AFRL

Control Theory in the age of Computation and Machine Learning

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- **Why am I here:** The general themes of this workshop have been relevant to my own research and to my current job as a program manager in computational mathematics.
- **My own research:** Computational methods in control of PDEs, and then numerical optimal control of nonlinear ODEs – relevance to astrodynamics.
- **Lessons learned:** Using generic numerical methods for solving control of PDEs/ODEs will not always work. These discretization methods need to satisfy certain properties of the original control system to achieve convergence.
    - We need more than convergence of the forward problem
    - convergence of the appropriate operators,
    - *convergence of the adjoint problem,*
    - preservation of stability (exponential) properties, and so on.
- **Scientific Challenges:** As more computational power becomes available, more is demanded in terms of complexity of models and mathematical analysis– from forward simulation of complex systems, to inverse problems, design and optimization, estimation, control

Air Force Office of Scientific Research

BAA: https://www.afrl.af.mil/AFOSR

Provides funding for Basic Research relevant to the Air Force and the Space Force

FIND

36 Program Officers (POs), **18** International Program Officers (IPOs) and **7** Program Coordinators (PCs) reaching scientists & engineers globally

FORM

Shape emerging science into high-performing teams and portfolios that address long-term basic science barriers to future AF capabilities

FUND

1,231 extramural research projects at U.S. universities in **45** states

201 intramural research projects at AFRL Technology Directorates

443 international efforts in **43** countries on **6** continents

FORWARD

Transition through AFRL Technology Directorates (TDs), Small Business Innovation Research & Small Business Technology Transfer (SBIR/STTR)

Basic Research Portfolios

Engineering and Complex Systems
- Dynamic Materials and Interactions
- GHz-THz Electronics and Materials
- Energy, Combustion, and Non-Equilibrium Thermodynamics
- Unsteady Aerodynamics and Turbulent Flows
- High-Speed Aerodynamics
- Aerospace Composite Materials
- Multiscale Structural Mechanics and Prognosis
- Space Propulsion and Power
- Agile Science of Test and Evaluation (T&E)

Information and Networks
- Computational Cognition and Machine Intelligence
- **Computational Mathematics**
- **Dynamical Systems and Control Theory**
- **Dynamic Data and Information Processing**
- Information Assurance and Cybersecurity
- **Mathematical Optimization**
- **Science of Information, Computation, Learning, and Fusion**
- Trust and Influence
- **Complex Networks**
- Cognitive and Computational Neurosciences

Physical Sciences
- Aerospace Materials with Extreme Properties
- Atomic and Molecular Physics
- Electromagnetics
- High Energy Radiation-Matter Systems (HERMeS)
- Optoelectronics and Photonics
- Quantum Information Sciences
- Physics of Remote Sensing
- Space Science
- Ultrashort Pulse Laser-Matter Interactions
- Condensed Matter Physics

Chemistry and Biological Sciences
- Biophysics
- Human Performance and Biosystems
- Mechanics of Multifunctional Materials and Microsystems
- Molecular Dynamics and Theoretical Chemistry
- Natural Materials and Systems
- Organic Materials Chemistry

Astrodynamics

International Office
- Asian Office of Aerospace R&D Tokyo
- European Office of Aerospace R&D London
- Southern Office of Aerospace R&D Santiago
- North America - Arlington

Mathematical Research is funded across all these different portfolios.

The National Defense Strategy emphasizes 8 areas: hypersonics, advanced computing, “big data” analytics, artificial intelligence, autonomy, robotics, directed energy, and biotechnology

Mission Statement of Computational Math Portfolio

Mission Statement: Discover and Develop Mathematical Algorithms and Computational Techniques that Provide *Accurate*, *Reliable*, and *Efficient* Algorithms for Modeling & Simulation, Design and Decision Making for Complex Systems for the DAF with radical cost and turn-time improvements.

Applications: Fluids, Structures, Plasmas, Materials, Quantum Systems, Biology, Social Systems, (and this year Space Systems)

Focus on algorithm development, no HPC research, no software, or hardware research

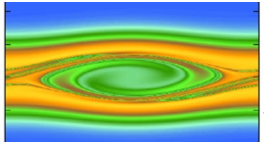
Emphasizing Fundamental, Cross-disciplinary Algorithm Development with Rigorous Analysis: error, convergence, stability, computational complexity

Technical Focus Areas of Computational Math

The Curse of Dimensionality
Effect **of uncertainty** ----high-dimensional problems, proper formulation
Multiscale Modeling
Understanding the Physics and Mathematical modeling before computing
Systems Modeling – Nonlinear, Dynamic Interactions between the components
Computational complexity
Convergence and Error Analysis

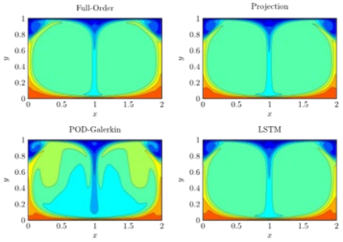
High-Order, High-Fidelity Numerical Methods

- Numerical Schemes of Order Accuracy Higher than 2 for Simulating Multiscale, Multi-Physics phenomena
- Turbulent High-Speed Flows, Structures, Plasma



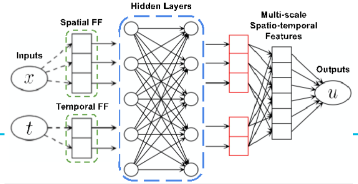
Dimensionality and Complexity Reduction

- **Reduced Order Modeling** for Analysis And Design
- **Uncertainty Quantification** – Model Error



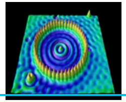
Data, Models, Learning

- Machine Learning, Deep Learning for Modeling Physical Systems
- Mean-Field Games, Optimal Transport
- Mathematics of “Digital Twins”



Emerging Applications

- Quantum Many-Body Systems
- Synthetic Biology
- Computational Social Science
- Space Science

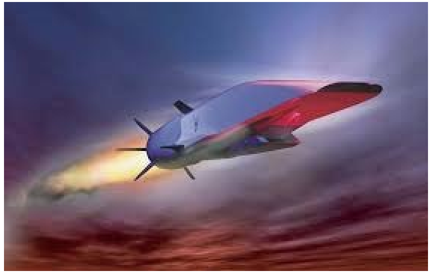


Big Trends

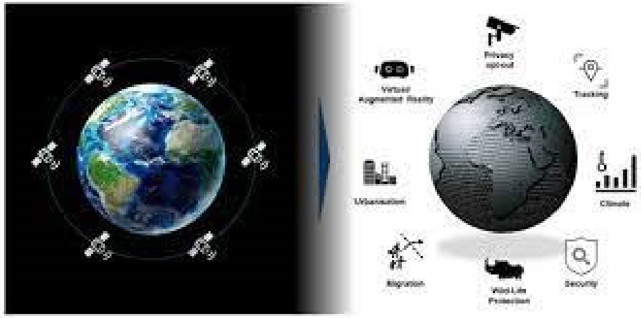
- Trends: AI/ML for scientific discovery, Modeling of systems, Emerging Applications-Biology, Quantum, Space --- DL has taken over analysis and computation
- Initial reactions of the comp math and controls community were negative – Black Box modeling
- Now everyone wants to know about mathematics of deep learning
- Also the effectiveness (and its limits) in discovering models using data
- The areas of ROMs, UQ (for model and parameter uncertainties), data assimilations are all using some variations of deep learning architectures and computing
- It has also encouraged multidisciplinary research among the optimization, computational math, and statistics communities – controls community is making contributions both in applications and theoretical levels
- It has also encouraged a computational way of thinking among the researchers in other areas of science – Scientific Machine Learning (SciML), ML for scientific discovery

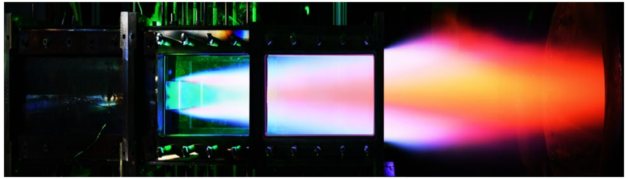
Digital Twins MURI – Background, Motivations

Need for New Paradigms for Modeling & Computation of Complex Systems



- Challenges in dealing with increasing complexity in models and requirements and faster innovation cycles for complex DoD systems and operations: Examples
  - *Hypersonic flight:* unknown physics, lack of mathematical models for physics at all relevant scales, uncertain operational environments
  - *Design of next generation of rockets and jet engines*: lack of multi-scale of models, lack of experimental data at local scales
  - *Autonomous* operations in contested, uncertain environments
  - *Space Domain operations*
- Existing modeling practices either rely on experiments that are either too costly, or cannot recreate the range of parameters and operational domain
  - OR
- Modeling is reliant on computational platforms that are still too costly and too time-consuming for exploring the relevant range of parameters and scenarios, AND also still not *Predictive*





HPC is NOT the only solution!

What Is Needed? Why Now?

- **Our Vision:** a computational model (or a set of coupled computational models) corresponding to multi-physics, multiscale, multi-components systems that evolves over time to persistently represent the structure, behavior, and context of a unique physical asset such as a component, system, or process.

- This vision is not yet realized in industrial or applied sectors:
  - Over-reliance and confidence on existing models that are super-expensive to run
  - Over-reliance on abundance of data to fix the models and parameters
  - The idea of multi-physics modeling as stitching existing single physics models together
  - Lack of Uncertainty Quantification practices in modeling
  - Insistence on one-off modeling and computing framework fine-tuned to a particular application

Recent Accomplishments:

- Multi-layered, rigorous complexity reduction techniques:
  - Reduced-Order modeling (ROM)
  - Physics-based Machine Learning (ML)
  - Automated discovery of dynamics (unknown physics, equations)
- Advanced hardware (neuromorphic, optical, quantum)
- Graph-based learning and data topology
- Bio-inspired Neural Networks
- New ideas in data-assimilation

We need to address the basic research needs to achieve this vision under our scientific leadership before the idea becomes co-opted by industry and turns into product development.

Topic Objective

Reduced Order Models for Multi-Physics Problems

While there is substantial recent work on surrogate models, little work is available for multi-physics/multi-scale problems

Reduced Order Models for Coupled Systems

The understanding of system behavior, derived from the understanding of several components, is very limited, yet essential to enable the modeling of complex multi-component systems and understand the risk of unintended consequences of couplings.

New Techniques for Sampling, Estimation, Risk Assessment for High-Dimensional Problems

Complex system behavior will depend on a large number of parameters,
Assessing risk and estimating behavior requires improved understanding of multi-fidelity models,
sampling and risk assessment in the context of high-dimensional problems.

Full Sensor Integration, Data Assimilation

Sensor integration plays a central role for the calibration of the Digital Twin, both initially and for updating information. For dynamic scenarios, data assimilation becomes a central tool to be used in close connection with the reduced models which serve as the backbone for data generation and model update.

Machine Learning

While much past work suggests that neural networks is sufficiently powerful to provide data-driven methodologies for decision support, much work is needed to understand the appropriate architecture for the applications being considered.

Validation on Complex Use Cases   ---- UQ of large complex systems

Benchmark demonstrations of the developed theory on computation for multiple applications are crucial.

Road Ahead

- Computational thinking has taken over --- as well as data-driven modeling
- Very interesting projects have started at the intersection of learning and control: Enrique's group, Miroslav Krstic's group, and G. Karniadakis' PINNs – Jerome Darbon (solving HJB equations)
- We are of the belief that math can bring more than rigor – also different ways of modeling and analysis: We need to be always aware of other areas in math (pure or applied) that could change and transform the field: algebraic topology, algebraic geometry, category theory
- But also functional analysis, approximation theory, probability and stochastic processes
- I cannot overstate the importance of foundations of control theory to all these areas of research – looking forward to the Thursday PM session