Adjoint Based Design Optimization of Systems With Time Dependent Physics and Probabilistically Modeled Uncertainties

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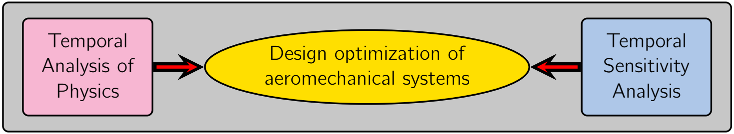
Summary of the Thesis – Main Contributions

1. Framework for design optimization of time dependent mechanical systems
   - enhanced existing implicit time marching methods
   - formulated time dependent adjoint for sensitivity analysis
   - demonstrated adjoint based optimization using **rotorcraft**

2. Framework for design optimization under uncertainties
   - quantified uncertainties using the stochastic Galerkin method
   - devised reuse of reusing deterministic finite element and adjoint
   - demonstrated optimization under uncertainty using **Canadarm**



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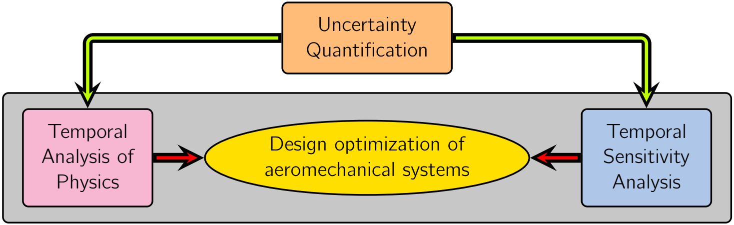


Section 2

Temporal Physics and Adjoint Based Optimization

Motivation : Consideration of time domain in structural design

Aircraft

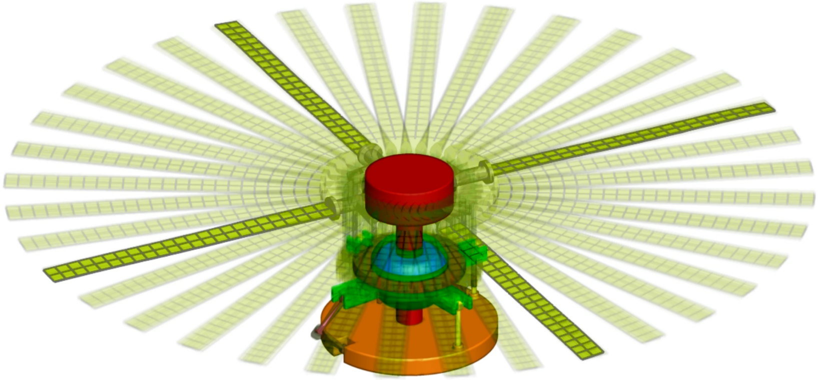
Rotorcraft

Wind farm

Tacomac bridge

Time dependent issues like flutter, large vibrations, whirling of shaft

Time domain simulation of collective blade pitch of rotorcraft system



flexible multibody dynamics of helicopter hub

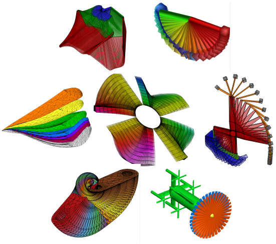
Key items for time domain simulation of structural systems

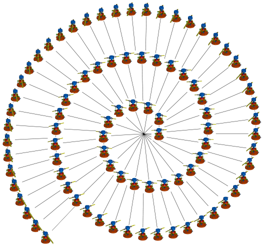
Computational Resources, Governing Equations (DAEs), Numerical Methods

1. Need high performance computing to perform high-fidelity time-domain analysis
2. Governing Euler–Lagrange equations: the states $u = (w, \ \mu)$, the DOFs w, constraints $g(w)$, multipliers μ, constraint Jacobian A, time t, design variables ξ

$$R(t, \xi, u(t,\xi), \dot{u}(t,\xi), \ddot{u}(t,\xi)) \triangleq \begin{bmatrix} \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{w}}\right) - \frac{\partial \mathcal{L}}{\partial w} - A^T\mu \\ g(w) \end{bmatrix} = 0$$

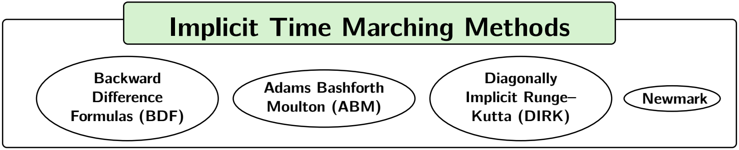
3. Implicit time marching methods due to the presence of constraints $g(w)$





Contribution : Time Marching in Natural Second Form (A Principle)

✈ We enhanced the **existing implicit time marching methods** to apply directly on second order form of governing equations



Advantages:

1. we can avoid algebraic conversion to first order form

$$\underbrace{R(t,\xi,u(t,\xi),\dot{u}(t,\xi),\ddot{u}(t,\xi))}_{natural\ \ second\ \ order} \xrightarrow[substitutions]{algebraic} \underbrace{S(t,\xi,v(t,\xi),\dot{v}(t,\xi))}_{first\ \ order}$$

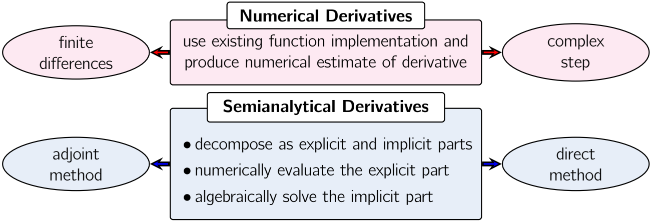
2. aligns with the “principle” of Newmark Family of integrators
3. makes the adjoint equations simpler
4. all time marching methods and adjoints can be implemented within a common framework

Subsection 2

Efficient Gradient Evaluation Methods

Motivation : Devise Efficient Gradient Evaluation Methods

Need gradients of metrics of interest with respect to design variables



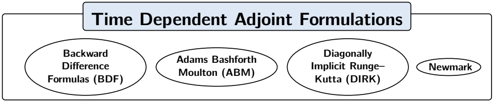
	adjoint method	direct method
solution variable	$\lambda_j = \frac{\partial F_j}{\partial u}\left[\frac{\partial R}{\partial u}\right]^{-1}$	$\phi_i = \left[\frac{\partial R}{\partial u}\right]^{-1} \frac{\partial R}{\partial \xi_i}$
accuracy	machine precision	machine precision
efficiency	more number of design variables $\xi = [\xi_1, \xi_2, \ldots]$	more number of functions $[F(\xi), G(\xi), H(\xi)]$

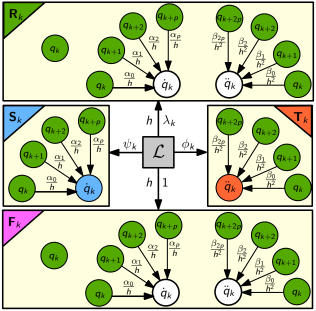
adjoint in conjunction with constraint aggregation in space and time domains

Contribution : Time Dependent Adjoint Sensitivity Formulations

✈ Developed adjoint equations for implicit time marching methods based on abstractions of

- governing equations $R(t, \xi, q, \dot{q}, \ddot{q})$
- metrics of interest $F(t, \xi, q, \dot{q}, \ddot{q})$





Time Dependent Lagrangian – BDF

✈ Verified the adjoint equations via complex-step method

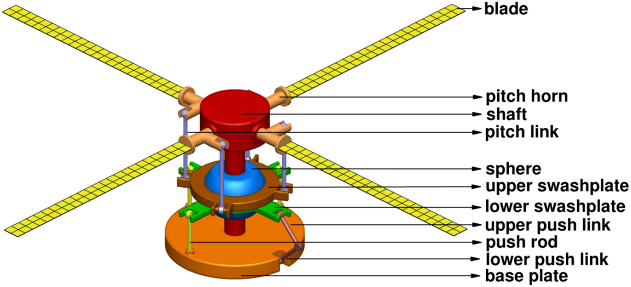
K. Boopathy and G. J. Kennedy, "Adjoint-based derivative evaluation methods for flexible multibody systems with rotorcraft applications", 55th AIAA Aerospace Sciences Meeting, Grapevine, Texas. AIAA Paper 2017-1671.

Subsection 3

Structural Optimization of Rotorcraft

- using time dependent analysis of rotorcraft
- using time dependent adjoint sensitivities

Model Problem: Rotorcraft Hub Assembly

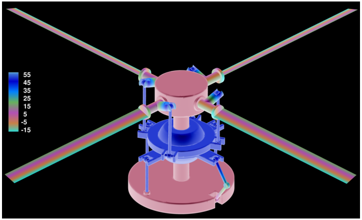


Sinusoidally modulated control amplitudes

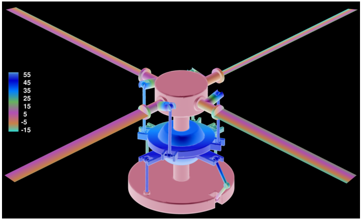
Blade Pitch Control	Motion	Push rod 1	Push rod 2	Push rod 3
collective	vertical	$0.050\sin(\Omega_t t)$	$0.050\sin(\Omega_t t)$	$0.050\sin(\Omega_t t)$
longitudinal cyclic	forward/pitch	$0.025\sin(\Omega_t t)$	$0.025\sin(\Omega_t t)$	$0.050\sin(\Omega_t t)$
lateral cyclic	sideways/roll	$0.025\sin(\Omega_t t)$	$0.050\sin(\Omega_t t)$	$0.025\sin(\Omega_t t)$

$$\Omega_{shaft} = 109.12 \; rad/s \; \ldots \; \Omega_t = 27.28 \; rad/s \; \ldots \; 28,640 \text{ DOF}$$

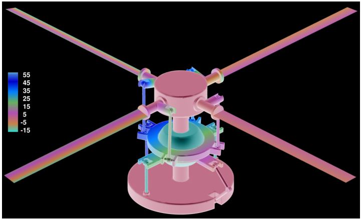
Vertical displacement of bodies



(a) collective



(b) longitudinal cyclic



(c) lateral cyclic

Deterministic Optimization – Stress Constrained Mass Minimization

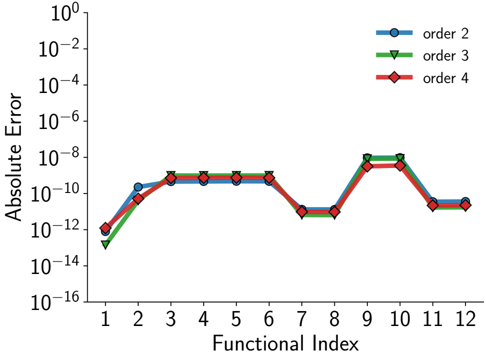
ξ_1	ξ_2	ξ_3	$\cdot$	$\cdot$	$\cdot$	$\cdot$	ξ_{46}	ξ_{47}	ξ_{48}

$$
\begin{aligned}
\underset{\xi}{\text{minimize}} \quad & \text{mass} = m(\xi), \\
\text{subject to} \quad & \bar{g}_1^k(\xi) = \xi_k - \xi_{k+1} \leq 1\,\text{mm}, \quad \forall k = 1, \ldots 47, \\
& \bar{g}_2^k(\xi) = \xi_{k+1} - \xi_k \leq 1\,\text{mm}, \quad \forall k = 1, \ldots 47, \\
& \bar{g}_3^k(\xi) = 1 - 4.0\frac{\sigma_{vm}^k}{\sigma_{max}^k} \geq 0, \quad \forall k = 1, \ldots 3, \\
\text{bounds} \quad & 10\,\text{mm} \leq \xi \leq 20\,\text{mm}.
\end{aligned}
$$

Blade Pitch Control	**Motion**	**Push rod 1**	**Push rod 2**	**Push rod 3**
g_3^1 – collective	vertical	$0.050\sin(\Omega_t t)$	$0.050\sin(\Omega_t t)$	$0.050\sin(\Omega_t t)$
g_3^2 – longitudinal cyclic	forward/pitch	$0.025\sin(\Omega_t t)$	$0.025\sin(\Omega_t t)$	$0.050\sin(\Omega_t t)$
g_3^3 – lateral cyclic	sideways/roll	$0.025\sin(\Omega_t t)$	$0.050\sin(\Omega_t t)$	$0.025\sin(\Omega_t t)$

Adjoint derivative verification using complex step method

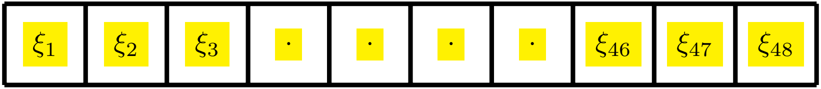
Functional	Complex-step	Adjoint
1. Structural Mass	250.0000000000000	249.9999999999999
2. Compliance	-0.008903780405108	-0.00890378045**7068**
3. Failure	-2.510549172940552	-2.51054917**3663148**

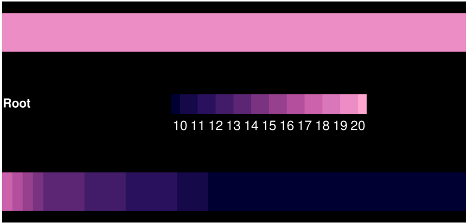


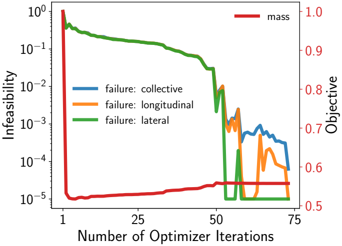
$$\frac{dF(\xi)}{d\xi} = \frac{F(\xi + \Delta\xi i)}{\Delta\xi}$$

$$\frac{dF(\xi)}{d\xi} = \frac{\partial F(\xi)}{\partial \xi} - \underbrace{\frac{\partial F}{\partial u}\left[\frac{\partial R}{\partial u}\right]^{-1}}_{adjoint\ \lambda} \frac{\partial R}{\partial \xi}$$

Optimization Results



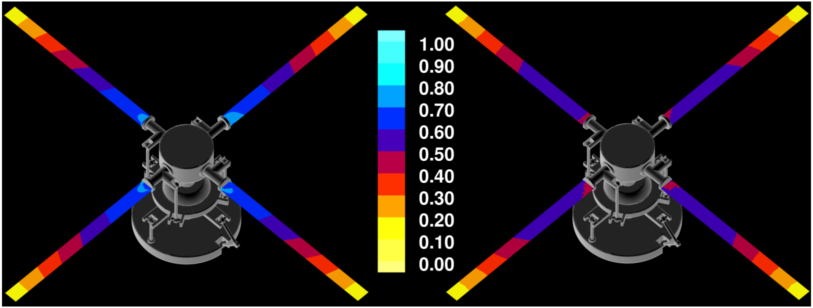




- initial uniform blade thickness of 2cm
- parallel analysis and sensitivity analysis using 5 processors for each flight mode (20 minutes per load case for analysis and adjoint)
- optimizer required 222 function and 88 gradient evaluations

Optimization Results

Contour plot of failure for lateral cyclic blade pitch



initial (left) and optimized designs (right)

✈ Optimized design has reduced stresses at the root of the blade

Summary : Adjoint Based Deterministic Optimization

❶ Implicit time marching methods for natural form of governing equations

Implicit Time Marching Methods

- Backward Difference Formulas (BDF)
- Adams Bashforth Moulton (ABM)
- Diagonally Implicit Runge–Kutta (DIRK)
- Newmark

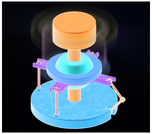
❷ Developed adjoint equations for implicit time marching methods

Time Dependent Adjoint Formulations

- Backward Difference Formulas (BDF)
- Adams Bashforth Moulton (ABM)
- Diagonally Implicit Runge–Kutta (DIRK)
- Newmark

❸ Demonstration using rotorcraft structural optimization

K. Boopathy and G. J. Kennedy, "Parallel Finite Element Framework for Rotorcraft Multibody Dynamics and Adjoint Sensitivities", AIAA Journal, Vol. 57, No. 8, pp. 3159–3172, 2019, DOI: 10.2514/1.J056585.



Section 3

Optimization Under Uncertainty

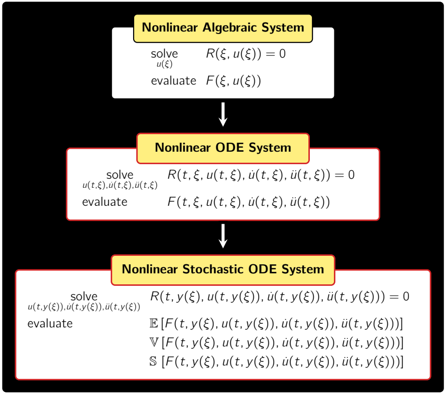
A product should be designed in such a way that makes its **performance insensitive to variation** *in variables beyond the control of the designer* — *Genichi Taguchi*

Uncertainties affecting Physics-Based Design

- The physics-based design of aerospace systems involves **solving differential equations** to obtain metrics of interest that guide the design process

- Sometimes inputs (coefficients, forcing, initial/boundary conditions) are difficult to be characterized as a deterministic value

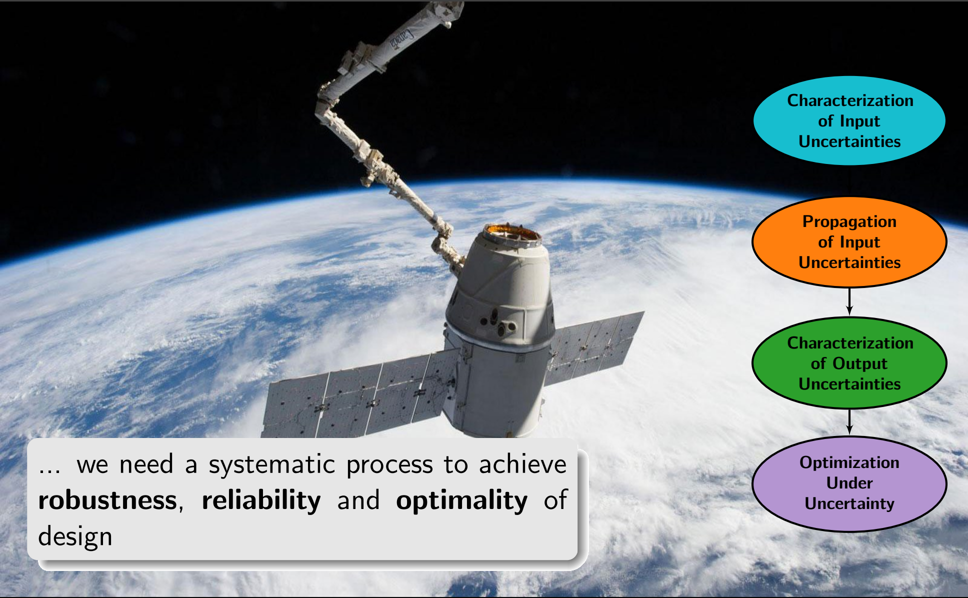
- The uncertainties in input parameters have a direct impact on the **output metrics of interest** which guide the system design process



Canadarm Example – A space system with uncertainty in operating conditions

- maximum payload mass $266,000$ kg for analysis by intuition/expert opinion
- distribution type: $\mathcal{U}(a = 0, b = 266,000)$, $\mathcal{N}(\mu = 100,000, \sigma = 50,000)$

Steps in Optimization Under Uncertainty



... we need a systematic process to achieve **robustness**, **reliability** and **optimality** of design

Characterization of Input Uncertainties

Propagation of Input Uncertainties

↓

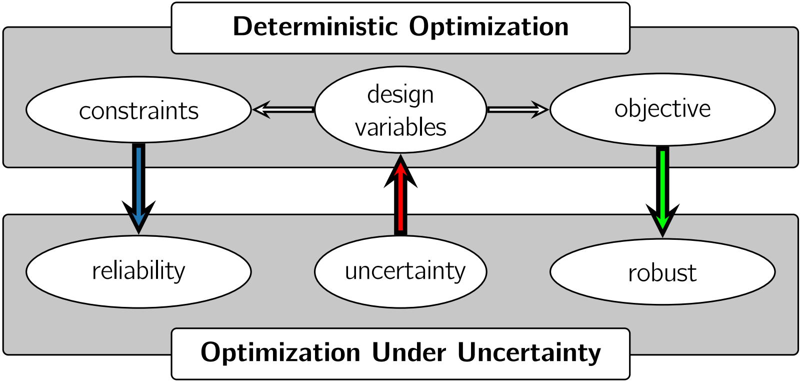
Characterization of Output Uncertainties

↓

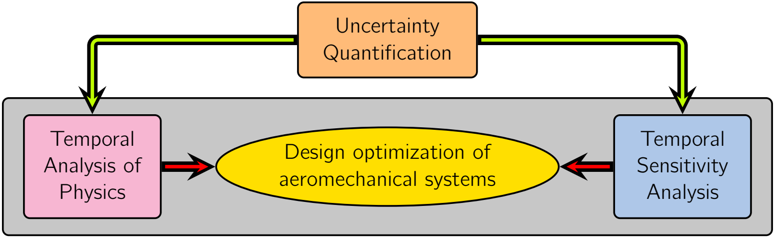
Optimization Under Uncertainty

Deterministic Optimization Problem

$$\begin{aligned} \underset{\xi}{\text{minimize}} \quad & F(\xi) \\ \text{subject to} \quad & G(\xi) \leq 0 \end{aligned}$$



Optimization Under Uncertainty Problem



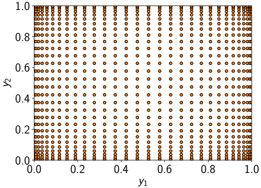
$$\underset{\xi}{\text{minimize}} \quad (1-\alpha)\cdot \mathbb{E}\left[F(y(\xi))\right] + \alpha \cdot \mathbb{S}\left[F(y(\xi))\right]$$

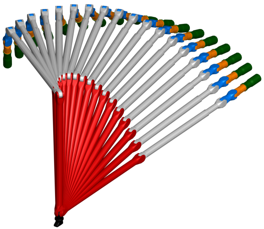
$$\text{subject to} \quad \mathbb{E}\left[G(y(\xi))\right] + \beta \cdot \mathbb{S}\left[G(y(\xi))\right] \leq 0$$

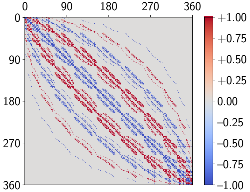
- objective and constraints are a linear combination of expectation and standard deviation; α – objective robustness, β – constraint reliability

Sampling and projection based uncertainty propagation

nonintrusive ← **Propagation of Input Uncertainties** → intrusive







quarature samples

projected Jacobian

nonintrusive		intrusive
repeated solutions smaller system	principle	one solution of bigger nonlinear system
no modifications (black box)	code	requires modifications

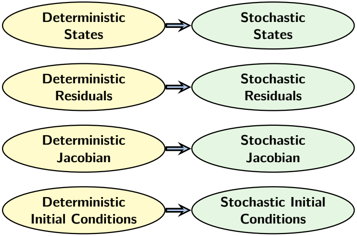
how to reuse deterministic FEA and adjoint code for projection?

Subsection 5

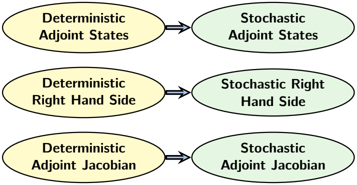
Semi-Intrusive Stochastic Galerkin Projection

Extending Deterministic Analysis to Stochastic Analysis

① Extending Time Domain Physical Analysis



② Extending Adjoint Sensitivity Analysis

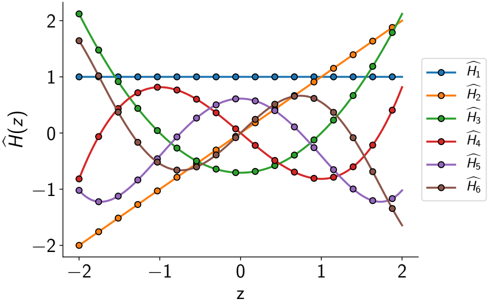


Probabilistic Space and Inner Product

- probabilistic function space is approximated with N basis entries

$$\mathcal{Y} \approx \text{span}\{\widehat{\psi}_1(y), \widehat{\psi}_2(y), \ldots, \widehat{\psi}_N(y)\}$$

- polynomial type based on the probability distribution type
  - Hermite, Legendre, Laguerre
  - Normal, Uniform, Exponential



- orthogonality + normality
- tensor product for multi-variate basis

Formation of Stochastic Physical States

The stochastic state vector is

$$u(t, y) \approx \sum_{i=1}^{N} U_i(t)\widehat{\psi}_i(y)$$

Core principles at play:

1. principle of variable separation – time and probabilistic domains
2. principle of superposition .... summation

- the state vector coefficients: $U(t) = [U_1(t), U_2(t), \ldots, U_N(t)]$ are available as guessed values from iterative solution
- the length of stochastic state vector is N times the length of deterministic state vector
- time derivatives $\dot{u}(t, y)$ and $\ddot{u}(t, y)$ are approximated similarly

Formation of Stochastic Residual

quadrature loop

$$\mathcal{Y} \approx \text{span}\{\widehat{\psi}_1(y), \widehat{\psi}_2(y), \dots, \widehat{\psi}_N(y)\}$$

$$\mathcal{R} = \begin{bmatrix} \mathcal{R}_1 \\ \mathcal{R}_2 \\ \vdots \\ \mathcal{R}_N \end{bmatrix} \quad \mathcal{R}_i \approx \sum_{q=1}^{Q} \underbrace{\alpha_q \widehat{\psi}_i(y_q)}_{\text{scalar}} \times \underbrace{R(t, y_q, u(t, y_q), \dot{u}(t, y_q), \ddot{u}(t, y_q))}_{\text{deterministic residual for } y_q}$$

- quadrature over deterministic residual implementations
- the length of stochastic residual vector is N times the length of deterministic residual vector
- need ability to update elements with new parameter values
- residuals can be system-wide or element-wise

Formation of Stochastic Jacobian

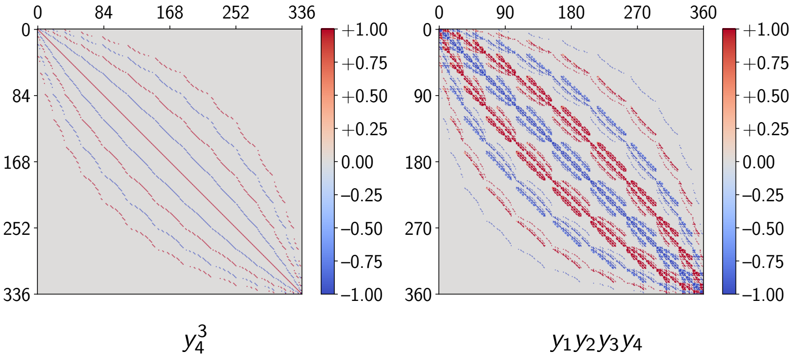
The stochastic Jacobian matrix is

$$\mathcal{J} = \begin{bmatrix} \mathcal{J}_{1,1} & \mathcal{J}_{1,2} & \cdots & \mathcal{J}_{1,N} \\ \mathcal{J}_{2\,1} & \mathcal{J}_{2,2} & \cdots & \mathcal{J}_{2,N} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{J}_{N,1} & \mathcal{J}_{N,2} & \cdots & \mathcal{J}_{N,N} \end{bmatrix}.$$

$$\mathcal{J}_{i,j} \approx \sum_{q=1}^{Q} \underbrace{\alpha_q \widehat{\psi}_i(y_q) \widehat{\psi}_j(y_q)}_{\text{scalar}} \times \underbrace{J(t, y_q, u(t, y_q), \dot{u}(t, y_q), \ddot{u}(t, y_q))}_{\text{deterministic Jacobian for } y_q}$$

- quadrature over deterministic jacobian implementations
- need ability to update element with new parameter values
- the size of stochastic Jacobian is N times the size of deterministic Jacobian
- applies to system-wide and element-wise Jacobians

Sparsity of Stochastic Jacobian Matrices



- sparsity patterns depend on the non-linearity parameter y
- can optimize the number of quadrature evaluations
- can determine the sparsity apriori

Formation of Stochastic Adjoint States

recall... stochastic physical state vector

$$U(t) = [U_1(t), U_2(t), \ldots, U_N(t)]$$

$$u(t, y) \approx \sum_{i=1}^{N} U_i(t)\widehat{\psi}_i(y)$$

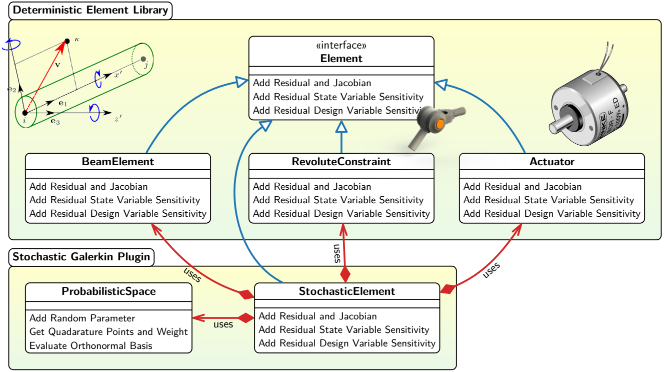
Stochastic Adjoint state vector is formed in a similar manner

$$\Lambda(t) = [\Lambda_1(t), \Lambda_2(t), \ldots, \Lambda_N(t)]$$

$$\lambda(t, y) \approx \sum_{i=1}^{N} \Lambda_i(t)\widehat{\psi}_i(y)$$

- ✔ transposed Jacobian matrix is formed similar to forward solve
- ✔ the right hand sides of the adjoint linear system are formed in a manner similar to residuals

Software Architecture for Stochastic Galerkin Method



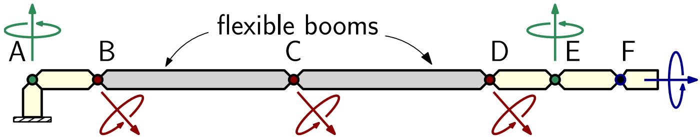
- ✔ `StochasticElement` –
  - **is an** `Element` by inheritance and also
  - **has an** *element* (deterministic) by composition
- ✔ `ProbabilisticSpace` – prob. quadrature and basis evaluations

Subsection 6

Canadarm Design Optimization Under Uncertainties

Canadarm Structural Model

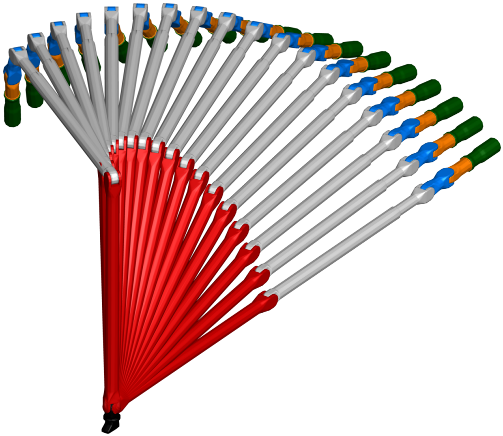
simplified model of flexible remote manipulator onboard space shuttle



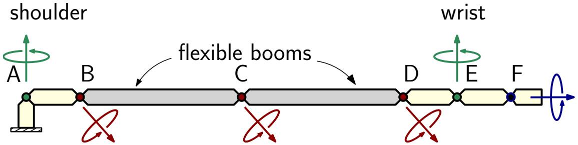
- 6 joint degrees of freedom (2 shoulder + 1 elbow + 3 wrist)
- The booms in Canadarm-I are made of graphite epoxy – we use material properties of steel
- 16 *m* long (foldable inside space shuttle) and 33 *cm* wide

Canadarm Time Lapse of Simulated Motion

Simulated motion of the Canadarm model



Optimization Problem Formulation



minimize	$\mathbb{E}[\text{mass}]$
design variable	width of bars
uncertainty	payload mass $\sim \mathcal{N}(\mu = 10^5, \sigma = 50,000)$ kg
subject to	$\mathbb{E}[\text{failure}] + \beta \cdot \mathbb{S}[\text{failure}] \leq 1$
bounds	$25cm \leq \text{width} \leq 50cm$

- Deterministic optimization with $mass = 10^5$ kg
- OUU with $\beta = 0, 1, 2, 3, 4, 5, 6$ (more constraint satisfaction)
- SGM for probabilistic moments of functions and adjoint-derivatives

The complex-step verification of adjoint derivatives for the Canadarm system

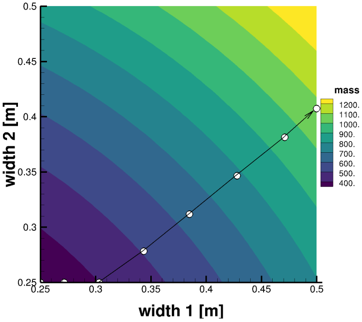
Quantity	Mass	Failure
adjoint $d\mathbb{E}[F]/d\xi$	$1.24800000000001979 \cdot 10^5$	-3.76597889920338691
complex $d\mathbb{E}[F]/d\xi$	$1.24800000000001819 \cdot 10^5$	-3.76596706242138746
relative error	$1.3 \cdot 10^{-15}$	$3.1 \cdot 10^{-6}$
adjoint $d\mathbb{V}[F]/d\xi$	N/A	$-4.46442271585651973 \cdot 10^{-1}$
complex $d\mathbb{V}[F]/d\xi$	N/A	$-4.46444953483493667 \cdot 10^{-1}$
relative error	N/A	$6.0 \cdot 10^{-6}$

- ✔ used complex-step method to verify the consistency of adjoint derivatives
- ✔ no variance derivative for mass due to the choice of random parameter

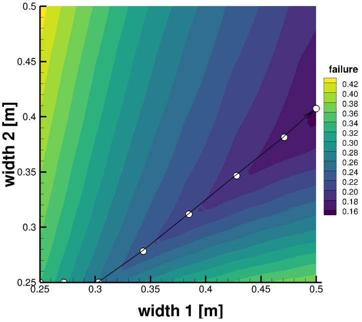
Optimization Results : Probabilistic and Deterministic

Quantity	Deterministic	$\beta = 0$	$\beta = 1$	$\beta = 2$	$\beta = 3$	$\beta = 4$	$\beta = 5$	$\beta = 6$
width 1 [m]	0.250	0.250	0.250	0.271	0.303	0.343	0.385	0.428
width 2 [m]	0.250	0.250	0.250	0.250	0.250	0.278	0.311	0.347
constraint activity %	34.1	72.9	92.6	100	100	100	100	100
$\mathbb{E}$[failure]	0.729	0.729	0.729	0.650	0.552	0.482	0.431	0.387

Recall: $\mathbb{E}[\text{failure}] + \beta \cdot \mathbb{S}[\text{failure}] \leq 1$



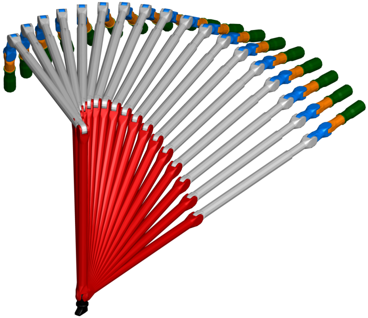
Objective



Failure

Summary : Optimization Under Uncertainty

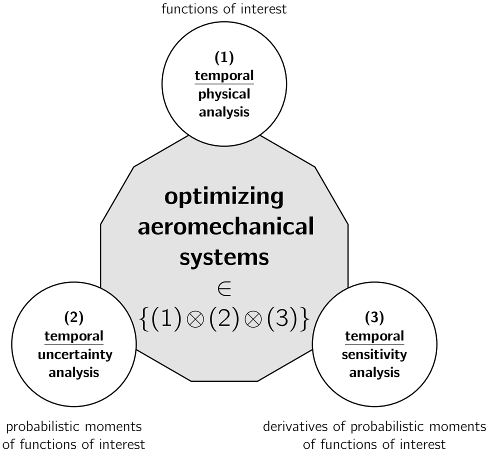
- Probabilistically modeled inputs
- Propagation of uncertainties via projection using the semi-intrusive Stochastic Galerkin method
- Reuse of deterministic forward analysis and adjoint capabilities
- Canadarm optimization under uncertain payloads



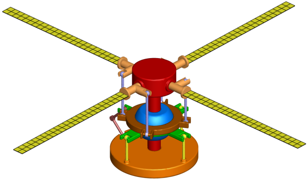
Section 4

Conclusion

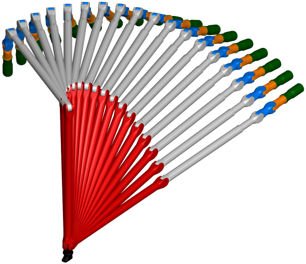
Mathematical Framework and Applications



Mathematical framework

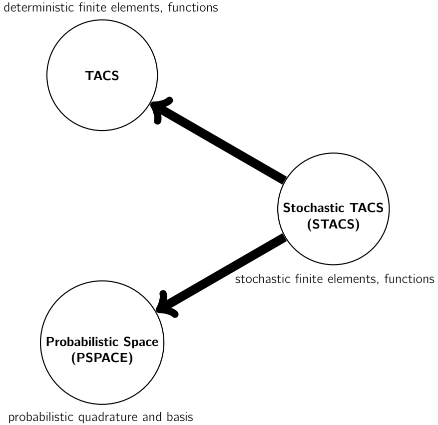


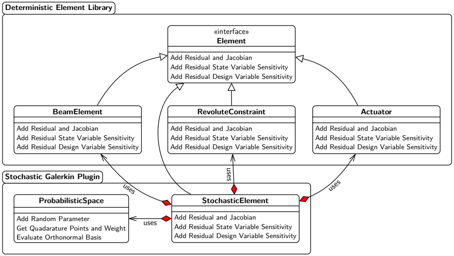
Rotorcraft design application



Canadarm design application

Computational Framework for UQ-OUU : Open Source Packages



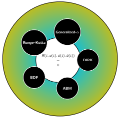


1. TACS finite element framework https://github.com/gjkennedy/tacs
2. Probabilistic Space PSPACE https://github.com/komahanb/pspace
3. Stochastic TACS framework STACS https://github.com/komahanb/stacs

Fundamental Contributions

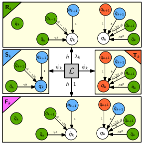
Enhanced Implicit Solution of DAEs

Implicit solution of initial value problems in natural descriptor representation (second order form)



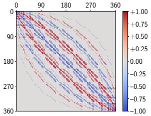
Generalized Adjoint Derivatives

Discrete adjoint sensitivity formulations for implicit BDF, ABM, DIRK and Newmark methods for abstract governing equations and functions of interest



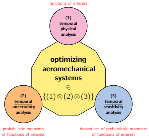
Novel Uncertainty Propagation Method

Semi-intrusive uncertainty propagation and adjoint sensitivity analysis using the stochastic Galerkin projection method



Design Under Uncertainty Framework

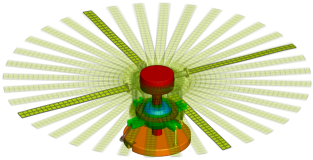
Unified framework featuring temporal analysis of physics, adjoint sensitivities and uncertainty quantification



Applied Contributions

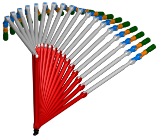
Rotorcraft Design Application

- Rotorcraft hub model with full control chain included in analysis



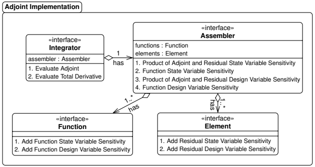
Canadarm Design Application

- Flexible remote manipulator with uncertain payload masses

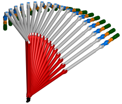


Architecture and Implementation

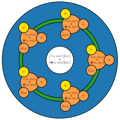
- Modular extensible time dependent adjoint framework
- Stochastic implementations from deterministic implementations



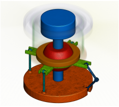
K. Boopathy and G. J. Kennedy, "Semi-Intrusive Stochastic Galerkin Method for Reusing Deterministic Finite Element and Adjoint Derivative Capabilities", AIAA Journal. In Progress.



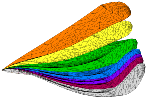
K. Boopathy and G. J. Kennedy, "Semi-Intrusive Uncertainty Propagation and Adjoint Sensitivity Analysis Using the Stochastic Galerkin Method", SciTech 2020, Orlando, Florida. AIAA Paper 2020-1146.



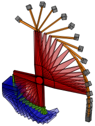
K. Boopathy and G. J. Kennedy, "Parallel Finite Element Framework for Rotorcraft Multibody Dynamics and Adjoint Sensitivities", AIAA Journal, Vol. 57, No. 8, pp. 3159–3172, 2019.



K. Boopathy and G. J. Kennedy, "Adjoint-based derivative evaluation methods for flexible multibody systems with rotorcraft applications", AIAA SciTech 2017, Grapevine, Texas. AIAA Paper 2017-1671.



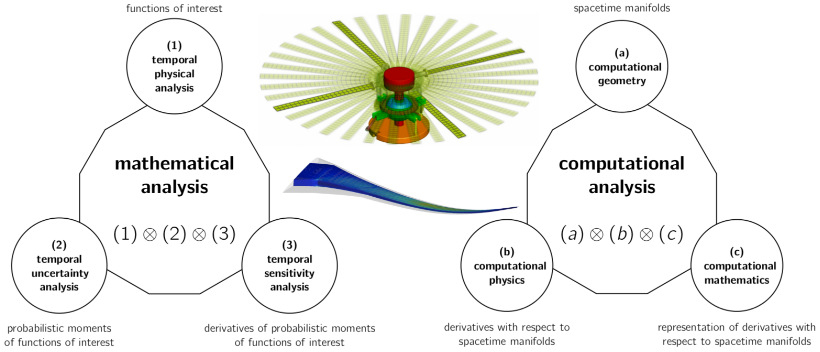
G. J. Kennedy and K. Boopathy, "A Scalable Adjoint Method for Coupled Flexible Multibody Dynamics", 57th AIAA/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference, San Diego, California, Jan 2016. AIAA Paper 2016-1907.



Thank You and Questions?

Acknowledgments

- National Institute of Aerospace
- NASA Langley Research Center



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