The Right Space (TRS)

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Information Session
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Since we cannot change reality, let us change the eyes with which we see reality
– Nikos Kazantzakis, *Report To Greco*, 1961

Clarification

If there is any discrepancy between what is presented today and the Disruption Opportunity (DO) DARPA-PA-24-04-07, the DO takes precedence.

Goal: Maximize pool of innovative proposal concepts for TRS

Objectives:

- Introduce the research community to TRS goals and objectives
- Identify scientific merits of a successful proposal
- Describe milestones, timeline, deliverables, and out of scope approaches
- Explain mechanisms of disruption opportunity
- Collect (send questions to TRS@darpa.mil) and publish Q&A (www.darpa.mil/work-with-us/opportunities)

Outline

- Motivation and Background
  - DoD Need
  - State of the practice
- Disruption Opportunity Description
  - Goals
  - Enabling Technologies
  - Milestones and Deliverables
- Administrative

Motivation and Background

The Right Space (TRS)

Core Hypothesis:

The right representation makes solving complex problems easier and potentially more interpretable

Objective: Systematically

(i) Discover new, insightful representations to solve DoD-relevant problems better and faster;

(ii) Find and analyze their limits of validity

Approach:

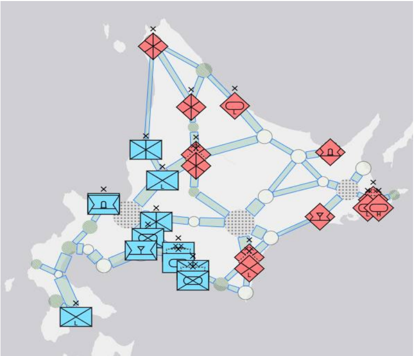
(i) Adopt and extend new mathematical methods originally developed for PDEs in high dimensions;

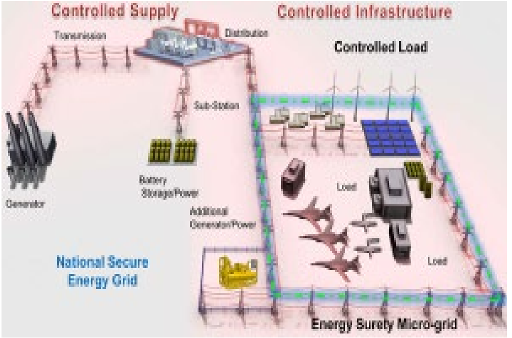
(ii) *Learn the equations in the transformed "Right Space";*

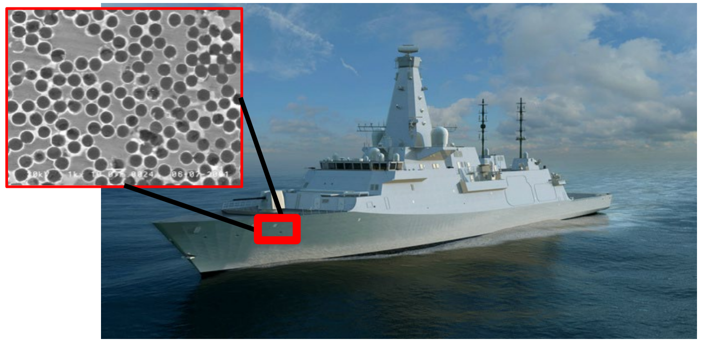
(ii) Develop Numerics for Singularities to *study the limits of transformation validity* - both deterministic and stochastic cases

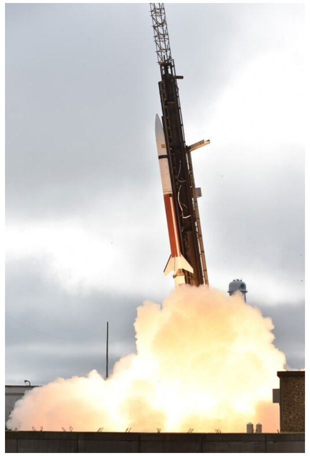
If Successful,

Drastically (>1000x) accelerate complex systems computation





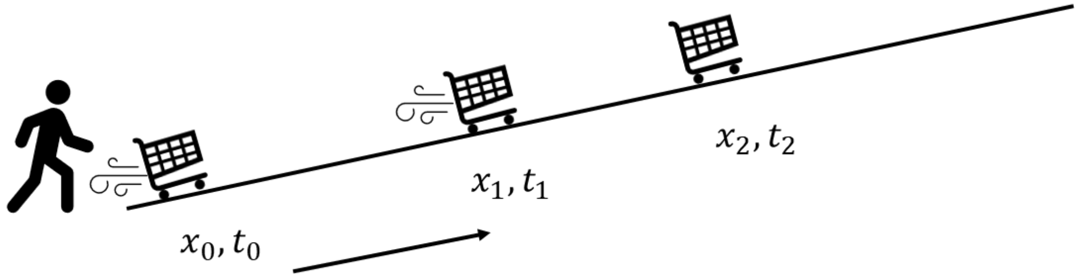


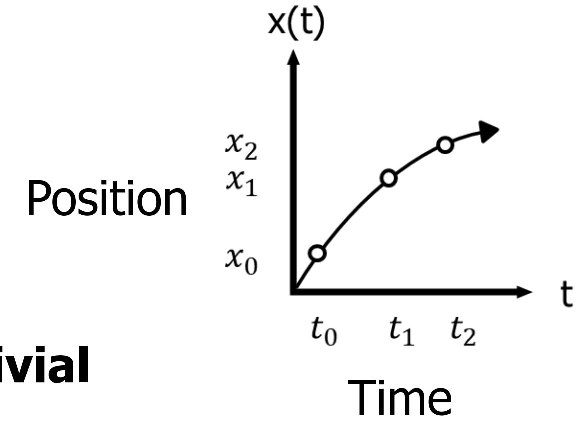


https://enerknol.com/us-armys-first-microgrid-enters-demonstration-phase/

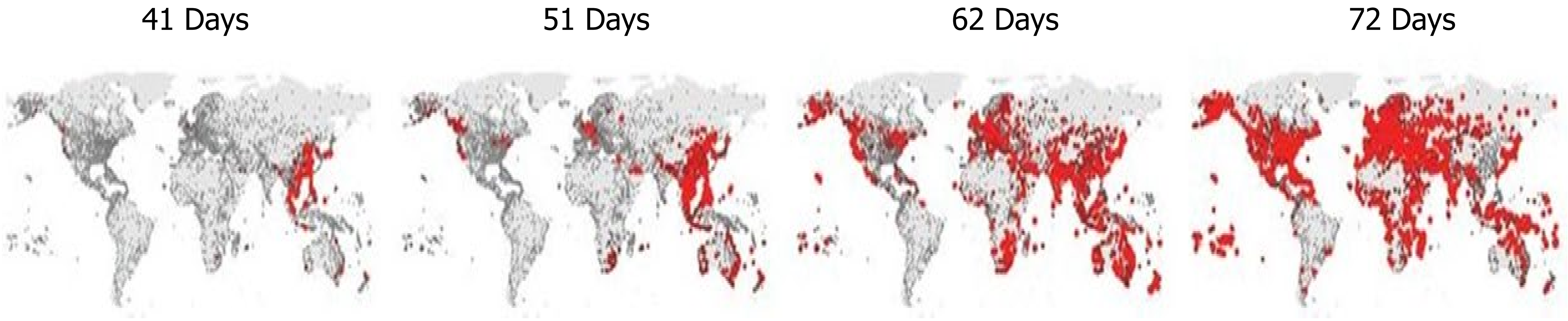
PDE: Partial Differential Equation

Example of Modeling Complex Dynamics





Learning to model/predict the position of the cart is trivial



Model of 2003 SARS Contagion

Learning to model/predict the spread of contagion is extremely challenging

SARS: Severe Acute Respiratory Syndrome

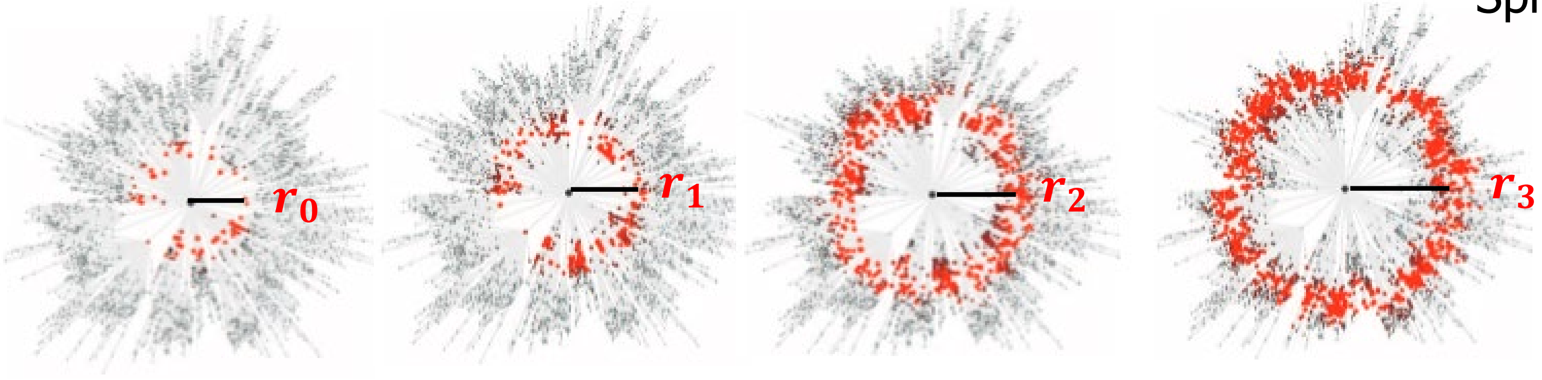
The Right Representation Enables Modeling/Prediction of 2003 SARS Contagion

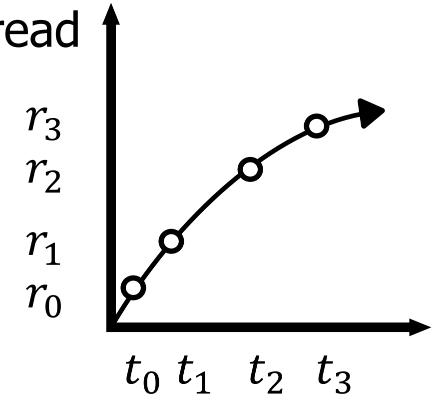
41 Days 51 Days 62 Days 72 Days

Effective Distance as a Global Mobility Network

Plot as a measure of distance from airport near outbreak epicenter

Brockmann, Dirk, and Dirk Helbing. "The hidden geometry of complex, network-driven contagion phenomena." science 342.6164 (2013): 1337-1342.





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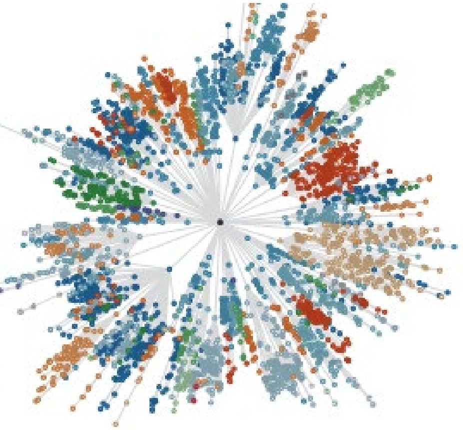
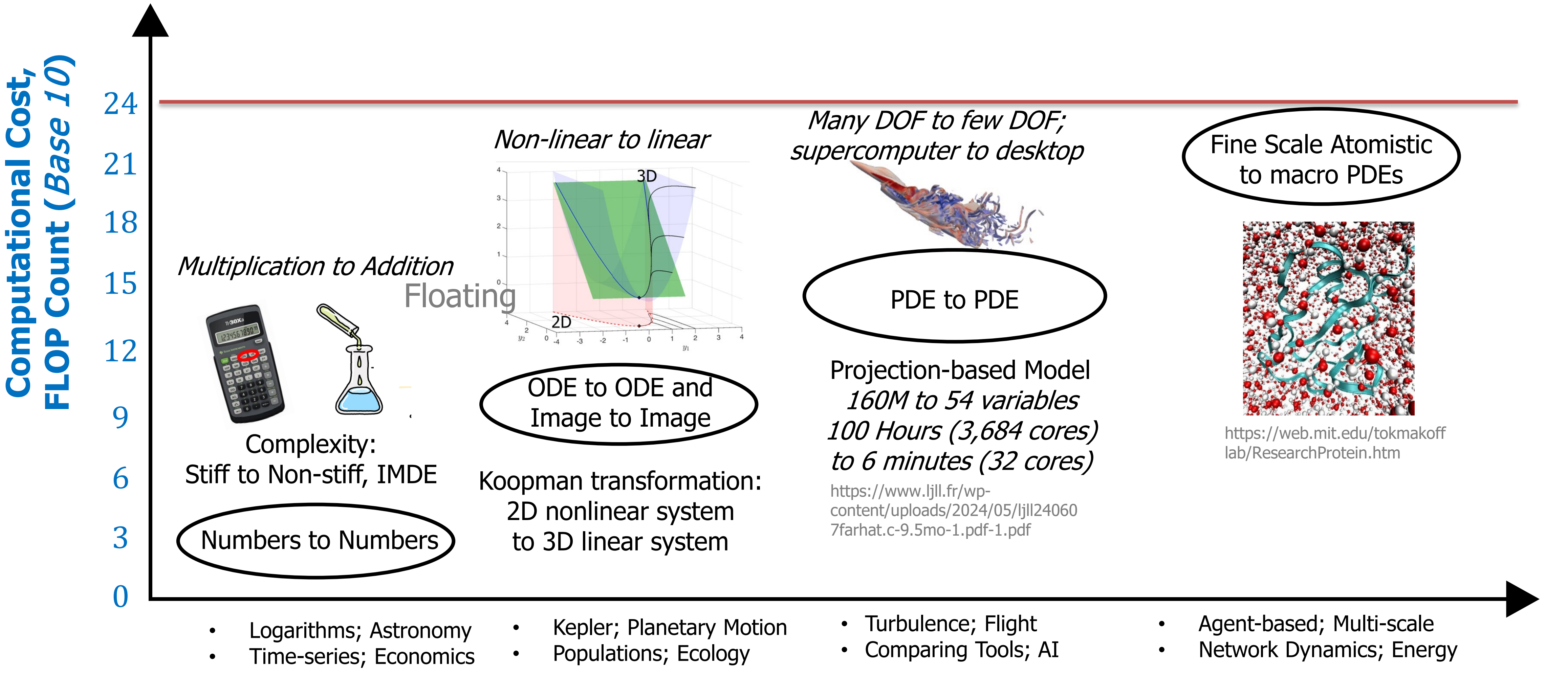


Accelerate Predicting Evolution of Contagion by finding the Right *smooth* Space where Dynamics required fewer DOF

DOF: Degrees Of Freedom
SARS: Severe Acute Respiratory Syndrome

The Cost of Modeling Complexity



Small/Macro

Complexity (DOF/Tasks)

Large/Nano

DOF: Degrees Of Freedom
ODE: Ordinary Differential Equation
PDE: Partial Differential Equation
IMDE: Inverse Modified Differential Equation
FLOPS: Floating point operations

Current Approaches are Brute Force

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CSTR[1]

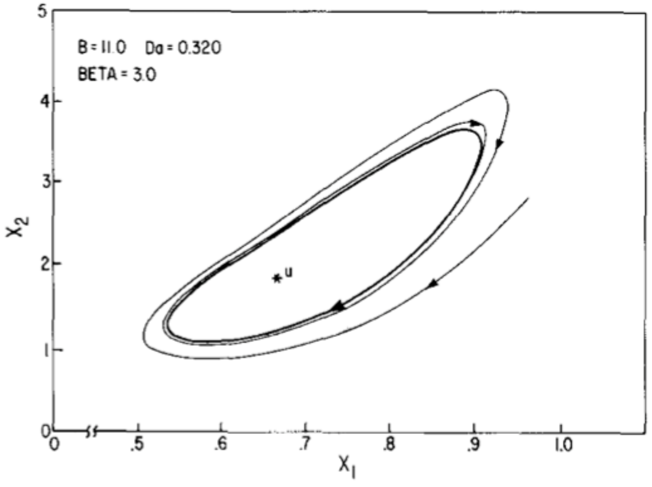


Fig. 25. Phase plane trajectories, case 6, $Da = 0{\cdot}320$.

$$\dot{x_1} = -x_1 + Da\,(1 - x_1)e^{\frac{x_2}{1+\frac{x_2}{\gamma}}}$$

$$\dot{x_2} = -x_2 + BDa\,(1 - x_1)e^{\frac{x_2}{1+\frac{x_2}{\gamma}}} - \beta(x_2 - x_{2c})$$

CSTR: Continuous Stirred Tank Reactors
DOF: Degrees Of Freedom

Normal form transformation

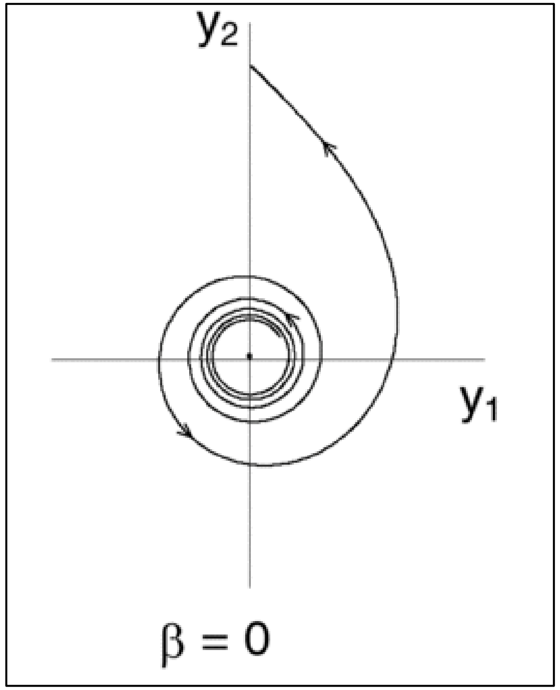
Solve a **Functional Equation**
(using local Taylor series)

$$Y_1 = f_1(x_1, x_2, Da) = a_{11}(x_1 - x_{10}) + a_{12} * (x_1 - x_{10})^2 + \cdots + b_{11}(x_2 - x_{20}) + b_{12}(x_2 - x_{20})^2 + \ldots + c_{11}(Da - Da_0) + c_{12}(Da - Da_0)^2 + \ldots$$

$$Y_2 = f_2(x_1, x_2, Da) = a_{21}(x_1 - x_{10}) + a_{22} * (x_1 - x_{10})^2 + \cdots + b_{21}(x_2 - x_{20}) + b_{22}(x_2 - x_{20})^2 + \ldots + c_{21}(Da - Da_0) + c_{22}(Da - Da_0)^2 + \cdots$$

$$\beta = \beta(Da) = d_1(Da - Da_0) + d_2(Da - Da_0)^2 + \ldots$$

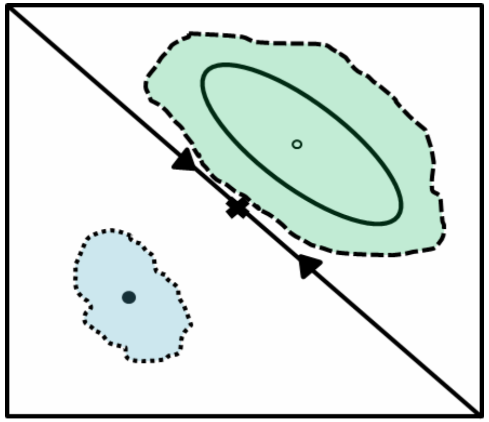
Hopf Normal Form[2]



$$\dot{y}_1 = \beta y_1 - y_2 + \sigma y_1(y_1^2 + y_2^2)$$

$$\dot{y}_2 = y_1 + \beta y_2 + \sigma y_2(y_1^2 + y_2^2)$$

Global Dynamics



Simplification methods are very local/few DOF/unwieldy and ….. ignore global dynamics

[1] A. Uppal, W. Ray, and A. Poore, "On the dynamic behavior of continuous stirred tank reactors," Chemical Engineering Science 29, 967–985 (1974).
[2] http://www.scholarpedia.org/article/Andronov-Hopf_bifurcation

Challenges in Constructing Transformations - and Why Now?

Challenge 1: ***Difficult*** to discover

- Huge search space and costly to compute

Insight 1*: Recent developments in solution operator approximations for nonlinear PDEs can be used to transform to systems with desirable properties and learn the dynamics in the transformed space*

- *e.g., **To Linear, to Non-Stiff, to Integrable, to Hamiltonian, to Smooth …***

Challenge 2: ***Intractable*** in high dimensions

- Real-world problems are complex and have high DOF; curse of dimensionality

Insight 2*: SciML algorithms, iteratively partitioning to smaller dimensions, enable transformation numerics*

- *e.g., Stochastic Dimension Stochastic Gradient Descent (SDSGD) for Hamilton Jacobi Bellman Equations in High Dimensions*
- *e.g., Deep Backward Stochastic Differential Equations for Score Based Generative Sampling Methods*

Challenge 3: ***Local***, unwieldy, and ignore global dynamics

- Brute force methods have regions of validity and do not generalize

Insight 3*: Flow-Box Theorem; singularities bound transformation validity; calibration IS a transformation*

- *e.g., neural network activations for singular function approximation*

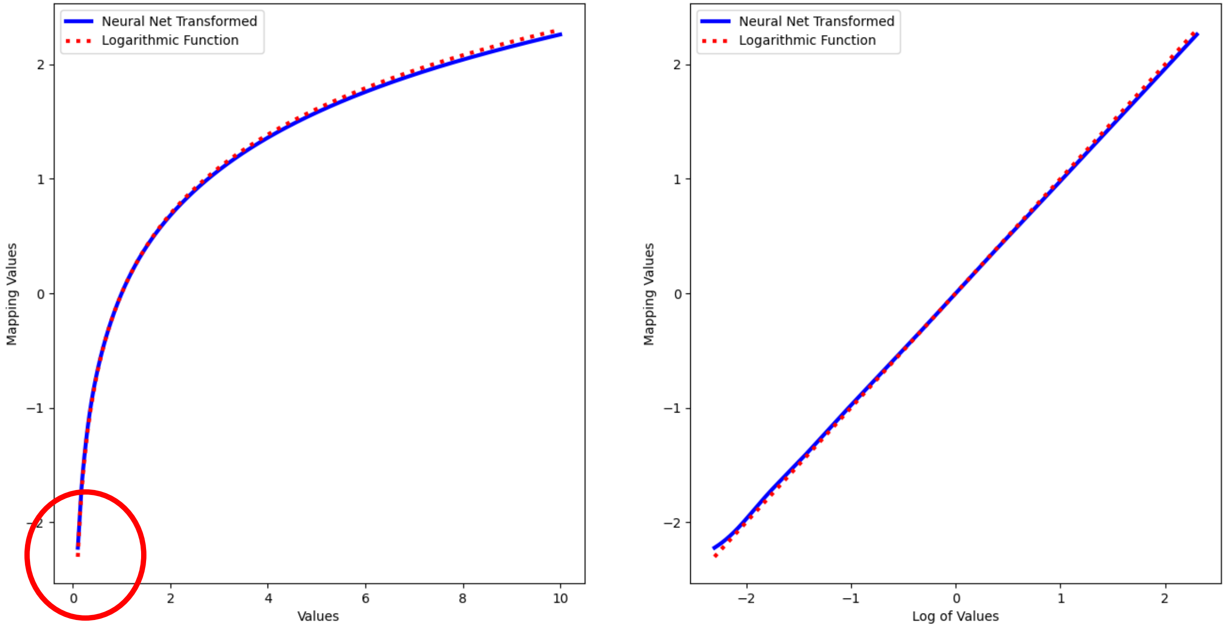
Recent advances in mathematics developed for scientific computing hold promise towards making transformations feasible

DOF: Degrees of Freedom
PDE: Partial Differential Equation
SciML: Scientific Machine Learning

Example 1: Reduce Search Space - Focus on Desirable Properties

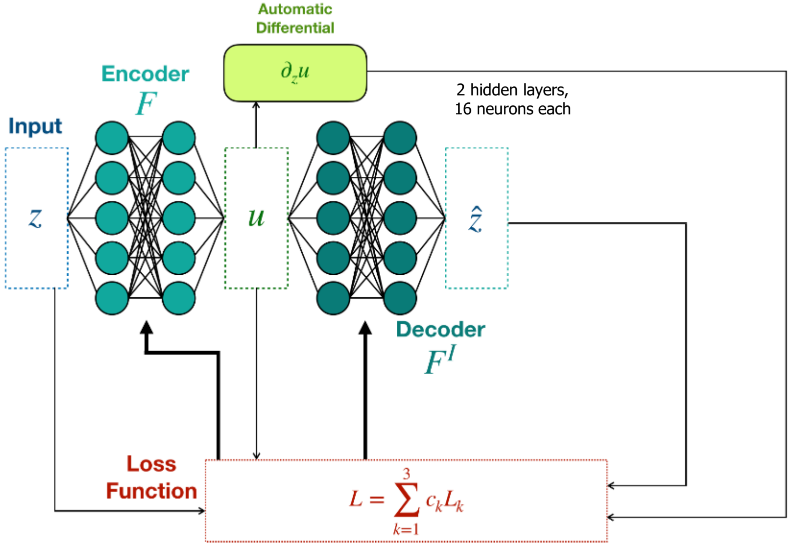
Multiplication z —— A logarithm transformation ——→ *Addition* $F(z)$

Functional Equation satisfies $F(z_1 z_2) = F(z_1) + F(z_2)$



Towards "learning logarithms" today

Learning architecture for neural networks



New Capability:

- *Where do logarithms fail?*
- *Where does the functional equation develop a singularity?*
- *Where does the transformation go to infinity?*

Disruption Opportunity Description

DO Goal and Objectives

Goal: Explore disruptive capabilities in the systematic discovery of transformations of a system's variables and parameters to representations that make solving complex modeling problems easier, faster, and potentially more interpretable

Objectives:

- Discover new, insightful representations to solve DoD-relevant problems better and faster;
- *Find and analyze their limits of validity*

Expected Program Outcomes

- Develop systematic tools for discovering local useful transformations
- Improve the real time accuracy of Digital Twins
- Develop algorithms (and SciML tools) for finding/analyzing obstacles to transformation validity
- Initiate the exploration of algorithm equivalence/AI-tool calibration
- Discover examples of techniques for mitigation of transformation failure (e.g., more variables)
- Chart the tradespace relating tools/feasible computations and useful applications

- Alter (add a new step to) scientific modeling process: learn new space before computing
- Create tools to systematically find *global* transformations
- Develop the Numerics for Singularities (especially for SciML)
- If the transformation is successful, we may even learn to think in these new spaces

Disruption Opportunity Program Structure

Proposed Complex System Classes

Discrete Interactions: Agent based, atomistic, networks
Continuum: Complex flows, microstructured materials

Stochastic equivalence: Optimization Algorithms, AI
Calibration: Accurate Digital Twins

Select an application in a class

Identify DoD relevance
Identify SotA/baseline (over a range of initial conditions, parameters, geometries)
Propose *tools*/algorithms to be developed/modified

Feasible:	Expected effort/time to transformation discovery
Extendable:	Expected limits of validity and their detection/mitigation
Generalizable:	Expected generalizability across problem classes
Useful:	Expected computational acceleration

Work with IV&V team

SotA: State-of-the-Art
IV&V: Independent Verification and Validation

Metrics & Schedule

Performance Metrics		
Metric	Description	Performance
Feasibility	Speed of Discovery	<1 Month
Extendibility	Limits of Validity: Singularities	Understand and explore mitigations, extend SotA range by at least 10x
Generalizability	Broad usefulness	Across and within problem classes
Usefulness	FLOP reduction	100-1,000x @ 99% accuracy

Phase 1 (12 Months) ≤$500,000				Phase 2 (12 Months) ≤$750,000			
FY25				FY26			
Q1	Q2	Q3 (a)	Q4 (b)	Q1	Q2 (c)	Q3	Q4 (d)
(a) Discover at least one new transformation (b) Enable 10x reduction and identify limits of validity				(c) Discover transformation in a new class and identify its limits (d) Enable 100-1000x reduction and attempt to mitigate failures			

Phase 1 Kickoff

IV&V to validate efforts

TRS + Government Modeling and Simulation Community Workshop

Program Completion

FLOP: Floating point operation
CFD: Computational Fluid Dynamics

System Classes by Phase

System Classes, Applications, and Instances by Phase			
	Phase 1	Phase 2	
Classes	Proposed system class	Phase 1 system class	New System class
Applications	One application in system class	Phase 1 application	New application (selected in coordination with IV&V)
Instances	Multiple Instances (defined by initial conditions, parameters, and geometries)	New instance (selected by IV&V)	Multiple Instances (selected in coordination with IV&V)

Out Of Scope

- Techniques that do not leverage scientific machine learning / scientific computing
- Approaches that do not generalize
- Manual transformation discovery
- Techniques that do not strive towards some form of human interpretability
- Approaches that do not strive to understand and mitigate the limits of validity of the transformations

"Proposed studies that do not leverage advances in SciML/scientific computing as well as those that do not strive towards generalizability, interpretability, and understanding and mitigating the limits of validity of transformations will be deemed out of scope and may be removed from consideration"

Schedule of milestones and payments

All proposals submitted in response to this announcement must comply with the content and format instructions in Section 5 of DARPA-PA-24-04 Amendment 1. All proposals must use the templates provided as Attachments to DARPA-PA-24-04 Amendment 1 and the DARPA Streamlined Cost Buildup Workbook Excel Attachment provided with this DO and follow the instructions therein.

Information not explicitly requested in DARPA-PA-24-04, its Attachments, or this announcement may not be evaluated.

Proposers must review the model OT for Prototype agreement provided as an attachment to DARPA-PA-24-04 Amendment 1 prior to submitting a proposal. DARPA has provided the model OT to expedite the negotiation and award process and ensure DARPA achieves the goal of Disruptioneering, which is to enable DARPA to initiate a new investment in less than 120 calendar days from idea inception. The model OT is representative of the terms and conditions that DARPA intends to include in all DO awards. The task description document, schedule of milestones and payments, and data rights assertions requested under Volumes 1, 2, and 3 will be included as attachments to the OT agreement upon negotiation and award.

DARPA has provided the schedule of fixed payable milestones in the solicitation.
Proposers should address these milestones in their proposals.

DO: Disruption Opportunity
OT: Other Transaction

Milestones: Phase 1

- Month 1:
  - Phase 1 project kick-off meeting to include presentation containing selected mathematical system class and selected target application. For the selected target application include DoD relevance, identification of SotA baseline, and all planned problem instances, defined by initial conditions, parameters, and geometries; timeline of testing proposed conditions, parameters, and geometries to be compared; list of tools/algorithms to be developed/modified and how they support your planned effort; and finally, proposed method to study limits of transformation validity with a notional example instantiated in the selected target application. All supporting positions identified in the proposal are assigned to personnel, and names are provided to the Government.
- Month 3:
  - Report on initial successes and/or failures in transformation effort for target application within first system class. Confirm all proposed personnel are working on the project at the planned level of effort.
- Month 6:
  - Demonstrate ability to create a useful transformation for at least one instance of conditions, parameters, and geometries for target application, or describe why systematic discovery of transformations for first system class failed and plans to mitigate failure.

Milestones: Phase 1

- Month 9:
  - Having demonstrated the ability to create a useful transformation in first system class, find and analyze the limits of validity for at least one instance of conditions, parameters, and geometries, or describe why systematic discovery of transformations and/or identifying limits of validity failed, and propose plans to mitigate this failure.
  - Provide transformation, documentation, and necessary data for first system class, application, and instances to the government evaluation team.
- Month 12
  - Demonstrate ability to systematically discover transformations for multiple instances within chosen system class and application, with a 2x increased region of validity and 10x (at 90% accuracy) reduction of floating-point operations (FLOP) over SotA; or describe why systematic discovery of transformations failed.

Milestones: Phase 2

- Month 13:
  - Phase 2 project kick-off meeting to include presentation containing (a) new selected mathematical system class and application; (b) DoD relevance and identification of SotA baseline; (c) all planned instances, defined by initial conditions, parameters, and geometries to be compared, including tentative timeline; (d) description of plan to extend Phase 1 work to generalize in the new system class.
- Month 16:
  - Report on initial successes and/or failures in transformation effort for second system class and ability to generalize approach.
- Month 18:
  - Demonstrate ability to create a useful transformation for at least one instance of conditions, parameters, and geometries in second system class or describe why systematic discovery of transformations failed and propose plans to mitigate failure
- Month 20:
  - Having demonstrated the ability to create a useful transformation in second system class, find and analyze the limits of validity for at least one instance of conditions, parameters, and geometries, or describe why systematic discovery of transformations and/or identifying limits of validity failed and propose plans to mitigate this failure.
  - Provide transformation, documentation, and necessary data to the government evaluation team.
- Month 24
  - Demonstrate ability of approach to generalize by systematically discovering transformations across and within first and second system classes, with a 10x increased region of validity and 100-1000x (at 99% accuracy) reduction of FLOP over SotA or describe why systematic discovery of transformations failed.

Deliverables

Performers will be expected to provide, at a minimum, the following deliverables:

- Negotiated deliverables specific to the objectives of the individual efforts. These may include registered reports; experimental protocols; publications; intermediate and final versions of software libraries, code, and APIs, including documentation and user manuals, and/or a comprehensive assemblage of design documents, models, modeling data, and results; SotA baseline values; discovered transformation and its limits of validity; and model validation data.

API: Application Programming Interface

Administrative

Questions & Answers

Questions can be submitted to TRS@darpa.mil, include [FAQ] in the subject line

Questions and answers are posted publicly (www.darpa.mil/work-with-us/opportunities);
do not include proprietary information

FAQ Submission Deadline: Questions submitted within seven (7) calendar days of the proposal due date may not be answered

Key Dates

Posting Date: Future Program Announcement 01/10/2025; Special Notice 2/26/2025; Solicitation 03/04/2025

Information Day: 03/12/2025 (Today)

Proposer Profile: No later than 4:00 PM on 03/13/2025, TRS@darpa.mil

- Contact information (name, organization, email, telephone number, mailing address, and organization website);
- a brief description of technical competencies;
- and, if applicable, desired expertise from other teams/organizations

Abstract Due Date: 03/24/2025 (Abstracts are **STRONGLY ENCOURAGED** but not required)

Full Proposal Due Date: 05/02/2025

Assumed Start Date of Successful Proposals: 06/30/2025

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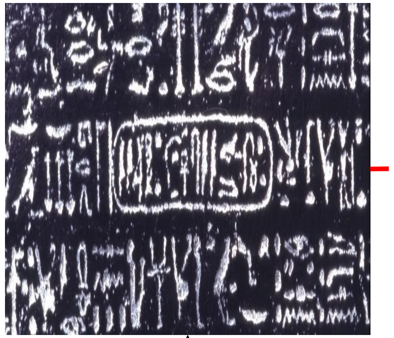
Translation: The Archetypal Facilitating Transformation

Egyptian hieroglyphs



Rosetta Stone

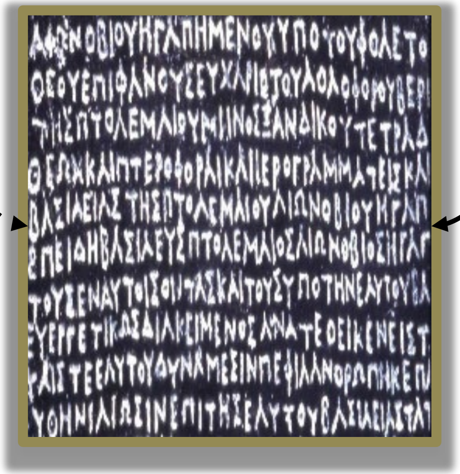
Impossible

Priests of a temple in Memphis support the reign of thirteen-year-old Ptolemy V, on the first anniversary of his coronation

Learnable

Easy

https://www.theguardian.com/culture/2020/aug/25/discovery-of-scholars-notes-shine-light-on-race-to-decipher-rosetta-stone



Ancient Greek