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SOFICS: Optimization Framework for Structures under Detonation-Induced Fluid Flows

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Summary

SOFICS (**S**tructural **O**ptimization through **F**luid-structure **I**nteraction and **C**oupled **S**imulations) is a software toolkit that optimizes the design of structures exposed to extreme pressure loads generated by detonations. It integrates the open-source fluid dynamics solver M2C and structural dynamics solver Aero-S to model the two-way interaction between fluid and structural dynamics. Leveraging Dakota, an open-source optimization tool, and Gmsh, an open-source finite element mesh generator, SOFICS explores various design options efficiently. By reusing a fixed fluid simulation setup and finite volume mesh across different design variations, SOFICS reduces computational costs while maintaining accuracy. SOFICS simplifies and streamlines the complex task of designing impact-resistant structures, making it accessible to a broad range of users.

Statement of need

Designing structures to withstand detonation-induced loads presents several critical challenges. Detonations produce traveling shock waves characterized by high density, velocity, and pressure in the surrounding fluid medium. When these shock waves impact a solid structure, they can cause significant, often permanent deformations, which, in turn, influence the dynamics of the surrounding fluid flow. This interaction creates a complex two-way coupling between the fluid and structural dynamics. The shared boundary between the fluid and the structure, known as the fluid-structure interface, evolves over time. As a result, the computational fluid dynamics solver must accommodate deforming boundaries. Additionally, the computational fluid and structural dynamics solvers must be able to exchange data in real-time following a predefined protocol. This ensures that the fluid solver receives the kinematics of the wetted surface of the structure, while the structural solver receives the transient pressure loads from the fluid.

Few open-source solutions exist that can simulate the highly nonlinear behavior of detonations and perform coupled fluid-structure simulations to evaluate the response of impacted structures. One possible approach involves coupling open-source finite volume solvers like OpenFOAM (Weller et al., 1998) with finite element solvers such as FEniCS (Alnaes et al., 2015) through a coupling library like preCICE (Chourdakis et al., 2022), which facilitates the transfer of structural velocities, fluid pressures, and shared fluid-structure interfaces between the two independent solvers. However, such a framework typically requires a moving, body-conforming fluid mesh to accurately communicate between solvers, resulting in the need for a unique fluid mesh for each design configuration. Additionally, optimization studies can introduce designs with complex features, such as sharp edges, narrow regions, and discontinuous geometry, which can lead to poor mesh quality and increased computational complexity.

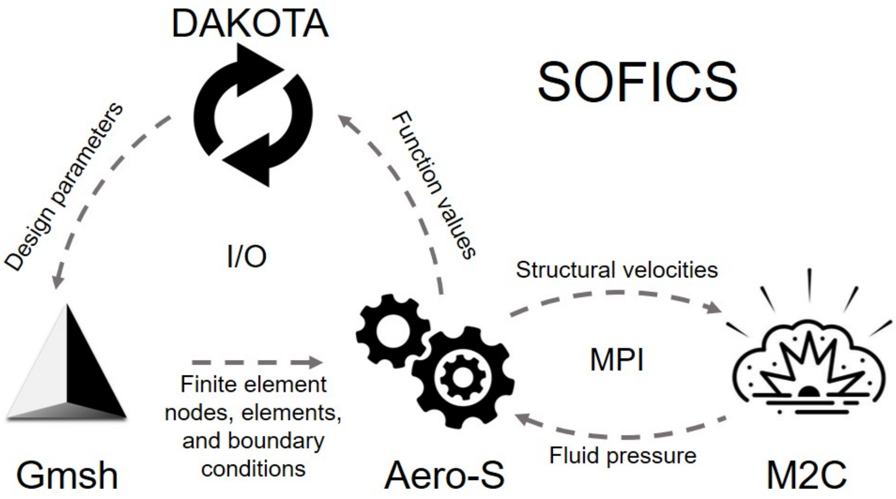

Figure 1: SOFICS Workflow: Coupling `Dakota` for optimization, `Gmsh` for finite-element meshing, `Aero-S` as the structural dynamics solver, and `M2C` as the fluid dynamics solver.

We develop `SOFICS`[1], shown in Figure 1, which streamlines the optimization of structures under detonation-induced fluid flows, providing a robust and flexible toolkit for researchers and engineers in the field. It is a utility written in Bash, that loosely-couples an optimizer and a simulation based evaluator that performs coupled fluid-structure simulations and computes the required objective and constraint values. It uses an in-house open-source fluid dynamics solver, `M2C`[2], developed in modern C++ with an Object-Oriented programming design. `M2C` solves the compressible Navier-Stokes equations using a high-resolution finite volume method. It supports a range of equations of state including, perfect gas, stiffened gas, and the Jones-Wilkins-Lee equation, which are widely used for simulating detonations in both air and underwater environments.

The advantages of using `M2C` for design optimization are three-fold. First, `M2C` is directly coupled with our open-source, finite element-based structural dynamics solver `Aero-S`[3] using the partitioned procedure (C. Farhat et al., 2010). Both solvers are designed for parallel computations, utilizing the Message Passing Interface (MPI) (2023) for efficient distributed processing. Second, we use the embedded boundary method (Ma et al., 2022; K. Wang et al., 2012; K. G. Wang et al., 2015) to accommodate large deflections. The method tracks the fluid-structure interface explicitly within a fixed, non-uniform, non-body conforming finite volume mesh, eliminating the need for mesh motion and frequent re-meshing. As a result, a single, fixed fluid mesh can be computed *a priori* and used consistently across different design configurations. Finally, `M2C` computes the interfacial mass, momentum, and energy fluxes across the fluid-structure interface using the **FI**nite **V**olume method with **E**xact multi-material **R**iemann problems (FIVER), which solves a 1D fluid-structure Riemann problem locally featuring a constant interface velocity obtained from the structural solver (Ma et al., 2022; K. Wang et al., 2012). The coupled fluid-structure simulation model has been validated for several multiphase flow and fluid-structure interaction problems. These include underwater and aerial explosions and implosions (C. Farhat et al., 2013; Ma et al., 2022; Narkhede et al., 2025), cavitation (S. Cao et al., 2021; Zhao et al., 2024), hypervelocity impacts (Islam et al., 2023a, 2023b), and shockwave and laser lithotripsy (Shunxiang Cao et al., 2019; Kevin G. Wang, 2017; Zhao et al., 2023).

`SOFICS` utilizes the open-source software `Dakota` (Adams et al., 2022) for the simulation-based

[1] https://github.com/anarkh97/sofics/tree/main
[2] https://github.com/kevinwgy/m2c
[3] https://github.com/anarkh97/aero-s-foam

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design optimization studies. Dakota was chosen because it provides a range of gradient-based and gradient-free optimization methods, along with robust asynchronous and parallel evaluation capabilities. It treats the fluid-structure simulation as a "black-box," using a user-defined analysis_driver – which can be an executable or a script – to generate a short results file containing the necessary objective and constraint values. It employs the operating system's fork interface to spawn child processes, on which the coupled fluid-structure simulations are performed.

To simplify usage, the analysis_driver is divided into three Bash scripts: pre_processor.sh, driver.sh, and post_processor.sh. The user can modify the pre- and post-processing scripts to fit their specific requirements. The pre-processing script reads the design parameter file from Dakota and generates the finite element mesh for the current structural design configuration using the open-source meshing tool, Gmsh (Geuzaine & Remacle, 2009). The driver script handles the execution of simulations across distributed processors. To prevent resource conflicts between concurrent design simulations, it dynamically identifies and allocates "idle" resources based on the evaluation ID assigned by Dakota and the computational requirements for each design evaluation. Finally, the post-processing script then reads the results from Aero-S, evaluates the objective and constrain value, and writes them to the results file provided by Dakota. Once all design configurations have been evaluated, Dakota advances to the next iteration. Figure 2 depicts the workflow for a generic optimization scheme in Dakota.

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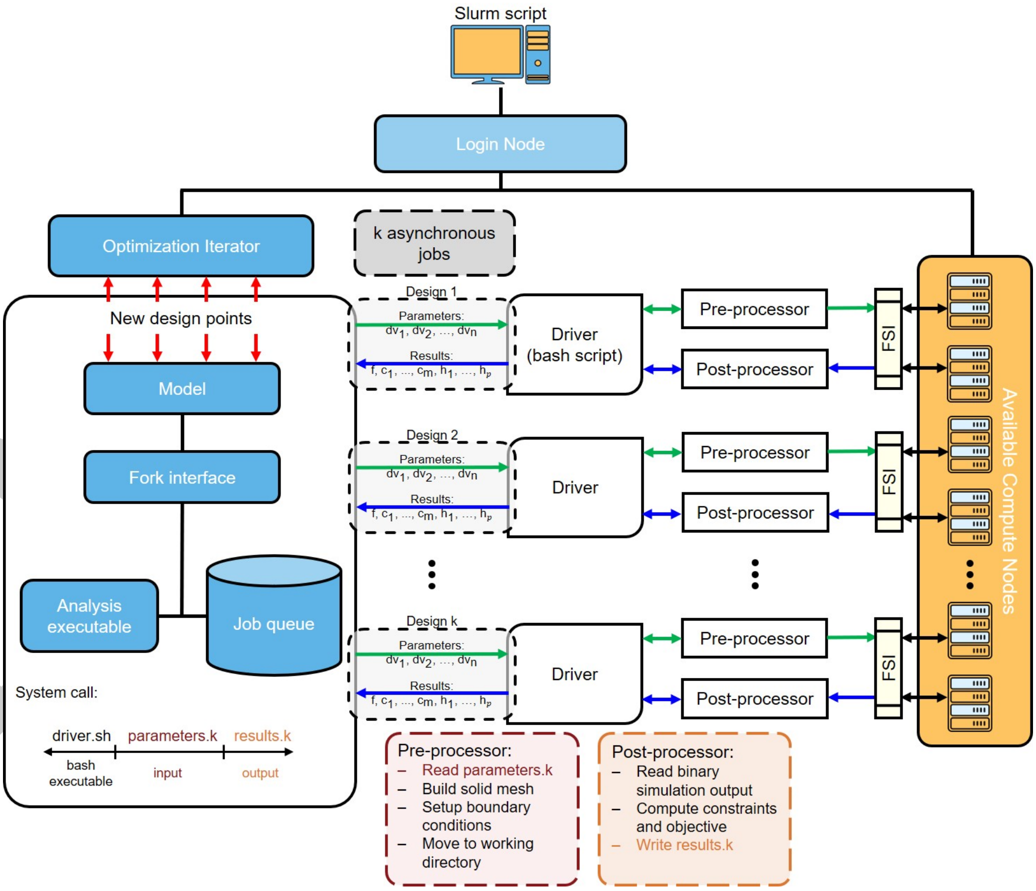

Figure 2: A high-level workflow of the asychrounous parallel optimization framework. The process begins with the Slurm script on the login node, distributing asynchronous optimization jobs across available compute nodes. Each design iteration involves pre-processing (e.g., parameter setup and meshing), running the driver script, fluid-structure interaction (FSI) simulations, and post-processing to compute constraints and objectives. Results are iteratively fed back into the optimization model via the fork interface.

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