I propose investigating airfoil shape optimization using a novel combination of recently developed techniques, including pseudospectral (PS), volume penalization, and adjoint looping optimization methods. I will perform simulations using the `Dedalus` PS python framework which I have used to study Rayleigh-Bénard convection and magnetohydrodynamics throughout the last two years. Volume penalization for external flow simulations has already been implemented with `Dedalus` [Hester 2020] and there exists a substantial body of airfoil shape optimization research for comparison. I am currently developing the necessary adjoint looping optimization infrastructure which uses `Dedalus` to solve the adjoint system, thereby allowing us to approximate gradients for arbitrary metrics. The proposed technique offers key advantages when compared to the conventional approach which relies on finite volume simulations and finite difference gradient-based optimization.

1. High-fidelity physics simulations: PS methods are well-suited for simulating turbulent fluid flow. Finite volume methods are subject to small grid-scale numerical errors which can excite nominally stable modes in turbulent shear flows, thereby triggering artificial instabilities [Lecoanet 2015]. In the context of shape optimization, these instabilities could propagate tremendous differences in the resulting optimized geometries.
2. Modular flow regimes: the `Dedalus` pseudospectral python framework interprets equations symbolically, allowing for rapid development and future shape optimization research in compressible, high-Mach number, multiphase, and combustive flow regimes using the same codes.
3. Efficient gradient-based optimization: adjoint looping allows us to approximate gradients rapidly and accurately in high dimensional parameter spaces [Lecoanet 2015]. The conventional finite difference method is costly (and sometimes inaccurate) because it involves a large number of simulations.
4. Flexible domain representation: the volume penalty method allows us to model external flows around an arbitrary spatial mask function, thereby eliminating the need to continuously remesh as the design is updated and ultimately reconstruct a palatable design from the optimized mesh.

Airfoils offer an ideal context for investigation because they operate in a wide range of flow regimes. Airfoil geometries are generally smooth, allowing us to represent them with truncated Fourier series. Smooth design representation has tangible benefits from an engineering perspective and it will allow us to analyze optimizated geometries from a scientific perspective. For instance, we will vary the system's Reynolds number and compare the optimized Fourier coefficient profiles.

Methods: The complicated domains necessary for shape optimization are difficult to represent via spectral basis functions. Volume penalization is the robust solution, where a time-invariant mask function Φ is included in the relevant PDE to represent the immersed solid. We combine this technique with the adjoint looping method, which has been used to optimize initial conditions in similar 2D incompressible flows [Kerswell 2014].

$$\partial_t \boldsymbol{u} + \boldsymbol{u}\cdot\boldsymbol{\nabla}\boldsymbol{u} + \frac{1}{\rho}\boldsymbol{\nabla} p = \nu\nabla^2\boldsymbol{u} - \frac{1}{\tau}\Phi(\boldsymbol{x};\boldsymbol{a})(\boldsymbol{u}-\boldsymbol{U}) \qquad \text{and} \qquad \boldsymbol{\nabla}\cdot\boldsymbol{u} = 0 \tag{1}$$

where $\boldsymbol{U} = \hat{\boldsymbol{x}}U$ is the airfoil's velocity frame; $\tau \ll 1$ is the damping timescale; and $\boldsymbol{u} = u\hat{\boldsymbol{x}} + v\hat{\boldsymbol{y}}$, p, ρ, and ν are the fluid's velocity, pressure, density, and viscosity respectively. The aerodynamic force acting on the immersed interface is given by $\boldsymbol{F} = F_D\hat{\boldsymbol{x}} + F_L\hat{\boldsymbol{y}} = \frac{\rho}{\tau}\langle\Phi(\boldsymbol{x};\boldsymbol{a})(\boldsymbol{u}-\boldsymbol{U})\rangle$ where $\langle\cdot\rangle$ denotes the spatial integral over the domain $-L_x/2 < x < L_x/2$, $-L_y/2 < y < L_y/2$.

Our optimization problem maximizes the mean lift to drag ratio $\overline{F_L/F_D} \equiv T^{-1}\int_0^T F_L/F_D\,dt$ where $T \gg U/L_x$. We use Γ's Fourier coefficients $\boldsymbol{a}$ as optimization parameters. The adjoint looping method involves differentiating a Lagrangian $\mathcal{L}$ to derive the adjoint system, which we solve backwards in time $t : T \to 0$, thereby allowing us to approximate $\boldsymbol{\nabla}_{\boldsymbol{a}}\mathcal{L}$.

The mask function is a smooth indicator $\Phi(\boldsymbol{x};\boldsymbol{a}) = \frac{1}{2}\big[1 - \tanh\big(d_r^{-1}\mathrm{SDF}(\boldsymbol{x};\boldsymbol{a},\theta)\big)\big]$ where d_r is proportional to the minimum resolvable length scale. The signed distance function $\mathrm{SDF}(\boldsymbol{x};\boldsymbol{a},\theta)$ can be treated analytically in terms of $\boldsymbol{a}$ but we must perform an eigenvalue decomposition at each spectral grid point to find the direction θ which minimizes the distance to Γ [Boyd 2006]. A small number ($n \sim 10$) of complex Fourier coefficients describe a large set of potential airfoil geometries. We employ Fourier and Chebyshev series spanning $-L_x/2 < x < L_x/2$ and $-L_y/2 < y < L_y$ respectively, along with stress-free impenetrable boundary conditions at $y = \pm L_y/2$. This formulation is nominally periodic in x, but when this is undesirable we implement spatial dampening to encourage $\boldsymbol{u} \to \boldsymbol{0}$ in the vicinity of $x = \pm L_x/2$. The source term containing Φ in 1 acts as a no-slip boundary condition proxy on Γ.

$$\mathcal{L}(\boldsymbol{u},p,\boldsymbol{a},\boldsymbol{\mu},\pi) = \int_0^T \Big\langle F_L(\boldsymbol{u};\boldsymbol{a})\Big\rangle dt - \Lambda\Big[\int_0^T \Big\langle F_D(\boldsymbol{u};\boldsymbol{a})\Big\rangle dt - \overline{F_D}\Big] + ...$$
$$\int_0^T \big\langle \boldsymbol{\mu}(\boldsymbol{x},t)\cdot\big(\partial_t\boldsymbol{u} + \boldsymbol{u}\cdot\boldsymbol{\nabla}\boldsymbol{u} + \frac{1}{\rho}\boldsymbol{\nabla}p - \nu\nabla^2\boldsymbol{u} + \frac{1}{\tau}\Phi(\boldsymbol{x};\boldsymbol{a})(\boldsymbol{u}-\boldsymbol{U})\big)\big\rangle dt + \int_0^T \big\langle \pi(\boldsymbol{x},t)\boldsymbol{\nabla}\cdot\boldsymbol{u}\big\rangle dt$$

where the first two terms, which we will call $\mathcal{J}$, is the scalar quantity to be maximized and the remaining terms impose the Navier-Stokes constraint. We aim to compute the complex Fourier coefficients $\boldsymbol{a}$ which maximize lift F_L while keeping the drag F_D in the approximate vicinity of some quantity $\overline{F_D}$. The function Λ is chosen to ensure that $\int_0^T \langle F_D\rangle dt \sim \overline{F_D}$ to a desired specificity.

From the corresponding Euler-Lagrange equations we derive the adjoint system

$$\boldsymbol{\nabla}\cdot\boldsymbol{\mu} = 0 \tag{2}$$
$$\partial_t\boldsymbol{\mu} + \boldsymbol{u}\cdot\boldsymbol{\nabla}\boldsymbol{\mu} - \boldsymbol{\mu}\cdot\big(\boldsymbol{\nabla}\boldsymbol{u}\big)^T + \boldsymbol{\nabla}\pi = -\nu\nabla^2\boldsymbol{\mu} + \frac{1}{\tau}\Phi\,\boldsymbol{\mu} + \frac{\delta\mathcal{J}}{\delta\boldsymbol{u}} \tag{3}$$

which is evolved backward in time $t : T \to 0$.

Given the airfoil curve coefficients $\boldsymbol{a}$, we compute the mask function's gradient $\nabla_{\boldsymbol{a}}\Phi$ numerically via finite differences. This calculation can be performed independently (embarrassingly-parallelizable) at each grid point by solving an eigenvalue problem of low rank.

The optimization loop is then performed as follows:

1. At iteration k, initialize with the previous iteration's end state $\boldsymbol{u}^{k-1}(T)$.
2. Solve 1 until a statistically-steady state is achieved, at which point ($t = 0$) we record the solution until $t = T$.
3. Initialize the adjoint system (3) at $t = T$ with $\boldsymbol{\mu}(\boldsymbol{x},T) = \boldsymbol{0}$.
4. Solve 3 backwards ($t : 0 \to T$)
5. Simultaneously solve for $\boldsymbol{\nabla}_{\boldsymbol{a}}\mathcal{L}$.
6. Evolve the Fourier coefficients by a magnitude of ε: $\boldsymbol{a}^{k+1} = \boldsymbol{a}^k + \varepsilon\boldsymbol{\nabla}_{\boldsymbol{a}}\mathcal{L}$.
7. Repeat until $|\mathcal{J}^{k+1} - \mathcal{J}^k|$ is less than some tolerance.