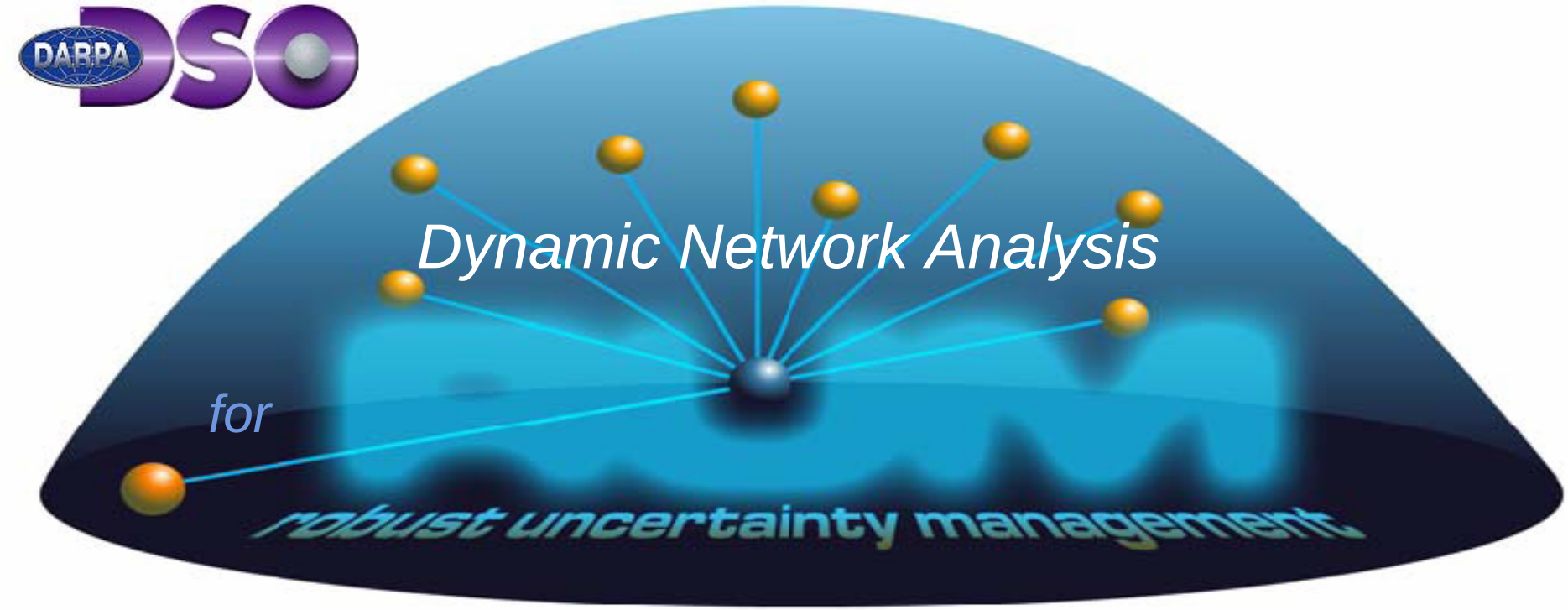


Andrzej Banaszuk
United Technologies Research Center

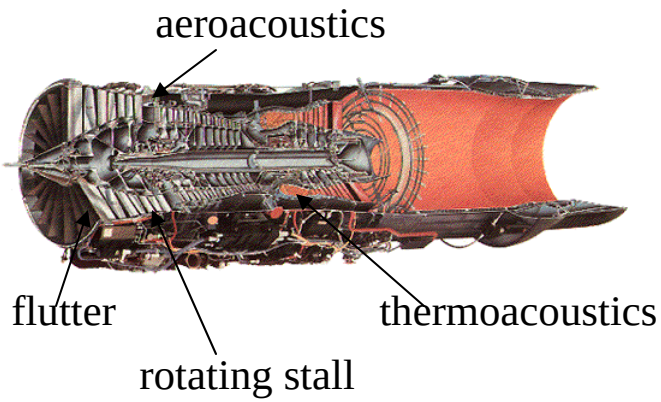
Outline

- 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

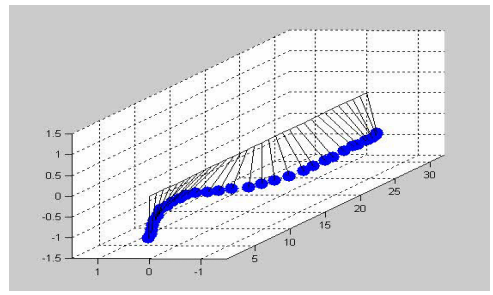
Dynamics at node + interconnection strength => emergent behavior

Imposing or breaking symmetry can enforce the desired behavior

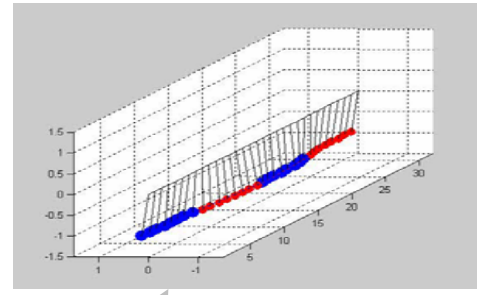


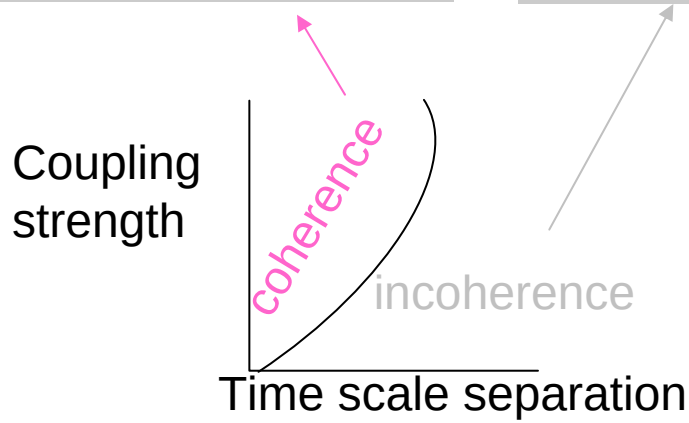
Pendula analog of engine dynamics

Symmetric => high amplitude wave



Mistuned => reduced amplitude



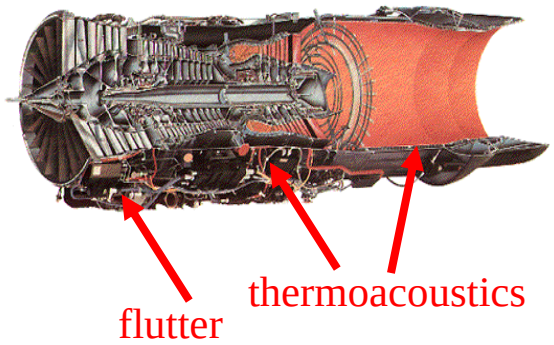


Exploit Interconnections

Analysis of symmetry => detrimental and beneficial interactions

Wave equation with skew-symmetric feedback

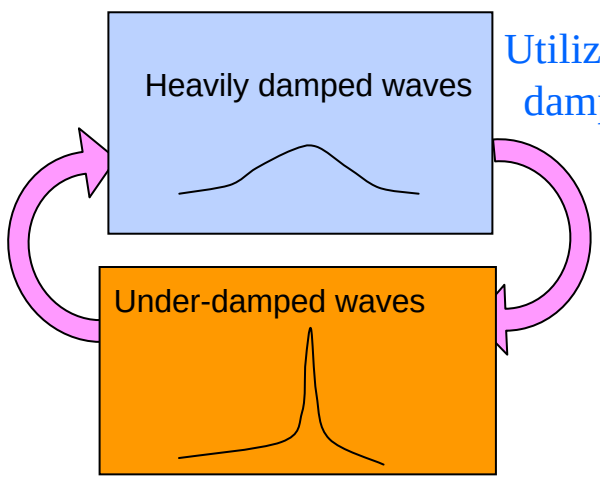
- Positive feedback => detrimental coupling
- Creates lightly and heavily damped spinning waves



Acoustics *Heat release* *Wave Speed Mistuning*

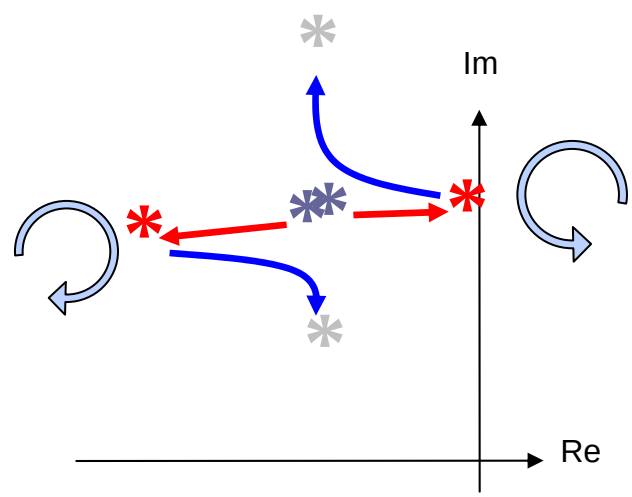
$$p_{tt} + \xi p_t - a_0^2 p_{\theta\theta} = F(p,\theta) + a^2(\theta) p_{\theta\theta}$$

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



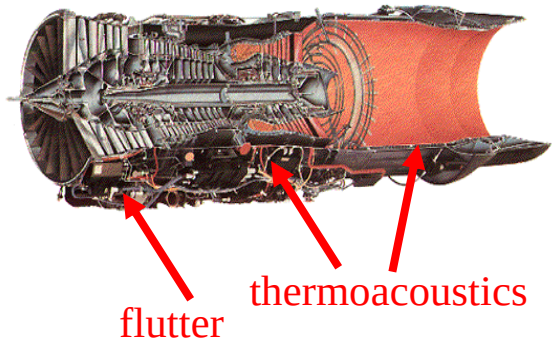
Utilized as dampers

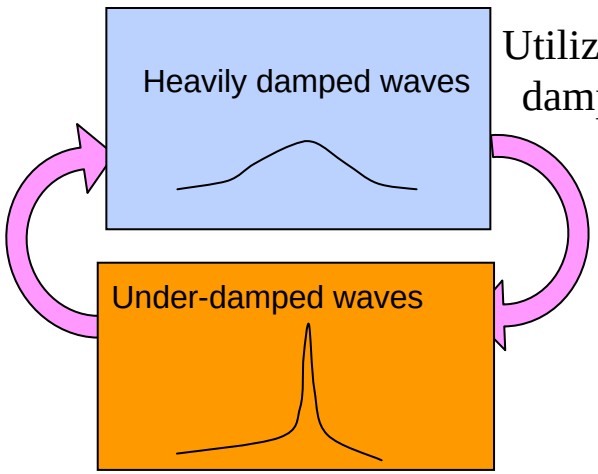
Wave mistuning creates beneficial coupling



Design Beneficial Interconnections

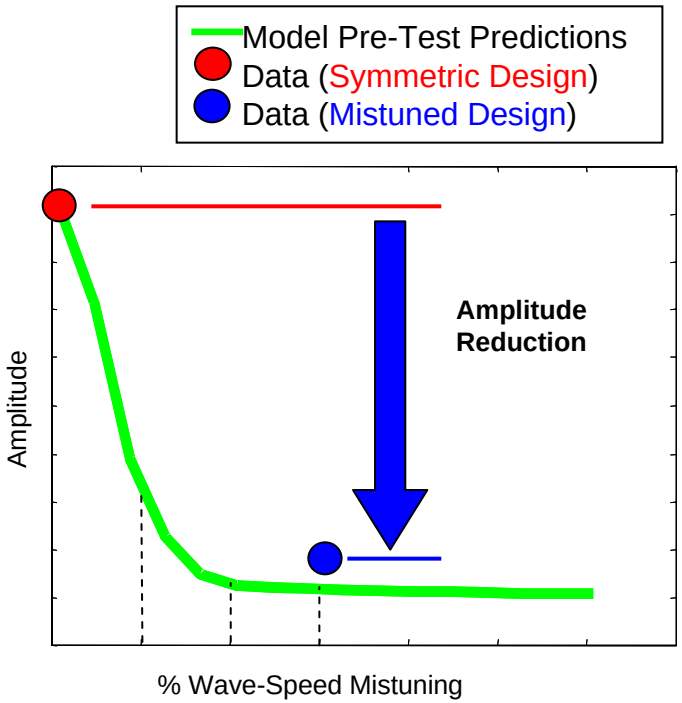
Engine problem eliminated by wave speed mistuning





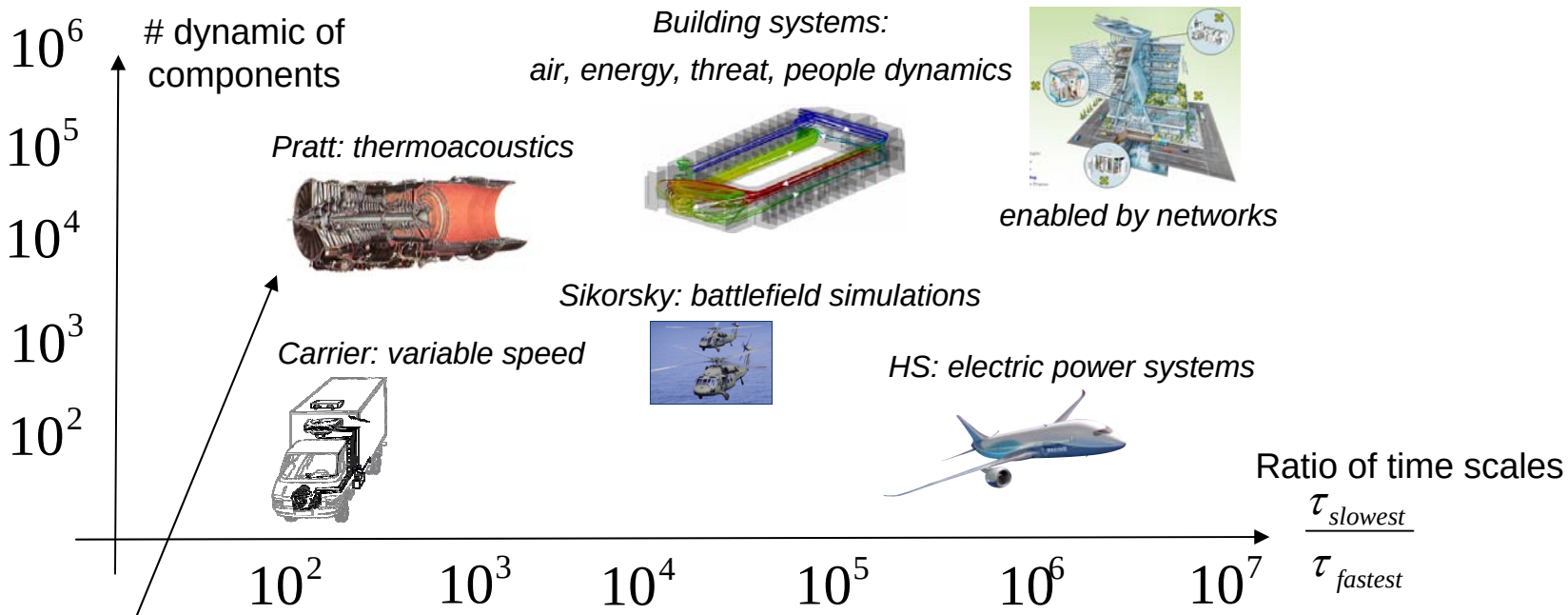
Utilized as dampers

Wave mistuning creates beneficial coupling



- 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



Acoustics Heat Release Turbulence

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

Large multi-scale Nonlinearity Delays Disturbance

Nontrivial dynamics Uncertain parameters

Sensitivity **Uncertainty**

Complexity

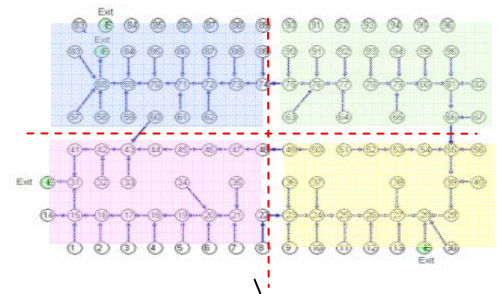
Multi-scale dynamical systems

barriers and enablers

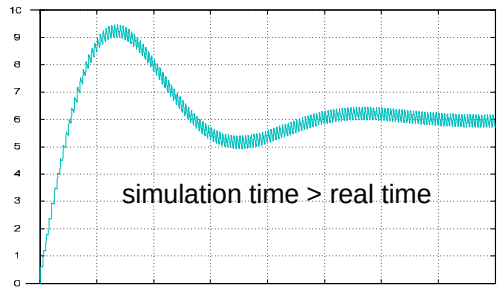
Computation cost $\sim n_{nodes} \bullet n_{links} \bullet n_{timesteps} \bullet n_{samples}$

Barriers

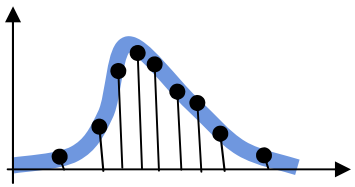
Large interconnected network



Multiple time scales



Uncertain parameters



Enablers

Coarse spatial variables

Coarse stochastic variables

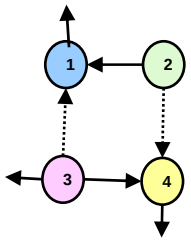
Coarse temporal integration

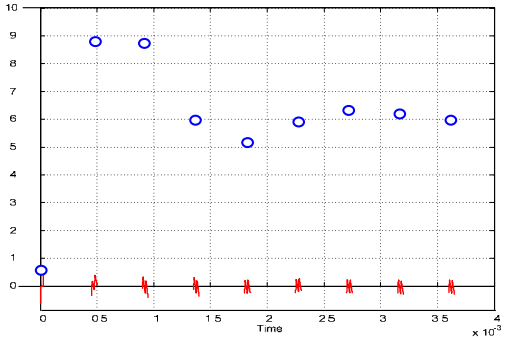
Network decomposition

Learn Model of Coarse Dynamics

Tractable description

- ***Simulations***
- ***Analysis***
- ***Design***

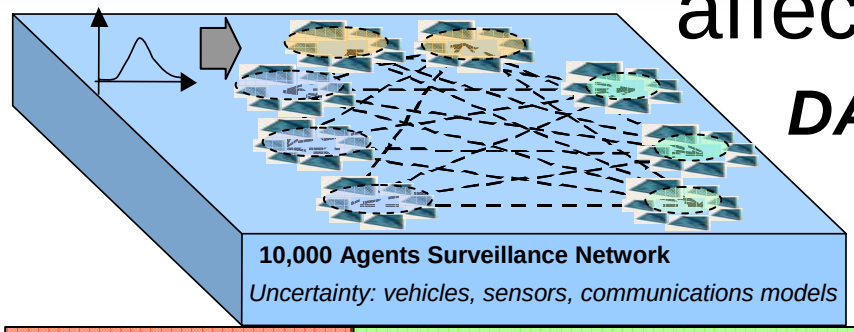




Exploit interconnections

Multi-scale complex dynamics affects DOD

DARPA DSO invests in Mathematics



Objectives:

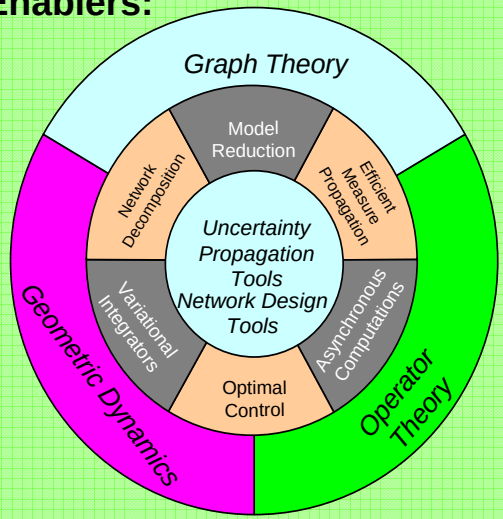
1. Develop analysis and design tools for Uncertainty Management
2. Demonstrate tools in a surveillance problem with > 10,000 agents

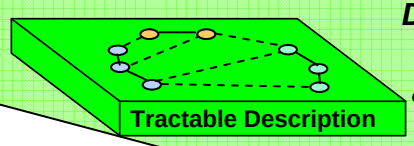
Barriers

- **Large Scale**
- **Multiscale**
- **Uncertainty**
- **Nontrivial Dynamics**

Uncertainty Propagation Intractable With Current Methods

Enablers:

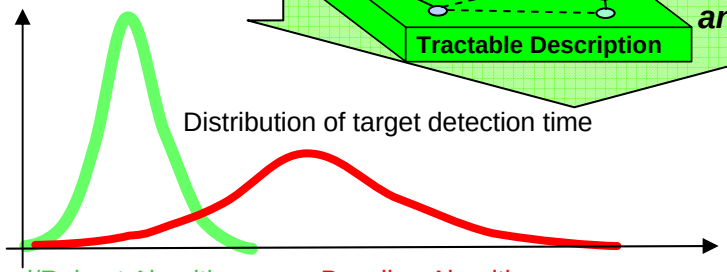




DYNARUM methods and tools

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 :

	Reduce computation time	Reduce average	Reduce standard deviation
Year 1	10x + validation on interacting particles challenge problem	-	-
Year 2	100x + validation on interacting particles challenge problem	10x	-
Year 3	100x + validation on surveillance problem	100x	10x

United Technologies Research Center

DyNARUM Team

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Simeon Grivopoulos

Bryan Eisenhower

Marko Budisic

Gunjan Thakur

Lan Yueheng

Jerry Marsden

Konda Reddy

Phillip Du Toit

Katalin Grubits

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Sigrid Leyendecker

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Bob LaBarre

George Mathew

Troy Smith

Jose Miguel Pasini

Sergey Shishkin

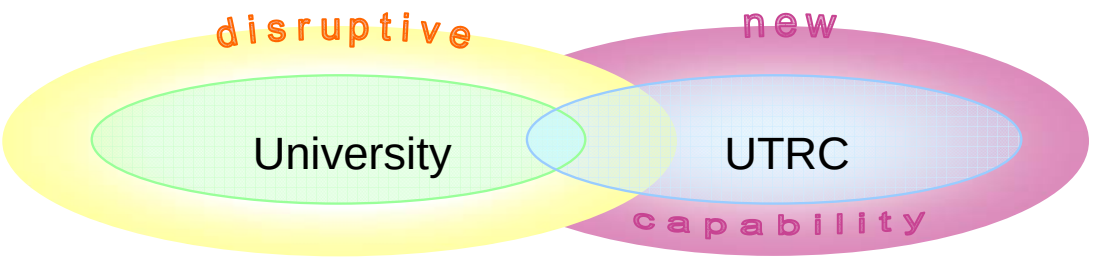
Sergei Burlatsky

Emrah Biyik (intern, RPI)

Vladimir Fonoberov

Caroline Cardonne

Eric Johnson



Basic Research:
Long range technology development

Applied Research:
Integrate, mature, and transfer technology to market opportunities

Yannis Kevrekidis (Princeton)

Gleb Oshanin (Univ. P&MCurie)

Sean Meyn (UIUC)

Michael Dellnitz (Paderborn)

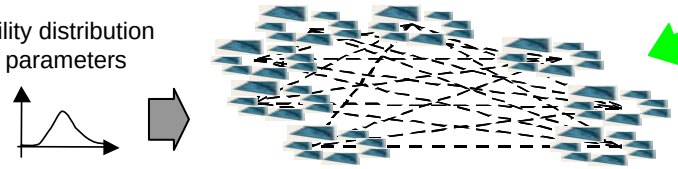
Mark Lutian

DyNARUM Approach

Approach:

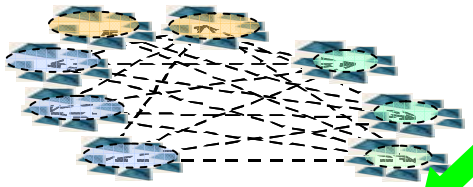
Challenge problem: 10,000 Agents Surveillance Network with uncertain vehicle and sensor models,

Probability distribution of input parameters



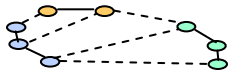
1. Decompose networks into components using Spectral Graph Theory.

Weak connections revealed, strongly connected components identified



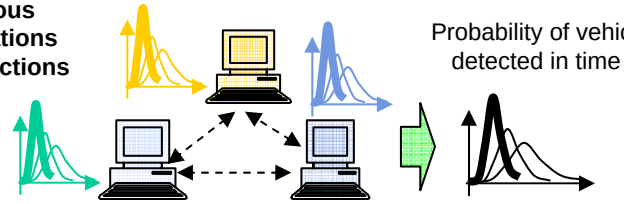
2. Propagate uncertainty through components using Operator Theory and Geometric Dynamics

Component measure propagation operators reduced, truncation error assessed



3. Iteratively aggregate component uncertainty

Parallel asynchronous computations, iterations across weak connections



Probability of vehicle detected in time T

Enabling technologies:

Design Tools

Geometric Dynamics and Optimal Control: design beneficial dynamics for robust surveillance with fast detection

Analysis Tools

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

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Outline

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  - And why UTC and DOD care
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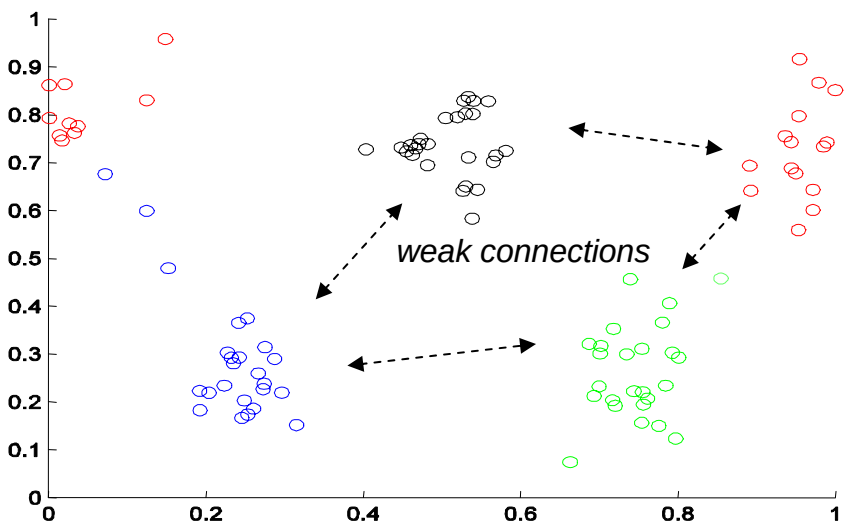
  - Efficient Uncertainty Quantification
- Future directions
  - Robust Surveillance and Distributed Estimation Networks
  - Cyber-Physical Systems

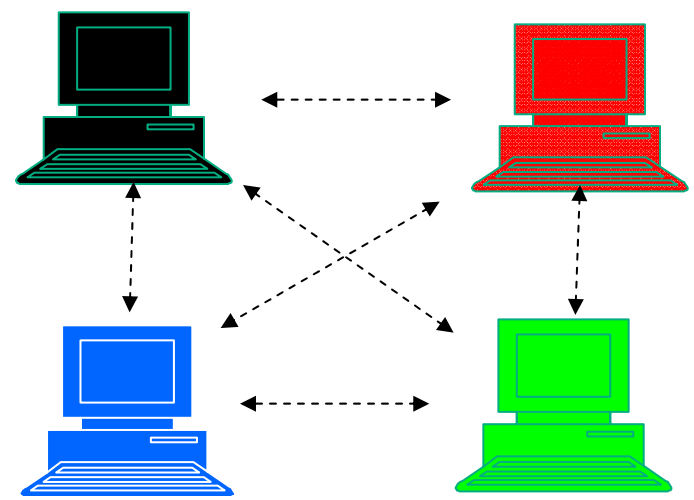
Decompose Networks

into weakly interacting sub-networks

=> speedup utilizing parallel computations

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





=> iterate for accuracy

$$\text{Error decays as } (Te^{TK^+}K^-)^N \leftarrow \text{\# iterations}$$

simulation time for one iteration

$$\sup\left\|\frac{\partial f_i}{\partial x_i}\right\| \qquad \sup\left\|\frac{\partial f_i}{\partial x_m}\right\|, i \neq m$$

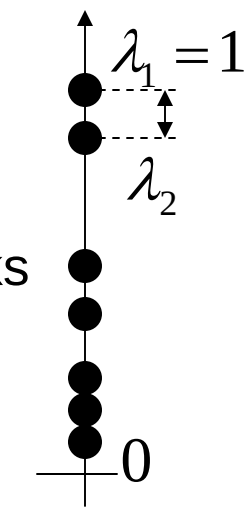
Decompose Networks

Enabler: Spectral Graph Theory

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

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

Eigenvalues



2. Small gaps between eigenvalues reveal weakly connected sub-networks

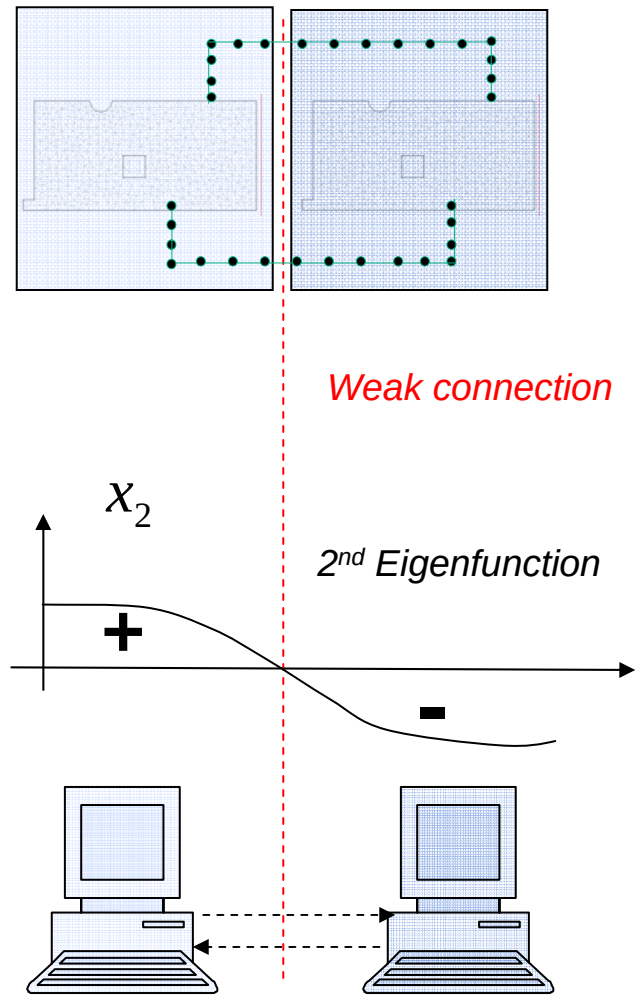
- Indicates transport bottleneck

3. Eigenfunctions sign change determines network decomposition

- 2nd eigenfunction is the slowest decaying pattern. Sign change is location of bottleneck.

Decomposition enables uncertainty propagation using parallel computations

Example: analysis of transport of species between coupled rooms



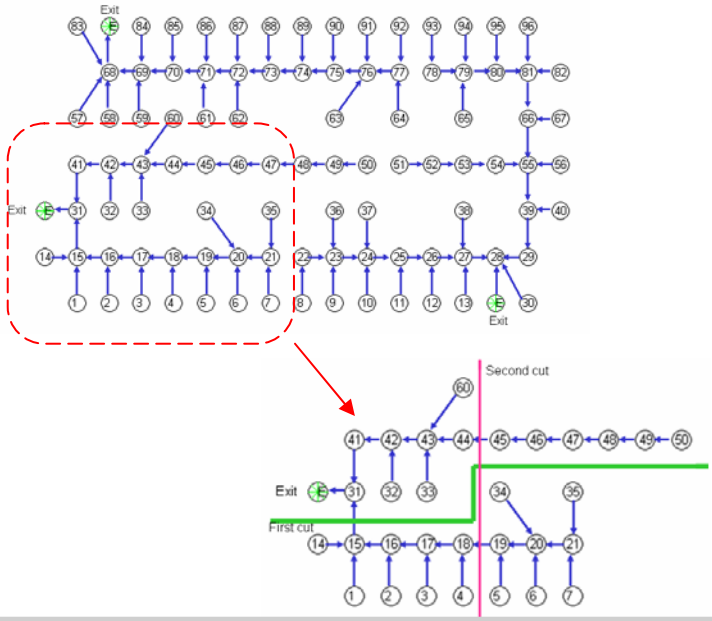
Decompose Networks

Application: analysis of people dynamics in buildings

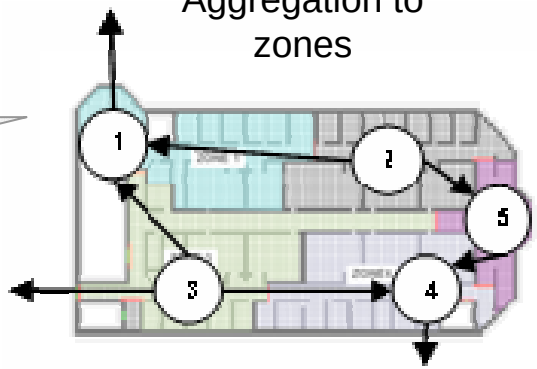
Fine-grained agent-based model computations ~ N^2

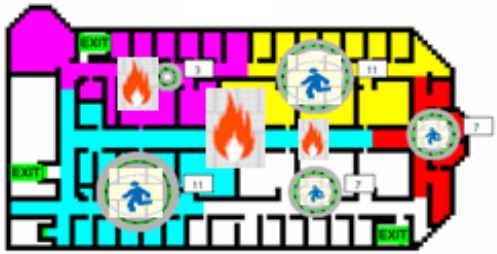
Enable model-based estimation of occupancy

Graph decomposition



Aggregation to zones





Identify strong and weak coupling to zone system and track movement between zones

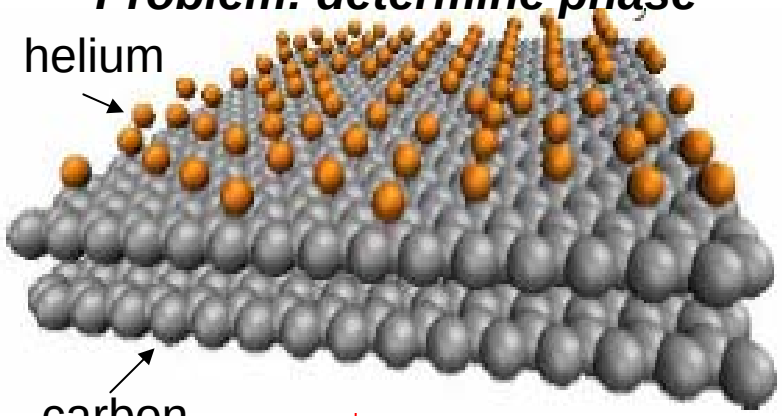
Learn Model of Coarse Dynamics

to reveal important time scales in the system

Choose local observable

measure local symmetry => average => phase

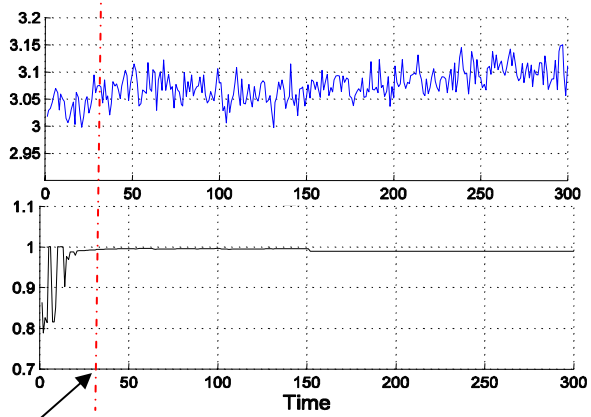
Problem: determine phase



Simulation with 2000 atoms

Average observable

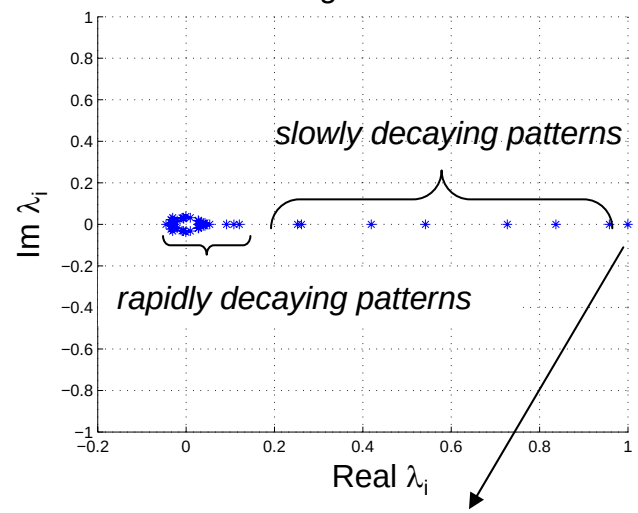
Learning of second eigenvalue of M



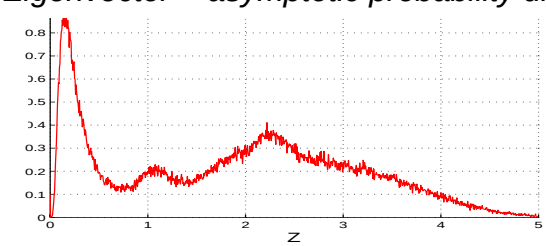
Learn its probability transition matrix

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

Eigenvalues of M



Eigenvector = asymptotic probability distribution



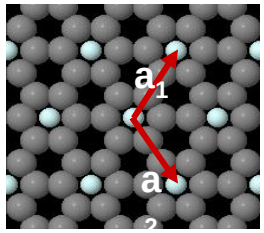
solid fluid observable

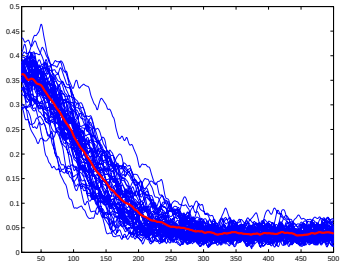
Learning completed = > <u>10x speedup</u> of phase determination

Equation-Free Coarse Temporal Integration

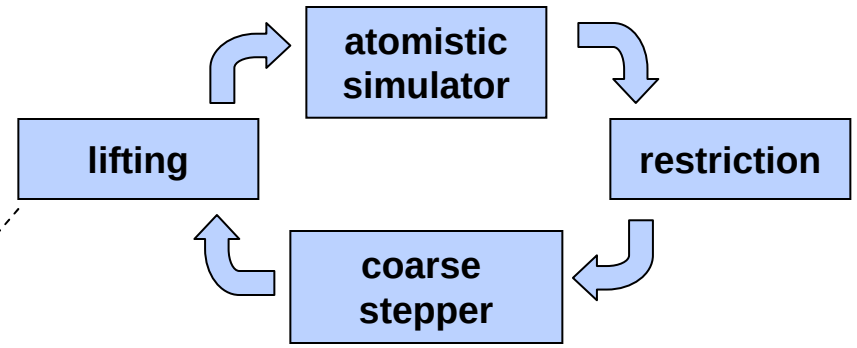
continuity of time scales reduces acceleration

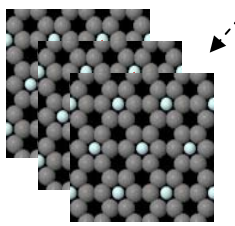
order parameter Ψ captures order-disorder transition



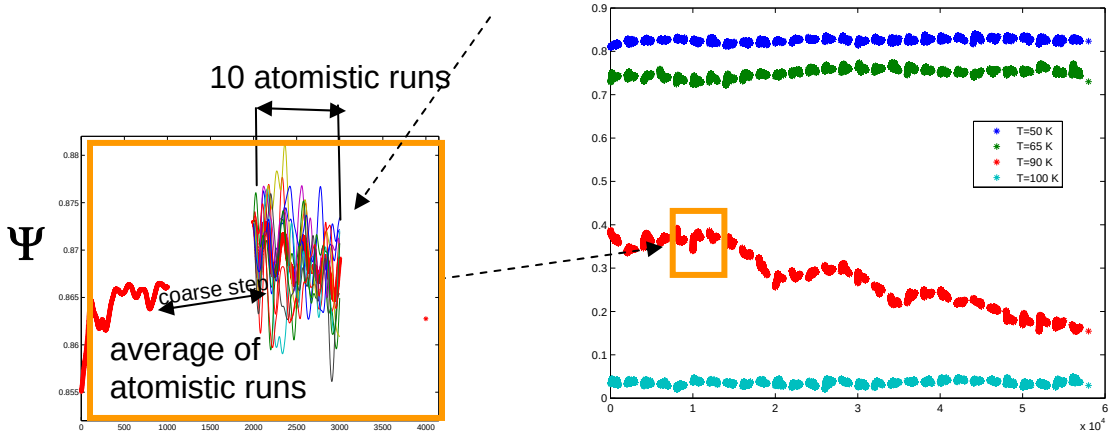


Procedure

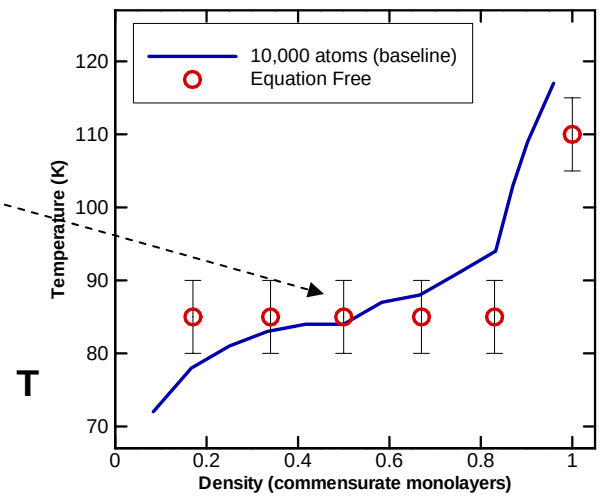




equation-free order parameter evolution at given density



calculated phase diagram



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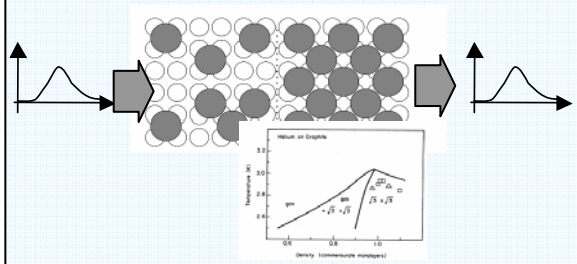
Midterm and final exams (and why we think we will pass)

2006	2007	2008	2009

Analysis Tools

Phase diagram (10K particles)



Coarse Variables
Model Reduction
Network Decomposition

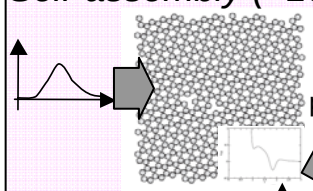
10x reduction of computation time

Stochastic Galerkin =>1000x faster than MC (Brown)
Equation-Free UQ => 3x faster than MC (Princeton)

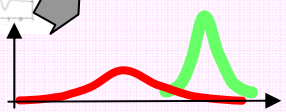
100x reduction of computation time over Monte-Carlo

Design Tools

Self-assembly (~100 particles)



Distribution of performance, stability measure



Baseline Algorithm Improved/Robust Algorithm

Quantify quality, stability, robustness

Coarse Variables
Model Reduction
Network Decomposition

Optimal Control

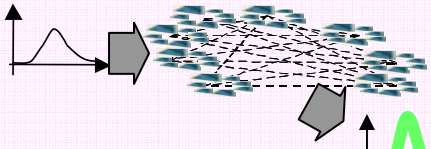
Geometric Dynamics
Chaotic search => exponentially fast coverage

10x better performance

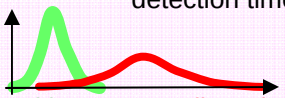
100x better performance

10x better robustness

Surveillance network (10K agents)



Distribution of target detection time

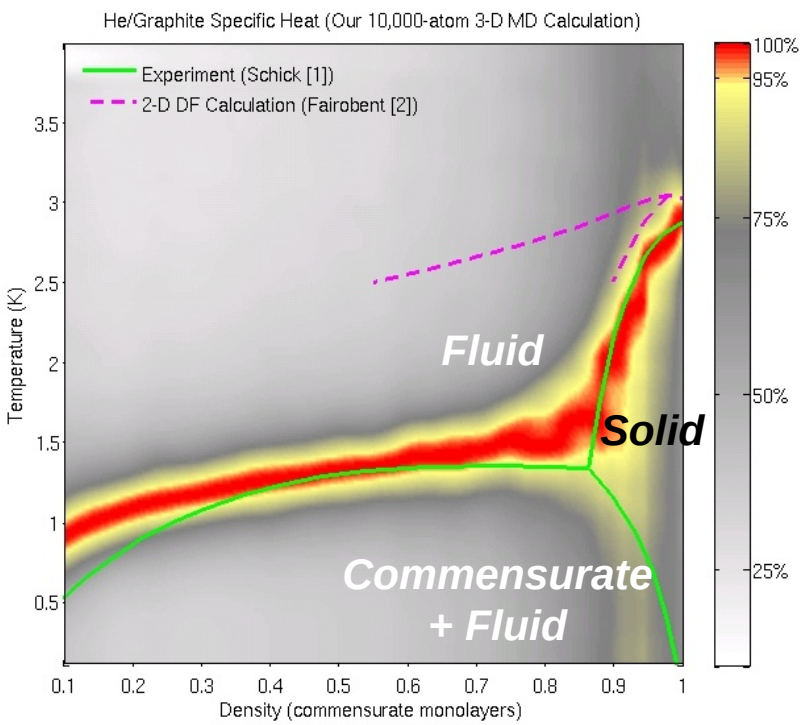


Optimal/Robust Algorithm Baseline Algorithm

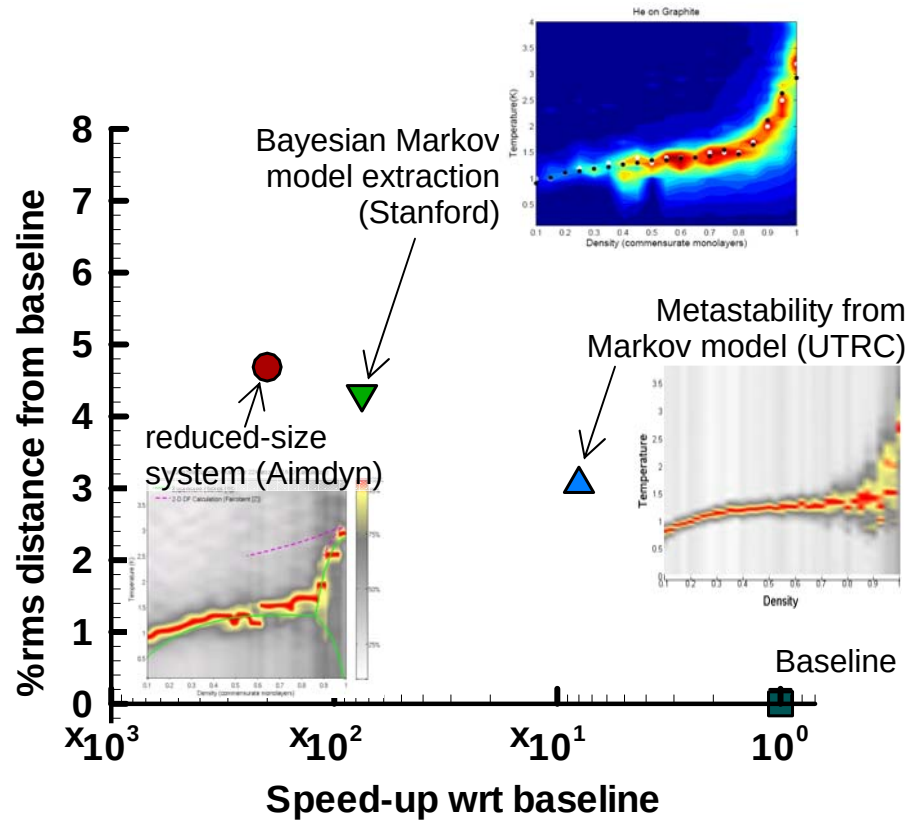
Milestone 1B: learning dynamics demonstrated on Phase Diagram problem

Baseline:

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

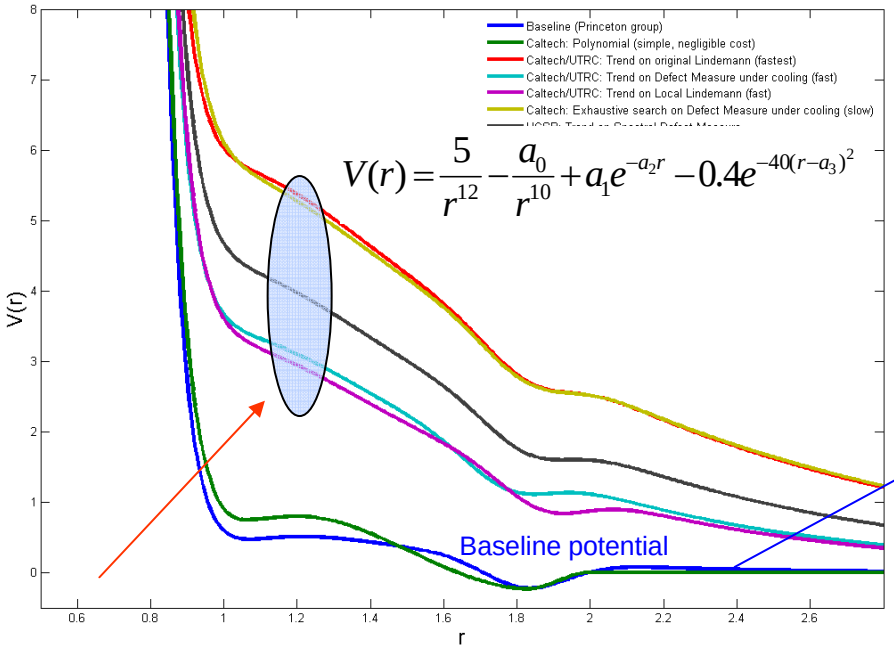


Phase diagrams obtained with RUM tools



Milestone 1A: new potential design method demonstrated in Self-Assembly problem

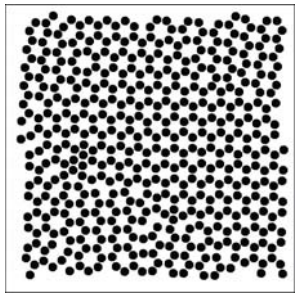
Particle interaction potentials



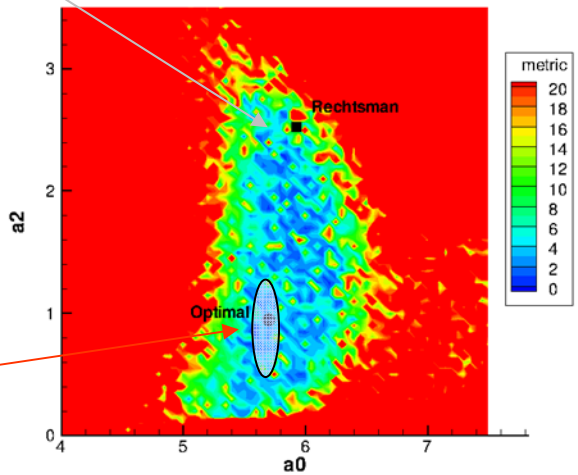
Goal: Design interaction potential so that 100 particles self-assemble to a honeycomb lattice

Baseline (Princeton 2005):

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



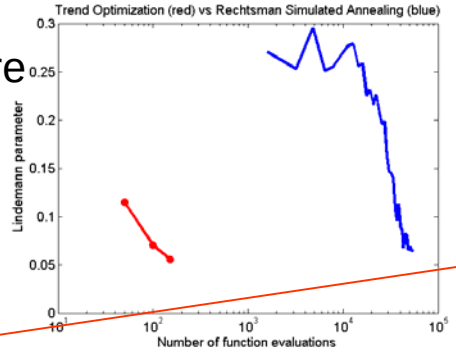
Defect measure

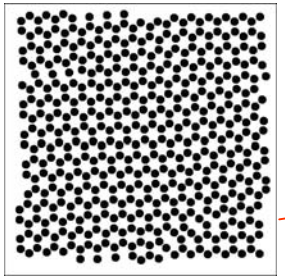


DyNARUM:

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

Defect measure





Molecular Dynamics runs

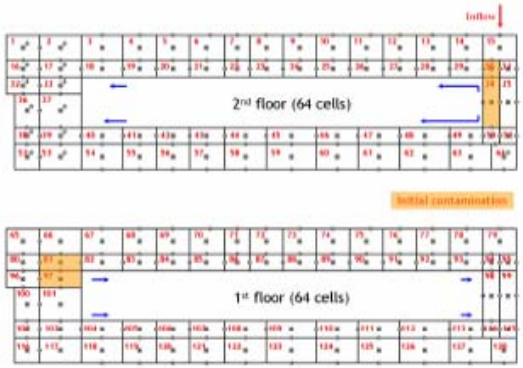
Outline

- 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

Future directions: distributed estimation

Distributed Estimators of Multiscale Phenomena

Estimate contaminant concentration in buildings



Estimator of physical dynamics

- Prediction

$$Y_i(t|t-1) = \left(F(t-1)Y_i^{-1}(t-1|t-1)F^T(t-1) + Q(t)\right)^{-1}$$
$$y_i(t|t-1) = Y_i(t|t-1)f\left(\hat{x}(t-1|t-1)\right)$$

- Measurement update

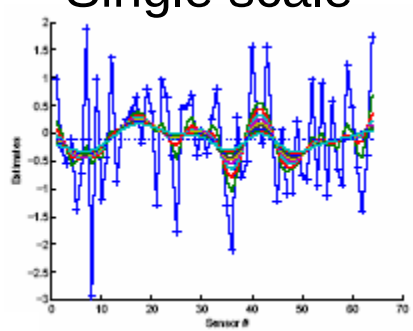
Multiscale

$$Y_i(t|t) = Y_i(t|t-1) + H^T(t)R^{-1}(t)H(t)$$
$$y_i(t|t) = y_i(t|t-1) + H^T(t)R^{-1}(t)\tilde{z}(t)$$

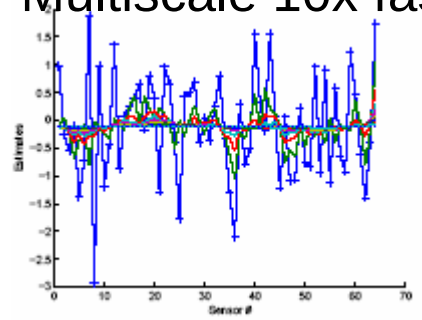
where $F(t)$ and $H(t)$ denote the Jacobian matrices, and
$\tilde{z}(t) = z(t) - h(\hat{x}(t|t-1)) + H(t)\hat{x}(t|t-1)$

Dynamics of consensus algorithm

Single scale



Multiscale 10x faster



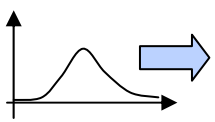
Challenge: Robust Cyber-Physical Systems

Codesign of Physical and IT Dynamics necessary

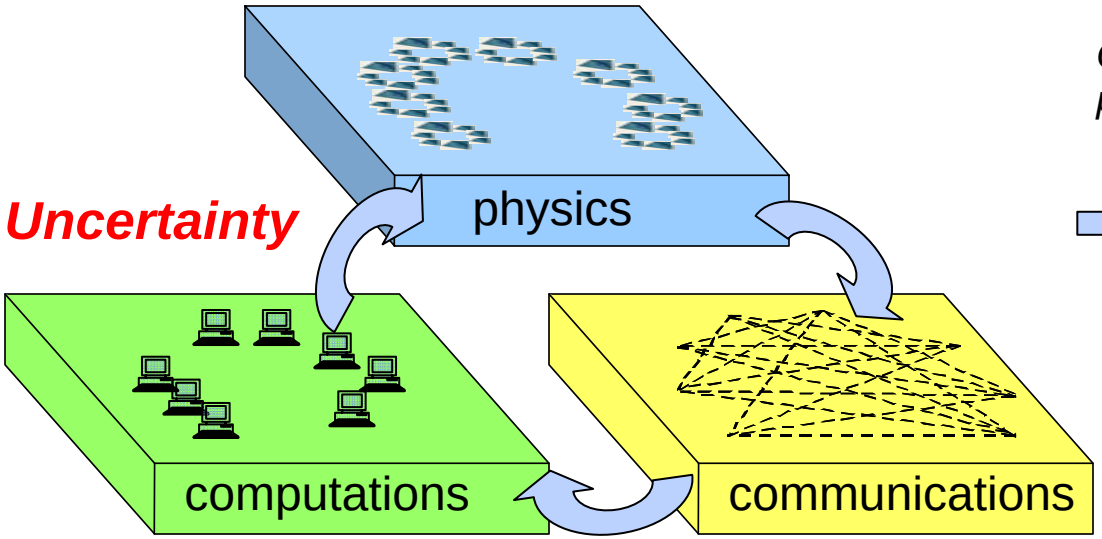
Power grid control | *City evacuation support* | *Building emergency response support* | *Surveillance networks*

Multiscale dynamics

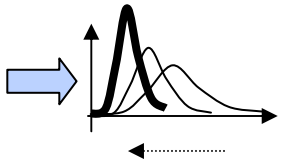
Input parameter probability distribution



Uncertainty



Output parameter probability distribution



Reduced uncertainty with robust design

No time scale separation

Summary

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  - Dynamics on Graphs
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  - And why UTC and DOD care
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