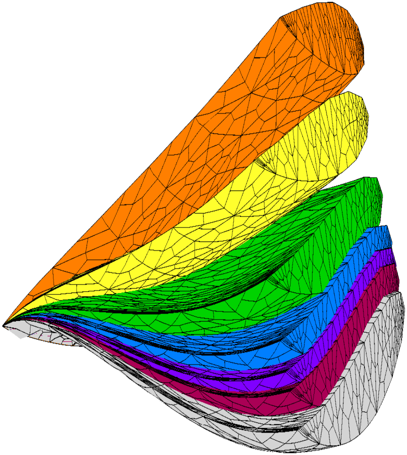

Adjoint-based derivative evaluation methods for flexible multibody systems with rotorcraft applications

Komahan Boopathy and
Graeme J. Kennedy
Georgia Tech

Motivation

Modeling Flexiblity

- Advanced lightweight materials enable more flexible aerospace structures
- Essential to model inertial loads and flexibility

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- Aero/elastic/dynamic rotorcraft simulations
- High-fidelity gradient-based optimization
- Parallel scalability is critical

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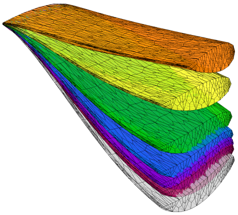
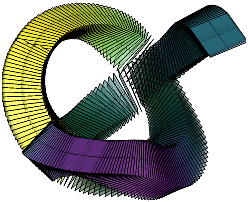
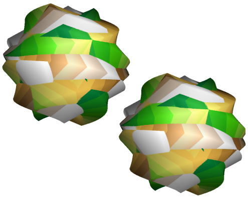
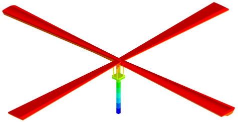
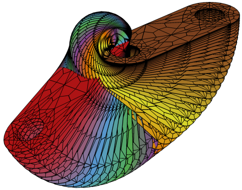
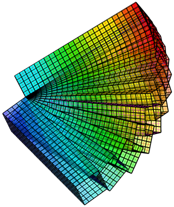
Current Focus

- Analysis and adjoint derivative capabilities for flexible multibody systems
- Enhance `Toolkit for the Analysis of Composite Structures (TACS)`
- `TACS` interfaces with `FUN3D` via `FUNtoFEM`

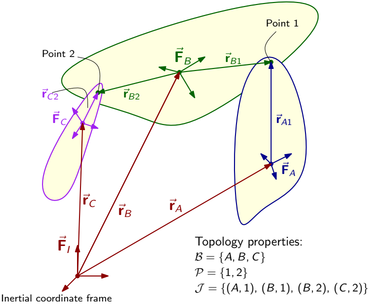
Some Dynamic Simulations in TACS

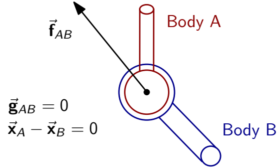







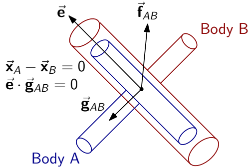
Equations of Motion $\mathrm{R}(\ddot{\mathrm{q}}, \dot{\mathrm{q}}, \mathrm{q}, \mathrm{x}, t) = 0$

Dynamics, Kinematics and Constraints

- Implicit function of state and design variables
- Leads to a descriptor system of Differential-Algebraic Equations (DAEs)
- Example: $\mathrm{R} = \mathrm{M}\ddot{\mathrm{q}} + \mathrm{C}\dot{\mathrm{q}} + \mathrm{K}\mathrm{q} - \mathcal{F}(t) = 0$







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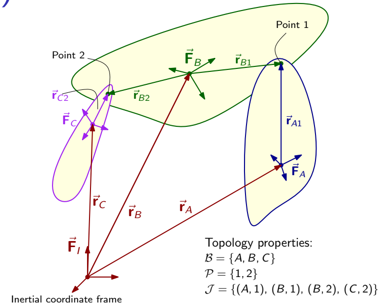
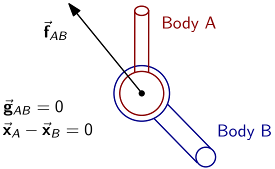
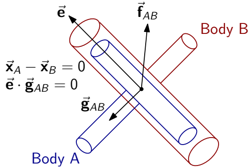


State Vector

- position variables
- rotational parametrization
- Lagrange multipliers





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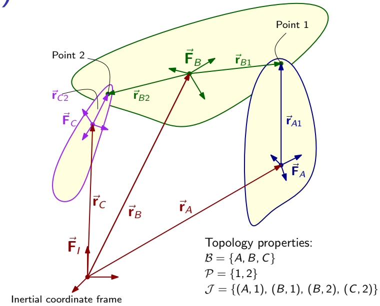

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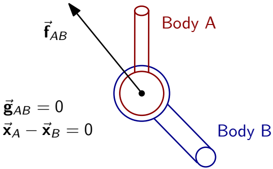
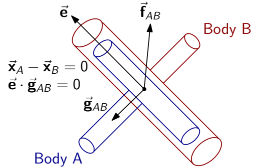


Natural vs. State-Space Form

We solve as *second-order equations*

- No state-space conversions
- Simpler adjoint developments
- Preserve the physical meaning of quantities



Solving the Coupled Flexible Multibody System

Time Marching Schemes

TACS supports different time integration schemes

1. Backward Difference Formulas (BDF)
2. Adams–Bashforth–Moulton (ABM)
3. Diagonally Implicit Runge–Kutta (DIRK)
4. Newmark

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Key issues

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- Multistage methods require more computations

multi-step-stage.pdf

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Forward Solution Mode

- March from the initial conditions $q_0, \dot{q}_0$
- Find state variables $\ddot{q}_k, \dot{q}_k, q_k$
- Newton's method based on linearization of governing equations

multi-step-stage.pdf

Time Marching: Matrix Structure

Banded lower triangular system solve to for state updates

$$
\begin{bmatrix}
\frac{\partial \mathbf{R}_k}{\partial \ddot{\mathbf{q}}_k} & & & & & & & & \\
\frac{\partial \mathbf{S}_k}{\partial \ddot{\mathbf{q}}_k} & \frac{\partial \mathbf{S}_k}{\partial \dot{\mathbf{q}}_k} & & & & & & & \\
\frac{\partial \mathbf{T}_k}{\partial \ddot{\mathbf{q}}_k} & \frac{\partial \mathbf{T}_k}{\partial \dot{\mathbf{q}}_k} & \frac{\partial \mathbf{T}_k}{\partial \mathbf{q}_k} & & & & & & \\
\frac{\partial \mathbf{R}_{k+1}}{\partial \ddot{\mathbf{q}}_k} & \frac{\partial \mathbf{R}_{k+1}}{\partial \dot{\mathbf{q}}_k} & \frac{\partial \mathbf{R}_{k+1}}{\partial \mathbf{q}_k} & \frac{\partial \mathbf{R}_{k+1}}{\partial \ddot{\mathbf{q}}_{k+1}} & & & & & \\
\frac{\partial \mathbf{S}_{k+1}}{\partial \ddot{\mathbf{q}}_k} & \frac{\partial \mathbf{S}_{k+1}}{\partial \dot{\mathbf{q}}_k} & \frac{\partial \mathbf{S}_{k+1}}{\partial \mathbf{q}_k} & \frac{\partial \mathbf{S}_{k+1}}{\partial \ddot{\mathbf{q}}_{k+1}} & \frac{\partial \mathbf{S}_{k+1}}{\partial \dot{\mathbf{q}}_{k+1}} & & & & \\
\frac{\partial \mathbf{T}_{k+1}}{\partial \ddot{\mathbf{q}}_k} & \frac{\partial \mathbf{T}_{k+1}}{\partial \dot{\mathbf{q}}_k} & \frac{\partial \mathbf{T}_{k+1}}{\partial \mathbf{q}_k} & \frac{\partial \mathbf{T}_{k+1}}{\partial \ddot{\mathbf{q}}_{k+1}} & \frac{\partial \mathbf{T}_{k+1}}{\partial \dot{\mathbf{q}}_{k+1}} & \frac{\partial \mathbf{T}_{k+1}}{\partial \mathbf{q}_{k+1}} & & & \\
\frac{\partial \mathbf{R}_{k+2}}{\partial \ddot{\mathbf{q}}_k} & \frac{\partial \mathbf{R}_{k+2}}{\partial \dot{\mathbf{q}}_k} & \frac{\partial \mathbf{R}_{k+2}}{\partial \mathbf{q}_k} & \frac{\partial \mathbf{R}_{k+2}}{\partial \ddot{\mathbf{q}}_{k+1}} & \frac{\partial \mathbf{R}_{k+2}}{\partial \dot{\mathbf{q}}_{k+1}} & \frac{\partial \mathbf{R}_{k+2}}{\partial \mathbf{q}_{k+1}} & \frac{\partial \mathbf{R}_{k+2}}{\partial \ddot{\mathbf{q}}_{k+2}} & & \\
\frac{\partial \mathbf{S}_{k+2}}{\partial \ddot{\mathbf{q}}_k} & \frac{\partial \mathbf{S}_{k+2}}{\partial \dot{\mathbf{q}}_k} & \frac{\partial \mathbf{S}_{k+2}}{\partial \mathbf{q}_k} & \frac{\partial \mathbf{S}_{k+2}}{\partial \ddot{\mathbf{q}}_{k+1}} & \frac{\partial \mathbf{S}_{k+2}}{\partial \dot{\mathbf{q}}_{k+1}} & \frac{\partial \mathbf{S}_{k+2}}{\partial \mathbf{q}_{k+1}} & \frac{\partial \mathbf{S}_{k+2}}{\partial \ddot{\mathbf{q}}_{k+2}} & \frac{\partial \mathbf{S}_{k+2}}{\partial \dot{\mathbf{q}}_{k+2}} & \\
\frac{\partial \mathbf{T}_{k+2}}{\partial \ddot{\mathbf{q}}_k} & \frac{\partial \mathbf{T}_{k+2}}{\partial \dot{\mathbf{q}}_k} & \frac{\partial \mathbf{T}_{k+2}}{\partial \mathbf{q}_k} & \frac{\partial \mathbf{T}_{k+2}}{\partial \ddot{\mathbf{q}}_{k+1}} & \frac{\partial \mathbf{T}_{k+2}}{\partial \dot{\mathbf{q}}_{k+1}} & \frac{\partial \mathbf{T}_{k+2}}{\partial \mathbf{q}_{k+1}} & \frac{\partial \mathbf{T}_{k+2}}{\partial \ddot{\mathbf{q}}_{k+2}} & \frac{\partial \mathbf{T}_{k+2}}{\partial \dot{\mathbf{q}}_{k+2}} & \frac{\partial \mathbf{T}_{k+2}}{\partial \mathbf{q}_{k+2}}
\end{bmatrix}
\begin{bmatrix}
\Delta\ddot{\mathbf{q}}_k \\ \Delta\dot{\mathbf{q}}_k \\ \Delta\mathbf{q}_k \\ \Delta\ddot{\mathbf{q}}_{k+1} \\ \Delta\dot{\mathbf{q}}_{k+1} \\ \Delta\mathbf{q}_{k+1} \\ \Delta\ddot{\mathbf{q}}_{k+2} \\ \Delta\dot{\mathbf{q}}_{k+2} \\ \Delta\mathbf{q}_{k+2}
\end{bmatrix}
= -
\begin{bmatrix}
\mathbf{R}_k \\ \mathbf{S}_k \\ \mathbf{T}_k \\ \mathbf{R}_{k+1} \\ \mathbf{S}_{k+1} \\ \mathbf{T}_{k+1} \\ \mathbf{R}_{k+2} \\ \mathbf{S}_{k+2} \\ \mathbf{T}_{k+2}
\end{bmatrix}
$$

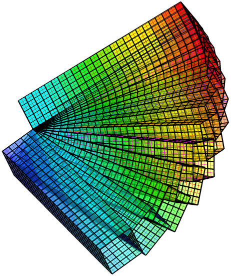
Representation of Functionals

Objective Function

Functionals that are an integral in time and dependent on the state and design variables:

$$f(\mathrm{x}) = \int_0^T F(\ddot{\mathrm{q}}, \dot{\mathrm{q}}, \mathrm{q}, \mathrm{x}, t)\ dt \approx \sum_{k=0}^{N} h\mathrm{F}_k(\ddot{\mathrm{q}}, \dot{\mathrm{q}}, \mathrm{q}, \mathrm{x}, t_k)$$

- Aggregation functionals such as p-norm and Kreisselmeier–Steinhauser (KS) provide smooth approximations
- Maximum value of the quantity of interest over the time interval $[0, T]$
- Other possibilities for functionals exist too



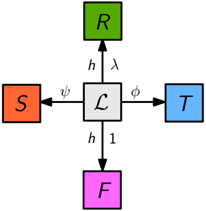
Adjoint Derivatives

Formation of the Lagrangian

Introduce λ_k, ψ_k and ϕ_k as the adjoint variables:

$$\mathcal{L} = \sum_{k=0}^{N} hF_k + \sum_{k=0}^{N} h\lambda_k^T \mathrm{R}_k + \sum_{k=0}^{N} \psi_k^T \mathrm{S}_k + \sum_{k=0}^{N} \phi_k^T \mathrm{T}_k$$

- Find adjoint variables λ, ψ and ϕ
- Use $\dfrac{\partial \mathcal{L}}{\partial \ddot{\mathrm{q}}_k}, \dfrac{\partial \mathcal{L}}{\partial \dot{\mathrm{q}}_k}, \dfrac{\partial \mathcal{L}}{\partial \mathrm{q}_k} = 0$
- Linear solve for each functional



Total Derivative

$$\frac{df(\mathrm{x})}{d\mathrm{x}} = \sum_{k=0}^{N} h\frac{\partial F_k}{\partial \mathrm{x}} + \sum_{k=0}^{N} h\lambda_k^T \frac{\partial \mathrm{R}_k}{\partial \mathrm{x}} + \sum_{k=0}^{N} \psi_k^T \cancelto{0}{\frac{\partial \mathrm{S}_k}{\partial \mathrm{x}}} + \sum_{k=0}^{N} \phi_k^T \cancelto{0}{\frac{\partial \mathrm{T}_k}{\partial \mathrm{x}}}$$

Discrete Adjoint: Matrix Structure

Banded upper triangular system with transposed Jacobian to solve for adjoint variables

$$
\begin{bmatrix}
\frac{\partial \mathbf{R}_k^T}{\partial \ddot{\mathbf{q}}_k} & \frac{\partial \mathbf{S}_k^T}{\partial \ddot{\mathbf{q}}_k} & \frac{\partial \mathbf{T}_k^T}{\partial \ddot{\mathbf{q}}_k} & \frac{\partial \mathbf{R}_{k+1}^T}{\partial \ddot{\mathbf{q}}_k} & \frac{\partial \mathbf{S}_{k+1}^T}{\partial \ddot{\mathbf{q}}_k} & \frac{\partial \mathbf{T}_{k+1}^T}{\partial \ddot{\mathbf{q}}_k} & \frac{\partial \mathbf{R}_{k+2}^T}{\partial \ddot{\mathbf{q}}_k} & \frac{\partial \mathbf{S}_{k+2}^T}{\partial \ddot{\mathbf{q}}_k} & \frac{\partial \mathbf{T}_{k+2}^T}{\partial \ddot{\mathbf{q}}_k} \\
 & \frac{\partial \mathbf{S}_k^T}{\partial \dot{\mathbf{q}}_k} & \frac{\partial \mathbf{T}_k^T}{\partial \dot{\mathbf{q}}_k} & \frac{\partial \mathbf{R}_{k+1}^T}{\partial \dot{\mathbf{q}}_k} & \frac{\partial \mathbf{S}_{k+1}^T}{\partial \dot{\mathbf{q}}_k} & \frac{\partial \mathbf{T}_{k+1}^T}{\partial \dot{\mathbf{q}}_k} & \frac{\partial \mathbf{R}_{k+2}^T}{\partial \dot{\mathbf{q}}_k} & \frac{\partial \mathbf{S}_{k+2}^T}{\partial \dot{\mathbf{q}}_k} & \frac{\partial \mathbf{T}_{k+2}^T}{\partial \dot{\mathbf{q}}_k} \\
 & & \frac{\partial \mathbf{T}_k^T}{\partial \mathbf{q}_k} & \frac{\partial \mathbf{R}_{k+1}^T}{\partial \mathbf{q}_k} & \frac{\partial \mathbf{S}_{k+1}^T}{\partial \mathbf{q}_k} & \frac{\partial \mathbf{T}_{k+1}^T}{\partial \mathbf{q}_k} & \frac{\partial \mathbf{R}_{k+2}^T}{\partial \mathbf{q}_k} & \frac{\partial \mathbf{S}_{k+2}^T}{\partial \mathbf{q}_k} & \frac{\partial \mathbf{T}_{k+2}^T}{\partial \mathbf{q}_k} \\
 & & & \frac{\partial \mathbf{R}_{k+1}^T}{\partial \ddot{\mathbf{q}}_{k+1}} & \frac{\partial \mathbf{S}_{k+1}^T}{\partial \ddot{\mathbf{q}}_{k+1}} & \frac{\partial \mathbf{T}_{k+1}^T}{\partial \ddot{\mathbf{q}}_{k+1}} & \frac{\partial \mathbf{R}_{k+2}^T}{\partial \ddot{\mathbf{q}}_{k+1}} & \frac{\partial \mathbf{S}_{k+2}^T}{\partial \ddot{\mathbf{q}}_{k+1}} & \frac{\partial \mathbf{T}_{k+2}^T}{\partial \ddot{\mathbf{q}}_{k+1}} \\
 & & & & \frac{\partial \mathbf{S}_{k+1}^T}{\partial \dot{\mathbf{q}}_{k+1}} & \frac{\partial \mathbf{T}_{k+1}^T}{\partial \dot{\mathbf{q}}_{k+1}} & \frac{\partial \mathbf{R}_{k+2}^T}{\partial \dot{\mathbf{q}}_{k+1}} & \frac{\partial \mathbf{S}_{k+2}^T}{\partial \dot{\mathbf{q}}_{k+1}} & \frac{\partial \mathbf{T}_{k+2}^T}{\partial \dot{\mathbf{q}}_{k+1}} \\
 & & & & & \frac{\partial \mathbf{T}_{k+1}^T}{\partial \mathbf{q}_{k+1}} & \frac{\partial \mathbf{R}_{k+2}^T}{\partial \mathbf{q}_{k+1}} & \frac{\partial \mathbf{S}_{k+2}^T}{\partial \mathbf{q}_{k+1}} & \frac{\partial \mathbf{T}_{k+2}^T}{\partial \mathbf{q}_{k+1}} \\
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 & & & & & & & & \frac{\partial \mathbf{T}_{k+2}^T}{\partial \mathbf{q}_{k+2}}
\end{bmatrix}
\begin{bmatrix}
\lambda_k \\ \psi_k \\ \phi_k \\ \lambda_{k+1} \\ \psi_{k+1} \\ \phi_{k+1} \\ \lambda_{k+2} \\ \psi_{k+2} \\ \phi_{k+2}
\end{bmatrix}
= -
\begin{bmatrix}
\frac{\partial F_k^T}{\partial \ddot{\mathbf{q}}_k} \\ \frac{\partial F_k^T}{\partial \dot{\mathbf{q}}_k} \\ \frac{\partial F_k^T}{\partial \mathbf{q}_k} \\ \frac{\partial F_{k+1}^T}{\partial \ddot{\mathbf{q}}_{k+1}} \\ \frac{\partial F_{k+1}^T}{\partial \dot{\mathbf{q}}_{k+1}} \\ \frac{\partial F_{k+1}^T}{\partial \mathbf{q}_{k+1}} \\ \frac{\partial F_{k+2}^T}{\partial \ddot{\mathbf{q}}_{k+2}} \\ \frac{\partial F_{k+2}^T}{\partial \dot{\mathbf{q}}_{k+2}} \\ \frac{\partial F_{k+2}^T}{\partial \mathbf{q}_{k+2}}
\end{bmatrix}
$$

Time Marching: Newmark Beta Gamma (NBG)

- Linear single step method
- β and γ are the coefficients of Newmark scheme
- Second time derivative of states, $\ddot{\mathrm{q}}_k$, are the primary unknowns

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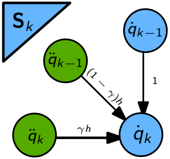

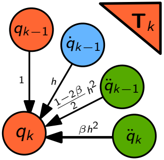

- First time derivative of states:

$$\dot{q}_k = \dot{q}_{k-1} + (1-\gamma)h\ddot{q}_{k-1} + \gamma h\ddot{q}_k + \mathcal{O}(h^p)$$

- State variables:

$$q_k = q_{k-1} + h\dot{q}_{k-1} + \frac{1-2\beta}{2}h^2\ddot{q}_{k-1} + \beta h^2\ddot{q}_k + \mathcal{O}(h^p)$$

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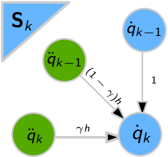

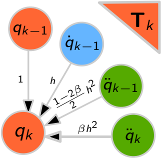

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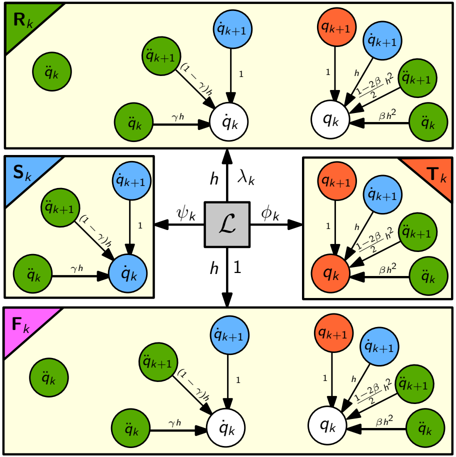
- Solve implicit system each step $\left[\frac{\partial R_k}{\partial \ddot{q}} + \gamma h \frac{\partial R_k}{\partial \dot{q}} + \beta h^2 \frac{\partial R_k}{\partial q}\right] \Delta\ddot{q}_k = -R_k$

The Lagrangian: Newmark Beta Gamma (NBG)



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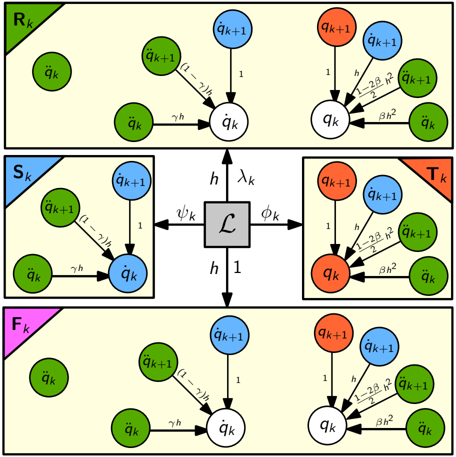

Formation of the Lagrangian

- S and T are the state approximation equations
- The residual R and the function F have same mathematical form
- The Lagrangian is a linear combination of equations

$$\mathcal{L} = \sum_{k=0}^{N} hF_k + \sum_{k=0}^{N} h\lambda_k^T \mathrm{R}_k + \sum_{k=0}^{N} \psi_k^T \mathrm{S}_k + \sum_{k=0}^{N} \phi_k^T \mathrm{T}_k$$

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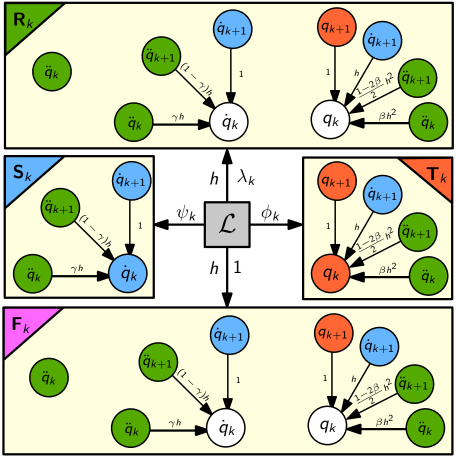

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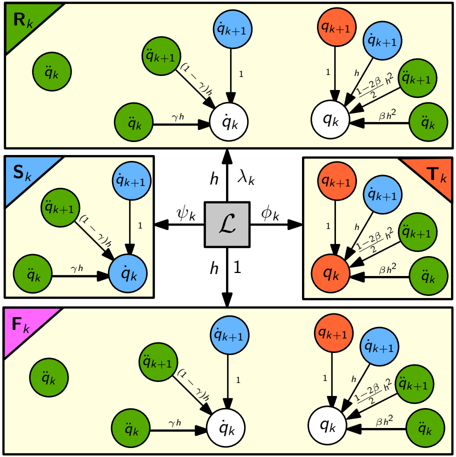
Find the adjoint variables

- Solve for ϕ_k using $\partial\mathcal{L}/\partial \mathrm{q}_k = 0$
- Solve for ψ_k using $\partial\mathcal{L}/\partial \dot{\mathrm{q}}_k = 0$
- Solve for λ_k using $\partial\mathcal{L}/\partial \ddot{\mathrm{q}}_k = 0$

The Lagrangian: Newmark Beta Gamma (NBG)



Formation of the Lagrangian

- S and T are the state approximation equations
- The residual R and the function F have same mathematical form
- The Lagrangian is a linear combination of equations

$$\mathcal{L} = \sum_{k=0}^{N} hF_k + \sum_{k=0}^{N} h\lambda_k^T R_k + \sum_{k=0}^{N} \psi_k^T S_k + \sum_{k=0}^{N} \phi_k^T T_k$$

Find the adjoint variables

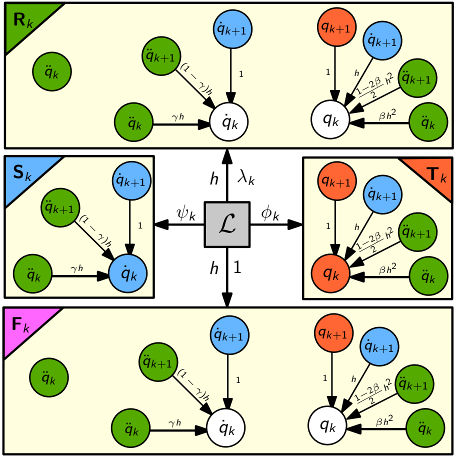
- Solve for ϕ_k using $\partial\mathcal{L}/\partial q_k = 0$
- Solve for ψ_k using $\partial\mathcal{L}/\partial \dot{q}_k = 0$
- Solve for λ_k using $\partial\mathcal{L}/\partial \ddot{q}_k = 0$

Total derivative

$$\frac{df(x)}{dx} = \sum_{k=0}^{N} h\frac{\partial F_k}{\partial x} + \sum_{k=0}^{N} h\lambda_k^T \frac{\partial R_k}{\partial x} + \sum_{k=0}^{N} \psi_k^T \cancelto{0}{\frac{\partial S_k}{\partial x}} + \sum_{k=0}^{N} \phi_k^T \cancelto{0}{\frac{\partial T_k}{\partial x}}$$

Discrete Adjoint: Newmark Beta Gamma (NBG)

$$\mathcal{L} = \sum_{k=0}^{N} hF_k + \sum_{k=0}^{N} h\lambda_k^T \mathrm{R}_k + \sum_{k=0}^{N} \psi_k^T \mathrm{S}_k + \sum_{k=0}^{N} \phi_k^T \mathrm{T}_k$$

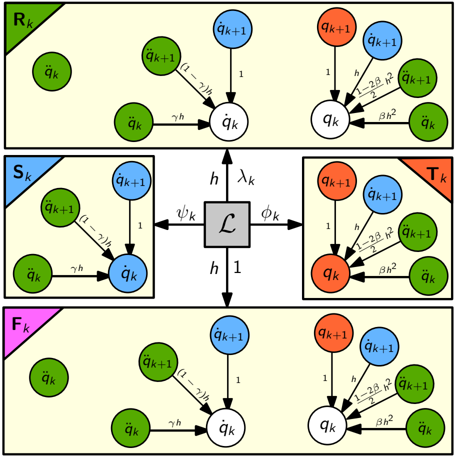


Solve for ϕ_k using $\partial\mathcal{L}/\partial \mathrm{q}_k = 0$

$$\phi_k = \phi_{k+1} + h\left[\frac{\partial \mathrm{R}_{k+1}}{\partial \mathrm{q}_{k+1}}\right]^T \lambda_{k+1} + h\left\{\frac{\partial F_{k+1}}{\partial \mathrm{q}_{k+1}}\right\}^T$$

Discrete Adjoint: Newmark Beta Gamma (NBG)

$$\mathcal{L} = \sum_{k=0}^{N} hF_k + \sum_{k=0}^{N} h\lambda_k^T \mathrm{R}_k + \sum_{k=0}^{N} \psi_k^T \mathrm{S}_k + \sum_{k=0}^{N} \phi_k^T \mathrm{T}_k$$



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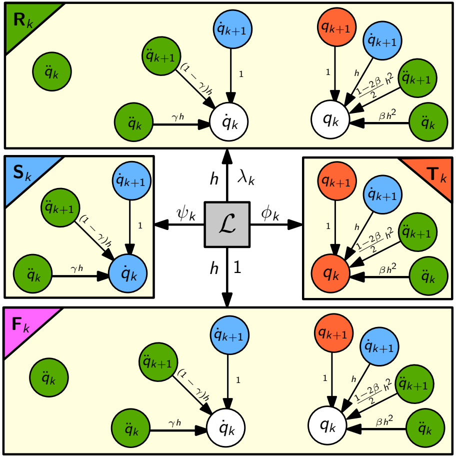
Four q_k

Discrete Adjoint: Newmark Beta Gamma (NBG)

$$\mathcal{L} = \sum_{k=0}^{N} hF_k + \sum_{k=0}^{N} h\lambda_k^T \mathrm{R}_k + \sum_{k=0}^{N} \psi_k^T \mathrm{S}_k + \sum_{k=0}^{N} \phi_k^T \mathrm{T}_k$$



Solve for ϕ_k using $\partial\mathcal{L}/\partial \mathrm{q}_k = 0$

$$\phi_k = \phi_{k+1} + h\left[\frac{\partial \mathrm{R}_{k+1}}{\partial \mathrm{q}_{k+1}}\right]^T \lambda_{k+1} + h\left\{\frac{\partial F_{k+1}}{\partial \mathrm{q}_{k+1}}\right\}^T$$

Four q_k

$$\frac{\partial \mathrm{T}_k}{\partial \mathrm{q}_k} = -\mathrm{I},$$

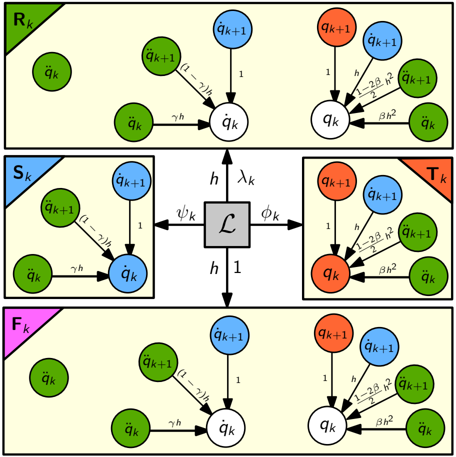
$$\frac{\partial \mathrm{T}_{k+1}}{\partial \mathrm{q}_k} = \mathrm{I}$$

$$\frac{\partial \mathrm{R}_{k+1}}{\partial \mathrm{q}_{k+1}} \rightarrow \text{stiffness matrix,}$$

$$\frac{\partial F_{k+1}}{\partial \mathrm{q}_{k+1}} \rightarrow \text{depends on the function}$$

Discrete Adjoint: Newmark Beta Gamma (NBG)

$$\mathcal{L} = \sum_{k=0}^{N} hF_k + \sum_{k=0}^{N} h\lambda_k^T \mathrm{R}_k + \sum_{k=0}^{N} \psi_k^T \mathrm{S}_k + \sum_{k=0}^{N} \phi_k^T \mathrm{T}_k$$

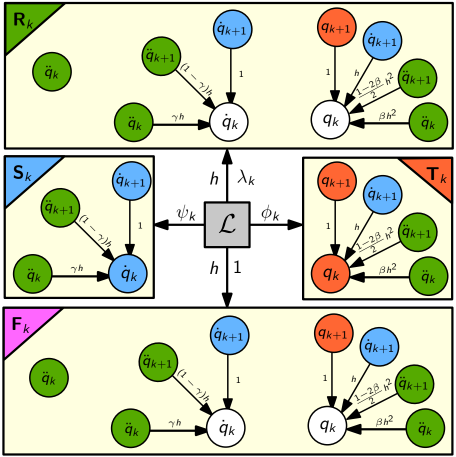


Solve for ψ_k using $\partial \mathcal{L} / \partial \dot{\mathrm{q}}_k = 0$

$$\begin{aligned}\psi_k &= \psi_{k+1} \\ &+ h\phi_{k+1} \\ &+ h\left[\frac{\partial \mathrm{R}_{k+1}}{\partial \dot{\mathrm{q}}_{k+1}} + h\frac{\partial \mathrm{R}_{k+1}}{\partial \mathrm{q}_{k+1}}\right]^T \lambda_{k+1} \\ &+ h\left\{\frac{\partial F_{k+1}}{\partial \dot{\mathrm{q}}_{k+1}} + h\frac{\partial F_{k+1}}{\partial \mathrm{q}_{k+1}}\right\}^T\end{aligned}$$

Discrete Adjoint: Newmark Beta Gamma (NBG)

$$\mathcal{L} = \sum_{k=0}^{N} hF_k + \sum_{k=0}^{N} h\lambda_k^T \mathrm{R}_k + \sum_{k=0}^{N} \psi_k^T \mathrm{S}_k + \sum_{k=0}^{N} \phi_k^T \mathrm{T}_k$$



Solve for ψ_k using $\partial\mathcal{L}/\partial\dot{\mathrm{q}}_k = 0$

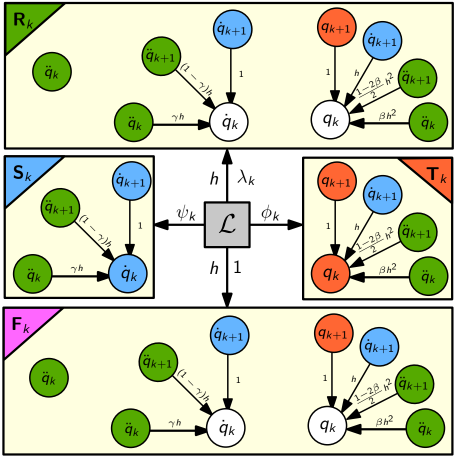
$$\begin{aligned}\psi_k &= \psi_{k+1} \\ &+ h\phi_{k+1} \\ &+ h\left[\frac{\partial \mathrm{R}_{k+1}}{\partial \dot{\mathrm{q}}_{k+1}} + h\frac{\partial \mathrm{R}_{k+1}}{\partial \mathrm{q}_{k+1}}\right]^T \lambda_{k+1} \\ &+ h\left\{\frac{\partial F_{k+1}}{\partial \dot{\mathrm{q}}_{k+1}} + h\frac{\partial F_{k+1}}{\partial \mathrm{q}_{k+1}}\right\}^T\end{aligned}$$

Seven $\dot{q}_k$

$\frac{\partial \mathrm{S}_k}{\partial \mathrm{q}_k} = -\mathrm{I}$ and $\frac{\partial \mathrm{S}_{k+1}}{\partial \mathrm{q}_k} = \mathrm{I}$

Discrete Adjoint: Newmark Beta Gamma (NBG)

$$\mathcal{L} = \sum_{k=0}^{N} hF_k + \sum_{k=0}^{N} h\lambda_k^T \mathrm{R}_k + \sum_{k=0}^{N} \psi_k^T \mathrm{S}_k + \sum_{k=0}^{N} \phi_k^T \mathrm{T}_k$$



Solve for λ_k using $\partial\mathcal{L}/\partial\ddot{\mathrm{q}}_k = 0$

$$\left[\frac{\partial \mathrm{R}_k}{\partial \ddot{\mathrm{q}}_k} + \gamma h \frac{\partial \mathrm{R}_k}{\partial \dot{\mathrm{q}}_k} + \beta h^2 \frac{\partial \mathrm{R}_k}{\partial \mathrm{q}_k}\right]^T \lambda_k =$$

$$- \left\{\frac{\partial F_k}{\partial \ddot{\mathrm{q}}_k} + \gamma h \frac{\partial F_k}{\partial \dot{\mathrm{q}}_k} + \beta h^2 \frac{\partial F_k}{\partial \mathrm{q}_k}\right\}^T$$

$$- \frac{1}{h}\left\{\gamma h \psi_k + \beta h^2 \phi_k\right\}$$

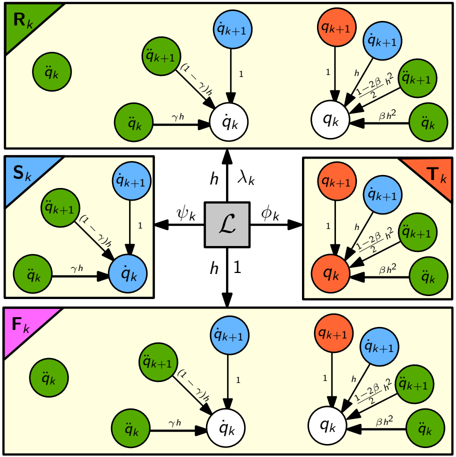
$$- \left[(1-\gamma)h \frac{\partial \mathrm{R}_{k+1}}{\partial \dot{\mathrm{q}}_{k+1}} + \frac{1-2\beta}{2} h^2 \frac{\partial \mathrm{R}_{k+1}}{\partial \mathrm{q}_{k+1}}\right]^T \lambda_{k+1}$$

$$- \left\{(1-\gamma)h \frac{\partial F_{k+1}}{\partial \dot{\mathrm{q}}_{k+1}} + \frac{1-2\beta}{2} h^2 \frac{\partial F_{k+1}}{\partial \mathrm{q}_{k+1}}\right\}^T$$

$$- \frac{1}{h}\left\{(1-\gamma)h\psi_{k+1} + \frac{1-2\beta}{2} h^2 \phi_{k+1}\right\}$$

Discrete Adjoint: Newmark Beta Gamma (NBG)

$$\mathcal{L} = \sum_{k=0}^{N} hF_k + \sum_{k=0}^{N} h\lambda_k^T \mathrm{R}_k + \sum_{k=0}^{N} \psi_k^T \mathrm{S}_k + \sum_{k=0}^{N} \phi_k^T \mathrm{T}_k$$



Solve for λ_k using $\partial \mathcal{L} / \partial \ddot{\mathrm{q}}_k = 0$

$$\left[\frac{\partial \mathrm{R}_k}{\partial \ddot{\mathrm{q}}_k} + \gamma h \frac{\partial \mathrm{R}_k}{\partial \dot{\mathrm{q}}_k} + \beta h^2 \frac{\partial \mathrm{R}_k}{\partial \mathrm{q}_k}\right]^T \lambda_k =$$

$$- \left\{\frac{\partial F_k}{\partial \ddot{\mathrm{q}}_k} + \gamma h \frac{\partial F_k}{\partial \dot{\mathrm{q}}_k} + \beta h^2 \frac{\partial F_k}{\partial \mathrm{q}_k}\right\}^T$$

$$- \frac{1}{h}\left\{\gamma h \psi_k + \beta h^2 \phi_k\right\}$$

$$- \left[(1-\gamma) h \frac{\partial \mathrm{R}_{k+1}}{\partial \dot{\mathrm{q}}_{k+1}} + \frac{1-2\beta}{2} h^2 \frac{\partial \mathrm{R}_{k+1}}{\partial \mathrm{q}_{k+1}}\right]^T \lambda_{k+1}$$

$$- \left\{(1-\gamma) h \frac{\partial F_{k+1}}{\partial \dot{\mathrm{q}}_{k+1}} + \frac{1-2\beta}{2} h^2 \frac{\partial F_{k+1}}{\partial \mathrm{q}_{k+1}}\right\}^T$$

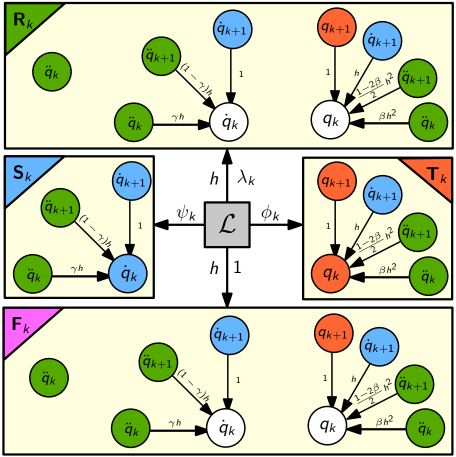
$$- \frac{1}{h}\left\{(1-\gamma) h \psi_{k+1} + \frac{1-2\beta}{2} h^2 \phi_{k+1}\right\}$$

Fourteen $\ddot{q}_k$

Coefficients from Newmark scheme

Discrete Adjoint: Newmark Beta Gamma (NBG)

$$\mathcal{L} = \sum_{k=0}^{N} hF_k + \sum_{k=0}^{N} h\lambda_k^T \mathrm{R}_k + \sum_{k=0}^{N} \psi_k^T \mathrm{S}_k + \sum_{k=0}^{N} \phi_k^T \mathrm{T}_k$$



Solve for λ_k using $\partial \mathcal{L}/\partial \ddot{\mathrm{q}}_k = 0$

$$\left[\frac{\partial \mathrm{R}_k}{\partial \ddot{\mathrm{q}}_k} + \gamma h \frac{\partial \mathrm{R}_k}{\partial \dot{\mathrm{q}}_k} + \beta h^2 \frac{\partial \mathrm{R}_k}{\partial \mathrm{q}_k}\right]^T \lambda_k =$$

$$- \left\{\frac{\partial F_k}{\partial \ddot{\mathrm{q}}_k} + \gamma h \frac{\partial F_k}{\partial \dot{\mathrm{q}}_k} + \beta h^2 \frac{\partial F_k}{\partial \mathrm{q}_k}\right\}^T$$

$$- \frac{1}{h}\left\{\gamma h \psi_k + \beta h^2 \phi_k\right\}$$

$$- \left[(1-\gamma)h \frac{\partial \mathrm{R}_{k+1}}{\partial \dot{\mathrm{q}}_{k+1}} + \frac{1-2\beta}{2} h^2 \frac{\partial \mathrm{R}_{k+1}}{\partial \mathrm{q}_{k+1}}\right]^T \lambda_{k+1}$$

$$- \left\{(1-\gamma)h \frac{\partial F_{k+1}}{\partial \dot{\mathrm{q}}_{k+1}} + \frac{1-2\beta}{2} h^2 \frac{\partial F_{k+1}}{\partial \mathrm{q}_{k+1}}\right\}^T$$

$$- \frac{1}{h}\left\{(1-\gamma)h\psi_{k+1} + \frac{1-2\beta}{2} h^2 \phi_{k+1}\right\}$$

Fourteen $\ddot{q}_k$

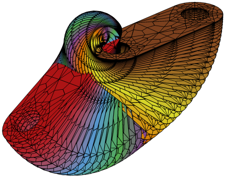
Coefficients from Newmark scheme

$$\frac{df(\mathrm{x})}{d\mathrm{x}} = \frac{\partial \mathcal{L}}{\partial \mathrm{x}} = \sum_{k=0}^{N} h \frac{\partial F_k}{\partial \mathrm{x}} + \sum_{k=0}^{N} h\lambda_k^T \frac{\partial \mathrm{R}_k}{\partial \mathrm{x}} + \sum_{k=0}^{N} \psi_k^T \underbrace{\frac{\partial \mathrm{S}_k}{\partial \mathrm{x}}}_{0} + \sum_{k=0}^{N} \phi_k^T \underbrace{\frac{\partial \mathrm{T}_k}{\partial \mathrm{x}}}_{0}$$

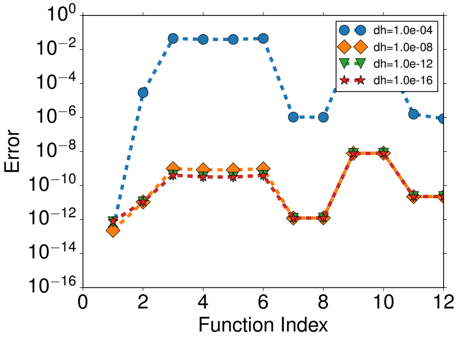
Complex-Step Verification of Newmark Adjoint

Complex-Step Verification of Newmark Adjoint

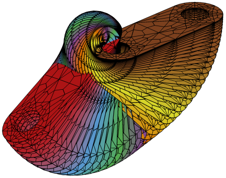
- Complex-step verification $\frac{\mathrm{d}f}{\mathrm{d}x_i} = \frac{\mathrm{Im} f(x+he_i)}{h}$
- Punched plate simulation run for 1000 time steps



Complex-Step Verification of Newmark Adjoint



- Complex-step verification $\frac{\mathrm{d}f}{\mathrm{d}x_i} = \frac{\mathrm{Im} f(x + he_i)}{h}$
- Punched plate simulation run for 1000 time steps
- $dh = 10^{-4}$, 10^{-8}, 10^{-12}, and 10^{-16}
- **Functionals:**
  - structural mass [1]
  - compliance [2]
  - KS von Mises failure [3, 4]
  - IE von Mises failure [5 − 12]
- Thickness design variables



Time Marching: Diagonally Implicit Runge–Kutta (DIRK)

Remarks

- Linear multi-stage method
- Primary unknowns are $\ddot{q}_{ki}$
- Not coupled like IRK

Butcher's Tableau

Stage	β_1	β_2	$\cdots$	β_s	
1	α_{11}	0	0	0	τ_1
2	α_{21}	α_{22}	0	0	τ_2
	$\vdots$	$\vdots$	$\ddots$	0	$\vdots$
s	α_{s1}	α_{s2}	$\cdots$	α_{ss}	τ_s

Time Marching: Diagonally Implicit Runge–Kutta (DIRK)

Stage Vectors

Stage Approximation Equations

$$\dot{u}_{ki} = \dot{q}_{k-1} + h\sum_{j=1}^{i} \alpha_{ij}\ddot{u}_{kj}$$
$$u_{ki} = q_{k-1} + h\sum_{j=1}^{i} \alpha_{ij}\dot{u}_{kj}$$

Remarks

- Linear multi-stage method
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	$\vdots$	$\vdots$	$\ddots$	0	$\vdots$
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Time Marching: Diagonally Implicit Runge–Kutta (DIRK)

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$u_{ki} = q_{k-1} + h \sum_{j=1}^{i} \alpha_{ij} \dot{u}_{kj}$

State Approximation Equations

$\ddot{q}_k = \sum_{i=1}^{s} \beta_i \ddot{u}_{ki}$

$\dot{q}_k = \dot{q}_{k-1} + h \sum_{i=1}^{s} \beta_i \ddot{u}_{ki}$

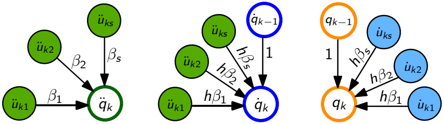
$q_k = q_{k-1} + h \sum_{i=1}^{s} \beta_i \dot{u}_{ki}$

Remarks

- Linear multi-stage method
- Primary unknowns are $\ddot{q}_{ki}$
- Not coupled like IRK

Stage Vectors

State Vectors



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Time Marching: Diagonally Implicit Runge–Kutta (DIRK)

Stage Approximation Equations

$$\dot{\text{u}}_{ki} = \dot{\text{q}}_{k-1} + h\sum_{j=1}^{i} \alpha_{ij}\ddot{\text{u}}_{kj}$$
$$\text{u}_{ki} = \text{q}_{k-1} + h\sum_{j=1}^{i} \alpha_{ij}\dot{\text{u}}_{kj}$$

State Approximation Equations

$$\ddot{\text{q}}_k = \sum_{i=1}^{s} \beta_i \ddot{\text{u}}_{ki}$$
$$\dot{\text{q}}_k = \dot{\text{q}}_{k-1} + h\sum_{i=1}^{s} \beta_i \ddot{\text{u}}_{ki}$$
$$\text{q}_k = \text{q}_{k-1} + h\sum_{i=1}^{s} \beta_i \dot{\text{u}}_{ki}$$

Linearization of $\text{R}_{ki}(\ddot{\text{q}}_{ki}, \dot{\text{q}}_{ki}, \text{q}_{ki}, \text{t}_{ki})$

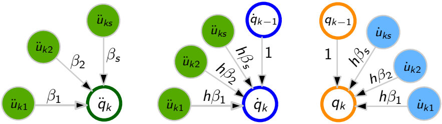
$$\left[\frac{\partial \text{R}_{ki}}{\partial \ddot{\text{u}}} + h\alpha_{ii}\frac{\partial \text{R}_{ki}}{\partial \dot{\text{u}}} + h^2\alpha_{ii}^2\frac{\partial \text{R}_{ki}}{\partial \text{u}}\right]\Delta\ddot{\text{u}}_{ki} = -\text{R}_{ki}$$

Remarks

- Linear multi-stage method
- Primary unknowns are $\ddot{\text{q}}_{ki}$
- Not coupled like IRK

Stage Vectors

State Vectors

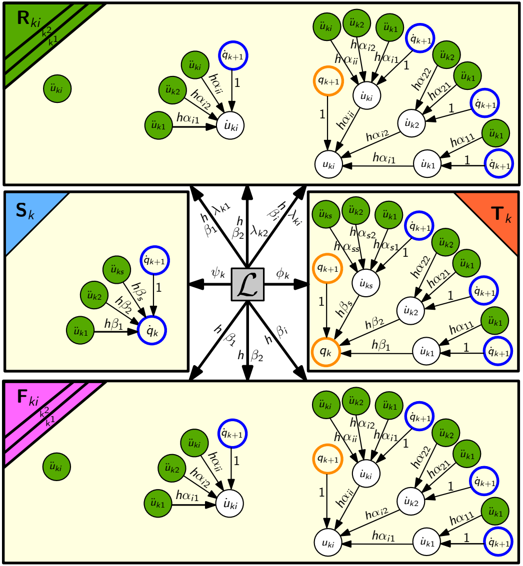


Butcher's Tableau

Stage	β_1	β_2	$\cdots$	β_s	
1	α_{11}	0	0	0	τ_1
2	α_{21}	α_{22}	0	0	τ_2
	$\vdots$	$\vdots$	$\ddots$	0	$\vdots$
s	α_{s1}	α_{s2}	$\cdots$	α_{ss}	τ_s

Discrete Adjoint: Diagonally Implicit Runge–Kutta (DIRK)

$$\mathcal{L} = \sum_{k=0}^{N} h \sum_{i=1}^{s} \beta_i F_{ki} + \sum_{k=0}^{N} h \sum_{i=1}^{s} \beta_i \lambda_{ki}^T \mathrm{R}_{ki} + \sum_{k=0}^{N} \psi_k^T \mathrm{S}_k + \sum_{k=0}^{N} \phi_k^T \mathrm{T}_k$$



Discrete Adjoint: Diagonally Implicit Runge–Kutta (DIRK)

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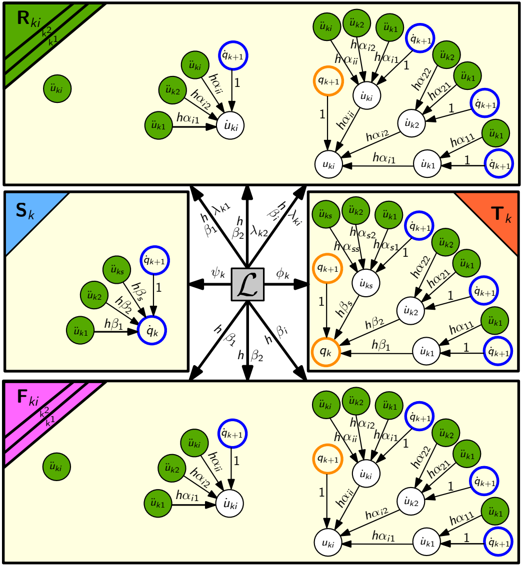
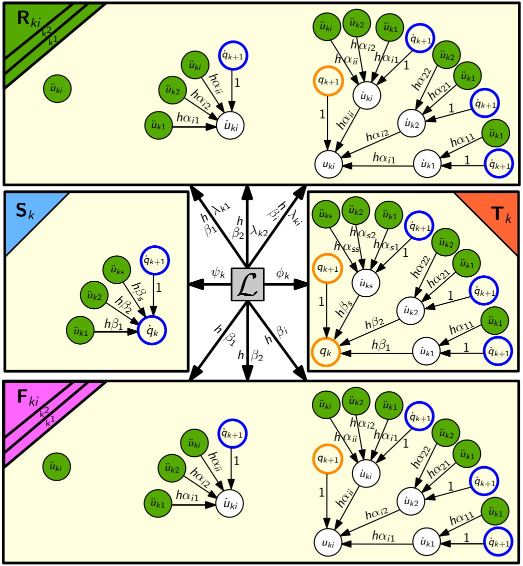


Solve for ϕ_k using $\partial\mathcal{L}/\partial \mathrm{q}_k = 0$

$$\phi_k = \phi_{k+1} + \sum_{i=1}^{s} h\beta_i \frac{\partial \mathrm{R}_{k+1,i}}{\partial \mathrm{u}_{k+1,i}}^T \lambda_{k+1,i} + \sum_{i=1}^{s} h\beta_i \frac{\partial F_{k+1,i}}{\partial \mathrm{u}_{k+1,i}}^T$$

Discrete Adjoint: Diagonally Implicit Runge–Kutta (DIRK)

$$\mathcal{L} = \sum_{k=0}^{N} h \sum_{i=1}^{s} \beta_i F_{ki} + \sum_{k=0}^{N} h \sum_{i=1}^{s} \beta_i \lambda_{ki}^T \mathrm{R}_{ki} + \sum_{k=0}^{N} \psi_k^T \mathrm{S}_k + \sum_{k=0}^{N} \phi_k^T \mathrm{T}_k$$



Solve for ϕ_k using $\partial\mathcal{L}/\partial \mathrm{q}_k = 0$

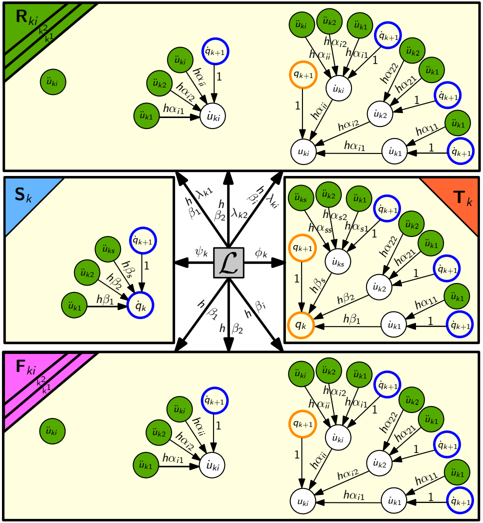
$$\phi_k = \phi_{k+1} + \sum_{i=1}^{s} h\beta_i \frac{\partial \mathrm{R}_{k+1,i}}{\partial \mathrm{u}_{k+1,i}}^T \lambda_{k+1,i} + \sum_{i=1}^{s} h\beta_i \frac{\partial F_{k+1,i}}{\partial \mathrm{u}_{k+1,i}}^T$$

Remarks

- q_k
- Number of terms: 2[T]+s[R]+s[F]
- Storage requirements: maximum number of stages

Discrete Adjoint: Diagonally Implicit Runge–Kutta (DIRK)

Lagrangian



Solve for ψ_k using $\partial \mathcal{L} / \partial \dot{\mathrm{q}}_k = 0$

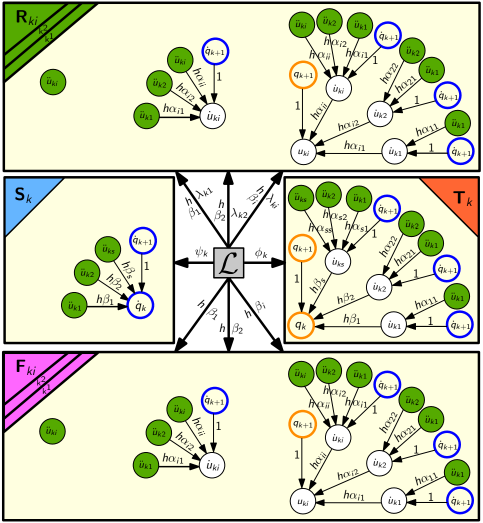
$$
\begin{aligned}
\psi_k &= \psi_{k+1} \\
&+ \sum_{i=1}^{s} h\beta_i \phi_{k+1} \\
&+ \sum_{i=1}^{s} h\beta_i \left[\frac{\partial \mathrm{R}_{k+1,i}}{\partial \dot{\mathrm{u}}_{k+1,i}} + h \sum_{j=1}^{i} \alpha_{ij} \frac{\partial \mathrm{R}_{k+1,i}}{\partial \mathrm{u}_{k+1,i}} \right]^T \lambda_{k+1,i} \\
&+ \sum_{i=1}^{s} h\beta_i \left\{ \frac{\partial F_{k+1,i}}{\partial \dot{\mathrm{u}}_{k+1,i}} + h \sum_{j=1}^{i} \alpha_{ij} \frac{\partial F_{k+1,i}}{\partial \mathrm{u}_{k+1,i}} \right\}^T
\end{aligned}
$$

Remarks

- $\dot{\mathrm{q}}_k$ is the primal variable for ψ_k
- Number of terms: 2[S]+s[T]+2s[R]+2s[F]
- **Storage requirements:**
  - s state vectors $\ddot{\mathrm{u}}_{ki}, \dot{\mathrm{u}}_{ki}, \mathrm{u}_{ki}$
  - adjoint vectors $\lambda_{ki}, \psi_k, \phi_k \in [1, s, s]$

Discrete Adjoint: Diagonally Implicit Runge–Kutta (DIRK)

Lagrangian



Solve for λ_{ki} using $\partial\mathcal{L}/\partial\ddot{u}_{ki}$

$$\beta_i \left[\frac{\partial R_{ki}}{\partial \ddot{u}_{ki}} + h\alpha_{ii}\frac{\partial R_{ki}}{\partial \dot{u}_{ki}} + h^2\alpha_{ii}^2 \frac{\partial R_{ki}}{\partial u_{ki}} \right]^T \lambda_{ki} =$$

$$- \beta_i \left\{ \frac{\partial F_{ki}}{\partial \ddot{u}_{ki}} + h^2\alpha_{ii}^2 \frac{\partial F_{ki}}{\partial \dot{u}_{ki}} + h^2\alpha_{ii}^2 \frac{\partial F_{ki}}{\partial u_{ki}} \right\}^T$$

$$- \sum_{j=i+1}^{s} \beta_j \left[h\alpha_{ji} \frac{\partial R_{kj}}{\partial \dot{u}_{kj}} + h^2 \sum_{p=i}^{j} \alpha_{jp}\alpha_{pi} \frac{\partial R_{kj}}{\partial u_{kj}} \right]^T \lambda_{kj}$$

$$- \sum_{j=i+1}^{s} \beta_j \left\{ h\alpha_{ji} \frac{\partial F_{kj}}{\partial \dot{u}_{kj}} + h^2 \sum_{p=i}^{j} \alpha_{jp}\alpha_{pi} \frac{\partial F_{kj}}{\partial u_{kj}} \right\}^T$$

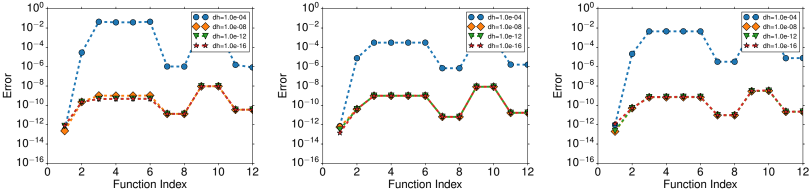
$$- \beta_i \psi_k - \sum_{j=i}^{s} \beta_j h\alpha_{ji}\phi_k$$

Remarks

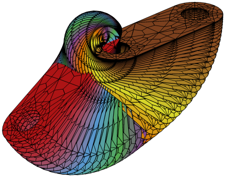
- $\ddot{u}_{ki}$ is the primal variable for λ_{ki}
- [s-i+1, 1, 2(s-i)+1, 2(s-i)+1]
- **Storage requirements:**
  - state vectors $\ddot{u}_{ki}, \dot{u}_{ki}, u_{ki} \in [s, s, s]$
  - adjoint vectors $\lambda_{ki}, \psi_k, \phi_k \in [s, 1, 1]$

Complex-Step Verification of DIRK Adjoint

DIRK Orders 2, 3 and 4

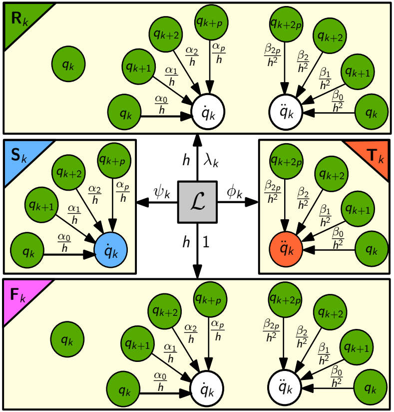


- Complex-step verification $\frac{\mathrm{d}f}{\mathrm{d}x_i} = \frac{\mathrm{Im} f(x + h e_i)}{h}$
- $dh = 10^{-4}$, 10^{-8}, 10^{-12}, and 10^{-16}
- Simulation run for 1000 time steps
- **Functionals:**
  - structural mass [1]
  - compliance [2]
  - KS von Mises failure [3, 4]
  - IE von Mises failure [5 − 12]
- Thickness design variables

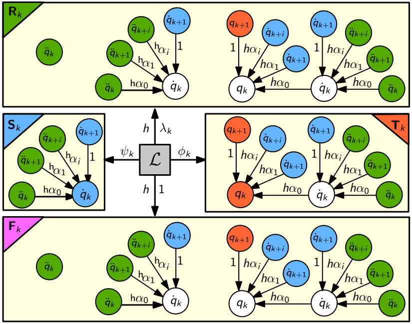


More Time Marching Methods...

Backwards Difference Formulas



Adams–Bashforth–Moulton

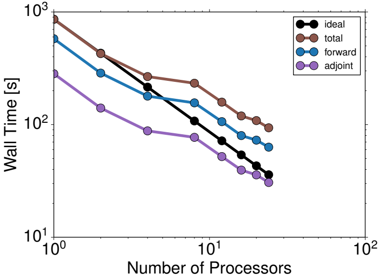


Parallel Scalability Assessment

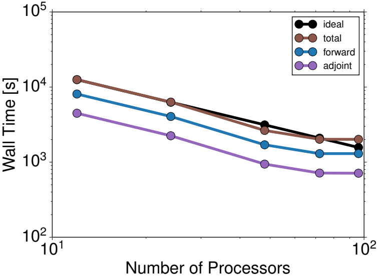
Highlevel Operations: Forward, Reverse and Total

Parallel Scalability Assessment

Highlevel Operations: Forward, Reverse and Total



192,000 DOF

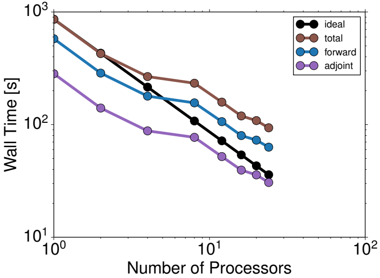


2 million DOF

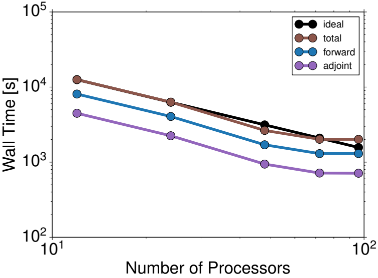
- Simulation on a *flexible plate* using *BDF* method
- Time taken for distributed operations on two problem sizes

Parallel Scalability Assessment

Highlevel Operations: Forward, Reverse and Total



192,000 DOF

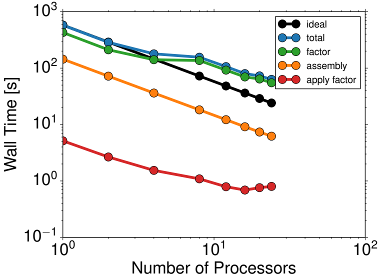


2 million DOF

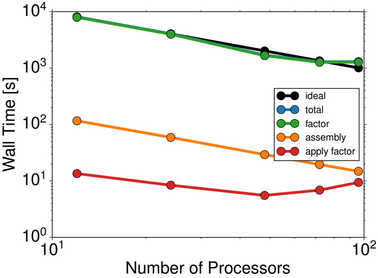
- Simulation on a *flexible plate* using *BDF* method
- Time taken for distributed operations on two problem sizes
  - **forward analysis:** nonlinear solution
  - **adjoint-derivative computations:** adjoint linear system, total-derivative computations
  - **Total** simulation time
  - **Ideal** expected scaling

Parallel Scalability Assessment

Forward Mode Operations



192,000 DOF

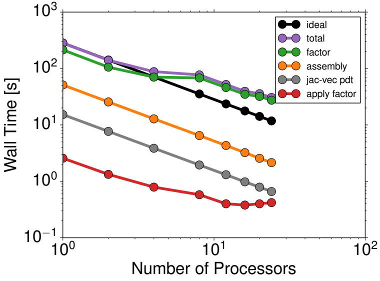


2 million DOF

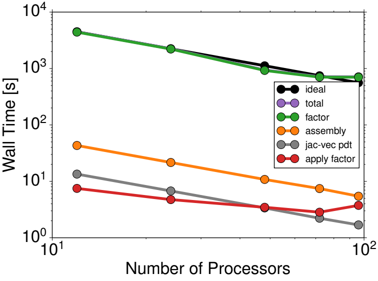
- **Assembly operations** for assembling the matrices and residuals
- **Factorization** of the linearized system at each Newton iteration
- **Applying the factorization** to solve for Newton update
- **Total** state variable solution time
- **Ideal** expected scaling

Parallel Scalability Assessment

Reverse Mode Operations



192,000 DOF

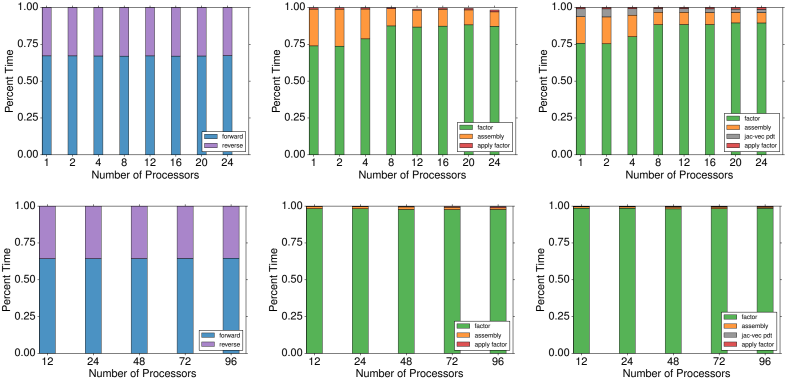


2 million DOF

- **Assembly operations** for setting up the transposed matrices and right-hand-side
- **Factorization** of the adjoint linear system
- **Applying the factorization** to solve for adjoint variables
- **Matrix-vector products** in computing the total derivative
- **Total** adjoint mode time
- **Ideal** expected scaling

Parallel Scalability Assessment

Percentage Time



Overall performance

Solution operations

Adjoint operations

- Percentage of time taken
- Matrix factorizations are the most expensive operation

Wrap Up

Descriptor & Natural Form of Governing Equations

Wrap Up

Descriptor & Natural Form of Governing Equations

Time Dependent Discrete Adjoint

- Multistep and multistage time marching: BDF, DIRK, ABM, Newmark
- Mathematical formulation, numerical verification, geometric interpretation of terms

Wrap Up

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Multibody Dynamics

- Simulations with key components for building complex and high-fidelity models

Wrap Up

Descriptor & Natural Form of Governing Equations

Time Dependent Discrete Adjoint

- Multistep and multistage time marching: BDF, DIRK, ABM, Newmark
- Mathematical formulation, numerical verification, geometric interpretation of terms

Multibody Dynamics

- Simulations with key components for building complex and high-fidelity models

Parallel Scalability

- Upto 2 million degrees of freedom with overall good scalability

Any Questions?

Time Marching: Backwards Difference Formula (BDF)

State Approximation Equations S_k and T_k

$$\dot{\mathrm{q}}_k = \frac{1}{h}\sum_{i=0}^{p}\alpha_i \mathrm{q}_{k-i} + \mathcal{O}(h^p)$$

$$\ddot{\mathrm{q}}_k = \frac{1}{h^2}\sum_{i=0}^{2p}\beta_i \mathrm{q}_{k-i} + \mathcal{O}(h^p)$$

Linearization of $\mathrm{R}_k(\ddot{\mathrm{q}}_k, \dot{\mathrm{q}}_k, \mathrm{q}_k, \mathrm{t}_k)$

$$\left[\frac{\beta_0}{h^2}\frac{\partial \mathrm{R}}{\partial \ddot{\mathrm{q}}} + \frac{\alpha_0}{h}\frac{\partial \mathrm{R}}{\partial \dot{\mathrm{q}}} + \frac{\partial \mathrm{R}}{\partial \mathrm{q}}\right]\Delta \mathrm{q}_k = -\mathrm{R}_k$$

Iterative Updates $\rightarrow \|R_k\| \leq \epsilon$

$$\mathrm{q}_k^{n+1} = \mathrm{q}_k^n + \Delta \mathrm{q}_k^n$$

$$\dot{\mathrm{q}}_k^{n+1} = \dot{\mathrm{q}}_k^n + \frac{\alpha_0}{h}\Delta \mathrm{q}_k^n$$

$$\ddot{\mathrm{q}}_k^{n+1} = \ddot{\mathrm{q}}_k^n + \frac{\beta_0}{h^2}\Delta \mathrm{q}_k^n$$

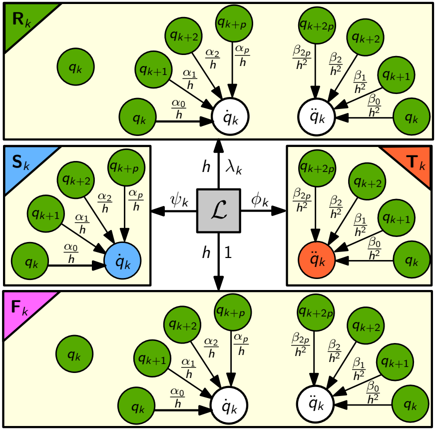
Linear Combination of State Vectors

Remarks

- Linear multistep method
- Differentiates the interpolating polynomial
- Primary unknowns are q_k

Discrete Adjoint: Backwards Difference Formula (BDF)

Linear Combination of Equations R, S, T and F

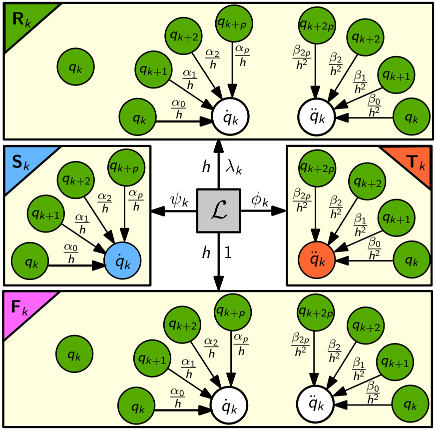


Solve for ϕ_k using $\partial \mathcal{L} / \partial \ddot{\mathrm{q}}_k = 0$

$$\frac{\partial \mathrm{T}_k}{\partial \ddot{\mathrm{q}}_k}^T \phi_k = 0 \implies \phi_k = 0$$

Discrete Adjoint: Backwards Difference Formula (BDF)

Linear Combination of Equations R, S, T and F

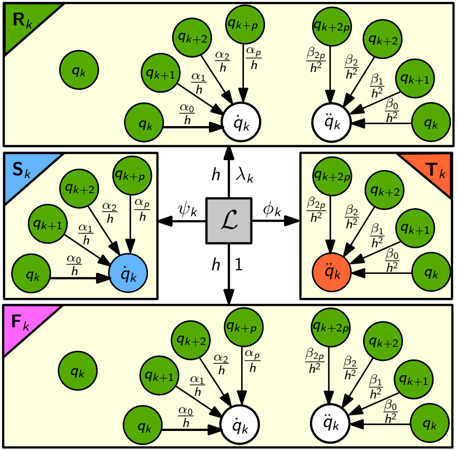


Solve for ψ_k using $\partial\mathcal{L}/\partial\dot{\mathrm{q}}_k = 0$

$$\frac{\partial \mathrm{S}_k}{\partial \dot{\mathrm{q}}_k}^T \psi_k = 0 \implies \psi_k = 0$$

Discrete Adjoint: Backwards Difference Formula (BDF)

Linear Combination of Equations



Solve for λ_k using $\partial\mathcal{L}/\partial \mathrm{q}_k = 0$

$$\left[\frac{\beta_0}{h^2}\frac{\partial \mathrm{R}_k}{\partial \ddot{\mathrm{q}}} + \frac{\alpha_0}{h}\frac{\partial \mathrm{R}_k}{\partial \dot{\mathrm{q}}} + \frac{\partial \mathrm{R}_k}{\partial \mathrm{q}}\right]^T \lambda_k =$$

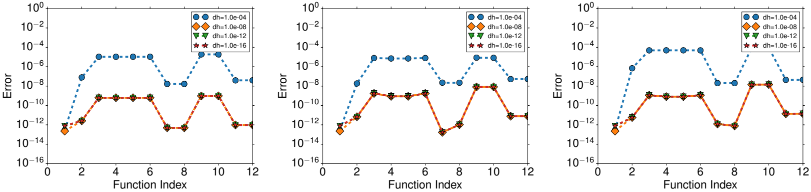
$$-\left\{\frac{\beta_0}{h^2}\frac{\partial F_k}{\partial \ddot{\mathrm{q}}} + \frac{\alpha_0}{h}\frac{\partial F_k}{\partial \dot{\mathrm{q}}} + \frac{\partial F_k}{\partial \mathrm{q}}\right\}$$

$$-\sum_{i=1}^{p}\frac{\alpha_i}{h}\frac{\partial \mathrm{R}_{k+i}}{\partial \dot{\mathrm{q}}_{k+i}}^T\lambda_{k+i} - \sum_{i=1}^{2p}\frac{\beta_i}{h^2}\frac{\partial \mathrm{R}_{k+i}}{\partial \ddot{\mathrm{q}}_{k+i}}^T\lambda_{k+i}$$

$$-\sum_{i=1}^{p}\frac{\alpha_i}{h}\frac{\partial F_{k+i}}{\partial \dot{\mathrm{q}}_{k+i}} - \sum_{i=1}^{2p}\frac{\beta_i}{h^2}\frac{\partial F_{k+i}}{\partial \ddot{\mathrm{q}}_{k+i}}$$

Complex-Step Verification of BDF Adjoint

Backwards Difference Formula: Orders 1, 2 and 3



Remarks

- Perturbation step sizes 10^{-4}, 10^{-8}, 10^{-12}, and 10^{-16}
- 1000 time steps
- **Functionals:**
  - structural mass [1]
  - compliance [2]
  - the KS aggregate of the von Mises failure criterion [3, 4]
  - the induced exponential aggregate of the von Mises failure criterion [5 − 12]
- Thickness design variables

Time Marching: Adams Bashforth Moulton (ABM)

State Approximation Equations S_k and T_k

$$\dot{q}_k = \dot{q}_{k-1} + \sum_{i=0}^{p-1} h\alpha_i \ddot{q}_{k-i} + \mathcal{O}(h^p)$$

$$q_k = q_{k-1} + \sum_{i=0}^{p-1} h\alpha_i \dot{q}_{k-i} + \mathcal{O}(h^p)$$

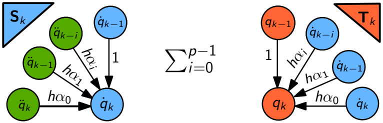
Linearization of $R_k(\ddot{q}_k, \dot{q}_k, q_k, t_k)$

$$\left[\frac{\partial R_k}{\partial \ddot{q}} + h\alpha_0 \frac{\partial R_k}{\partial \dot{q}} + h^2\alpha_0^2 \frac{\partial R_k}{\partial q}\right] \Delta\ddot{q}_k = -R_k$$

Iterative Updates $\rightarrow \|R_k\| \leq \epsilon$

$$\ddot{q}_k^{n+1} = \ddot{q}_k^n + \Delta\ddot{q}_k^n$$
$$\dot{q}_k^{n+1} = \dot{q}_k^n + h\alpha_0 \Delta\ddot{q}_k^n$$
$$q_k^{n+1} = q_k^n + h^2\alpha_0^2 \Delta\ddot{q}_k^n$$

Linear Combination of State Vectors



Adams–Moulton Coefficients α_i

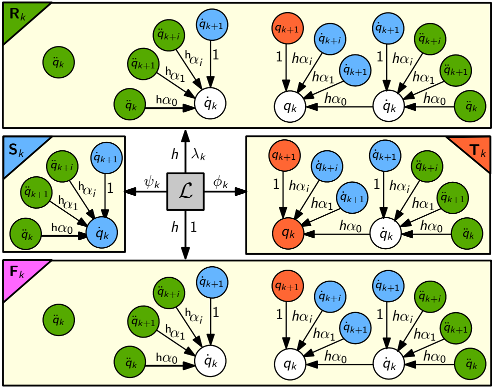
$p\backslash i$	0	1	2
1	1		
2	1/2	1/2	
3	5/12	8/12	-1/12

Remarks

- Linear multistep method
- Integrates the interpolating polynomial
- Primary unknowns are $\ddot{q}_k$

Discrete Adjoint: Adams–Bashforth–Moulton (ABM)

Linear Combination of Equations R, S, T and F

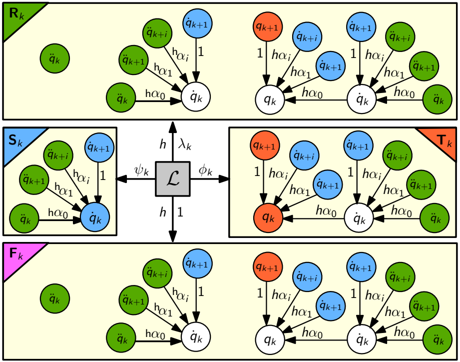


Solve for ϕ_k using $\partial \mathcal{L}/\partial \mathrm{q}_k = 0$

$$\phi_k = \phi_{k+1} + h \left[\frac{\partial \mathrm{R}_{k+1}}{\partial \mathrm{q}_{k+1}} \right]^T \lambda_{k+1} + h \left\{ \frac{\partial F_{k+1}}{\partial \mathrm{q}_{k+1}} \right\}^T$$

Discrete Adjoint: Adams–Bashforth–Moulton (ABM)

Linear Combination of Equations R, S, T and F



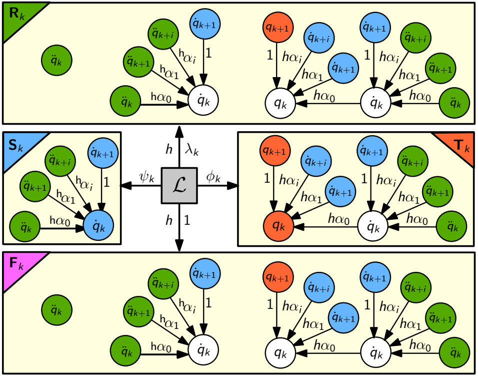
Solve for ψ_k using $\partial\mathcal{L}/\partial\dot{\mathsf{q}}_k = 0$

$$\psi_k = \psi_{k+1} + h\alpha_0\phi_{k+1} + h\left[\frac{\partial \mathsf{R}_{k+1}}{\partial \dot{\mathsf{q}}_{k+1}} + h\alpha_0 \frac{\partial \mathsf{R}_{k+1}}{\partial \mathsf{q}_{k+1}}\right]^T \lambda_{k+1} + h\left\{\frac{\partial F_{k+1}}{\partial \dot{\mathsf{q}}_{k+1}} + h\alpha_0 \frac{\partial F_{k+1}}{\partial \mathsf{q}_{k+1}}\right\}^T$$

$$+ h\sum_{i=1}^{p-1} \alpha_i \phi_{k+i} + h\sum_{i=1}^{p-1}\left[h\alpha_i \frac{\partial \mathsf{R}_{k+i}}{\partial \mathsf{q}_{k+i}}\right]^T \lambda_{k+i} + h\sum_{i=1}^{p-1}\left\{h\alpha_i \frac{\partial F_{k+i}}{\partial \mathsf{q}_{k+i}}\right\}^T$$

Discrete Adjoint: Adams–Bashforth–Moulton (ABM)

Linear Combination of Equations



Solve for λ_k using $\partial \mathcal{L}/\partial \ddot{\mathrm{q}}_k = 0$

$$\left[\frac{\partial \mathrm{R}_k}{\partial \ddot{\mathrm{q}}_k} + h\alpha_0 \frac{\partial \mathrm{R}_k}{\partial \dot{\mathrm{q}}_k} + h^2\alpha_0^2 \frac{\partial \mathrm{R}_k}{\partial \mathrm{q}_k}\right]^T \lambda_k =$$

$$- \left\{\frac{\partial F_k}{\partial \ddot{\mathrm{q}}_k} + h\alpha_0 \frac{\partial F_k}{\partial \dot{\mathrm{q}}_k} + h^2\alpha_0^2 \frac{\partial F_k}{\partial \mathrm{q}_k}\right\}^T$$

$$- \frac{1}{h}\left\{h\alpha_0\psi_k + h^2\alpha_0^2\phi_k\right\}$$

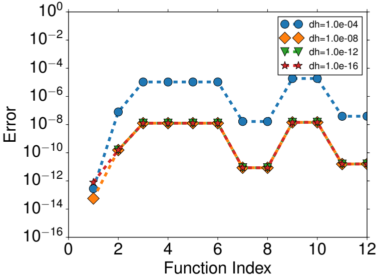
$$- \sum_{i=1}^{p-1}\left[h\alpha_i \frac{\partial \mathrm{R}_{k+i}}{\partial \dot{\mathrm{q}}_{k+i}} + h\alpha_0 h\alpha_i \frac{\partial \mathrm{R}_{k+i}}{\partial \mathrm{q}_{k+i}}\right]^T \lambda_{k+i}$$

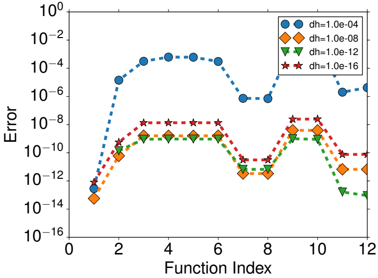
$$- \sum_{i=1}^{p-1}\left\{h\alpha_i \frac{\partial F_{k+i}}{\partial \dot{\mathrm{q}}_{k+i}} + h\alpha_0 h\alpha_i \frac{\partial F_{k+i}}{\partial \mathrm{q}_{k+i}}\right\}^T$$

$$- \frac{1}{h}\sum_{i=1}^{p-1}\left\{h\alpha_i\psi_{k+i} + h\alpha_0 h\alpha_i\phi_{k+i}\right\}$$

Complex-Step Verification of ABM Adjoint

ABM Orders 1 and 2





Remarks

- Perturbation step sizes 10^{-4}, 10^{-8}, 10^{-12}, and 10^{-16}
- 1000 time steps
- **Functionals:**
  - structural mass [1]
  - compliance [2]
  - the KS aggregate of the von Mises failure criterion [3, 4]
  - the induced exponential aggregate of the von Mises failure criterion [5 − 12]
- Thickness design variables