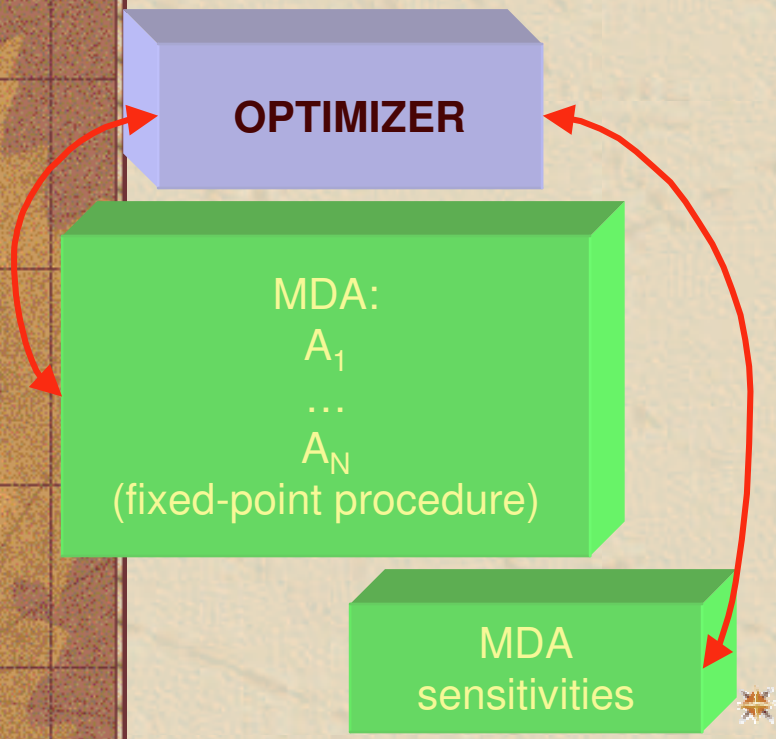
(CO not included here; will consider FIO, DAO, SAND)

MDO Problem Synthesis / Implementation

Problem:
design for objective f with



i = 1, …, N



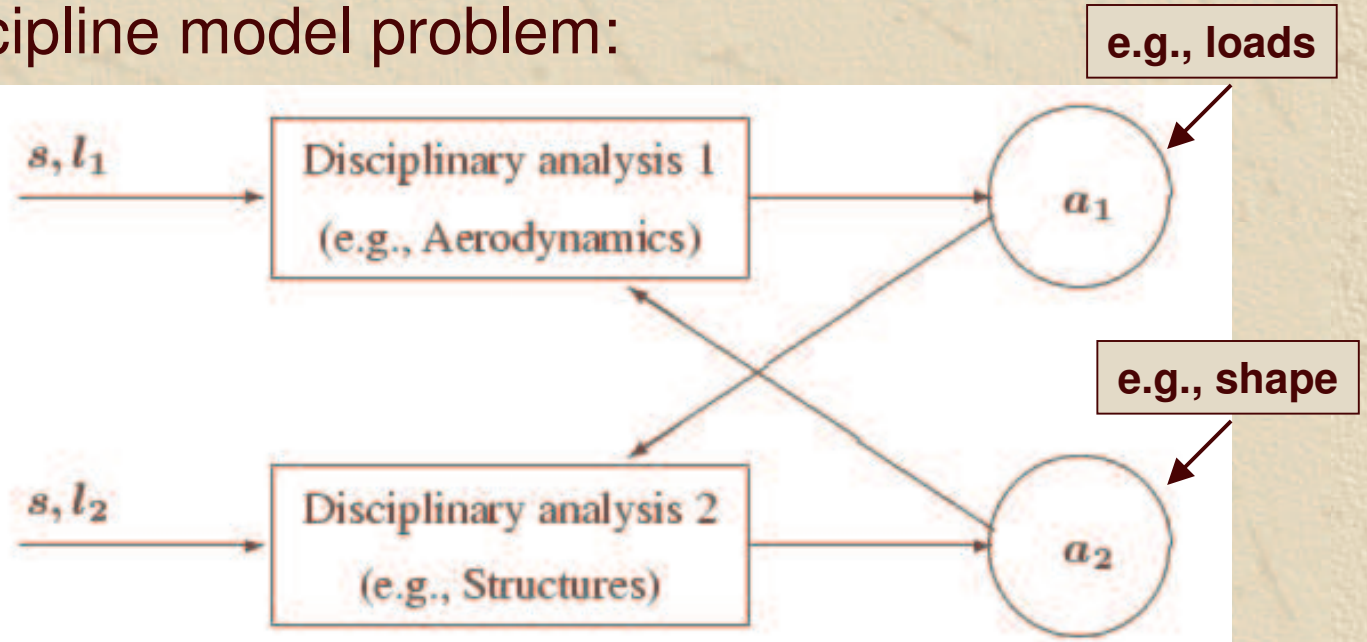
- Successful MDO-NLP usually in academic environments (simulation codes open to modification) or via *ad hoc* approaches
- Realistic MDO
  - Heroic software integration for MDA
  - MDA = (usually) fixed-point iteration; too rigid
  - May leave no resources for computing derivatives or experimenting with optimization
  - Difficult to get MDA-based objectives and constraints *automatically*
  - To reformulate the problem, need to "unscramble" codes
- ∴One-of-a-kind, monolithic implementations
- Want flexible and/or hybrid re-formulations

Algorithmic perspective

- Formulation vs. algorithm
- Start with the abilities of available algorithms; devise formulations amenable to algorithms
  - May not satisfy all organizational needs
- Develop reconfigurable approach to synthesis
  - All MDO formulations are related and share the same basic computational components
  - Appropriate implementation enables re-use of components in a straightforward way
- Tools for formulation analysis and matching with algorithms can be included in future computational frameworks

Origins of reconfigurability

- The capacity for reconfigurability stems from the relationship among formulations
- Two-discipline model problem:



- Coupled MDA $\sim$ the physical requirement that a solution satisfy both analyses
- Given $x = (s, l_1, l_2)$, we have

$$
\begin{aligned}
a_1 &= A_1(s, l_1, a_2) \\
a_2 &= A_2(s, l_2, a_1)
\end{aligned}
$$

Origins of reconfigurability: SAND

Write MDA as

$$
\begin{aligned}
a_1 &= A_1(s, l_1, t_2) \\
a_2 &= A_2(s, l_2, t_1) \\
t_1 &= a_1 \\
t_2 &= a_2
\end{aligned}
$$

Start with Simultaneous Analysis and Design (SAND) formulation:

(AKA All-at-Once, SAD, etc.)

$$
\begin{aligned}
\underset{s, l_1, l_2, a_1, a_2, t_1, t_2}{\text{minimize}} \quad & f(s, t_1, t_2) \\
\text{subject to} \quad & \\
& c_1(s, l_1, a_1) \geq 0 \\
& c_2(s, l_2, a_2) \geq 0 \\
& a_1 = A_1(s, l_1, t_2) \\
& a_2 = A_2(s, l_2, t_1) \\
& t_1 = a_1 \\
& t_2 = a_2
\end{aligned}
$$

disciplinary constraints

analysis constraints

consistency constraints

Origins of reconfigurability, cont.

- All other formulations may be viewed as derived from the SAND formulation by eliminating a particular set of independent variables from the optimization problem via closing a particular set of constraints or solving optimization problems.

Origins of reconfigurability: DAO

Distributed Analysis Optimization

(AKA Individual Discipline Feasible, In-Between, etc.)

A DAO formulation is

$$\begin{aligned} \underset{s,l_1,l_2,t_1,t_2}{\text{minimize}} \quad & f(s,t_1,t_2) \\ \text{subject to} \quad & \left.\begin{aligned} c_1(s,l_1,t_1) &\geq 0 \\ c_2(s,l_2,t_2) &\geq 0 \end{aligned}\right\} \text{disciplinary constraints} \\ & \text{consistency constraints} \left\{\begin{aligned} t_1 &= a_1(s,l_1,t_2) \\ t_2 &= a_2(s,l_2,t_1), \end{aligned}\right. \end{aligned}$$

where the disciplinary responses $a_1(s,l_1,t_2)$ and $a_2(s,l_2,t_1)$ are found by closing the disciplinary analysis constraints

$$\begin{aligned} a_1 &= A_1(s,l_1,t_2) \\ a_2 &= A_2(s,l_2,t_1). \end{aligned}$$

Origins of reconfigurability: FIO

Fully Integrated Optimization (straightforward approach)

The corresponding FIO formulation is

$$\begin{aligned} \underset{s,l_1,l_2}{\text{minimize}} \quad & f(s, t_1(s,l_1,l_2), t_2(s,l_1,l_2)) \\ \text{subject to} \quad & c_1(s, l_1, t_1(s,l_1,l_2)) \geq 0 \\ & c_2(s, l_2, t_2(s,l_1,l_2)) \geq 0 \end{aligned}$$

where we compute $t_1(s,l_1,l_2)$ and $t_2(s,l_1,l_2)$ by solving the MDA

$$\begin{aligned} a_1 &= A_1(s,l_1,t_2) & t_1 &= a_1 \\ a_2 &= A_2(s,l_2,t_1) & t_2 &= a_2. \end{aligned}$$

Origins of reconfigurability, cont.

- Other formulations further eliminate local design variables by solving disciplinary optimization subproblems
  - Need more work to derive reconfigurable relations
  - Computational components remain unchanged
- Standard results on reduced derivatives will tell us that the sensitivities in DAO and FIO are related to those in SAND *via variable reduction*
- Therefore, computational components of one formulation can be reconfigured to yield those of another

Reduced derivatives

Let

$$\Phi(x) = \phi(x, v(x)).$$

Given x, $v(x)$ is computed from

$$S(x, v(x)) = 0.$$

Let W be the *injection operator* (W^T is the reduction operator):

$$W = W(x, v) = \begin{pmatrix} I \\ -S_v^{-1}(x, v) S_x(x, v) \end{pmatrix}.$$

Define λ by

$$\lambda = \lambda(x, v) = -\left(S_v(x, v)\right)^{-T} \nabla_v \phi(x, v)$$

and the Lagrangian $L(x, v; \lambda)$ by

$$L(x, v; \lambda) = \phi(x, v) + \lambda^T S(x, v).$$

Reduced derivatives

The derivatives of ϕ and Φ are related as follows:

$$\nabla_x \Phi(x) = \underbrace{W^T(x, v(x)) \nabla_{(x,v)} \phi(x, v(x)).}_{\text{Reduced gradient}}$$

$$\nabla^2_{xx} \Phi(x) = \underbrace{W^T \left(\nabla^2_{(x,v)} \phi + \nabla^2_{(x,v)} S \cdot \lambda \right) W,}_{\text{Reduced Hessian of the Lagrangian}}$$

where

$$\begin{aligned} W &= W(x, v(x)) \\ \nabla^2_{(x,v)} \phi &= \nabla^2_{(x,v)} \phi(x, v(x)) \\ \nabla^2_{(x,v)} S \cdot \lambda &= \nabla^2_{(x,v)} S(x, v(x)) \cdot \lambda(x, v(x)) \\ &= \sum_{i=1}^{n} \lambda_i \nabla^2_{(x,v)} S_i. \end{aligned}$$

Barrier-SQP approach to SAND

Now illustrate reconfigurability in the context of a specific class of algorithms: barrier-SQP methods

Let

$$F_{\text{SAND}}(s, l_1, l_2, t_1, t_2) = f(s, t_1, t_2) - \mu \left[\sum_i \ln c_1^i(s, l_1, t_1) + \sum_j \ln c_2^j(s, l_2, t_2) \right]$$

Barrier-SQP solves a sequence of subproblems of the form:

$$\begin{aligned} \underset{s, l_1, l_2, t_1, t_2, a_1, a_2}{\text{minimize}} \quad & F_{\text{SAND}}(s, l_1, l_2, t_1, t_2) \\ \text{subject to} \quad & a_1 = A_1(s, l_1, t_2) \\ & a_2 = A_2(s, l_2, t_1) \\ & t_1 = a_1 \\ & t_2 = a_2, \end{aligned}$$

Barrier-SQP approach to DAO

Let

$$F_{\text{DAO}}(s, l_1, l_2, t_1, t_2) = f(s, t_1, t_2) - \mu \left[\sum_i \ln c_1^i(s, l_1, t_1) + \sum_j \ln c_2^j(s, l_2, t_2) \right]$$

Barrier subproblem for DAO is

$$\begin{aligned} \underset{s, l_1, l_2, t_1, t_2}{\text{minimize}} \quad & F_{\text{DAO}}(s, l_1, l_2, t_1, t_2) \\ \text{subject to} \quad & t_1 = a_1(s, l_1, t_2) \\ & t_2 = a_2(s, l_2, t_1), \end{aligned}$$

where the disciplinary responses $a_1(s, l_1, t_2)$ and $a_2(s, l_2, t_1)$ are computed via the disciplinary analyses:

$$\begin{aligned} a_1 &= A_1(s, l_1, t_2) \\ a_2 &= A_2(s, l_2, t_1). \end{aligned}$$

Relationship among SAND, DAO, FIO Sensitivities

Then setting an appropriate (x, v) for each formulation, we have

$$\nabla_{(s,l_1,l_2,t_1,t_2)} F_{\text{DAO}} = W_{\text{DAO}}^T \nabla_{(s,l_1,l_2,t_1,t_2,a_1,a_2)} F_{\text{SAND}}$$

and

$$\nabla^2_{(s,l_1,l_2,t_1,t_2)} F_{\text{DAO}} = W_{\text{DAO}}^T \nabla^2_{(s,l_1,l_2,t_1,t_2,a_1,a_2)} F_{\text{SAND}} W_{\text{DAO}}.$$

A similar relationship exists between the sensitivities for solving the barrier-SQP subproblems for SAND and FIO:

$$\nabla_{(s,l_1,l_2)} F_{\text{FIO}} = W_{\text{FIO}}^T \nabla_{(s,l_1,l_2,t_1,t_2,a_1,a_2)} F_{\text{SAND}}$$

and

$$\nabla^2_{(s,l_1,l_2)} F_{\text{FIO}} = W_{\text{FIO}}^T \nabla^2_{(s,l_1,l_2,t_1,t_2,a_1,a_2)} F_{\text{SAND}} W_{\text{FIO}},$$

where the expressions for the reduction operators W_{FIO}^T and W_{DAO}^T are given in the paper.

Solving barrier-SQP subproblem

Solving barrier subproblem is an iterative process, in which we approximately solve

$$\begin{array}{ll} \text{minimize} & \frac{1}{2}p^T H p + g^T p \\ \text{subject to} & \nabla S^T p + S = 0 \end{array}$$

H - approximation to the Hessian of the Lagrangian

g - is the gradient of the Lagrangian

p - step in the iterative process

Reduced-basis approach to barrier-SQP subproblem

- For a specific choice of algorithm for solving the barrier-SQP subproblem, can say even more about the relationship among the computational elements needed to solve the three formulations
- The relationship among the sensitivities means that it is possible to implement an optimization algorithm for SAND so that with a single modification we obtain an algorithm for DAO or FIO

Reduced-basis barrier-SQP for SAND

Algorithm 1: Reduced-basis algorithm for SAND

Initialization: Choose an initial (x_c, v_c).

Until convergence, do {

1. Compute the multiplier $\lambda_{SAND} = -S_v^{-1}\nabla_v F_{\text{SAND}}$.
2. Test for convergence.
3. Construct a local model of L about (x_c, v_c).
4. Take a step p^{LF} to improve linear feasibility:

$$p^{LF} = \alpha \begin{pmatrix} 0 \\ -S_v^{-1} S \end{pmatrix}.$$

5. Subject to the improved linear feasibility, improve optimality:

$$\begin{array}{ll} \text{minimize} & \frac{1}{2} q^T W^T H W q + (g + H p_{LF})^T W^T q \\ \text{subject to} & \| p_{LF} + W q \| \leq r. \end{array}$$

6. Set $p = (p_x, p_v) = p_{LF} + W q$.
7. Evaluate $(x_+, v_+) = (x_c, v_c) + (p_x, p_v)$ and update $(x_c, v_c), r$. }

Reduced-basis SQP for FIO and DAO

Algorithm 2: Reduced-basis algorithm for SAND + analysis = FIO

Initialization: Choose an initial x_c.

Analysis: Solve $S_{\text{no}}(x_c, v_c(x_c)) = 0$ for $v_c(x_c)$.

Until convergence, do {

1–6. These steps remain unchanged.

7. **Analysis: Solve $S_{\text{no}}(x_+, v_+) = 0$ for $v_+(x_+)$; evaluate (x_+, v_+).**

8. This step remains unchanged.

}

Algorithm 3: Reduced-basis algorithm for SAND + analysis = DAO

Initialization: Choose an initial (x_c, v_c).

Analysis: Solve $S_{\text{no}}(x_c, v_c(x_c)) = 0$ for $v_c(x_c)$.

Until convergence, do {

1–6. These steps remain unchanged.

7. **Analysis: Solve $S_{\text{no}}(x_+, v_+) = 0$ for $v_+(x_+)$; evaluate (x_+, v_+).**

8. This step remains unchanged.

}

Other algorithms

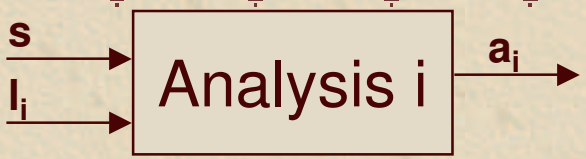
- Outlined reconfigurable scheme should work for other methods that handle inequalities via a penalty function (e.g., augmented Lagrangian)
- Active set methods are likely to take more work

Concluding remarks

- MDO problem formulation directly affects the tractability of the problem
- There are many formulations with a spectrum of benefits
- Regardless of the formulation or even the paradigm, there is a clear need for flexible problem synthesis and easy reconfiguration
- Basic computational components combined with transformations within specific algorithms form a promising approach
- Plan: develop tools for analysis of problems in terms of formulation and algorithm matching

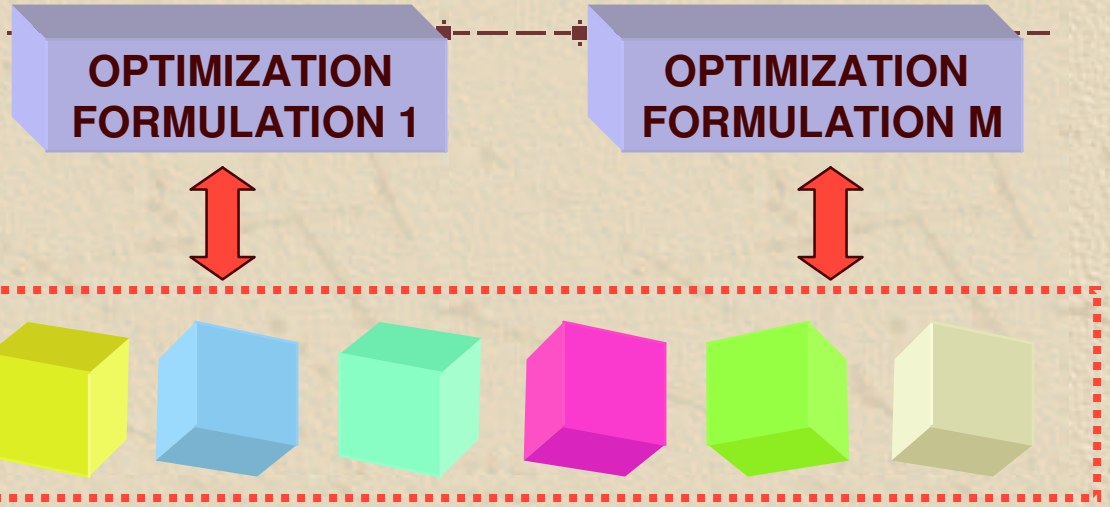
MDO Problem Synthesis / Implementation

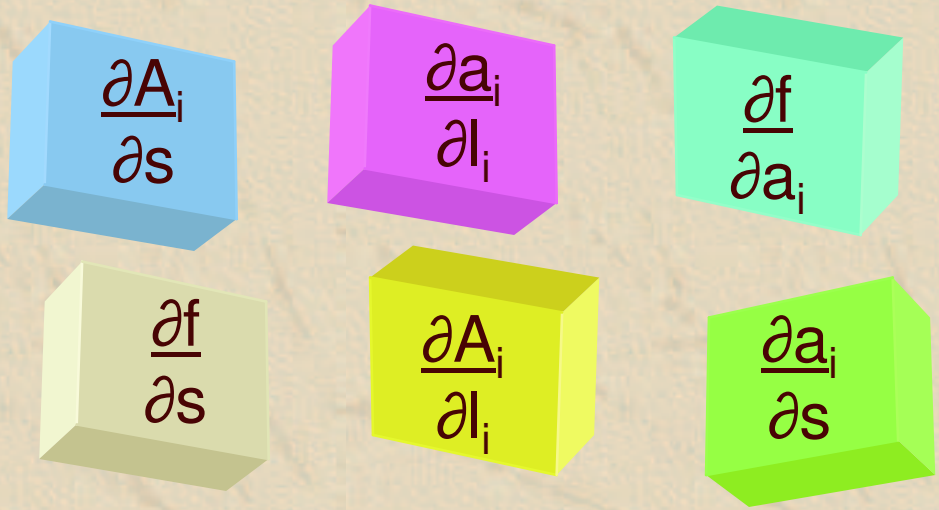
Problem:
design for objective f with



i = 1, …, N

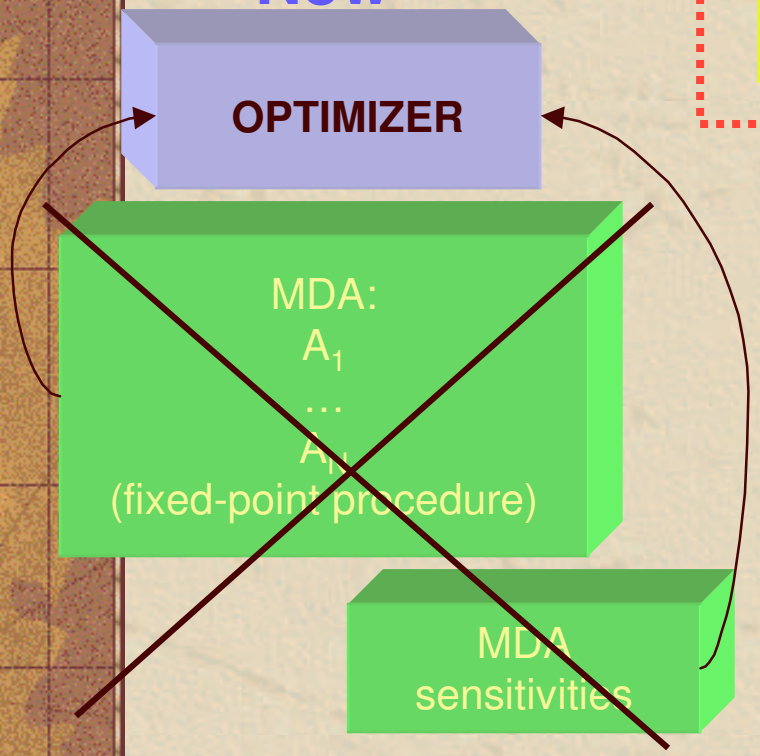
Future





Expend the effort at the outset to implement appropriate function and derivative components; straightforward to transform and expand: an opportunity for a general framework

Now



Laborious, expensive, one-time integration, difficult to transform/ expand