A Convex Optimization Framework for Generating Finite Difference Schemes for Arbitrary PDEs (Discovered or Derived)

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Research Summary

Fundamental Research

Uncertainty Propagation
Nonlinear & non Gaussian

State Estimation
Sparse & multi-rate sensor fusion

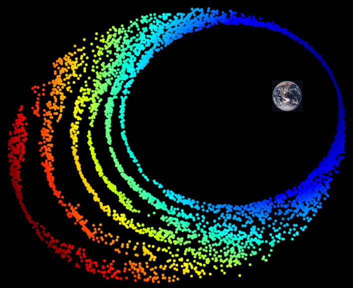
Integrated Design Optimization
Sensing & control architecture

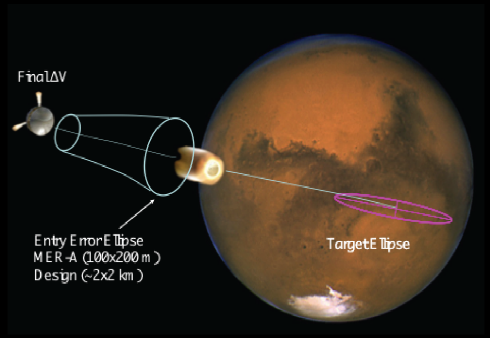
Control with Uncertainty
Nonlinear robust control

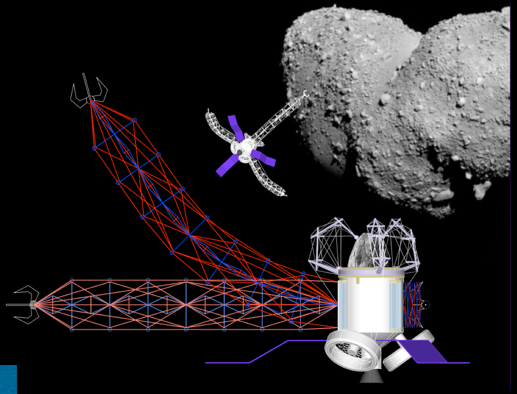
Numerical Algorithms
High performance computing

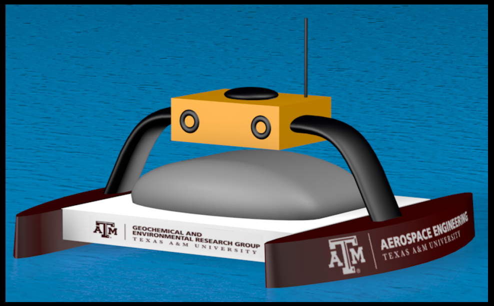
Uncertainty Quantification & Mitigation

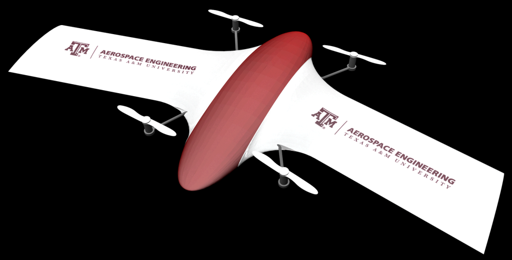
Applications







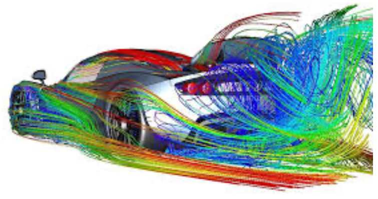
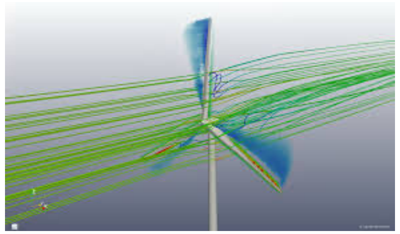
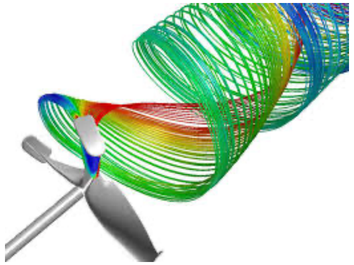


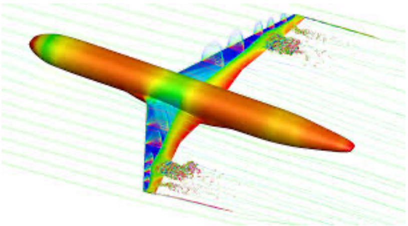
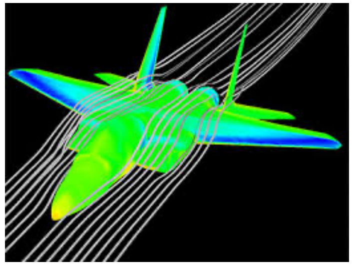


Scientific Machine Learning

Focus on solving PDEs

- Model based design
  - Speed up
  - Less expensive
- Digital twins
  - Predict failures
  - Refine design
- Uncertainty Propagation
  - Nonlinear estimation

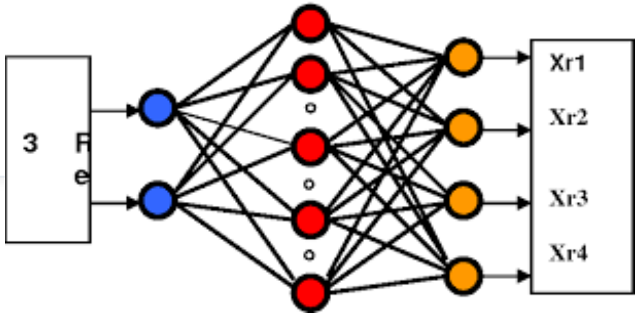




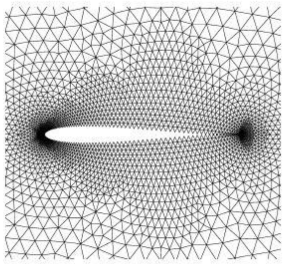
Images: Google images

Scientific Machine Learning

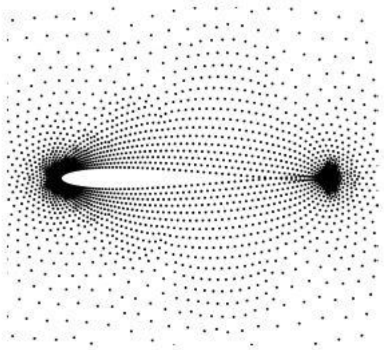
Focus on solving PDEs



- **Mesh**
  - Finite-difference
  - Finite-element/volume



- **Machine learning**
  - Address the representation problem
  - Automate/learn basis functions (NN)
  - Adapt to solution, etc.



- **Meshfree**
  - RBF
  - Maximum-entropy basis functions

- **This talk**
  - Automate generation of finite-difference schemes
  - PDE specific FD-scheme
  - Optimize for boundary condition, geometry, and PDE.
  - Needs pre-specified mesh

Images: Google images

Discretization of PDEs

Current Approach

- Choose temporal and spatial discretization (mostly adhoc)
- Discretization is PDE independent!
- Work with dt, dx to get acceptable errors and stability
- Many moving parts!

This talk: Present a Unified Framework!

Automated Discretization of PDEs

A Unified Framework – Convex optimization formulation

Mesh

i

General PDE

$$\mathbb{D}_t f = \mathbb{D}_x f$$

Discretize Operator

$$f_i^{(d)} = \frac{1}{(\Delta x)^d} \sum_{m=-\eta}^{\eta} a_m f_{i+m}$$

$$\boxed{\frac{\partial f}{\partial t} = \sum_{d=1}^{D} \beta_d \frac{\partial^d f}{\partial^d x}.}$$

Discrete Time Dynamical System

$$\mathbf{F}^{k+1} = \left(\mathbf{I} + \Delta t \sum_{d=1}^{D} \frac{\beta_d}{(\Delta x)^d} \mathbf{A}_d\right) \mathbf{F}^k$$

Determine coefficients by optimizing performance with stability constraints

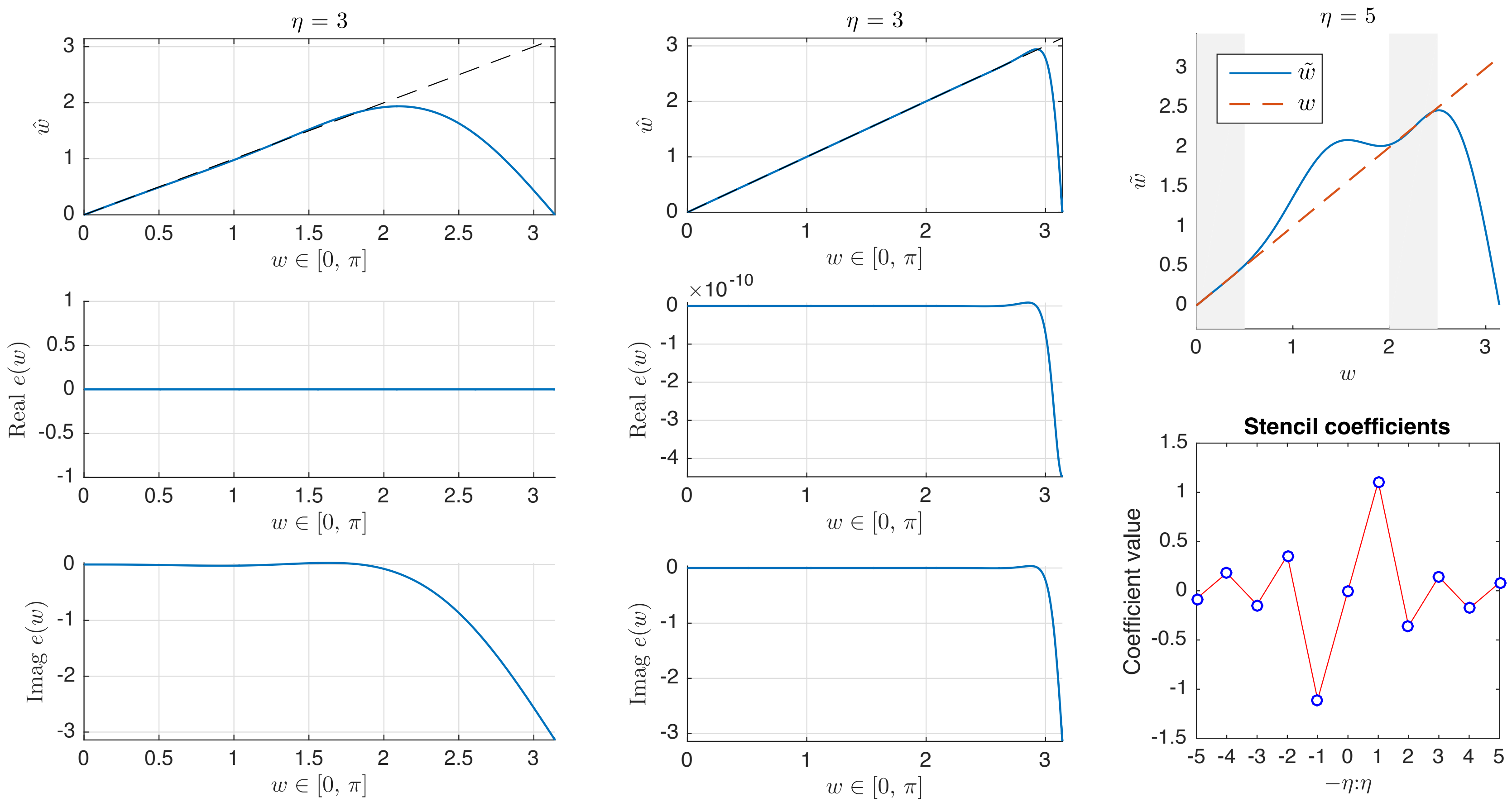
$$\min_{\mathbf{a} \in \mathbb{R}^{2\eta+1}} \|e(w)\|^2_{\mathcal{L}_2}$$

$$\mathbf{A}_d \mathbf{X}_d = \mathbf{Y}_d$$ Order

$$\left\| \left(\mathbf{I} + \Delta t \sum_{d=1}^{D} \frac{\beta_d}{(\Delta x)^d} \mathbf{A}_d\right) \right\|_2 \leq 1$$ Stability

Automated Discretization of PDEs (contd.)

Superior accuracy with low order approximation



a) **Explicit Scheme:** Minimum spectral error with 7 point stencil. First derivative, with second order accuracy.

b) **Implicit Scheme:** Minimum spectral error with 7 point stencil. First derivative, with second order accuracy.

c) **Multi-band Spectral Accuracy:** Explicit scheme with 11 point stencil. First derivative, with second order accuracy.

Summary

- Treat coefficients of finite-difference scheme as unknowns
- Over parameterize
- Solve minimized error (spectral) subject to stability and accuracy constraints
- Coefficients are "Control Variables"
  - Formulation similar to State-Feedback control
- Powerful connection
  - We can formulate finite-difference schemes as a control problem
  - Guarantee transient and steady-state behaviour of numerical method
  - Robustness to uncertainties, quantization error, etc.
  - Nonlinear extensions

1. A unified framework to generate optimized compact finite difference schemes, Authors: Vedang M. Deshpande, Raktim Bhattacharya, Diego A. Donzis
2. A Unified Approach for Deriving Optimal Finite Differences, Authors: Komal Kumari, Raktim Bhattacharya, Diego A. Donzis