Tangent and Adjoint Problems in Partially Converged Flows

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Outline

- Motivation/introduction
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- Explanation of steady-state adjoint and tangent problems
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• Derivation and investigation of the pseudo-time accurate adjoint and tangent problems
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  - Derivation, verification, and investigation of Forward Euler
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  - Derivation, verification, and investigation for Newton’s Method
- Application of pseudo-time accurate approach to a well converging but truncated simulation
- Application of pseudo-time accurate approach to a non-converging primal problem in transonic flow
- Conclusions/future work
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- The adjoint and tangent problems are derived from $R = 0$.
- When simulating problems with blunt or complex geometries or higher order spatial discretizations this constraint can be difficult to satisfy.
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- The adjoint system is difficult to solve and the results are sensitive to when the simulation is terminated.
  - This is an issue, as when a simulation mimics the physical unsteadiness by entering limit-cycle oscillations, no state is more valid than another.
- The time accurate approach is the proper way to view these problems as the steady-state converged problem is unphysical and provides very different sensitivities than the time-accurate averaged case.
Motivation: Mishra et al. 2015

- Mishra et al. show that for time-dependent rotorcraft optimization, partial convergence of the implicit system at each time-step leads to growing adjoint sensitivity error.
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When taken in combination with Krakos and Darmofal, this shows that a time accurate approach is appropriate, but when we move to the time accurate approach, the cost of deep convergence is generally prohibitive.
Motivation: Luers et al. 2018

- Volumetric optimization of a CRESCENDO turbine with objective function and constraint
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- Volumetric optimization of a CRESCENDO turbine with objective function and constraint
- four order of magnitude residual decrease, and seemingly converged objective function and constraint values
- close qualitative agreement between adjoint and finite-difference computed sensitivities
- better final design from finite-difference computed sensitivities than the adjoint-computed ones
We employ a pseudo-time accurate approach that applies the unsteady adjoint to the steady state problem.
Introduction: Pseudo-Time Accurate Approach

- We employ a pseudo-time accurate approach that applies the unsteady adjoint to the steady state problem.
- In the tangent problem we take the derivative of every step used to solve the primal to march forward in pseudo-time.
- These are not chaotic flows, as is shown in the results section the sensitivities do not diverge.
We employ a pseudo-time accurate approach that applies the unsteady adjoint to the steady state problem. In the tangent problem we take the derivative of every step used to solve the primal to march forward in pseudo-time. In the adjoint problem, we transpose those derivatives to march back in pseudo-time.
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- These are not chaotic flows, as is shown in the results section the sensitivities do not diverge.
Steady-State Tangent and Adjoint Problems
We begin with an objective functional $L(u(D), x(D))$, whose derivative is the sensitivity equation and is expressed as:

$$\frac{dL}{dD} = \frac{\partial L}{\partial x} \frac{dx}{dD} + \frac{\partial L}{\partial u} \frac{du}{dD} \quad (1)$$

We can calculate everything except for $\frac{du}{dD}$ by differentiating subroutines in the code. $\frac{du}{dD}$ is obtained by solving the tangent system.
To develop the tangent system, we begin with our zero residual constraint:

\[ R(u(D), x(D)) = 0 \]  

(2)
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$$R(u(D), x(D)) = 0$$  \hspace{1cm} (2)

Then we take the total derivative, which must be equal to zero

$$\left[ \frac{\partial R}{\partial u} \right] \frac{du}{dD} + \left[ \frac{\partial R}{\partial x} \right] \frac{dx}{dD} = 0$$  \hspace{1cm} (3)
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\[
\left[ \frac{\partial R}{\partial u} \right] \frac{du}{dD} + \left[ \frac{\partial R}{\partial x} \right] \frac{dx}{dD} = 0
\]  \hspace{1cm} (3)

We have a system of linear equations that scales with the number of design variables:

\[
\left[ \frac{\partial R}{\partial u} \right] \frac{du}{dD_i} = - \left[ \frac{\partial R}{\partial x} \right] \frac{dx}{dD_i}
\]  \hspace{1cm} (4)

The calculated values of \( \frac{du}{dD} \) can be substituted into the objective functional derivative to return the sensitivities.
Beginning from the objective function, we add a constraint and a lagrange multiplier:

\[ J(u(D), x(D)) = L(u(D), x(D)) + \Lambda^T R(u(D), x(D)) \] (5)
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(5)

we can take the derivative of both sides to obtain the sensitivity equation:

\[ \frac{dJ}{dD} = \left( \frac{\partial L}{\partial x} + \Lambda^T \frac{\partial R}{\partial x} \right) \frac{dx}{dD} + \left( \frac{\partial L}{\partial u} + \Lambda^T \frac{\partial R}{\partial u} \right) \frac{du}{dD} \]  

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We choose \( \Lambda \) such that we do not have to calculate \( \frac{du}{dD} \):

\[ \left[ \frac{\partial R}{\partial u} \right]^T \Lambda = - \left[ \frac{\partial L}{\partial u} \right]^T \]  \hspace{1cm} (7)
Pseudo-Time Accurate Tangent and Adjoint Formulation Derivation and Investigation
Derivation for Forward Euler
As in the steady-state tangent system we want to solve for \( \frac{du}{dD} \). To that end we look at our pseudo-time evolution equation:

\[
    u^k = u^{k-1} + CFL\Delta t(u^{k-1}(D), x(D))R(u^{k-1}(D), x(D))
\]

(8)

where \( \Delta t \) is the local time step.
As in the steady-state tangent system we want to solve for $\frac{du}{dD}$. To that end we look at our pseudo-time evolution equation:

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where $\Delta t$ is the local time step.

We take the derivative and obtain a pseudo-time evolution equation:

$$\frac{du^k}{dD} = \frac{du^{k-1}}{dD} + CFL\Delta t \left[ \frac{\partial R}{\partial x} \frac{dx}{dD} + \frac{\partial R}{\partial u} \frac{du}{dD} \right] + CFL \left[ \frac{\partial \Delta t}{\partial x} \frac{dx}{dD} + \frac{\partial \Delta t}{\partial u} \frac{du^{k-1}}{dD} \right] R(u^{k-1}) \quad (9)$$

By running this relation through pseudo-time we can obtain the exact sensitivities at every pseudo-time step.
For an objective functional dependent on the last $m$ states for a simulation that runs $n$ time steps:

$$L = L(u^n, u^{n-1}, ..., u^{n-m}, D) \quad (10)$$
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the sensitivity equation is:

$$\frac{dL}{dD} = \frac{\partial L}{\partial x} \frac{dx}{dD} + \frac{\partial L}{\partial u^n} \frac{du^n}{dD} + \frac{\partial L}{\partial u^{n-1}} \frac{du^{n-1}}{dD} + ... + \frac{\partial L}{\partial u^{n-m}} \frac{du^{n-m}}{dD}$$  \hspace{1cm} (11)

And we can substitute the pseudo-time accurate tangent provided values for $\frac{du^k}{dD}$
Here we begin with an objective functional dependent on the last $m$ states for a simulation that runs $n$ time steps:

$$L = L(u^n, u^{n-1}, ..., u^{n-m}, D)$$  \hspace{1cm} (12)
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$$L = L(u^n, u^{n-1}, ..., u^{n-m}, D)$$ \hspace{1cm} (12)

with the pseudo-time constraint of:

$$G^k(u^k(D), u^{k-1}(D), D) = u^k - u^{k-1} - CFL\Delta t R(u^{k-1}) = 0$$ \hspace{1cm} (13)
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(13)

We then form our augmented objective functional with the above constraint and a corresponding adjoint for each pseudo-time step:

$$J(D, u^n, u^{n-1}, ..., \Lambda^n, \Lambda^{n-1}, ...) = L(u^n, u^{n-1}, ..., u^{n-m}, D) + \Lambda^n^T G^n(u^n(D), u^{n-1}(D), D) + \Lambda^{n-1}^T G^{n-1}(u^{n-1}(D), u^{n-2}(D), D) + ... + \Lambda^1^T G^1(u^1(D), u^0(D), D)$$

(14)
Taking the derivative of the augmented objective functional yields:

\[
\frac{dJ}{dD} = \frac{\partial L}{\partial x} \frac{dx}{dD} + \frac{\partial L}{\partial u^n} \frac{du^n}{dD} + \frac{\partial L}{\partial u^{n-1}} \frac{du^{n-1}}{dD} + \ldots + \frac{\partial L}{\partial u^{n-m}} \frac{du^{n-m}}{dD} \\
+ \Lambda^{nT} \left( \frac{\partial G^n}{\partial x} \frac{dx}{dD} + \frac{\partial G^n}{\partial u^n} \frac{du^n}{dD} + \frac{\partial G^n}{\partial u^{n-1}} \frac{du^{n-1}}{dD} \right) \\
+ \Lambda^{n-1T} \left( \frac{\partial G^{n-1}}{\partial x} \frac{dx}{dD} + \frac{\partial G^{n-1}}{\partial u^{n-1}} \frac{du^{n-1}}{dD} + \frac{\partial G^{n-1}}{\partial u^{n-2}} \frac{du^{n-2}}{dD} \right) \\
+ \ldots \\
+ \Lambda^{1T} \left( \frac{\partial G^1}{\partial x} \frac{dx}{dD} + \frac{\partial G^1}{\partial u^1} \frac{du^1}{dD} + \frac{\partial G^1}{\partial u^0} \frac{du^0}{dD} \right)
\]  

(15)
As in the steady-state adjoint we take the total derivatives, and choose the adjoint variable such that we do not have to calculate \( \frac{du^k}{dD} \), which returns a series of adjoint recurrence relations:

\[
\frac{\partial L}{\partial u^{k-1}} + \Lambda^k T \frac{\partial G^k}{\partial u^{k-1}} + \Lambda^{k-1} T \frac{\partial G^{k-1}}{\partial u^{k-1}} = 0
\]

with \( \Lambda^{n+1} T = 0 \)
As in the steady-state adjoint we take the total derivatives, and choose the adjoint variable such that we do not have to calculate \( \frac{du^k}{dD} \), which returns a series of adjoint recurrence relations:

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\]  

(16)

with \( \Lambda^{n+1} T = 0 \)

We can plug in the constraint derivative to the recurrence relation and obtain:

\[
[I] \Lambda^{k-1} = - \left[ -I - CFL \Delta t^{k-1} \frac{\partial R(u^{k-1})}{\partial u^{k-1}} - CFL \frac{\partial \Delta t}{\partial u^{k-1}} R(u^{k-1}) \right]^T \Lambda^k
\]

\[
- \left[ \frac{\partial L}{\partial u^{k-1}} \right]^T
\]

(17)
The sensitivity equation with the terms that vanish due to the choice of adjoint variable is expressed as:

\[
\frac{dJ}{dD} = \frac{\partial L}{\partial D} + \Lambda^n \frac{\partial G^n}{\partial D} + \Lambda^{n-1} \frac{\partial G^{n-1}}{\partial D} + \Lambda^{n-2} \frac{\partial G^{n-2}}{\partial D} + \ldots \quad (18)
\]
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\]

Plugging in the constraint derivative values we get:

\[
\frac{dJ}{dD} = \frac{\partial L}{\partial D} - \Lambda^n T \left[ CFL \Delta t^{n-1} \frac{\partial R(u^{n-1})}{\partial D} + CFL \frac{\partial \Delta t}{\partial D} R(u^{n-1}) \right] \\
- \Lambda^{n-1} T \left[ CFL \Delta t^{n-2} \frac{\partial R(u^{n-2})}{\partial D} + CFL \frac{\partial \Delta t}{\partial D} R(u^{k-2}) \right] \\
- \ldots \\
- \Lambda^1 T \left[ CFL \Delta t^0 \frac{\partial R(u^0)}{\partial D} + CFL \frac{\partial \Delta t}{\partial D} R(u^0) \right]
\tag{19}
\]
• Tangent equations march forward in time similarly to the primal problem.
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• The adjoint equations march backwards in time in the reverse of the primal problem, accumulating the sensitivities through the backwards in time integration.
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• The adjoint equations march backwards in time in the reverse of the primal problem, accumulating the sensitivities through the backwards in time integration.
• Each tangent/adjoint pseudo-time step equation is cheap, and is the result of a few matrix vector multiplications and additions, rather than a full linear system solution.
Verification and Investigation of Forward Euler and RK5
Design variables are two equally spaced Hicks-Henne bump functions.

$Mach = .6, \alpha = 1^\circ$

Spring analogy used for mesh motion and mesh sensitivities

Objective function is a weighted combination of lift and drag
Primal Problem Convergence
Residual vs. Iterations

Residual convergence
Tangent System for Forward Euler (Verification)

Difference between pseudo-time accurate tangent sensitivities and complex sensitivities for forward Euler pseudo-time evolution with linearized time-step

Differences are of the order of machine zero for all iterations in pseudo-time. (Implementation is verified)
Comparison of adjoint and complex-step computed sensitivities

- Here we show the verification for a low storage five stage explicit RK scheme looking at the first design variable.
  - The derivation for the RK5 method can be found in our paper: "Toward a Pseudo-Time Accurate Formulation of the Adjoint and Tangent Systems".
PTA Adjoint System RK5 Investigation

(a) Residual Convergence

Residual convergence and adjoint magnitude behavior for RK5 scheme

The adjoint at a pseudo-time step relates a perturbation in the constraint of that pseudo-time step to a change in the objective function.
(a) Tangent Sensitivity Convergence  
(b) Adjoint Sensitivity Convergence

Sensitivity convergence for RK5 scheme
Derivation for Newton’s Method
As previously, we try to solve for $\frac{dU}{dD}$. Looking at our primal solver:

$$u^k = u^{k-1} + [P_{k-1}]^{-1} R(u^{k-1}(D), X(D))$$ (20)

where $P_k$ is defined as:

$$P_k = \frac{\partial R}{\partial u} + M$$ (21)

Where $\frac{\partial R}{\partial u}$ is an approximation to the jacobian and $M$ is a suitable mass matrix:

$$M = \frac{vol}{\Delta t}$$ (22)
PTA Tangent system for Newton’s Method

Taking the derivative of the nonlinear solver gives:

\[
\frac{du^k}{dD} = \frac{du^{k-1}}{dD} + \frac{d[P_{k-1}]^{-1} R(u^{k-1}, D)}{dD}
\] (23)
PTA Tangent system for Newton’s Method

Taking the derivative of the nonlinear solver gives:

\[
\frac{du^k}{dD} = \frac{du^{k-1}}{dD} + \frac{d[P_{k-1}]^{-1}}{dD} R(u^{k-1}, D)
\]  

(23)

If a Newton-Chord method is used, the derivative of the augmented jacobian inverse can be neglected:

\[
\frac{du^k}{dD} = \frac{du^{k-1}}{dD} + [P_{k-1}]^{-1} \left[ \frac{dR(u^{k-1}, D)}{dD} \right]
\]  

(24)
Taking the derivative of the nonlinear solver gives:

\[
\frac{d u^k}{dD} = \frac{d u^{k-1}}{dD} + \frac{d [P_{k-1}]^{-1} R(u^{k-1}, D)}{dD} \tag{23}
\]

If a Newton-Chord method is used, the derivative of the augmented jacobian inverse can be neglected:

\[
\frac{d u^k}{dD} = \frac{d u^{k-1}}{dD} + [P_{k-1}]^{-1} \left[ \frac{d R(u^{k-1}, D)}{dD} \right] \tag{24}
\]

Otherwise, the derivative must be computed:

\[
\frac{d u^k}{dD} = \frac{d u^{k-1}}{dD} + [P_{k-1}]^{-1} \left[ \frac{d R(u^{k-1}, D)}{dD} \right] \\
+ \frac{d [P_{k-1}]^{-1}}{dD} R(u^{k-1}, D) \tag{25}
\]
• fully linearizing the linear system solve is not feasible, especially for more complicated linear solvers, e.g. GMRES
• fully linearizing the linear system solve is not feasible, especially for more complicated linear solvers, e.g. GMRES
• There are two ways to tackle the linearization of the matrix inverse

\[
\begin{align*}
\frac{d}{dx} \left( A^{-1} \right) &= -A^{-1} \frac{dA}{dx} A^{-1}
\end{align*}
\]
• fully linearizing the linear system solve is not feasible, especially for more complicated linear solvers, e.g. GMRES
• There are two ways to tackle the linearization of the matrix inverse
• the first way is to use complex perturbations in the conservative variable and the nodal coordinate vectors to obtain the Frechet derivative
• fully linearizing the linear system solve is not feasible, especially for more complicated linear solvers, e.g. GMRES
• There are two ways to tackle the linearization of the matrix inverse
• the first way is to use complex perturbations in the conservative variable and the nodal coordinate vectors to obtain the Frechet derivative
• the second way is to use an identity for the derivative of the matrix inverse, this will not be exact, but it is less expensive and simpler:
\[
\frac{dA^{-1}}{dx} = -A^{-1} \frac{dA}{dx} A^{-1}
\]
Newton-Chord:

\[
\frac{du^k}{dD} = \frac{du^{k-1}}{dD} + [P_{k-1}]^{-1} \left[ \frac{\partial R}{\partial u^{k-1}} \frac{du^{k-1}}{dD} + \left[ \frac{\partial R}{\partial x} \right] \frac{dx}{dD} \right]
\]  

(26)
Newton-Chord:

\[
\frac{du^k}{dD} = \frac{du^{k-1}}{dD} + [P_{k-1}]^{-1} \left[ \frac{\partial R}{\partial u^{k-1}} \frac{du^{k-1}}{dD} + \left[ \frac{\partial R}{\partial x} \right] \frac{dx}{dD} \right] \tag{26}
\]

Inverse Identity:

\[
\frac{du^k}{dD} = \frac{du^{k-1}}{dD} + [P_{k-1}]^{-1} \left[ \frac{\partial R}{\partial u^{k-1}} \frac{du^{k-1}}{dD} + \left[ \frac{\partial R}{\partial x} \right] \frac{dx}{dD} \right] - [P_{k-1}]^{-1} \left[ \frac{d[P_{k-1}]}{dD} \right] [P_{k-1}]^{-1} R(u^{k-1}, D) \tag{27}
\]
Newton-Chord:

$$\frac{d u^k}{dD} = \frac{d u^{k-1}}{dD} + [P_{k-1}]^{-1} \left[ \frac{\partial R}{\partial u^{k-1}} \frac{d u^{k-1}}{dD} + \left[ \frac{\partial R}{\partial x} \right] \frac{d x}{dD} \right]$$

Inverse Identity:

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As in the forward euler adjoint there is a series of adjoint recurrence relations:

\[
\frac{\partial L}{\partial u^{k-1}} + \Lambda^k \frac{\partial G^k}{\partial u^{k-1}} + \Lambda^{k-1} \frac{\partial G^{k-1}}{\partial u^{k-1}} = 0
\]  

with \( \Lambda^{n+1} = 0 \)
As in the forward euler adjoint there is a series of adjoint recurrence relations:

\[
\frac{\partial L}{\partial u^{k-1}} + \Lambda^k \nabla \frac{\partial G^k}{\partial u^{k-1}} + \Lambda^{k-1} \nabla \frac{\partial G^{k-1}}{\partial u^{k-1}} = 0 \tag{28}
\]

with \( \Lambda^{n+1} = 0 \)

Plugging in the constraint derivatives from Newton’s method:

\[
[I] \Lambda^{k-1} = - \left[ -I - \frac{\partial [P_{k-1}]^{-1} R(u_{k-1})}{\partial u^{k-1}} \right]^T \Lambda^k
\]

\[
- \left[ \frac{\partial L}{\partial u^{k-1}} \right]^T
\]

(29)
Newton-Chord:

$$[I] \Lambda^{k-1} = - \left[ -I - [P_{k-1}]^{-1} \frac{\partial R(u^{k-1})}{\partial u^{k-1}} \right]^T \Lambda^k - \left[ \frac{\partial L}{\partial u^{k-1}} \right]^T$$ (30)
Newton-Chord:

\[
[I] \Lambda^{k-1} = - \left[ -I - [P_{k-1}]^{-1} \frac{\partial R(u^{k-1})}{\partial u^{k-1}} \right]^T \Lambda^k - \left[ \frac{\partial L}{\partial u^{k-1}} \right]^T
\]  

Inverse identity:

\[
[I] \Lambda^{k-1} = - \left[ -I - [P_{k-1}]^{-1} \frac{\partial R(u^{k-1})}{\partial u^{k-1}} - \frac{\partial [P_{k-1}]^{-1}}{\partial u^{k-1}} R(u^{k-1}) \right]^T \Lambda^k - \left[ \frac{\partial L}{\partial u^{k-1}} \right]^T
\]  

(31)
PTA Adjoint System for Newton’s Method (Derivation)

Newton-Chord:

\[
[I] \Lambda^{k-1} = - \left( -I - [P_{k-1}]^{-1} \frac{\partial R(u^{k-1})}{\partial u^{k-1}} \right)^T \Lambda^k - \left[ \frac{\partial L}{\partial u^{k-1}} \right]^T
\]  

Inverse identity:

\[
[I] \Lambda^{k-1} = - \left( -I - [P_{k-1}]^{-1} \frac{\partial R(u^{k-1})}{\partial u^{k-1}} + [P_{k-1}]^{-1} \frac{\partial P_{k-1}}{\partial u^{k-1}} \Delta u \right)^T \Lambda^k - \left[ \frac{\partial L}{\partial u^{k-1}} \right]^T
\]
Define a secondary adjoint variable:

\[ [P_{k-1}]^T \psi^k = \Lambda^k \]  

(32)
Define a secondary adjoint variable:

\[
[P_{k-1}]^T \psi^k = \Lambda^k
\]  

(32)

Newton-Chord:

\[
\Delta \Lambda^{k-1} = \left[ \frac{\partial R(u^{k-1})}{\partial u^{k-1}} \right]^T \psi^k - \left[ \frac{\partial L}{\partial u^{k-1}} \right]^T
\]

(33)
Define a secondary adjoint variable:

\[ [P_{k-1}]^T \psi^k = \Lambda^k \] (32)

Newton-Chord:

\[ \Delta \Lambda^{k-1} = \left[ \frac{\partial R(u^{k-1})}{\partial u^{k-1}} \right]^T \psi^k - \left[ \frac{\partial L}{\partial u^{k-1}} \right]^T \] (33)

Inverse identity:

\[ \Delta \Lambda^{k-1} = \left[ \frac{\partial R(u^{k-1})}{\partial u^{k-1}} - \frac{\partial P_{k-1}}{\partial u^{k-1}} \Delta u \right]^T \psi^k - \left[ \frac{\partial L}{\partial u^{k-1}} \right]^T \] (34)
Beginning with the constraint based expression of the sensitivity equation as we did for forward euler:

\[
\frac{dJ}{dD} = \frac{\partial L}{\partial D} + \Lambda^n \frac{\partial G^n}{\partial D} + \Lambda^{n-1} \frac{\partial G^{n-1}}{\partial D} + \Lambda^{n-2} \frac{\partial G^{n-2}}{\partial D} + \ldots \tag{35}
\]
PTA Adjoint System for Newton’s Method (Derivation)

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$$\frac{dJ}{dD} = \frac{\partial L}{\partial D} + \Lambda^n \frac{\partial G^n}{\partial D} + \Lambda^{n-1} \frac{\partial G^{n-1}}{\partial D} + \Lambda^{n-2} \frac{\partial G^{n-2}}{\partial D} + \ldots$$  \hspace{1cm} (35)

Plugging in the constraint derivative values for the Newton-Chord method:

$$\frac{dJ}{dD} = \frac{\partial L}{\partial D} - \Lambda^n \left[ [P_{n-1}]^{-1} \frac{\partial R(u^{n-1})}{\partial D} \right]
- \Lambda^{n-1} \left[ [P_{n-2}]^{-1} \frac{\partial R(u^{n-2})}{\partial D} \right]
- \Lambda^{n-2} \left[ [P_{n-3}]^{-1} \frac{\partial R(u^{n-3})}{\partial D} \right]
- \ldots
- \Lambda \left[ P_0 \right]^{-1} \frac{\partial R(u^0)}{\partial D}$$ \hspace{1cm} (36)
Beginning with the constraint based expression of the sensitivity equation as we did for forward euler:

$$\frac{dJ}{dD} = \frac{\partial L}{\partial D} + \Lambda^n T \frac{\partial G^n}{\partial D} + \Lambda^{n-1} T \frac{\partial G^{n-1}}{\partial D} + \Lambda^{n-2} T \frac{\partial G^{n-2}}{\partial D} + ... \tag{35}$$

Plugging in the constraint derivative values for the Newton-Chord method:

$$\frac{dJ}{dD} = \frac{\partial L}{\partial D} - \psi^n T \left[ \frac{\partial R(u^{n-1})}{\partial D} \right] - \psi^{n-1} T \left[ \frac{\partial R(u^{n-2})}{\partial D} \right] - ... - \psi^1 T \left[ \frac{\partial R(u^0)}{\partial D} \right] \tag{36}$$
Referencing the constraint based expression of the sensitivity equation as we did for forward euler:

$$\frac{dJ}{dD} = \frac{\partial L}{\partial D} + \Lambda^n T \frac{\partial G^n}{\partial D} + \Lambda^{n-1} T \frac{\partial G^{n-1}}{\partial D} + \Lambda^{n-2} T \frac{\partial G^{n-2}}{\partial D} + \ldots$$  \hspace{1cm} (37)

Plugging in the constraint derivative values using the inverse identity:

$$\frac{dJ}{dD} = \frac{\partial L}{\partial D} - \Lambda^n T \left[ [P_{n-1}]^{-1} \frac{\partial R(u^{n-1})}{\partial D} - [P_{n-1}]^{-1} \frac{\partial [P_{n-1}] \Delta u^{n-1}}{\partial D} \right]$$

$$- \Lambda^{n-1} T \left[ [P_{n-2}]^{-1} \frac{\partial R(u^{n-2})}{\partial D} - [P_{n-2}]^{-1} \frac{\partial [P_{n-2}] \Delta u^{n-2}}{\partial D} \right]$$

$$- \ldots$$

$$- \Lambda^1 T \left[ [P_0]^{-1} \frac{\partial R(u^0)}{\partial D} - [P_0]^{-1} \frac{\partial [P_0] \Delta u^0}{\partial D} \right]$$  \hspace{1cm} (38)
Referencing the constraint based expression of the sensitivity equation as we did for forward euler:

\[
\frac{dJ}{dD} = \frac{\partial L}{\partial D} + \Lambda^{nT} \frac{\partial G^n}{\partial D} + \Lambda^{n-1T} \frac{\partial G^{n-1}}{\partial D} + \Lambda^{n-2T} \frac{\partial G^{n-2}}{\partial D} + \ldots \tag{37}
\]

Plugging in the constraint derivative values using the inverse identity:

\[
\frac{dJ}{dD} = \frac{\partial L}{\partial D} - \psi^n \left[ \frac{\partial R(u^{n-1})}{\partial D} - \frac{\partial [P_{n-1}]}{\partial D} \Delta u^{n-1} \right]
- \psi^{n-1} \left[ \frac{\partial R(u^{n-2})}{\partial D} - \frac{\partial [P_{n-2}]}{\partial D} \Delta u^{n-2} \right]
- \ldots
- \psi^0 \left[ \frac{\partial R(u^0)}{\partial D} - \frac{\partial [P_0]}{\partial D} \Delta u^0 \right] \tag{38}
\]
Verification and Investigation of Newton’s Method
Comparison of adjoint and complex-step computed sensitivities

- Here we show the sensitivity comparison between the Newton-Chord (NC) and quasi-Newton inverse identity (QNII) adjoints and complex sensitivities to verify the implementation.

- For the Newton-Chord method, the solver must be done with a dual solver, here with block Jacobi.

- For the Quasi-Newton method, the solver does not need to be a dual solver and is done primarily with block Gauss-Seidel.

| Scheme | Steps | Complex Sensitivity | Adjoint Sensitivity | || Residual ||₂ |
|--------|-------|---------------------|---------------------|------------------|
| NC     | 10    | -2.344315562026746  | -2.344315562026735  | 0.3205858355993253E-03 |
| NC     | 20    | -5.117070610162804  | -5.5117070610162807 | 0.2522158472255535E-03 |
| QNII   | 10    | -3.482196439075767  | -3.482196439075786  | 0.2982633094835574E-03 |
| QNII   | 20    | -2.264493935071775  | -2.264493935071703  | 0.1691766297621063E-03 |
Residual convergence and adjoint magnitude behavior for Quasi-Newton scheme

(a) Residual Convergence

(b) Adjoint Magnitude Behavior

The adjoint at a pseudo-time step relates a perturbation in the constraint of that pseudo-time step to a change in the objective function.
PTA Adjoint System Quasi-Newton Investigation

(a) Tangent Sensitivity Convergence

(b) Adjoint Sensitivity Convergence

Sensitivity convergence for Quasi-Newton scheme
PTA Tangent Behavior for Linear Tolerance = 1e-1

(a) Design Variable 1
(b) Design Variable 2

Sensitivity convergence for linear tolerance, 1e-1
PTA Tangent Behavior for Linear Tolerance $= 1e-1$

(a) Design Variable 1
Iterative sensitivity difference for linear tolerance, $1e-1$

(b) Design Variable 2
PTA Tangent Behavior for Linear Tolerance $= 1e-4$

(a) Design Variable 1

(b) Design Variable 2

Sensitivity convergence for linear tolerance, $1e-4$
PTA Tangent Behavior for Linear Tolerance $= 1e-4$

(a) Design Variable 1

(b) Design Variable 2

Iterative sensitivity difference for linear tolerance, $1e-4$
PTA Tangent Behavior as a function of linear tolerance

Maximum iterative difference vs. linear tolerance
Results
Results for a Truncated Simulation
Density field for NACA0012 airfoil in \( Mach = 0.85, \alpha = 3 \)
Results: Steady-State Residual and Steady-State Adjoint Convergence

(a) Primal Convergence

(b) Adjoint Linear Convergence

Residual and steady-state adjoint convergence

• The primal problem residual has decreased by three orders of magnitude.
• The adjoint problem has converged by 8 orders of magnitude, and is sufficiently accurate for this comparison.
Why is Angle Important?

The angle $\theta$ is calculated as follows, with $u$ and $v$ being the sensitivity vectors:

$$ a = \frac{u \cdot v}{\|u\| \|v\|} $$  \hspace{1cm} (39)

$$ \theta = \arccos(a), \theta \leq 180 $$

$$ \theta = 360 - \arccos(a), \theta > 180 $$  \hspace{1cm} (40)
Why is Angle Important?

The angle $\theta$ is calculated as follows, with $u$ and $v$ being the sensitivity vectors:

$$a = \frac{u \cdot v}{\|u\| \|v\|}$$  \hspace{1cm} (39)

$$\theta = \arccos(a), \; \theta \leq 180$$  \hspace{1cm} (40)

$$\theta = 360 - \arccos(a), \; \theta > 180$$

- The important thing about the sensitivity vector is the direction.
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- The important thing about the sensitivity vector is the direction.
- If the direction is off, then the optimizer takes a suboptimal path and this leads to greater expense and possibly suboptimal designs.
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(40)

- The important thing about the sensitivity vector is the direction.
- If the direction is off, then the optimizer takes a suboptimal path and this leads to greater expense and possibly suboptimal designs.
- If the magnitude is off, then through the line search maybe the step isn’t as large, but that’s not a large issue for an optimizer.
### Results: Truncated Simulation Sensitivity Vectors

<table>
<thead>
<tr>
<th>Design Variable</th>
<th>Steady-State Value</th>
<th>Pseudo-Time Accurate Value</th>
<th>Percent Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-38.9168562768552</td>
<td>-34.07260014448312</td>
<td>14.2%</td>
</tr>
<tr>
<td>2</td>
<td>-58.8314866801896</td>
<td>-62.28918541979274</td>
<td>5.6%</td>
</tr>
<tr>
<td>3</td>
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<td>-70.15517817818902</td>
<td>26.0%</td>
</tr>
<tr>
<td>4</td>
<td>-69.3520141341324</td>
<td>-95.35571541527936</td>
<td>27.3%</td>
</tr>
</tbody>
</table>

Comparison of pseudo-time accurate adjoint and steady-state adjoint computed sensitivities for truncated primal simulation

The angle between the two sensitivity vectors is $\theta = 8.652^\circ$. 
### Results: Truncated Simulation Sensitivity Vectors

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Comparison of pseudo-time accurate adjoint and steady-state adjoint computed sensitivities for truncated primal simulation

The angle between the two sensitivity vectors is $\theta = 8.652^\circ$. 
Results for Non-Converging Transonic Simulation
Results: Non-Converging Transonic Case Introduction

(a) Mesh

Fine mesh for NACA0012 airfoil cut off at 97% chord length

(b) Trailing Edge

- Design variables are three Hicks-Henne bump functions.
- $Mach = .7, \alpha = 2^\circ$
- Explicit inverse distance weighting used for mesh motion and mesh sensitivities
Results: Primal Behavior of Non-Converging Transonic Simulation

Primal convergence for cut-off NACA0012 airfoil at $\text{Mach} = .7$, $\alpha = 2^\circ$
Using instantaneous objective functionals in oscillatory flows can provide sensitivities with a high dependence on the initial conditions and the design variables, this is not true for the averaged objective functional.
• Using instantaneous objective functionals in oscillatory flows can provide sensitivities with a high dependence on the initial conditions and the design variables, this is not true for the averaged objective functional.

• The averaged objective functional, for a statistically converged average shows low dependence on the initial condition, which could allow for partial backwards in time integration for cheaper evaluation of the sensitivities.
Results: Running Average of Force Coefficients

(a) $C_L$ over different averaging windows

(b) $C_D$ over different averaging windows

Force coefficient averaging over different windows

- 250 and 1000 iteration averaging windows do not damp out oscillations sufficiently
- The 10000 averaging window appears to be statistically converged. We will use 20000 iteration averaging window going forward.
Results: Sensitivities for Final State Objective Functional

(a) Sensitivities

(b) Angle Convergence

Sensitivities integrated through pseudo-time

- The sensitivities are highly oscillatory.
- The angle fails to converge well as we integrate back.
Results: Sensitivities for 250 Iteration Window Averaged Objective Functional

Sensitivities integrated through pseudo-time

- The sensitivities are highly oscillatory, but less oscillatory than the instantaneous objective case.
- The angle is better behaved, but fails to converge.
Results: Sensitivities for 20000 Iteration Window Averaged Objective Functional

(a) Sensitivities

(b) Angle Convergence

Sensitivities integrated through pseudo-time

- The sensitivities are well behaved and converge to a final value outside of the averaging window
- The angle is well behaved, lending credence to partial backwards-in-pseudo-time integration, as was previously theorized.
Results: Convergence for Steady-State Adjoint systems

(a) Final State

Steady-State adjoint convergence for $Mach = .7$, $\alpha = 2^\circ$

- Both systems take many iterations to converge, this follows the conclusions of Krakos and Darmofal.
- The average state converges slightly faster.

(b) Average State

<table>
<thead>
<tr>
<th>Iterations</th>
<th>2-Norm of Linear System Residual</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>$10^{-12}$</td>
</tr>
<tr>
<td>5e+05</td>
<td>$10^{-6}$</td>
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<td>$10^{-3}$</td>
</tr>
<tr>
<td>1.5e+06</td>
<td>$10^{-1}$</td>
</tr>
<tr>
<td>2e+06</td>
<td>$10^{-0}$</td>
</tr>
<tr>
<td>2.5e+06</td>
<td>$10^{1}$</td>
</tr>
<tr>
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Results: Sensitivity Vector Comparison of Final State Steady State Adjoint to PTA Adjoint

<table>
<thead>
<tr>
<th>Design Variable</th>
<th>Steady-State Value (Final State)</th>
<th>Pseudo-Time Accurate Value</th>
<th>Percent Difference</th>
</tr>
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<tbody>
<tr>
<td>1</td>
<td>44.5805974889098</td>
<td>38.03996816573513</td>
<td>17.19%</td>
</tr>
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<td>2</td>
<td>14.0224144011606</td>
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<td>21.79%</td>
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<td>3</td>
<td>-1.27443407446669</td>
<td>0.2080948770865852</td>
<td>712.43%</td>
</tr>
</tbody>
</table>

Comparison of sensitivity vectors for steady-state and pseudo-time accurate (20000 iteration averaging window) adjoints
Comparison of sensitivity vectors for steady-state and pseudo-time accurate (20000 iteration averaging window) adjoints

The angle between the two sensitivity vectors is $\theta = 7.98972^\circ$
Results: Sensitivity Vector Comparison of Averaged State Steady State Adjoint to PTA Adjoint

<table>
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<tr>
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<tbody>
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<td>43.3642585762660</td>
<td>38.03996816573513</td>
<td>14.00%</td>
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<tr>
<td>2</td>
<td>16.9218981680917</td>
<td>17.92859539270058</td>
<td>5.62%</td>
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<tr>
<td>3</td>
<td>-9.717943674789181E-002</td>
<td>0.2080948770865852</td>
<td>146.70%</td>
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Results: Sensitivity Vector Comparison of Averaged State Steady State Adjoint to PTA Adjoint

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Comparison of sensitivity vectors for steady-state and pseudo-time accurate (20000 iteration averaging window) adjoints

The angle between the two sensitivity vectors is $\theta = 3.93855^\circ$
Conclusions and Future Work
Conclusions

- For Newton’s Method we can compute the adjoint and tangent systems without full solution of the linear system and obtain error estimates on the sensitivity.

- For non-converging or truncated simulations, the pseudo-time accurate sensitivities are significantly different than the steady-state sensitivities when linearized about the final state and the pseudo-time averaged state.

- Increasing the functional averaging window provides better sensitivity behavior.

- The pseudo-time accurate sensitivities converge to approximately the final values after integrating through the functional averaging window (for long windows).

- We do not address chaotic flows where the sensitivity computation diverges.
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• Application to error estimation (underway)
Future Work

- Application to error estimation (underway)
- Test cases with design cycles
Future Work

- Application to error estimation (underway)
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- Applications to unsteady simulations and adjoints
Thank you!