Dynamic Network Analysis for robust uncertainty management

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Outline

• DyNARUM origin
  • Dynamics on Graphs
  • Beneficial and detrimental interconnection
  • and why UTC and DOD care

• Multiscale Complex Dynamics: Barriers and Enablers
  • Graph Decomposition
  • Learning Models of Coarse Dynamics
  • Coarse Temporal Integration
  • Efficient Uncertainty Quantification

• Future directions
  • Robust Surveillance and Distributed Estimation Networks
  • Cyber-Physical Systems
Dynamics on Graphs

Dynamics at node + interconnection strength => emergent behavior

Imposing or breaking symmetry can enforce the desired behavior

Pendula analog of engine dynamics

Symmetric => high amplitude wave
Mistuned => reduced amplitude

Flutter
Rotating stall
Aeroacoustics
Thermoacoustics

Coupling strength

Coherence
Incoherence
Time scale separation
Exploit Interconnections

Analysis of symmetry => detrimental and beneficial interactions

Wave equation with skew-symmetric feedback

- Positive feedback => detrimental coupling
- Creates lightly and heavily damped spinning waves

\[ p_{tt} + \xi p_t - a_0^2 p_{\theta\theta} = F(p, \theta) + a^2(\theta)p_{\theta\theta} \]

Use coarse variables (modes +1, -1)
=> simple model => analysis tractable

Heavily damped waves
- Utilized as dampers

Under-damped waves
- Wave mistuning creates beneficial coupling

Acoustics
Heat release
Wave Speed Mistuning

flutter
thermoacoustics

***
Engine problem eliminated by wave speed mistuning

- Inspiration: 2004 study of symmetry of DNA molecules (I. Mezic)
- From initial concept to engine test in 18 months
- Passive solution: no extra hardware necessary
Multi-scale complex dynamics affects United Technologies

- **Pratt: thermoacoustics**
- **Sikorsky: battlefield simulations**
- **HS: electric power systems**

Building systems: air, energy, threat, people dynamics

- **Carrier: variable speed**
- **Pratt: thermoacoustics**
- **Sikorsky: battlefield simulations**
- **HS: electric power systems**

Ratio of time scales

\[ \frac{\tau_{\text{slowest}}}{\tau_{\text{fastest}}} \]

Acoustics

\[ x_{tt} - a^2 \Delta x = F(x(t), x(t - \tau), \mu) + n(t) \]

Large multi-scale
Nontrivial dynamics

Heat Release
Nonlinearity
Delays
Uncertain parameters

Turbulence
Disturbance

Sensitivity

Complexity

Uncertainty
Multi-scale dynamical systems

barriers and enablers

Computation cost \( \sim n_{\text{nodes}} \cdot n_{\text{links}} \cdot n_{\text{timesteps}} \cdot n_{\text{samples}} \)

**Barriers**

- Large interconnected network
- Multiple time scales
- Uncertain parameters

**Enablers**

- Coarse spatial variables
- Coarse temporal integration
- Coarse stochastic variables

**Tractable description**

- Simulations
- Analysis
- Design

Exploit interconnections

Learn Model of Coarse Dynamics

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Multi-scale complex dynamics affects DOD

DARPA DSO invests in Mathematics

Objectives:
1. Develop analysis and design tools for Uncertainty Management
2. Demonstrate tools in a surveillance problem with > 10,000 agents

Approach:
1. Decompose networks into components using Spectral Graph Theory.
2. Propagate uncertainty through components using Operator Theory and Geometric Dynamics
3. Iteratively aggregate component uncertainty

Program Metrics:

<table>
<thead>
<tr>
<th>Year</th>
<th>10x validation on interacting particles challenge problem</th>
<th>Reduce average</th>
<th>Reduce standard deviation</th>
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<tbody>
<tr>
<td>Year 1</td>
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<tr>
<td>Year 2</td>
<td>100x validation on interacting particles challenge problem</td>
<td>10x</td>
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<tr>
<td>Year 3</td>
<td>100x validation on surveillance problem</td>
<td>100x</td>
<td>10x</td>
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DyNARUM Approach

Approach:

1. Decompose networks into components using Spectral Graph Theory.
   - Weak connections revealed, strongly connected components identified

2. Propagate uncertainty through components using Operator Theory and Geometric Dynamics
   - Component measure propagation operators reduced, truncation error assessed

3. Iteratively aggregate component uncertainty
   - Parallel asynchronous computations, iterations across weak connections

Enabling technologies:

- **Geometric Dynamics and Optimal Control**: design beneficial dynamics for robust surveillance with fast detection
- **Spectral Graph Theory methods**: analysis of spectrum of Markov matrix associated with network reveals interconnection structure, strong and weak connections
- **Coarse Variables and Symmetry**: exploit symmetry to decouple slow and fast scales, enable network decomposition, model reduction, asynchronous parallel computations
- **Geometric Dynamics and Measure Propagation**: Efficient choice of basis for measure propagation for networks with nontrivial component dynamics
- **Variational Integrators and Asynchronous Computations**: preserve energy, probability measures, exploit time scale separation for efficient computing
- **Operator Theory and Model Reduction**: use eigenfunctions of Markov matrices associated with components for model reduction while keeping track of truncation error, prove convergence of iterative methods for measure propagation

Challenge problem: 10,000 Agents Surveillance Network with uncertain vehicle and sensor models, probability distribution of input parameters

Parallel asynchronous computations, iterations across weak connections
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Decompose Networks into weakly interacting sub-networks

$\dot{X} = F(X) \Rightarrow \frac{\partial F}{\partial X}$

$\frac{d}{dt} (x_i)^{k+1}(t) = f_i((x_1)^k, ..., (x_i)^{k+1}, ..., (x_m)^k)$

$\Rightarrow$ iterate for accuracy

Error decays as $(Te^{TK})^N \Rightarrow$ # iterations

simulation time for one iteration

$\sup ||\frac{\partial f_i}{\partial x_i}||, i \neq m$
Decompose Networks

Enabler: Spectral Graph Theory

1. Local dynamics + interconnection structure => Markov chain on graph

\[ \mu_{n+1} = M\mu_n \quad \Rightarrow \quad \lambda x = Mx \]

2. Small gaps between eigenvalues reveal weakly connected sub-networks
   • Indicates transport bottleneck

3. Eigenfunctions sign change determines network decomposition
   • 2\textsuperscript{nd} eigenfunction is the slowest decaying pattern. Sign change is location of bottleneck.

Example: analysis of transport of species between coupled rooms

Decomposition enables uncertainty propagation using parallel computations
Fine-grained agent-based model computations $\sim N^2$

Enable model-based estimation of occupancy

Aggregation to zones

Graph decomposition

Identify strong and weak coupling to zone system and track movement between zones
Learn Model of Coarse Dynamics to reveal important time scales in the system

Choose local observable

*measure local symmetry* $\Rightarrow$ *average* $\Rightarrow$ *phase*

**Problem:** determine phase

Simulation with 2000 atoms

Average observable

Learning of second eigenvalue of $M$

Learning completed $\Rightarrow$ 10x speedup of phase determination

Learn its probability transition matrix

$$\mu_{n+1} = M \mu_n$$

Eigenvalues of $M$

- Rapidly decaying patterns
- Slowly decaying patterns

Eigenvector $= \text{asymptotic probability distribution}$
Equation-Free Coarse Temporal Integration

continuity of time scales reduces acceleration

order parameter $\Psi$ captures order-disorder transition

Procedure

atomistic simulator

lifting

restriction

course stepper

equation-free order parameter evolution at given density

calculated phase diagram
Midterm and final exams (and why we think we will pass)

### Analysis Tools

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- Stochastic Galerkin $\Rightarrow$ 1000x faster than MC (Brown)
- Equation-Free UQ $\Rightarrow$ 3x faster than MC (Princeton)

### Design Tools

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- Optimal Control
- Geometric Dynamics
- Chaotic search $\Rightarrow$ exponentially fast coverage

### Phase diagram (10K particles)

- 10x reduction of computation time

### Self-assembly (~100 particles)

- Distribution of performance, stability measure
- Baseline Algorithm $\Rightarrow$ Improved/Robust Algorithm
- Quantify quality, stability, robustness

### Surveillance network (10K agents)

- Distribution of target detection time
- Baseline Algorithm $\Rightarrow$ Optimal/Robust Algorithm
- 10x better performance
- 100x better performance
- 10x better robustness
Milestone 1B: learning dynamics demonstrated on Phase Diagram problem

Baseline:
Phase diagrams from 10,000 Helium atoms on C 2000 simulations, total 100 hours (12 CPUs)

Phase diagrams obtained with RUM tools

Bayesian Markov model extraction (Stanford)

Metastability from Markov model (UTRC)

Reduced-size system (Aimdyn)
Milestone 1A: new potential design method demonstrated in Self-Assembly problem

**Goal**: Design interaction potential so that 100 particles self-assemble to a honeycomb lattice

**Baseline** (Princeton 2005):
- Final lattice still has defects
- Computationally expensive (Simulated Annealing gets stuck in local minima of a defect measure)

**DyNARUM**:
- Repulsive potentials avoids defects produced by local minima
- Trend-based optimization 100x faster than Simulated Annealing

Particle interaction potentials

\[
V(r) = \frac{5}{r^{12}} - \frac{d_0}{r^{10}} + a_1 e^{-a_2 r} - 0.4e^{-40(r-a_3)^2}
\]

Defect measure

# Molecular Dynamics runs
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Future directions: distributed estimation

Distributed Estimators of Multiscale Phenomena

Estimator of physical dynamics

- **Prediction**
  \[
  Y_i(t|t-1) = (F(t-1)Y_i(t-1|t-1)F^T(t-1) + Q(t))^{-1}
  \]
  \[
  y_i(t|t-1) = Y_i(t|t-1)f(\hat{z}(t-1|t-1))
  \]

- **Measurement update**
  \[
  Y_i(t|t) = Y_i(t|t-1) + H^T(t)R^{-1}(t)H(t)
  \]
  \[
  y_i(t|t) = y_i(t|t-1) + H^T(t)R^{-1}(t)\tilde{z}(t)
  \]

where \(F(t)\) and \(H(t)\) denote the Jacobian matrices, and
\[
\tilde{z}(t) = z(t) - h(\hat{z}(t|t-1)) + H(t)\tilde{\hat{z}}(t|t-1)
\]

Dynamics of consensus algorithm

**Single scale**

**Multiscale 10x faster**
Challenge: Robust Cyber-Physical Systems

Codesign of Physical and IT Dynamics necessary

Input parameter probability distribution

Output parameter probability distribution

Reduced uncertainty with robust design

No time scale separation

Power grid control
City evacuation support
Building emergency response support
Surveillance networks

Multiscale dynamics

Uncertainty
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