Enabling Multidisciplinary Design Optimization: Inexact-Newton-Krylov and the Individual-Discipline-Feasible Formulation

Alp Dener (Graduate Student) and Jason Hicken (PI)
Department of Mechanical, Aerospace, and Nuclear Engineering
Rensselaer Polytechnic Institute

Rensselaer

optimal.design.lab

Acknowledgments

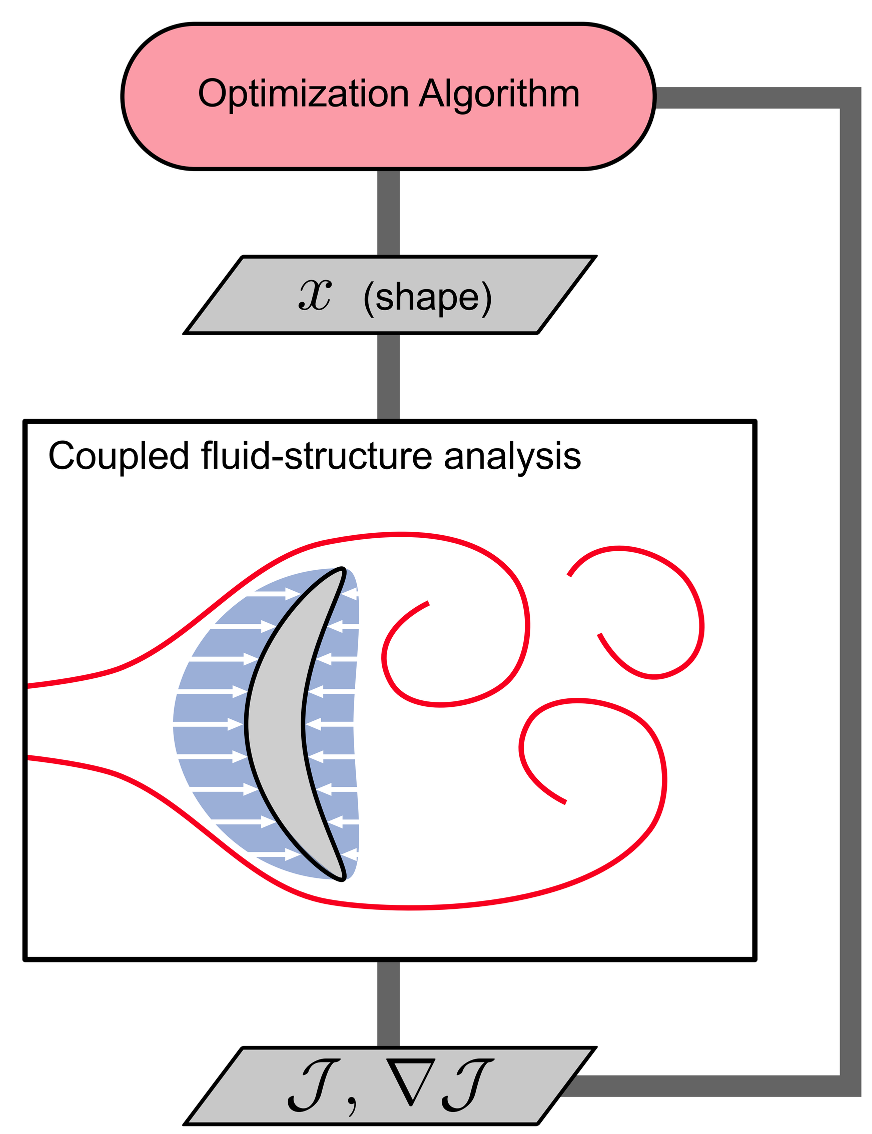
This material is based upon work supported by the National Science Foundation under Grant No. 1332819.

Presented at the Engineering Design and Systems Engineering Foundations Workshop at Clemson University, Nov. 14-17, 2015. The accompanying YouTube video is accessible via the QR code on the right.

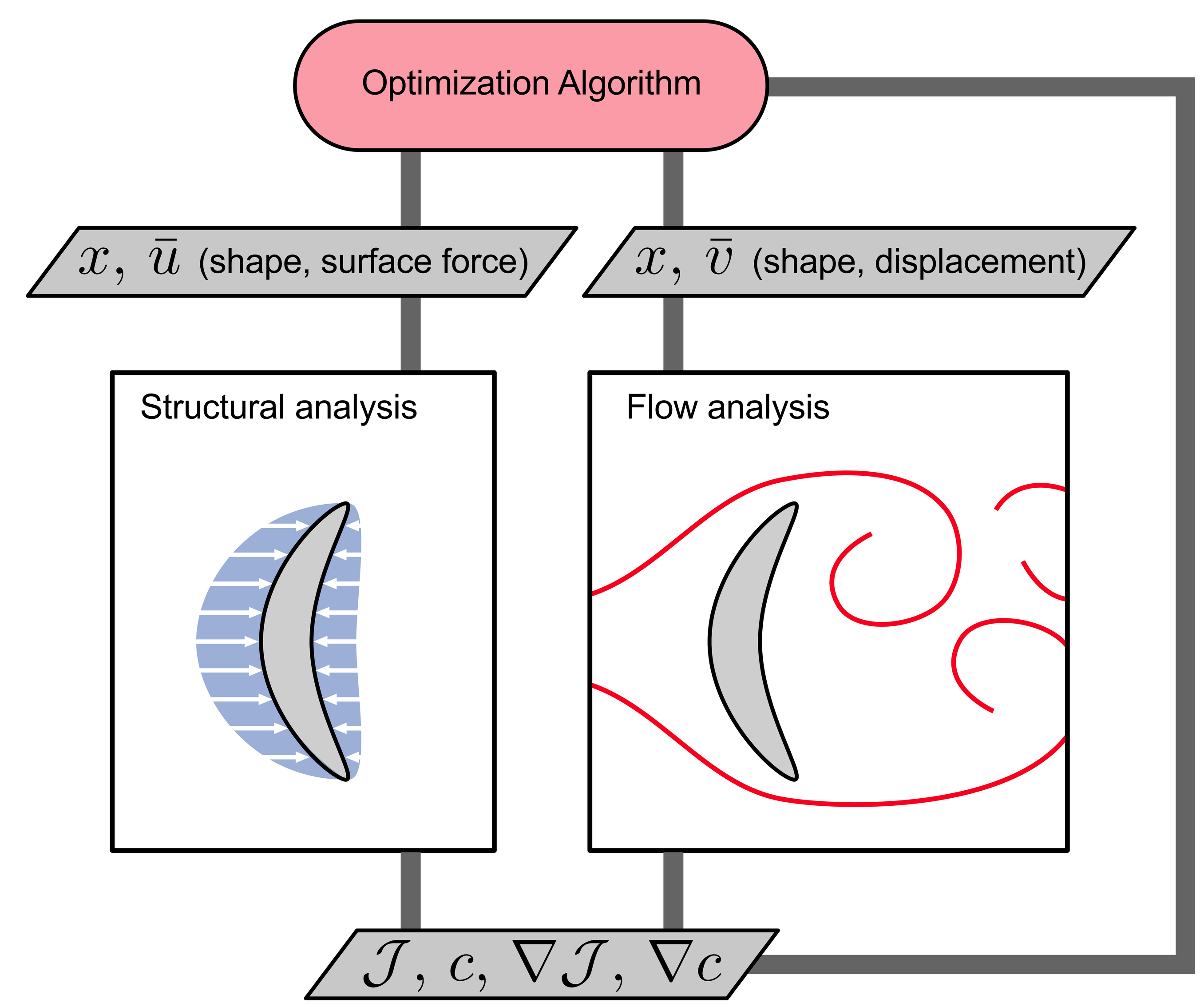
Motivation

- Engineering systems governed by complex multi-physics are challenging to design, because they often exhibit subtle tradeoffs and defy our intuition.
- High-fidelity Multi-disciplinary Design Optimization (MDO), based on physics-based simulations, can help guide and inform the design of complex engineering systems.
- Few high-fidelity multi-disciplinary analysis codes are available to industry: **how can we couple existing disciplinary codes to enable industrial MDO?**

Multidisciplinary Feasible (MDF)



Individual-discipline Feasible (IDF)



On-going and future work

- Implement a matrix-free interior-point algorithm to handle inequality constraints.
- Benchmark inexact-Newton-FLECS, using the MDF-based preconditioner, against conventional optimization methods on a large-scale aero-structural IDF problem.

References cited

[1] Cramer, E. J., Dennis, J. E., Frank, P. D., Lewis, R. M., and Shubin, G. R., "Problem Formulation for Multidisciplinary Optimization," *SIAM Journal on Optimization*, Vol. 4, No. 4, Nov. 1994, pp. 754-776.

[2] Hicken, J. E. and Dener, A., "A Flexible Iterative Solver for Nonconvex, Equality-Constrained Quadratic Subproblems," *SIAM Journal on Scientific Computing*, Vol. 37, No. 4, July 2015, pp. A1801-A1824.

[3] *Dener, A. and Hicken, J. E.*, "Revisiting Individual Discipline Feasible using matrix-free Inexact-Newton-Krylov," *10th AIAA Multidisciplinary Design Optimization Conference, American Institute of Aeronautics and Astronautics, Jan. 2014, paper number AIAA-2014-0110.*

[4] Biros, G. and Ghattas, O., "Parallel Lagrange-Newton-Krylov-Schur methods for PDE-constrained optimization. Part I: the Krylov-Schur solver," *SIAM Journal on Scientific Computing*, Vol. 27, 2005, pp. 687-713.

The individual-discipline-feasible (IDF) formulation offers a possible solution

- Consider a two discipline optimization problem:

$$\min_{x} \quad \mathcal{J}(x, u(x), v(x))$$
$$\text{governed by} \quad \begin{cases} \mathcal{R}_u(x,u,v) = 0 \\ \mathcal{R}_v(x,v,u) = 0 \end{cases}$$

coupled PDEs

- The IDF formulation [1] introduces coupling variables, $\bar{u}$ and $\bar{v}$ below, that eliminate the need for a full multidisciplinary analysis at each optimization iteration:

$$\min_{x,\bar{u},\bar{v}} \quad \mathcal{J}(x, u(x,\bar{v}), v(x,\bar{u}))$$
$$\text{subject to} \quad c(x,\bar{u},\bar{v}) = \begin{bmatrix} \bar{u} - u(x,\bar{v}) \\ \bar{v} - v(x,\bar{u}) \end{bmatrix} = 0$$
$$\text{governed by} \quad \begin{cases} \mathcal{R}_u(x,u,\bar{v}) = 0 \\ \mathcal{R}_v(x,v,\bar{u}) = 0 \end{cases}$$

uncoupled PDEs

- This simplifies the solution of MDO problems by maintaining modularity of the disciplinary software; however, **the large number of IDF coupling variables and constraints poses a challenge to conventional (matrix-based) optimization methods**.

Matrix-free Newton-Krylov can solve the IDF formulation without explicit constraint Jacobians

- We favor derivative-based methods for large (> 10^2) design problems. Thus, we need to solve linear systems based on the primal-dual matrix:

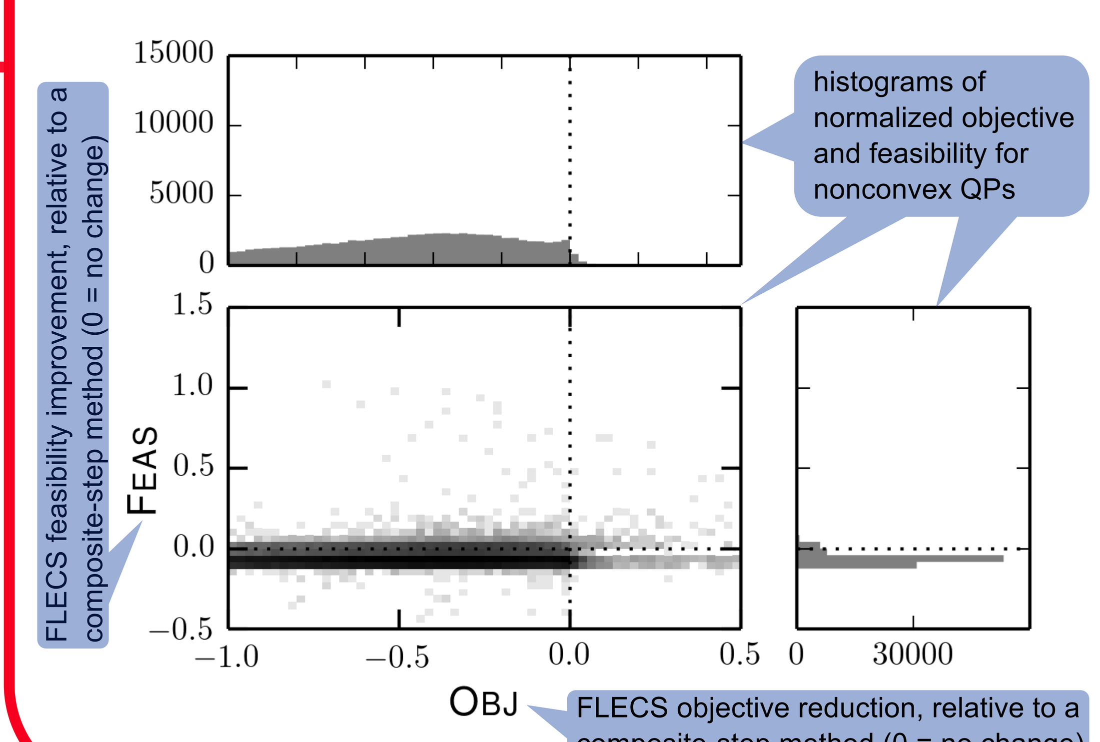
$$\mathsf{K} = \begin{bmatrix} \mathsf{W} & \mathsf{A}^T \\ \mathsf{A} & 0 \end{bmatrix}$$

Primal-dual matrix; Hessian of the Lagrangian; IDF constraint Jacobian

- Conventional algorithms require the user to provide A explicitly, and this is a problem for IDF: each row of A requires a PDE solution, and it is common to have thousands of rows.
- In contrast, Krylov methods only require products of the form $\mathsf{K}z$, where z is arbitrary; these products can be formed using two second-order adjoints, i.e. no Jacobians are required.

Challenge 1: nonconvexity in the context of a matrix-free algorithm

- Newton's method does not distinguish between stationary points, so we need to prevent convergence to local maxima. This is difficult to do matrix-free.
- To cope with such nonconvexity, we created the FLexible Equality-Constrained Subproblem solver, or FLECS [2].
- Numerical experiments indicate that FLECS outperforms composite-step algorithms based on the projected Steihaug conjugate-gradient method.



Challenge 2: matrix-free preconditioning of the primal-dual matrix

- The primal-dual matrix must be preconditioned. Most preconditioners are based on matrix factorizations, but we do not have a matrix.
- Our approach is to construct a preconditioner based on an approximation of multi-disciplinary feasible (MDF) [3]. This preconditioner is inspired by the reduced-space preconditioner used in one-shot methods [4].
- The MDF-based preconditioner is effective and scales well as the number of design and coupling variables increases.