

Time-Dependent Adjoint Methods for Single and Multi-Disciplinary Problems

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Motivation

- Computational fluid dynamics analysis capabilities commonplace today
- In addition to analysis capability, sensitivity capability is highly desirable
 - Design optimization
 - Error estimation
 - Parameter sensitivity
- Sensitivities may be obtained by:
 - Perturb input, rerun analysis code (Finite difference)
 - Linearizing analysis code (tangent method)
 - Good for 1 input, many outputs
 - Adjoint method (Pironneau, Jameson, many others...)
 - Good for many inputs, one output

Objective

- Demonstrate methodical approach for formulating and implementing discrete adjoint to increasingly complex problems
- Progressively more complex simulation sensitivity formulations
 - Steady-state aerodynamics
 - Time-dependent aerodynamics (2D)
 - Time-dependent coupled aero-elastic (3D)
- Focus
 - Adjoint formulation
 - Hand coded (occasional use of AD)
 - Same data structures/solution techniques as analysis
 - Verification
 - Exact full sensitivities in all cases
 - Optimization examples are mostly illustrative



- **Time-dependent**
- Aeroelastic
- **Overset meshes**
- **Adaptive meshes**



Outline

- General unsteady tangent/adjoint formulations
 - Backward time integration
- Specific Case
 - Time-dependent aerodynamic shape optimization
 - 2D pitching airfoil optimization
- Generalized multidisciplinary formulation
 - Time-dependent aerodynamic shape optimization
 - Time-dependent aeroelastic shape optimization
- Aeroelastic rotor optimization example
- Conclusions

Adjoint Sensitivity Formulation

- Continuous vs. Discrete Adjoint Approaches
 - Continuous: Linearize then discretize
 - Discrete: Discretize then Linearize
- Continuous Approach:
 - More flexible adjoint discretizations
 - Framework for non-differentiable tasks (limiters)
 - Often invoked using flow solution as constraint using Lagrange multipliers
- Discrete Approach:
 - Reproduces exact sensitivities of code
 - Verifiable through finite differences
 - Relatively simple implementation (but tedious)
 - Chain rule differentiation of analysis code
 - Transpose these derivatives
 - (transpose and reverse order)
 - Includes boundary conditions
 - Automation possible (but use judiciously for efficiency reasons)

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Adjoint Formulation (chain rule approach)

- Objective: L = L(D, u(D))
- Subject to: R(u(D), D) = 0
 - R = 0: flow solution converged
 - u : flow variables (solution)
 - D: design parameters (shape parameters)



Adjoint Formulation

• Sensitivity equation:



Evaluate first, define as Λ^T

- Adjoint equation:
 - No dependence on D

$$\frac{\partial R}{\partial u} \bigg|^T \Lambda = - \bigg[\frac{\partial L}{\partial u} \bigg]^T$$

- Dependence on L
- Final form: $\frac{dL}{dD} = \frac{\partial L}{\partial D} + \Lambda^T \frac{\partial R}{\partial D}$
- Cost is independent of number of D's
- dL/dD are then used by a gradient based optimizer to find next best shape

KKT/Lagrange Multiplier Adjoint Formulation

$$J(D, \mathbf{U}, \Lambda) = L(\mathbf{U}(D), D) + \Lambda^T \mathbf{R}(\mathbf{U}(D), D)$$

$$J_{min} = \min_{D \in I} J(D)$$

subject to $\mathbf{R}(\mathbf{U}(\mathbf{D}), \mathbf{D}) = 0$

$$\frac{\partial J}{\partial D} = \frac{\partial L}{\partial D} + \Lambda^T \frac{\partial \mathbf{R}}{\partial D} = 0$$
$$\frac{\partial J}{\partial \mathbf{U}} = \frac{\partial L}{\partial \mathbf{U}} + \Lambda^T \frac{\partial \mathbf{R}}{\partial \mathbf{U}} = 0$$
$$\frac{\partial J}{\partial \Lambda} = \mathbf{R}(\mathbf{U}) = 0$$

Sensitivity equation

Adjoint equation

Constraint equation

Optimization for Time Dependent Problems

- Using chain rule linearization
 - New time-step values depend on previous time step values
 - Integrate linearized equation in time (tangent problem)
 - Transpose all to get adjoint (and reverse order of matrix multiplication) $[[A][B]]^T = [B]^T [A]^T$
 - Integrate backwards in time
 - Requires storing entire time history (to disk)
 - 10 8-Byte variables per grid point per time step
 - Advantage of using large time steps with good implicit solver
 - Use local node disks on parallel computer (>1TB each node)
- Simple derivation of time-dependent adjoint
 - Chain rule linearization
 - Lagrange multipliers

Time Dependent Problems: Forward Sensitivity

- Time integrated objective functional $L = L(\mathbf{u}^n(D), \mathbf{u}^{n-1}(D), \mathbf{u}^{n-2}(D), ..., \mathbf{u}^0(D), D)$
- Unsteady Residual (BDF1 for simplicity) $\mathbf{R}^{n}(\mathbf{u}^{n}(D), \mathbf{u}^{n-1}(D), D) = 0$

• Sensitivity of objective (chain rule) $\frac{dL}{dD} = \frac{\partial L}{\partial D} + \frac{\partial L}{\partial \mathbf{u}^n} \frac{\partial \mathbf{u}^n}{\partial D} + \frac{\partial L}{\partial \mathbf{u}^{n-1}} \frac{\partial \mathbf{u}^{n-1}}{\partial D} + \frac{\partial L}{\partial \mathbf{u}^{n-2}} \frac{\partial \mathbf{u}^{n-2}}{\partial D} + \dots + \frac{\partial L}{\partial \mathbf{u}^0} \frac{\partial \mathbf{u}^0}{\partial D}$

Time Dependent Problems: Forward Sensitivity

$$\mathbf{R}^n(\mathbf{u}^n(D),\mathbf{u}^{n-1}(D),D)=0$$

Obtain flow sensitivity by differentiating residual



Substitute into objective sensitivity equation

 $\frac{dL}{dD} = \frac{\partial L}{\partial D} + \frac{\partial L}{\partial \mathbf{u}^n} \frac{\partial \mathbf{u}^n}{\partial D} + \frac{\partial L}{\partial \mathbf{u}^{n-1}} \frac{\partial \mathbf{u}^{n-1}}{\partial D} + \frac{\partial L}{\partial \mathbf{u}^{n-2}} \frac{\partial \mathbf{u}^{n-2}}{\partial D} + \ldots + \frac{\partial L}{\partial \mathbf{u}^0} \frac{\partial \mathbf{u}^0}{\partial D}$

Time Dependent Problems: Adjoint Formulation

 $L = L(\mathbf{u}^{n}(D), \mathbf{u}^{n-1}(D), \mathbf{u}^{n-2}(D), ..., \mathbf{u}^{0}(D), D)$

$\mathbf{R}^n(\mathbf{u}^n(D),\mathbf{u}^{n-1}(D),D) = 0$

- n constraints (1 per time step)
- n Lagrange multipliers

$$\begin{split} J(D, \mathbf{u}^{n}, \mathbf{u}^{n-1}, ..., \mathbf{\Lambda}^{n}, \mathbf{\Lambda}^{n-1}, ...) &= L(\mathbf{u}^{n}(D), \mathbf{u}^{n-1}(D), \mathbf{u}^{n-2}(D), ..., \mathbf{u}^{0}(D), D) \\ &+ \mathbf{\Lambda}^{nT} \mathbf{R}^{n}(\mathbf{u}^{n}(D), \mathbf{u}^{n-1}(D), D) \\ &+ \mathbf{\Lambda}^{n-1T} \mathbf{R}^{n-1}(\mathbf{u}^{n-1}(D), \mathbf{u}^{n-2}(D), D) \\ &+ ... \\ &+ \mathbf{\Lambda}^{1T} \mathbf{R}^{n}(\mathbf{u}^{1}(D), \mathbf{u}^{0}(D), D) \end{split}$$

Time Dependent Problems: Adjoint Formulation

Constraint equation(s)

$$\frac{\partial J}{\partial \Lambda^n} = \mathbf{R}^n(\mathbf{u}^n, \mathbf{u}^{n-1}, D) = 0$$
$$\frac{\partial J}{\partial \Lambda^{n-1}} = \mathbf{R}^{n-1}(\mathbf{u}^{n-1}, \mathbf{u}^{n-2}, D) = 0$$

$$\frac{\partial J}{\partial \Lambda^1} = \mathbf{R}^1(\mathbf{u}^1, \mathbf{u}^0, D) = 0$$

. . .

Sensitivity equation(s)

$$\frac{\partial J}{\partial D} = \frac{\partial L}{\partial D} + \Lambda^{nT} \frac{\partial \mathbf{R}^{n}}{\partial D} + \Lambda^{n-1T} \frac{\partial \mathbf{R}^{n-1}}{\partial D} + \Lambda^{n-2T} \frac{\partial \mathbf{R}^{n-2}}{\partial D} + \dots = 0$$

Time Dependent Problems: Adjoint Formulation

Adjoint equations

$$\begin{aligned} \frac{\partial J}{\partial \mathbf{u}^{n}} &= \frac{\partial L}{\partial \mathbf{u}^{n}} + \Lambda^{nT} \frac{\partial \mathbf{R}^{n}}{\partial \mathbf{u}^{n}} = 0\\ \frac{\partial J}{\partial \mathbf{u}^{n-1}} &= \frac{\partial L}{\partial \mathbf{u}^{n-1}} + \Lambda^{nT} \frac{\partial \mathbf{R}^{n}}{\partial \mathbf{u}^{n-1}} + \Lambda^{n-1T} \frac{\partial R^{n-1}}{\partial \mathbf{u}^{n-1}} = 0\\ \frac{\partial J}{\partial \mathbf{u}^{n-2}} &= \frac{\partial L}{\partial \mathbf{u}^{n-2}} + \Lambda^{n-1T} \frac{\partial \mathbf{R}^{n-1}}{\partial \mathbf{u}^{n-2}} + \Lambda^{n-2T} \frac{\partial \mathbf{R}^{n-2}}{\partial \mathbf{u}^{n-2}} = 0\\ \dots\\ \frac{\partial J}{\partial \mathbf{u}^{1}} &= \frac{\partial L}{\partial \mathbf{u}^{1}} + \Lambda^{2T} \frac{\partial \mathbf{R}^{2}}{\partial \mathbf{u}^{1}} + \Lambda^{1T} \frac{\partial \mathbf{R}^{1}}{\partial \mathbf{u}^{1}} = 0 \end{aligned}$$

$$\begin{bmatrix} \frac{\partial \mathbf{R}^{n}}{\partial \mathbf{u}^{n}} \end{bmatrix}^{T} \mathbf{\Lambda}^{n} = -\frac{\partial L}{\partial \mathbf{u}^{n}}^{T}$$
$$\begin{bmatrix} \frac{\partial \mathbf{R}^{n-1}}{\partial \mathbf{u}^{n-1}} \end{bmatrix}^{T} \mathbf{\Lambda}^{n-1} = -\frac{\partial L}{\partial \mathbf{u}^{n-1}}^{T} - \mathbf{\Lambda}^{nT} \frac{\partial \mathbf{R}^{n}}{\partial \mathbf{u}^{n-1}}$$

- Reverse recurrence relation
 - Solved by back-substitution
 - Requires u at each time level

Generalized Discrete Sensitivities

• Consider a multi-phase analysis code:

$$\mathbf{L}(\mathbf{D}) = \mathbf{L}(F_{n-1}(F_{n-2}(...,F_2(F_1(\mathbf{D}))....))))$$

- -L = Objective(s)
- D = Design variable(s)
- Sensitivity Analysis
 Using chain rule:

$$\delta \mathbf{L} = \frac{d\mathbf{L}}{d\mathbf{D}} \delta \mathbf{D}$$

$$\frac{d\mathbf{L}}{d\mathbf{D}} = \frac{\partial \mathbf{L}}{\partial F_{n-1}} \cdot \frac{\partial F_{n-1}}{\partial F_{n-2}} \cdot \dots \cdot \frac{\partial F_2}{\partial F_1} \cdot \frac{\partial F_1}{\partial \mathbf{D}}$$

Tangent Model

- Special Case:
 - 1 Design variable D, many objectives L
- Precompute all stuff depending on single D
- Construct dL/dD elements as:

$$\frac{d\mathbf{L}}{d\mathbf{D}} = \frac{\partial \mathbf{L}}{\partial F_{n-1}} \cdot \left[\frac{\partial F_{n-1}}{\partial F_{n-2}} \left[\dots \left[\frac{\partial F_2}{\partial F_1} \left[\frac{\partial F_1}{\partial \mathbf{D}} \right] \right] \right] \right]$$

Adjoint Model

- Special Case:
 - 1 Objective L, Many Design Variables D
 - Would like to precompute all left terms

$$\frac{d\mathbf{L}}{d\mathbf{D}} = \frac{\partial \mathbf{L}}{\partial F_{n-1}} \cdot \frac{\partial F_{n-1}}{\partial F_{n-2}} \cdot \dots \cdot \frac{\partial F_2}{\partial F_1} \cdot \frac{\partial F_1}{\partial \mathbf{D}}$$

– Transpose entire equation:

$$\frac{d\mathbf{L}}{d\mathbf{D}}^{T} = \frac{\partial F_{1}}{\partial \mathbf{D}}^{T} \cdot \frac{\partial F_{2}}{\partial F_{1}}^{T} \cdot \frac{\partial F_{n-1}}{\partial F_{n-2}}^{T} \dots \frac{\partial \mathbf{L}}{\partial F_{n-1}}^{T}$$

Adjoint Model

- Special Case:
 - 1 Objective L, Many Design Variables D
 - Would like to precompute all left terms

$$\frac{d\mathbf{L}}{d\mathbf{D}} = \frac{\partial \mathbf{L}}{\partial F_{n-1}} \cdot \frac{\partial F_{n-1}}{\partial F_{n-2}} \dots \cdot \frac{\partial F_2}{\partial F_1} \cdot \frac{\partial F_1}{\partial \mathbf{D}}$$

– Transpose entire equation: precompute as:

$$\frac{d\mathbf{L}}{d\mathbf{D}}^{T} = \frac{\partial F_{1}}{\partial \mathbf{D}}^{T} \cdot \left[\frac{\partial F_{2}}{\partial F_{1}}^{T} \cdot \left[\frac{\partial F_{n-1}}{\partial F_{n-2}}^{T} \cdot \left[\dots \left[\frac{\partial \mathbf{L}}{\partial F_{n-1}}^{T} \right] \right] \right]$$

Steady-State Shape Optimization Problem

• Multi-phase process:

$$\mathbf{L}(\mathbf{D}) = \mathbf{L}(F_3(F_2(F_1(\mathbf{D}))))$$

$$\mathbf{x}_{surf} = F_1(\mathbf{D})$$
$$\mathbf{x}_{int} = F_2(\mathbf{x}_{surf})$$
$$\mathbf{w} = F_3(\mathbf{x}_{int})$$
$$L = L(\mathbf{w}, \mathbf{x}_{int})$$

Tangent Problem

 $d\mathbf{D}$

- 1: Surface mesh sensi
- 2: Interior mesh sensi
- 3: Residual sensitivity
- 4: Flow variable sensitive
- 5: Final sensitivity

tivity:
$$\frac{\partial \mathbf{x}_{surf}}{\partial \mathbf{D}}$$

tivity:
$$\begin{bmatrix} K \end{bmatrix} \frac{\partial \mathbf{x}_{int}}{\partial \mathbf{D}} = \frac{\partial \mathbf{x}_{surf}}{\partial \mathbf{D}}$$

$$\begin{pmatrix} \vdots & \frac{\partial \mathbf{R}}{\partial \mathbf{D}} = \frac{\partial \mathbf{R}}{\partial \mathbf{x}_{int}} \cdot \frac{\partial \mathbf{x}_{int}}{\partial \mathbf{D}}$$

itivity:
$$\begin{bmatrix} \frac{\partial \mathbf{R}}{\partial \mathbf{w}} \end{bmatrix} \frac{\partial \mathbf{w}}{\partial \mathbf{D}} = -\frac{\partial \mathbf{R}}{\partial \mathbf{D}}$$

$$d\mathbf{L} \quad \partial \mathbf{L} \quad \partial \mathbf{w} \qquad \partial \mathbf{L} \quad \partial \mathbf{x}_{int}$$

 $= \overline{\partial \mathbf{w}} \cdot \overline{\partial \mathbf{D}}$

 $O\mathbf{L}$

 $\overline{\partial \mathbf{x}_{int}}$

 $O\mathbf{X}_{int}$

Adjoint Problem

- 1: Objective flow sensitivity:
- 2: Flow adjoint:

$$\begin{bmatrix} \frac{\partial \mathbf{R}}{\partial \mathbf{w}} \end{bmatrix}^T \mathbf{\Lambda}_w = \frac{\partial \mathbf{L}}{\partial \mathbf{w}}^T$$

 $d\mathbf{x}^*_{\mathbf{int}}$

 $\partial \mathbf{L}$

 $\frac{d\mathbf{L}}{d\mathbf{x}_{int}^*}^T = \frac{\partial \mathbf{L}}{\partial \mathbf{x}_{int}}^T$

T

- 3:Objective sens. wrt mesh:
- $[K]^T \mathbf{\Lambda}_x = \frac{d\mathbf{L}}{\mathbf{L}_x}$ • 4: Mesh adjoint:
- 5: Final sensitivity:

$$\frac{d\mathbf{L}^{T}}{d\mathbf{D}} = \frac{\partial \mathbf{x}_{surf}}{\partial \mathbf{D}}^{T} \mathbf{\Lambda}_{x}$$

$$- rac{\partial \mathbf{R}}{\partial \mathbf{x}_{int}}^T \mathbf{\Lambda}_w$$

T

General Approach

- Linearize each subroutine/process individually in analysis code (tangent or forward model)
 - Check linearization by finite difference/complex variables/dual numbers/AD
 - Transpose to get adjoint, and check duality relation
 - Should reproduce same sensitivities to machine precision
- Build up larger components
 - Check linearization, duality relation
- Check entire process for FD/Complex and duality
- Use single modular solver for all phases
- Maintaining forward linearization has advantages
 - Cases with few design variables, many objectives
 - Debugging adjoint code
 - Enables exact Jacobian/vector products for Krylov solve
 - Facilitates Hessian calculations (later...)

Verification: Complex Step

- Finite difference approach is plagued by round-off error (small ε) versus non-linear error (large ε)
 - Must find range of ε that gives accurate sensitivities
 - Sometimes no such range exists
- Complex variable approach:
 - Replace f(x) with complex function $f(x+i\epsilon)$
 - Then $df/dx = Im(f(x+i\varepsilon))/\varepsilon$
 - Can take $\varepsilon = 1.e-100$ (no roundoff error)
 - Very accurate gradients (machine precision)

General Duality Relation

•Analysis Routine:

$$f = f(x)$$

•Tangent Model:

•Adjoint Model:



•Duality Relation:

 $\partial f_2^T \cdot \partial f_1 = \partial x_2^T \cdot \partial x_1$

- Necessary but not sufficient test
 - Check using series of arbitrary input vectors

General Duality Relation

•Analysis Routine:

•Tangent Model:

•Adjoint Model:

•Duality Relation:



- Necessary but not sufficient test
 - Check using series of arbitrary input vectors



Time Dependent & Moving Mesh Shape Optimization Problem

- Flow equations written in ALE form
- Functional dependence of residual (BDF2)
- Functional dependence of mesh motion equations (same as before)

$$R^{n}(U^{n}, U^{n-1}, U^{n-2}, x^{n}, x^{n-1}, x^{n-2}) = 0$$

$$G(x^n, x_{surf}^n(D)) = 0 \implies [K] \delta x = \delta x_{surf}$$

Time Dependent & Moving Mesh Shape Optimization Problem

- Flow equations written in ALE form
- Using space-time notation
 - U = solution over all space and time
 - R = residuals over all space and time

$$\begin{bmatrix} \frac{\partial \mathbf{R}}{\partial \mathbf{U}} \end{bmatrix} = \begin{bmatrix} \ddots & 0 & 0 & 0 & 0 \\ \ddots & \ddots & 0 & 0 & 0 \\ \frac{\partial \mathbf{R}^{n-2}}{\partial \mathbf{U}^{n-4}} & \frac{\partial \mathbf{R}^{n-2}}{\partial \mathbf{U}^{n-3}} & \frac{\partial \mathbf{R}^{n-2}}{\partial \mathbf{U}^{n-2}} & 0 & 0 \\ 0 & \frac{\partial \mathbf{R}^{n-1}}{\partial \mathbf{U}^{n-3}} & \frac{\partial \mathbf{R}^{n-1}}{\partial \mathbf{U}^{n-2}} & \frac{\partial \mathbf{R}^{n-1}}{\partial \mathbf{U}^{n-1}} & 0 \\ 0 & 0 & \frac{\partial \mathbf{R}^{n}}{\partial \mathbf{U}^{n-2}} & \frac{\partial \mathbf{R}^{n}}{\partial \mathbf{U}^{n-1}} & \frac{\partial \mathbf{R}^{n}}{\partial \mathbf{U}^{n}} \end{bmatrix}$$

$$\begin{bmatrix} \frac{\partial \mathbf{R}}{\partial \mathbf{x}} \end{bmatrix} = \begin{bmatrix} \ddots & 0 & 0 & 0 & 0 \\ \ddots & \ddots & 0 & 0 & 0 \\ \frac{\partial \mathbf{R}^{n-2}}{\partial \mathbf{x}^{n-4}} & \frac{\partial \mathbf{R}^{n-2}}{\partial \mathbf{x}^{n-3}} & \frac{\partial \mathbf{R}^{n-2}}{\partial \mathbf{x}^{n-2}} & 0 & 0 \\ 0 & \frac{\partial \mathbf{R}^{n-1}}{\partial \mathbf{x}^{n-3}} & \frac{\partial \mathbf{R}^{n-1}}{\partial \mathbf{x}^{n-2}} & \frac{\partial \mathbf{R}^{n-1}}{\partial \mathbf{x}^{n-1}} & 0 \\ 0 & 0 & \frac{\partial \mathbf{R}^{n}}{\partial \mathbf{x}^{n-2}} & \frac{\partial \mathbf{R}^{n}}{\partial \mathbf{x}^{n-1}} & \frac{\partial \mathbf{R}^{n}}{\partial \mathbf{x}^{n}} \end{bmatrix}$$

Time Dependent & Moving Mesh Shape Optimization Problem

- Flow adjoint solved by backsubstitution
 - Using 2 previous levels in time (BDF2)

$$\left[\frac{\partial R^{n}}{\partial U^{n}}\right]^{T} \Lambda_{u}^{n} = -\left[\frac{\partial L}{\partial U^{n}}\right]^{T} + \left[\frac{\partial R^{n+1}}{\partial U^{n}}\right]^{T} \Lambda_{u}^{n+1} + \left[\frac{\partial R^{n+2}}{\partial U^{n}}\right] \Lambda_{u}^{n+2}$$

 Interior mesh sensitivities : dR/dX inner product (2 levels back in time)

$$\begin{bmatrix} K \end{bmatrix}^T \Lambda_x^n = \begin{bmatrix} \frac{\partial L}{\partial x^n} \end{bmatrix}^T + \begin{bmatrix} \frac{\partial R^n}{\partial x^n} \end{bmatrix}^T \Lambda_u^n + \begin{bmatrix} \frac{\partial R^{n+1}}{\partial x^n} \end{bmatrix}^T \Lambda_u^{n+1} + \begin{bmatrix} \frac{\partial R^{n+2}}{\partial x^n} \end{bmatrix} \Lambda_u^{n+2}$$

• Final (surface) sensitivity - Single mesh adjoint problem $\frac{dL}{dD} = \Lambda_x^n \frac{\partial x_{surf}}{\partial D} + \Lambda_x^{n-1} \frac{\partial x_{surf}}{\partial D} + \dots$

Time-Integrated Objective Formulation



Pitching airfoil time histories of CL and CD

Optimization Procedure



(or provide gradient to optimizer)

Unsteady Flow Solution

Pressure Contours for Pitching Airfoils $M_{inf} = 0.755$, $\alpha_0 = 0.016^\circ$, $\alpha_{max} = 2.51^\circ$, $\omega = 0.1628$, t=0 to 54 27 time-steps with dt=2.0



NACA0012 Baseline Airfoil



Optimized Airfoil

Time-Dependent Load Convergence



Dynamic Stall Optimization





Optimized airfoil performance: Objective=Minimize moment excursions at constant lift



Generalized Form for Multidisciplinary **Unsteady Coupled Equations**

m coupled disciplines=> L is a functional computed using multidisciplinary solution set:

 $L = L(D, \mathcal{U}_1, \mathcal{U}_2, \cdots, \mathcal{U}_m)$ U over all space and time **m**th discipline Linearize using chain rule with respect to **D**:

$$\frac{dL}{dD} = \frac{\partial L}{\partial D} + \frac{\partial L}{\partial \mathcal{U}_1} \frac{\partial \mathcal{U}_1}{\partial D} + \frac{\partial L}{\partial \mathcal{U}_2} \frac{\partial \mathcal{U}_2}{\partial D} + \dots + \frac{\partial L}{\partial \mathcal{U}_m} \frac{\partial \mathcal{U}_m}{\partial D}$$

$$\frac{dL}{dD} = \frac{\partial L}{\partial D} + \frac{\partial L}{\partial \mathcal{U}_1} \frac{\partial \mathcal{U}_1}{\partial D} + \frac{\partial L}{\partial \mathcal{U}_2} \frac{\partial \mathcal{U}_2}{\partial D} + \dots + \frac{\partial L}{\partial \mathcal{U}_m} \frac{\partial \mathcal{U}_m}{\partial D}$$

Inner-product form:

Tranpose for adjoint total sensitivity:
Residual equations for *m* disciplines:

$$\mathcal{R}_1(D, \mathcal{U}_1, \mathcal{U}_2, \cdots, \mathcal{U}_m) = 0$$

$$\mathcal{R}_2(D, \mathcal{U}_1, \mathcal{U}_2, \cdots, \mathcal{U}_m) = 0$$

$$\mathscr{R}_m(D, \mathscr{U}_1, \mathscr{U}_2, \cdots, \mathscr{U}_m) = 0$$

Linearize with respect to **D**:

$rac{\partial \mathscr{R}_1}{\partial D}$	$+ rac{\partial \mathscr{R}_1}{\partial \mathscr{U}_1} rac{\partial \mathscr{U}_1}{\partial D}$	$+ \frac{\partial \mathscr{R}_1}{\partial \mathscr{U}_2} \frac{\partial \mathscr{U}_2}{\partial D} + \cdots$	$+\frac{\partial \mathcal{R}_1}{\partial \mathcal{U}_m}\frac{\partial \mathcal{U}_m}{\partial D} = 0$
$rac{\partial \mathscr{R}_2}{\partial D}$	$+ rac{\partial \mathscr{R}_2}{\partial \mathscr{U}_1} rac{\partial \mathscr{U}_1}{\partial D}$	$+\frac{\partial \mathscr{R}_2}{\partial \mathscr{U}_2}\frac{\partial \mathscr{U}_2}{\partial D}+\cdots$	$+\frac{\partial \mathscr{R}_2}{\partial \mathscr{U}_m}\frac{\partial \mathscr{U}_m}{\partial D}=0$
			:
$rac{\partial \mathscr{R}_m}{\partial D} +$	$-rac{\partial \mathscr{R}_m}{\partial \mathscr{U}_1}rac{\partial \mathscr{U}_1}{\partial D}+$	$+ rac{\partial \mathscr{R}_m}{\partial \mathscr{U}_2} rac{\partial \mathscr{U}_2}{\partial D} + \cdots +$	$+\frac{\partial \mathscr{R}_m}{\partial \mathscr{U}_m}\frac{\partial \mathscr{U}_m}{\partial D}=0$

Write in combined matrix form:

$rac{\partial \mathscr{R}_1}{\partial \mathscr{U}_1}$	$rac{\partial \mathscr{R}_1}{\partial \mathscr{U}_2}$	 $\frac{\partial \boldsymbol{\mathscr{R}}_1}{\partial \boldsymbol{\mathscr{U}}_m}$	$\frac{\partial \mathscr{U}_1}{\partial D}$		$-\frac{\partial \mathscr{R}_1}{\partial D}$
$rac{\partial \mathscr{R}_2}{\partial \mathscr{U}_1}$	$rac{\partial \mathscr{R}_2}{\partial \mathscr{U}_2}$	 $\frac{\partial \boldsymbol{\mathscr{R}}_2}{\partial \boldsymbol{\mathscr{U}}_m}$	$rac{\partial \mathscr{U}_2}{\partial D}$	=	$-rac{\partial \mathscr{R}_2}{\partial D}$
÷			÷		÷
$rac{\partial \mathscr{R}_m}{\partial \mathscr{U}_1}$	$rac{\partial \mathscr{R}_m}{\partial \mathscr{U}_2}$	 $rac{\partial {\mathscr R}_m}{\partial {\mathscr U}_m}$	$rac{\partial \mathscr{U}_m}{\partial D}$		$-rac{\partial \mathscr{R}_m}{\partial D}$

Transpose and rearrange for vector of state sensitivity matrices:

$$\begin{bmatrix} \frac{\partial \mathcal{U}_{1}}{\partial D}^{T} & \frac{\partial \mathcal{U}_{2}}{\partial D}^{T} & \dots & \frac{\partial \mathcal{U}_{m}}{\partial D}^{T} \end{bmatrix} = \\ -\begin{bmatrix} \frac{\partial \mathcal{R}_{1}}{\partial D}^{T} & \frac{\partial \mathcal{R}_{2}}{\partial D}^{T} & \dots & \frac{\partial \mathcal{R}_{m}}{\partial D}^{T} \end{bmatrix} \begin{bmatrix} \frac{\partial \mathcal{R}_{1}}{\partial \mathcal{U}_{1}}^{T} & \frac{\partial \mathcal{R}_{2}}{\partial \mathcal{U}_{1}}^{T} & \dots & \frac{\partial \mathcal{R}_{m}}{\partial \mathcal{U}_{1}}^{T} \\ \frac{\partial \mathcal{R}_{1}}{\partial \mathcal{U}_{2}}^{T} & \frac{\partial \mathcal{R}_{2}}{\partial \mathcal{U}_{2}}^{T} & \dots & \frac{\partial \mathcal{R}_{m}}{\partial \mathcal{U}_{2}}^{T} \\ \vdots & & & \\ \frac{\partial \mathcal{R}_{1}}{\partial \mathcal{U}_{m}}^{T} & \frac{\partial \mathcal{R}_{2}}{\partial \mathcal{U}_{m}}^{T} & \dots & \frac{\partial \mathcal{R}_{m}}{\partial \mathcal{U}_{m}}^{T} \end{bmatrix}^{-1}$$

Substitute into adjoint total sensitivity equation:

 $\frac{dL}{dD}^{T} = \frac{\partial L}{\partial D}^{T} \begin{bmatrix} \frac{\partial \mathscr{R}_{1}}{\partial D}^{T} & \frac{\partial \mathscr{R}_{2}}{\partial D}^{T} & \dots & \frac{\partial \mathscr{R}_{m}}{\partial D}^{T} \end{bmatrix} \begin{bmatrix} \frac{\partial \mathscr{R}_{1}}{\partial \mathscr{U}_{1}}^{T} & \frac{\partial \mathscr{R}_{2}}{\partial \mathscr{U}_{1}}^{T} & \dots & \frac{\partial \mathscr{R}_{m}}{\partial \mathscr{U}_{1}}^{T} \\ \frac{\partial \mathscr{R}_{1}}{\partial \mathscr{U}_{2}}^{T} & \frac{\partial \mathscr{R}_{2}}{\partial \mathscr{U}_{2}}^{T} & \dots & \frac{\partial \mathscr{R}_{m}}{\partial \mathscr{U}_{2}}^{T} \\ \vdots & & & & \\ \frac{\partial \mathscr{R}_{1}}{\partial \mathscr{U}_{m}}^{T} & \frac{\partial \mathscr{R}_{2}}{\partial \mathscr{U}_{m}}^{T} & \dots & \frac{\partial \mathscr{R}_{m}}{\partial \mathscr{U}_{m}}^{T} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial L}{\partial \mathscr{U}_{1}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{1}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{2}}^{T} \\ \vdots \\ \frac{\partial \mathcal{R}_{1}}{\partial \mathscr{U}_{m}}^{T} & \frac{\partial \mathscr{R}_{2}}{\partial \mathscr{U}_{m}}^{T} & \dots & \frac{\partial \mathscr{R}_{m}}{\partial \mathscr{U}_{m}}^{T} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial L}{\partial \mathscr{U}_{1}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{2}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial L}{\partial \mathscr{U}_{1}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{2}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial L}{\partial \mathscr{U}_{1}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{2}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial L}{\partial \mathscr{U}_{1}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{2}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial L}{\partial \mathscr{U}_{1}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{2}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{2}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial L}{\partial \mathscr{U}_{1}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{2}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{2}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial L}{\partial \mathscr{U}_{1}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{2}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{2}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial L}{\partial \mathscr{U}_{2}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{2}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{2}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial L}{\partial \mathscr{U}_{2}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{2}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{2}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial L}{\partial \mathscr{U}_{2}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{2}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial L}{\partial \mathscr{U}_{2}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial L}{\partial \mathscr{U}_{2}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T}$

Define vector of disciplinary adjoint variables:

Rearrange to recover linear adjoint system:

$$\begin{bmatrix} \Lambda_{\mathscr{U}_{1}} \\ \Lambda_{\mathscr{U}_{2}} \\ \vdots \\ \Lambda_{\mathscr{U}_{m}} \end{bmatrix} = -\begin{bmatrix} \frac{\partial \mathscr{R}_{1}^{T}}{\partial \mathscr{U}_{1}} & \frac{\partial \mathscr{R}_{2}^{T}}{\partial \mathscr{U}_{1}} & \cdots & \frac{\partial \mathscr{R}_{m}^{T}}{\partial \mathscr{U}_{1}} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial L}{\partial \mathscr{U}_{1}}^{T} \\ \frac{\partial \mathscr{R}_{1}^{T}}{\partial \mathscr{U}_{2}} & \frac{\partial \mathscr{R}_{2}^{T}}{\partial \mathscr{U}_{2}} & \cdots & \frac{\partial \mathscr{R}_{m}^{T}}{\partial \mathscr{U}_{2}} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial L}{\partial \mathscr{U}_{1}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{2}}^{T} \\ \vdots \\ \frac{\partial \mathscr{R}_{1}}{\partial \mathscr{U}_{m}}^{T} & \frac{\partial \mathscr{R}_{2}}{\partial \mathscr{U}_{m}}^{T} & \cdots & \frac{\partial \mathscr{R}_{m}}{\partial \mathscr{U}_{m}}^{T} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial L}{\partial \mathscr{U}_{1}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{2}}^{T} \\ \vdots \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial L}{\partial \mathscr{U}_{1}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{2}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial L}{\partial \mathscr{U}_{m}}^{T} \\ \frac{\partial L}{\partial \mathscr{U}_{m}}^{T}$$

$$\begin{bmatrix} \frac{\partial \mathcal{R}_{1}}{\partial \mathcal{U}_{1}}^{T} & \frac{\partial \mathcal{R}_{2}}{\partial \mathcal{U}_{1}}^{T} & \cdots & \frac{\partial \mathcal{R}_{m}}{\partial \mathcal{U}_{1}}^{T} \\ \frac{\partial \mathcal{R}_{1}}{\partial \mathcal{U}_{2}}^{T} & \frac{\partial \mathcal{R}_{2}}{\partial \mathcal{U}_{2}}^{T} & \cdots & \frac{\partial \mathcal{R}_{m}}{\partial \mathcal{U}_{2}}^{T} \\ \vdots & & & \\ \frac{\partial \mathcal{R}_{1}}{\partial \mathcal{U}_{m}}^{T} & \frac{\partial \mathcal{R}_{2}}{\partial \mathcal{U}_{m}}^{T} & \cdots & \frac{\partial \mathcal{R}_{m}}{\partial \mathcal{U}_{m}}^{T} \end{bmatrix} \begin{bmatrix} \Lambda_{\mathcal{U}_{1}} \\ \Lambda_{\mathcal{U}_{2}} \\ \vdots \\ \Lambda_{\mathcal{U}_{m}} \end{bmatrix} = -\begin{bmatrix} \frac{\partial L}{\partial \mathcal{U}_{1}}^{T} \\ \frac{\partial L}{\partial \mathcal{U}_{2}}^{T} \\ \vdots \\ \frac{\partial L}{\partial \mathcal{U}_{m}}^{T} \end{bmatrix}$$

Γ.

		·	0	0	0	
General Jacobian matrix when	$\partial \mathcal{R}$		$\frac{\partial \mathscr{R}^{n-2}}{\partial \mathscr{U}^{n-2}}$	0	0	
expanded discretely in time is lower triangular due to	$\overline{\partial \mathcal{U}} =$		$\frac{\partial \mathscr{R}^{n-1}}{\partial \mathscr{U}^{n-2}}$	$\frac{\partial \mathscr{R}^{n-1}}{\partial \mathscr{U}^{n-1}}$	0	
hyperbolic nature of time:			$\frac{\partial \mathscr{R}^n}{\partial \mathscr{U}^{n-2}}$	$rac{\partial \mathscr{R}^n}{\partial \mathscr{U}^{n-1}}$	$rac{\partial \mathscr{R}^n}{\partial \mathscr{U}^n}$	
	F	L	I	٦	-	1
$\begin{bmatrix} \frac{\partial \mathcal{R}_{1}^{n-1}}{\partial \mathcal{U}_{1}^{n-1}} & \frac{\partial \mathcal{R}_{1}^{n}}{\partial \mathcal{U}_{1}^{n-1}} \end{bmatrix} \begin{bmatrix} \frac{\partial \mathcal{R}_{1}^{n-1}}{\partial \mathcal{U}_{2}^{n-1}} & \frac{\partial \mathcal{R}_{1}^{n}}{\partial \mathcal{U}_{2}^{n-1}} \end{bmatrix}$	$\frac{\partial L}{\mathcal{U}_1^{n-1}}^T \left[\frac{\partial \mathcal{R}_1^{n-1}}{\partial \mathcal{U}_1^{n-1}} \right]$	$\frac{\partial \mathscr{R}_1^{n-1}}{\partial \mathscr{U}_2^{n-1}}$	$\frac{\partial \mathscr{R}_1^n}{\partial \mathscr{U}_1^{n-1}}^T$	$\left. \frac{\partial \mathcal{R}_1^n}{\partial \mathcal{U}_2^{n-1}} \right _{\Gamma}$	n-1]	$\frac{\partial L}{\partial \boldsymbol{\mathscr{U}}_1^{n-1}}^T$
$\begin{bmatrix} 1 & 1 \\ 0 & \frac{\partial \mathscr{R}_1^n}{\partial \mathscr{U}_1^n} \end{bmatrix} \begin{bmatrix} 2 & 2 \\ 0 & \frac{\partial \mathscr{R}_1^n}{\partial \mathscr{U}_2^n} \end{bmatrix} \begin{bmatrix} \Lambda_{\mathscr{U}_1}^{n-1} \\ \Lambda_{\mathscr{U}_1}^n \end{bmatrix} \begin{bmatrix} \frac{\partial \mathscr{R}_1^n}{\partial \mathscr{U}_2^n} \end{bmatrix}$	$\frac{\partial L}{\partial \boldsymbol{\mathcal{U}}_1^n}^T \qquad \qquad \frac{\partial \boldsymbol{\mathcal{R}}_2^{n-1}}{\partial \boldsymbol{\mathcal{U}}_1^{n-1}}$	$\frac{\partial \mathscr{R}_2^{n-1}}{\partial \mathscr{U}_2^{n-1}}$	$\frac{\partial \mathscr{R}_2^n}{\partial \mathscr{U}_1^{n-1}}^T$	$\frac{\partial \mathscr{R}_2^n}{\partial \mathscr{U}_2^{n-1}} \begin{bmatrix} I \\ I \\ I \end{bmatrix}$	$ \begin{bmatrix} \mathbf{A}_{\mathcal{U}_1} \\ \mathbf{A}_{\mathcal{U}_2}^{n-1} \end{bmatrix} = - \mathbf{A}_{\mathcal{U}_2}^{n-1} $	$\frac{\partial L}{\partial \boldsymbol{\mathscr{U}}_2^{n-1}}^T$
$\frac{1}{\frac{\partial \mathcal{R}_{2}^{n-1}}{\partial \mathcal{U}_{1}^{n-1}}} \frac{\partial \mathcal{R}_{2}^{n}}{\partial \mathcal{U}_{1}^{n-1}} \frac{1}{\partial \mathcal{R}_{2}^{n-1}} \frac{\partial \mathcal{R}_{2}^{n-1}}{\partial \mathcal{U}_{2}^{n-1}} \frac{\partial \mathcal{R}_{2}^{n}}{\partial \mathcal{U}_{2}^{n-1}} \left \frac{1}{\Lambda_{\mathcal{U}_{2}}^{n}} \right = - \left \frac{1}{\frac{\partial \mathcal{R}_{2}^{n}}{\partial \mathcal{U}_{2}^{n}}} \right $	$\frac{\overline{\partial L}^{T}}{\mathcal{U}_{2}^{n-1}}$ 0	0	$\frac{\partial \boldsymbol{\mathscr{R}}_1^n}{\partial \boldsymbol{\mathscr{U}}_1^n}^T$	$\frac{\partial \mathscr{R}_1^n T}{\partial \mathscr{U}_2^n} \qquad \qquad$	$egin{array}{c} \mathbf{\Lambda}^n_{\mathscr{U}_1} \ \mathbf{\Lambda}^n_{\mathscr{U}_2} \end{array}$	$\frac{\partial L}{\partial \mathscr{U}_1^n}^T$
$\begin{bmatrix} 1 & 1 & 1 & 2 & 2 \\ 0 & \frac{\partial \mathcal{R}_2^n}{\partial \mathcal{U}_1^n} & 0 & \frac{\partial \mathcal{R}_2^n}{\partial \mathcal{U}_2^n} \end{bmatrix} \begin{bmatrix} \mathcal{M}_{\mathcal{U}_2} \end{bmatrix} \begin{bmatrix} \frac{\partial \mathcal{R}_2^n}{\partial \mathcal{U}_2^n} \end{bmatrix}$	$\frac{\partial L}{\partial \mathcal{U}_2^n}^T \qquad \qquad$	0	$\frac{\partial \mathscr{R}_2^n{}^T}{\partial \mathscr{U}_1^n}$	$rac{\partial \mathscr{R}_2^n ^T}{\partial \mathscr{U}_2^n}$	-	$\frac{\partial L}{\partial \boldsymbol{\mathscr{U}}_2^n}^T$

Swap rows and columns to obtain an upper triangular linear system that can be solved by back substitution

ы

Finally, substitute vector of disciplinary adjoint variables into total sensitivity equation to obtain gradient

$$\frac{dL}{dD}^{T} = \frac{\partial L}{\partial D}^{T} + \begin{bmatrix} \frac{\partial \Re_{1}}{\partial D}^{T} & \frac{\partial \Re_{2}}{\partial D}^{T} & \dots & \frac{\partial \Re_{m}}{\partial D}^{T} \end{bmatrix} \begin{bmatrix} \Lambda_{\mathscr{U}_{1}} \\ \Lambda_{\mathscr{U}_{2}} \\ \dots \\ \Lambda_{\mathscr{U}_{m}} \end{bmatrix}$$

Extension to Multidisciplinary Problems: Time-Dependent Aeroelasticity

- Fully coupled problem involves 4 modules:
 - Flow solver
 - Structural Solver
 - Mesh deformation
 - Fluid-structure interface (FSI)
- Adjoint formulation leads to :
 - Disciplinary adjoints: Fluids, Structures, Mesh, FSI
 - Disciplinary adjoints are coupled at each time step
 - Coupled adjoint solver analogous (transpose) of coupled aeroelastic analysis solver

Forward Flight Flexible Rotor Optimization

- 4 bladed Hart-II rotor in forward flight:
 - Rigid & Flexible; $M_{tip} = 0.64$; 1040 RPM; $\mu=0.15 (M_{\infty}\sim0.1); \alpha=5.4^{\circ}$
- CFD/CSD specifications:
 - 2.32 million grid nodes (prisms, pyramids, tets)
 - 20 beam elements per blade
- Tight CFD/CSD coupling
 - 2 rotor revs
 - 2.32M : $\Delta t=2^{\circ}$
 - 6 coupling per time step, 10 CFD and 20 CSD non-linear iterations per coupling
 - ~40 min/rev with 1024 cores
 - Control Inputs:
 - Collective (θ_0) and Cyclics (θ_{1c}, θ_{1s})

$$\theta_{pitch} = \theta_O + \theta_{1c} \cos \psi + \theta_{1s} \sin \psi$$



Aerodynamic Solver: NSU3D

- 3D unstructured mesh finite-volume RANS solver
- 2nd –order accurate in space and time.
- One equation Spalart-Allmaras turbulence model.
- Deforming mesh capability with GCL compliance
- Fully implicit discretization solved using Newton's method at each time-step as:

$$\mathbf{R}^n = A \frac{\partial \mathbf{U}}{\partial t} + \mathbf{S}(\mathbf{x}^n, \dot{\mathbf{x}}^n, \mathbf{U}^n) = 0$$

$$\begin{bmatrix} \frac{\partial \mathbf{R}(\mathbf{U}^k)}{\partial \mathbf{U}^k} \end{bmatrix} \delta \mathbf{U}^k = -\mathbf{R}(\mathbf{U}^k)$$
$$\mathbf{U}^{k+1} = \mathbf{U}^k + \delta \mathbf{U}^k$$



- Preconditioned GMRES used for linear system
 - Forward linearization used for exact Jacobian-vector products
- Linear agglomeration multigrid for preconditioner
- Line implicit solver as smoother for linear multigrid



Structural Analysis: Beam Model

- Hodges-Dowell type finite element based solver
- 15 degrees of freedom (flap, lag, axial and torsion)
- First order system: $\mathbf{Q} = [\mathbf{q}, \dot{\mathbf{q}}]^T$ where, $\mathbf{J} = [I] \dot{\mathbf{Q}} + [A] \mathbf{Q} - \mathbf{F} = 0$
- J = Residual of structural equation
- **q** = blade dof (displacements)
- **F** = beam (aero) forcing
- Solved via direct inversion



Comparison of Hart-II Natural Frequencies

Modes	Present Model	UMARC	DLR
Flap 1	1.104	1.112	1.125
Flap 2	2.802	2.843	2.835
Flap 3	5.010	5.189	5.168
Torsion 1	3.878	3.844	3.845

Mesh Deformation

- Propagates surface displacements to interior mesh
 - Deflections from structural model at each time step (xⁿ)
 - Design shape changes (D)
- Based on linear elasticity analogy
 - (more robust than spring analogy)
- Solved using line-implicit agglomeration multigrid (analogous to flow solver)

$G(x^n, x^n_{surf}, D) = 0$





Fluid-Structure Interface (FSI)

- Cloud of surface points associated with beam element
- Forces projected onto beam element shape functions

$$F_{beam} = [T(Q)]F_{cfd}(x,u) \quad S(F_{beam}, Q, F_{cfd}(x,u)) = 0$$

 Displacements projected back to CFD surface points using transpose

$$x_{surf} = [T(Q)]^T Q$$
$$S'(x_{surf}, Q) = 0$$



CFD/CSD Coupling Time Integration Methodology

- Outer loop over physical time steps
 - Coupling iterations per time step :
 - Mesh:
 - Line implicit multigrid
 - Flow:
 - Implicit BDF2 Newton iterations (GMRES)
 - Linear agglomeration multi-grid
 - FSI (Fluid to structure)
 - Explicit assignment
 - Structure:
 - Implicit BDF2 newton iteration (direct inversion)
 - FSI (Structure to fluid)
 - Explicit assignment

Analysis Convergence

Rigid blade convergence



- 60 non-linear iterations per time step •
- 3 multigrid cycles/iteration
- Convergence by 2 orders of magnitude

Flexible blade convergence



- 6 coupling cycles per time step
- 10 non-linear iterations/coupling with 3 multi-grid cycles/iteration
- Convergence by 2 orders of magnitude

Convergence continued...



Mesh solves upto 60 iterations or 1x10⁻⁹ (whichever earlier) per coupling

Mesh convergence by 10 orders of magnitude per time step (6 coupling cycles)

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Beam convergence to machine precision (faster convergence)



Blade Tip Time History



• Blade flaps to high values, but converges to a lower value after 2 revs

Aerodynamic Sensitivity: Tangent

• Time-dependent objective function:

$$L = L(u^{n}, u^{n-1}, \dots, u^{0}, x^{n}, x^{n-1}, \dots, x^{0})$$

• Linearizing w.r.t design variable 'D':

$$\frac{dL}{dD} = \frac{\partial L}{\partial u^n} \frac{\partial u^n}{\partial D} + \frac{\partial L}{\partial u^{n-1}} \frac{\partial u^{n-1}}{\partial D} + \dots + \frac{\partial L}{\partial x^n} \frac{\partial x^n}{\partial D} + \frac{\partial x^{n-1}}{\partial D} + \dots$$

 General expression for forward linearization of objective function w.r.t design variables:

$$\frac{dL}{d\mathbf{D}} = \begin{bmatrix} \frac{\partial L}{\partial \mathbf{x}} & \frac{\partial L}{\partial \mathbf{U}} \end{bmatrix} \begin{bmatrix} \frac{\partial \mathbf{x}}{\partial \mathbf{D}} \\ \frac{\partial \mathbf{U}}{\partial \mathbf{D}} \end{bmatrix}$$

Represents inner product over space and time

Aero Sensitivity: Tangent

Constraint equation to be satisfied: Implicit residual at each time-step.

$$G(x, D) = 0$$
$$R(U, x) = 0$$

Writing in generalized matrix form:



Solution involves integrating forward over entire time domain

Aero Sensitivitiy: Adjoint

Adjoint equations:

Solution involves integrating backward over entire time domain

Equations independent of **D**

• Solve adjoint system:



Structural Sensitivity

- Objective function L, $\frac{dL}{dD} = \frac{\partial L}{\partial D} + \frac{\partial L}{\partial Q} \frac{\partial Q}{\partial D}$
- Constraint: J(Q,F) = 0
- Tangent: $\begin{bmatrix} \frac{\partial J}{\partial Q} \end{bmatrix} \frac{\partial Q}{\partial D} = -\frac{\partial J}{\partial F} \frac{\partial F}{\partial D} \frac{\partial J}{\partial D}$ • Adjoint: $\begin{bmatrix} \frac{\partial J}{\partial Q} \end{bmatrix}^T \Lambda_Q = \frac{\partial L}{\partial Q}^T$



 'D' can be structural or geometric shape parameters

Fully Coupled Fluid-Structure Analysis

General solution



Fully Coupled Fluid-Structure Sensitivity: Tangent

 $\partial \mathbf{x}$ $\overline{\partial D}$ $\partial \mathbf{U}$ $\overline{\partial D}$

 $\partial \mathbf{F}$ $\overline{\partial D}$

Functional sensitivity:

Solve:

 $\frac{dL}{d\mathbf{D}} = \begin{bmatrix} \frac{\partial L}{\partial \mathbf{x}} & \frac{\partial L}{\partial \mathbf{U}} & 0 & 0 & 0 \end{bmatrix}$ ∂F_B ∂D 9G ∂G ∂х 0 ∂x. $\partial \mathbf{Q}$ дx <u>9D</u> $\overline{\partial D}$ ∂R ∂R **∂**G ∂u 0 0 0 0 $\partial \mathbf{x_s}$ <u>du</u> дx <u>9D</u> <u>9D</u> ∂D ∂F ∂F ∂F 0 0 0 0 **Per coupling** dx du <u>9D</u> 0 $\frac{\partial S}{\partial F}$ $\frac{\partial S}{\partial F_{h}}$ $\frac{\partial \mathbf{S}}{\partial \mathbf{Q}}$ ∂Fb cycle 0 0 0 9D 0 $\frac{\partial J}{\partial F_b}$ $\frac{\partial \mathbf{J}}{\partial \mathbf{Q}}$ ∂Q 0 0 0 0 9D 0 $\frac{\partial \mathbf{S}'}{\partial \mathbf{Q}}$ $\partial \mathbf{x}_{\mathbf{s}}$ ∂S′ 0 0 0 <u>9D</u> ∂x. ∂S ∂S $\partial \mathbf{F_b}^c$ $\partial \mathbf{S} \partial \mathbf{F}^{c}$ ∂Fb 90 $\overline{\partial \mathbf{F}} \overline{\partial \mathbf{D}}$ $\partial \mathbf{x_s}^c$ $\partial \mathbf{S}' \, \partial \mathbf{Q}^c$

Fully Coupled Fluid-Structure Sensitivity: Adjoint

• Solve:



$$\begin{bmatrix} \frac{\partial \mathbf{G}}{\partial \mathbf{x}}^T & \frac{\partial \mathbf{R}}{\partial \mathbf{x}}^T \\ \mathbf{0} & \frac{\partial \mathbf{R}}{\partial \mathbf{u}}^T \end{bmatrix} \begin{bmatrix} \Lambda_{\mathbf{x}}^c \\ \Lambda_{\mathbf{u}}^c \end{bmatrix} = \begin{bmatrix} \frac{\partial L}{\partial \mathbf{x}}^T + \frac{\partial \mathbf{F}}{\partial \mathbf{x}}^T \Lambda_{\mathbf{F}}^c \\ \frac{\partial L}{\partial \mathbf{u}}^T + \frac{\partial \mathbf{F}}{\partial \mathbf{u}}^T \Lambda_{\mathbf{F}}^c \end{bmatrix}$$

Fully Coupled Fluid-Structure Sensitivity: Adjoint

Solve:



 $\Lambda_{\mathbf{Q}}$

Coupling Schematic



Blade Geometry Parametrization



Hicks-Henne bump functions

- Master blade shape defined by Hicks-Henne bump functions and twist
 - Defined by high-resolution structured mesh (in black)
 - Shape changes interpolated onto unstructured CFD surface mesh
- 115 design parameters
 - 10 Hicks-Henne bump fcts per blade section, 11 blade sections (110)
 - Twist at blade root and tip (2) and 3 pitch parameters





Unsteady Objective Function

$$\min L = L_{power} + \omega L_{trim}$$

 $L_{trim} = \omega_1$

$$L_{trim} \qquad L_{power} = \frac{1}{T} \sum_{n=1}^{n-N} \Delta t \left[\delta C_Q^n \right]^2$$

$$\frac{1}{T} \sum_{n=1}^{n-N} \Delta t \left[\delta C_T^n \right]^2 + \omega_2 \left[\delta \overline{C}_{Mx} \right]^2 + \omega_3 \left[\delta \overline{C}_{My} \right]$$

$$\delta C_Q^n = (C_Q^n - C_{Q_{TARGET}}^n)$$

$$\delta C_T^n = (C_T^n - \overline{C}_{T_{TARGET}}^n)$$

$$\delta \overline{C}_{My} = \frac{1}{T} \sum_{n=1}^{n=N} \Delta t (C_{My}^n - C_{My_{TARGET}}^n)$$

$$\delta \overline{C}_{Mx} = \frac{1}{T} \sum_{n=1}^{n=N} \Delta t (C_{Mx}^n - C_{Mx_{TARGET}}^n)$$

- Trim Target thrust = 4.4e-3 Target C_{Mx} C_{My}=0.0
- Performance
 - Target power = 0.0_{63}

Unsteady Strongly Coupled CFD/CSD Adjoint Sensitivity Verification

- Tangent and adjoint verification by perturbing collective pitch (i.e. D=θ₀)
- Complex perturbation of value 1x10⁻¹⁰⁰
- $\frac{\partial L^n}{\partial D}$ from tangent and adjoint verified with complex step method every time step
- Three sensitivity analysis formulations converged to machine zero every time step

Verification of Strongly Coupled CFD/CSD Adjoint Formulation

- Verified to 10 significant digits
- Verified over multiple time steps
- Accuracy preserved over multiple timesteps

Time	Method	∂L^n
step		<u></u> <i>∂D</i>
1	Complex	7.56981714367 3123 E-005
	Tangent	7.56981714367 3061 E-005
	Adjoint	7.56981714367 2761 E-005
2	Complex	6.040142774935 852 E-005
	Tangent	6.040142774935 835 E-005
	Adjoint	6.040142774935 570 E-005
3	Complex	-4.95990987078 6381 E-006
	Tangent	-4.95990987078 7765 E-006
	Adjoint	-4.95990987078 5228 E-006
5	Complex	-1.142069116982 308 E-004
	Tangent	-1.142069116982 308 E-004
	Adjoint	-1.142069116982 432 E-004
180	Complex	-5.17618942743 9016 E-003
	Tangent	-5.17618942743 9005 E-003
	Adjoint	-5.17618942743 4507 E-003

Optimization Procedure

- 1:Trim rotor
 - Minimize L_{trim} (drive to 0)
 - Using only control inputs as design parameters
- 2: Perform optimization
 - Minimze L_{design} = $L_{performance}$ + L_{trim}
 - Using shape parameters + control inputs (design)
- 3: Retrim shape-optimized rotor
 - L_{trim}=0 not maintained exactly in design process (implemented as penalty term)
- First perform for rigid rotor, then flexible rotor

Strongly Coupled Optimization on Hart-II Rotor: 2.32M Grid

- Optimization (trim/shape) over 2 rev: $\Delta t=2.0^{\circ}$
- Optimizer: L-BFGS-B bounded reduced Hessian
- Bounds for shape parameters:
 - $-\pm5\%$ chord on airfoil section
 - $-\pm1.0^{\circ}$ twist
- Bounds for control inputs
 - $-\theta_{o}, \theta_{1c}, \theta_{1s}: \pm 5.0^{o}$
- 6 CFD-CSD coupling cycles/time-step, 10 Newton cycles/coupling
- Run in parallel using 1024 cores
 70 minutes per rotor revolution

Flexible Hart-II Forward Flight Trim



Thrust vs time

Lateral Moment vs time

Long. Moment vs time

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Trimmed to target mean thrust (Ct=4.4e-3), zero moments (~1e-5)

Pitch (deg)	Experiment	HOST	Present (Flexible)
$\theta_{\rm O}$ (Collective)	3.20	4.91	4.56
θ_{1c} (Lat. Cyclic)	2.00	1.41	1.28
θ_{1s} (Long. Cyclic)	-1.10	-1.34	-2.72

Flexible Rotor Trim Convergence



- Gradient drops more than 2 orders
- Objective converges by ~15 iterations
- Consistent pitch parameter convergence

Flexible Hart-II Shape Optimization

Power vs time Thrust vs time .00028 0.0055 .00026 0.005 .00024 \mathbf{c} 0.0045 S .00022 0.004 0.0002-**Baseline Shape Flexible** 0.0035 **Baseline Shape Flexible Optimized Shape Flexible Optimized Shape Flexible Optimized Shape Retrim Flexible Optimized Shape Retrim Flexible** 00018 0.003 0.5 1.5 2 0.5 1.5 2 Revs Revs

- Trimmed to target mean thrust (Ct=4.4e-3), zero moments (~1e-5)
- Overall ~3.1% power reduction w/ shape optimization after retrim

Flexible Optimized Blade Shape



5000.0 Functional

0.0004 LL

5



1 and ¹/₂ order gradient drop, objective plateaus

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10 Iterations

10⁻⁵ 20

Conclusions

- Adjoint methods can be extended to problems of arbitrary complexity
 - Time-dependent
 - Multidisciplinary
- Requires methodical approach
 - Analogous to analysis formulation
 - Same data-structures
 - Reuse coupled disciplinary solvers
- Using discrete adjoint
 - Straight forward conceptually
 - Tedious
Conclusions

- Reverse time integration not large issue for URANS calculations with large implicit time steps
- Accuracy of gradients with partial convergence remains poorly understood



- Chaotic adjoint behavior possible with time-dependent problems
 - Not likely for URANS with large separation of scales
 - Occurs for turbulence resolving scales (LES)
 - Additional techniques required (Q. Wang 2013)