ADJOINT METHODS IN A HIGHER-ORDER SPACE-TIME DISCONTINUOUS-GALERKIN SOLVER FOR TURBULENT FLOWS

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Motivation

• Perform detailed time-accurate scale-resolving simulations of practical, complex, compressible flows

• High-Reynolds-number separated flows involving large-scale unsteadiness, where RANS models are unreliable
Approach

• Turbulent flows involve a large range of spatial and temporal scales which need to be resolved
• Efficient algorithms and implementation necessary for wall-resolved high Reynolds number flows
• Numerical method must be capable of handling complex geometry
• Numerical method must be “robust”

Developed higher-order space-time discontinuous-Galerkin spectral element framework
Approach

- Gradient computation needed for error-estimation, adaptation, design, sensitivity analysis, etc.
- Tangent and adjoint methods have been successfully applied to a variety of steady and unsteady flows
- High-fidelity simulations we are targeting are chaotic
- Can traditional tangent/adjoint methods work?
- Develop efficient implementation of tangent and adjoint method in space-time discontinuous solver
- Assess the applicability of traditional adjoint and tangent methods for chaotic flows
Outline

• Space-time DG formulation
  • Discrete primal formulation
  • Discrete tangent and adjoint formulations
• NACA0012
  • Flow sensitivity with increasing Reynolds number
  • Properties of adjoint for chaotic flows
• T106a LPT
  • Adjoint solutions corresponding to a practical simulation
• Summary/Outlook
Space-Time Discontinuous-Galerkin (DG) Formulation

- Compressible Navier-Stokes Equations:
  \[ \frac{\partial u}{\partial t} + \nabla \cdot F(u, \nabla u) = 0 \]

- Space-Time Discontinuous-Galerkin Discretization:
  - Entropy variables: Hughes (1986)
    \[ A_o v_{,t} + A_i v_{,i} - (K_{ij} v_{,j})_{,i} = 0 \]
  - Inviscid Flux: Ismail & Roe (2009)
  - Integrals evaluated using numerical quadrature with 2N points
    \[ (\rho s)_{,t} + \left( \frac{q_i}{c_v T} \right)_{,i} = v^T_{,i} K_{ij} v_{,j} \geq 0 \]
Discrete Formulation

• Discrete system solved each time-slab:

\[ R^n(u^n, w^n) + G^n(u^{n-1}, w^n) = 0 \]

• where:

\[
R^n(u^n, w^n) = \sum_{\kappa} \left\{ \int_I \int_{\kappa} - \left( \frac{\partial w}{\partial t} u + \nabla w \cdot F \right) + \int_I \int_{\partial \kappa} w \overline{F \cdot n} + \int_{\kappa} w(t_{n+1})u(t_{n+1}) \right\}
\]

\[
G^n(u^{n-1}, w^n) = \sum_{\kappa} \left\{ \int_{\kappa} -w(t_+^n)u(t_-^n) \right\}
\]

• beginning/end of time-slab

\[ w(t_+^n) = I_s w^n \quad w(t_-^{n+1}) = I_e w^n \]
Discrete Tangent formulation

Output: \( J(u; \alpha) \)

- where \( \alpha \) is a parameter (i.e. angle of attack, Reynolds number etc.)

Compute sensitivity of output to parameters:

\[
\frac{dJ}{d\alpha} = \frac{\partial J}{\partial \alpha} + \frac{\partial J}{\partial u} \frac{\partial u}{\partial \alpha} = \frac{\partial J}{\partial \alpha} + \frac{\partial J}{\partial R} \frac{\partial R}{\partial \alpha}
\]

Tangent equation:

\[
\frac{\partial R^n}{\partial u^n} (\delta u^n, w^n) + \frac{\partial G^n}{\partial u^{n-1}} (\delta u^{n-1}, w^n) = - \frac{\partial R^n}{\partial \alpha}
\]

Matrix form:

\[
\begin{bmatrix}
\frac{\partial R^{n-1}}{\partial u^{n-1}} & 0 & 0 \\
\frac{\partial G^n}{\partial u^n} & \frac{\partial R^n}{\partial u^n} & 0 \\
0 & \frac{\partial G^{n+1}}{\partial u^{n+1}} & \frac{\partial R^{n+1}}{\partial u^{n+1}}
\end{bmatrix}
\begin{bmatrix}
\delta u^{n-1} \\
\delta u^n \\
\delta u^{n+1}
\end{bmatrix} = -
\begin{bmatrix}
\frac{\partial R^{n-1}}{\partial u^{n-1}} \\
\frac{\partial R^n}{\partial u^n} \\
\frac{\partial R^{n+1}}{\partial u^{n+1}}
\end{bmatrix}
\]
Discrete Adjoint Formulation

- **Lagrangian:** \[ \mathcal{L}(u, \psi; \alpha) = J(u; \alpha) + \psi^T \bar{R}(u; \alpha) \]

- **Stationarity of Lagrangian:**
  \[ \delta \mathcal{L} = \left( \left. \frac{\partial J^T}{\partial u} \right|_\alpha + \psi^T \left. \frac{\partial \bar{R}}{\partial u} \right|_\alpha \right) \delta u + \left( \left. \frac{\partial J^T}{\partial \alpha} \right|_u + \psi^T \left. \frac{\partial \bar{R}}{\partial \alpha} \right|_u \right) \delta \alpha = 0 \]

- **Adjoint equation:**
  \[ \frac{\partial R^n}{\partial u^n} (w^n, \psi^n) + \frac{\partial G^n}{\partial u^{n-1}} (w^{n-1}, \psi^n) = - \frac{\partial J^n}{\partial u^n} (\psi^n) \]

- **Matrix Form:**
  \[
  \begin{bmatrix}
    \frac{\partial R^{n-1}}{\partial u^{n-1}}^T & \frac{\partial G^n}{\partial u^{n-1}}^T & 0 \\
    0 & \frac{\partial R^n}{\partial u^n}^T & \frac{\partial G^{n+1}}{\partial u^n}^T \\
    0 & 0 & \frac{\partial R^{n+1}}{\partial u^{n+1}}^T
  \end{bmatrix}
  \begin{bmatrix}
    \psi^{n-1} \\
    \psi^n \\
    \psi^{n+1}
  \end{bmatrix}
  = - \begin{bmatrix}
    \frac{\partial J^{n-1}}{\partial u^{n-1}} \\
    \frac{\partial J^n}{\partial u^n} \\
    \frac{\partial J^{n+1}}{\partial u^{n+1}}
  \end{bmatrix}
  \]
Primal Solver: Implementation Details

- Efficient implementation of higher order DG
  - Tensor-product basis
  - Take advantage of hardware (SIMD/optimized kernels)
  - Jacobian-free Approximate Newton-Krylov solver
  - Tensor-product based ADI-preconditioner

- Primal Residual Evaluation:
  1. Evaluate state/gradient at quadrature points
  2. Evaluate flux at quadrature points
  3. Weight fluxes with gradient of test functions

Optimized sum-factorization
Vectorized Kernels
Tangent/Adjoint: Implementation Details

• Reuse optimization from primal for tangent and adjoint

  • Tangent Residual Evaluation:
    1. Evaluate state/gradient and update/gradient at quadrature points
    2. Evaluate linearized flux at quadrature points
    3. Weight fluxes with gradient of test functions

  • Adjoint Residual Evaluation:
    4. Evaluate state/gradient and adjoint/gradient at quadrature points
    5. Evaluate adjoint flux at quadrature points
    6. Weight fluxes with gradient of test functions
NACA0012, $\alpha = 10$

- At high angle of attack, flow over NACA0012 airfoil exhibits vortex shedding which become chaotic with increasing Reynolds number. (Pulliam 1993)

- Examine primal and adjoint solutions
NACA0012, $\text{Re} = 800$, $\alpha = 10$

- Unsteady shedding gives periodic output signal
- Adjoint solution also periodic (after initial transient)
NACA0012, $Re = 1600$, $\alpha = 10$

- With increasing Reynolds number force has multiple frequencies
- Adjoint solution still essentially appears periodic
NACA0012, Re = 2400, \( \alpha = 10 \)

Directional Force Output

- With increasing Reynolds number simulated flow become chaotic
- Adjoint solution begins to grow unboundedly
NACA0012, $Re = 800-2400$, $\alpha = 10$

- With increasing Reynolds number simulated flow become chaotic
- Adjoint solution begins to grow unboundedly
NACA0012, Re = 800-2400, \( \alpha = 10 \)

- Solution is in fact chaotic at Re = 1600, but growth rate is much slower than at Re = 2400
- Windowing approaches may be successful at Re = 800, 1600
T106c Low Pressure Turbine

- $\text{Re} = 80,000$, $M_{\text{inflow}} = 0.243$, $\alpha = 32.7$, $M_{\text{exit}} = 0.65$
- Periodic BCs in span-wise and pitch-wise directions
- No free-stream turbulence
- Spanwise domain is 20% of chord
Primal Solution

- Nearly steady flow upstream and over first 2/3 of blade
- Separation leading to transition/vortex shedding on suction-side of blade
- Fully turbulent wake
Sensitivity to Inflow Boundary Condition

- Modify inlet flow angle from $\alpha = 32.7$ to $\alpha = 32.701$
Sensitivity to Inflow Boundary Condition

Convective disturbance hits leading edge

Acoustic disturbance hits leading edge

Domain flow-through time
Adjoint of mean Axial Force

- Output is integrated axial force

\[ \bar{J} = \frac{1}{T} \int_{0}^{T} F_x(u(\tau)) d\tau \]

- Also define output without temporal normalization

\[ J(t) = \int_{0}^{t} F_x(u(\tau)) d\tau \]

Range: \([-1e6, 1e6]\)
Sensitivity computed using adjoint

\[
\Delta J(t) = J(t; \alpha + \Delta \alpha) - J(t; \alpha) = \int_0^t F_x(u(\tau; \alpha + \Delta \alpha)) - F_x(u(\tau; \alpha)) d\tau \\
\approx \int_0^t \Psi(\tau; t, \alpha)^T R(u(\tau); \alpha + \Delta \alpha)
\]
Sensitivity computed using adjoint

\[ \Delta F_x(\tau) = F_x(u(\tau; \alpha + \Delta \alpha)) - F_x(u(\tau; \alpha)) \]

\[ ?? \approx \Psi(t - \tau; t, \alpha)^T R(u; \alpha + \Delta \alpha) \]

- Approximation holds since flow upstream of blade is essentially time-independent
- Adjoint correctly captures sensitivity in part of flow upstream of separation
Sensitivity computed using adjoint

- Sensitivity computed using adjoint only valid for very short time windows
- Adjoint computed using long time window blows up
- Sensitivity computed using short time window, not representative long time behaviour
Graphical demonstration of concepts

• Adjoint correctly captures sensitivity in part of flow upstream of separation

• Sensitivity computed using adjoint only valid for very short time windows

• Sensitivity computed using short time window, not representative long time behaviour
Adjoint-based Error Estimation

- Estimate error using dual-weighted residual method (Becker & Rannacher 1995)

$$\epsilon = J(u) - J(u_H) \approx R_H(u_H, \psi_h)$$

- Localize error

$$\epsilon_\kappa \equiv R_H(u_H, \psi_h|_\kappa)$$

- Flag elements with largest error for refinement

Primal Solution

Element-based error-indicator
• Unbounded adjoint not useful for error estimation
• Estimate is orders of magnitude larger than actual signal
• Error localization simply flags regions where adjoint is large
Adjoint growth with mesh resolution

- Refined mesh has essentially double mesh resolution near separation region.
- Increase mesh resolution results in faster growth of adjoint (i.e. larger Lyapunov exponent).
- Adaptation mechanism is not convergent.
Summary

• Presented space-time adjoint solver for turbulent compressible flows
• Confirmed failure of traditional sensitivity methods for chaotic flows
• Assessed rate of exponential growth of adjoint for practical 3D turbulent simulation
• Demonstrated failure of short-window sensitivity approximations.
Questions??

Outlook/Future Work:

• Lyapunov exponents, least-square shadowing and beyond…