

The Right Space (TRS)

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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







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-withus/opportunities)





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





Motivation and Background





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:

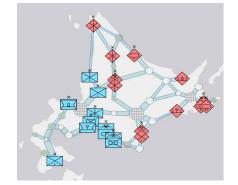
(i) Adopt and extend new mathematical methods originally developed for PDEs in high dimensions;

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

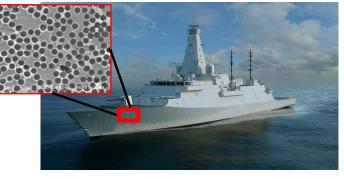
(ii) Develop Numerics for Singularities to study the limits of transformation validity - both deterministic and stochastic cases

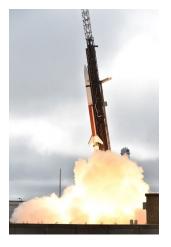
If Successful,

Drastically (>1000x) accelerate complex systems computation







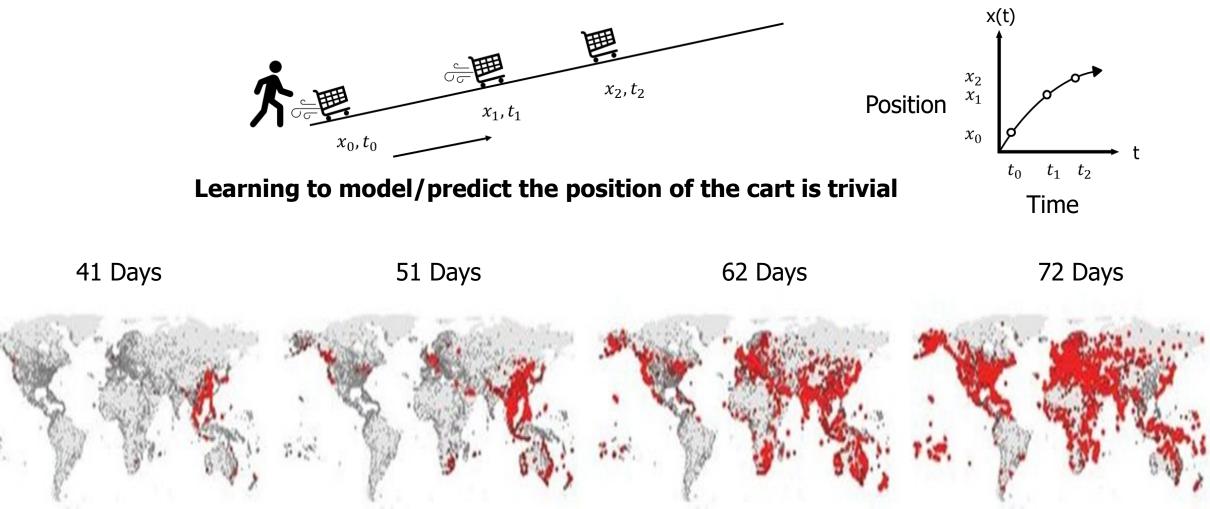


https://enerknol.com/us-armys-first-microgrid-enters-demonstration-phase/



Example of Modeling Complex Dynamics





Model of 2003 SARS Contagion

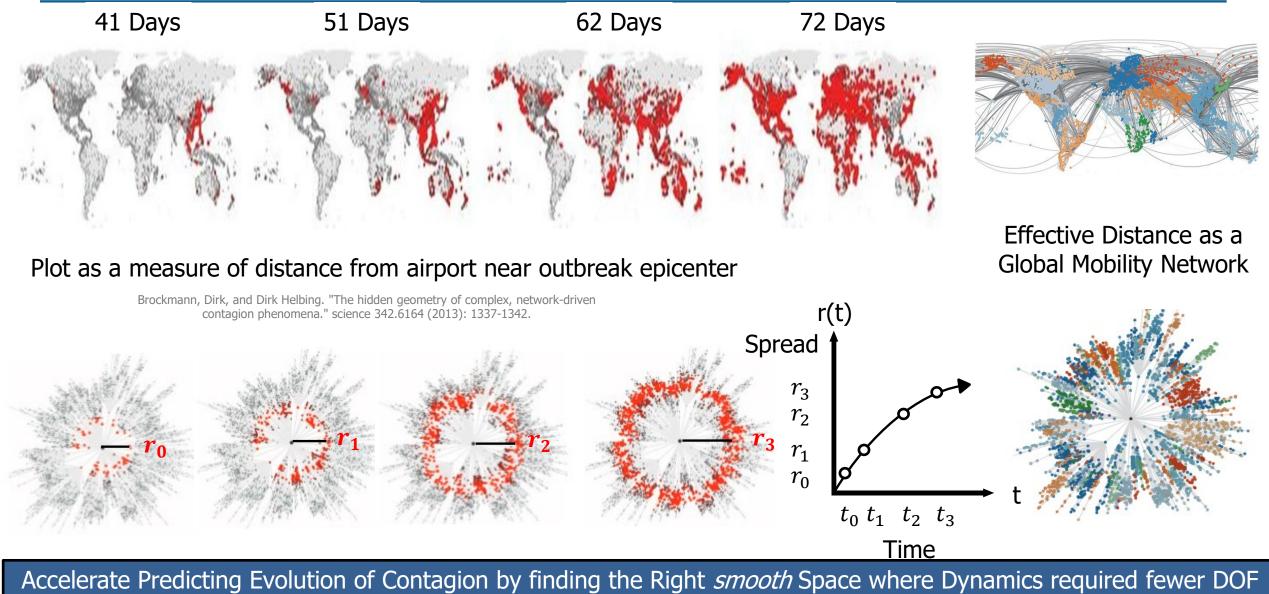
Learning to model/predict the spread of contagion is extremely challenging

SARS: Severe Acute Respiratory Syndrome



The Right Representation Enables Modeling/Prediction of 2003 SARS Contagion

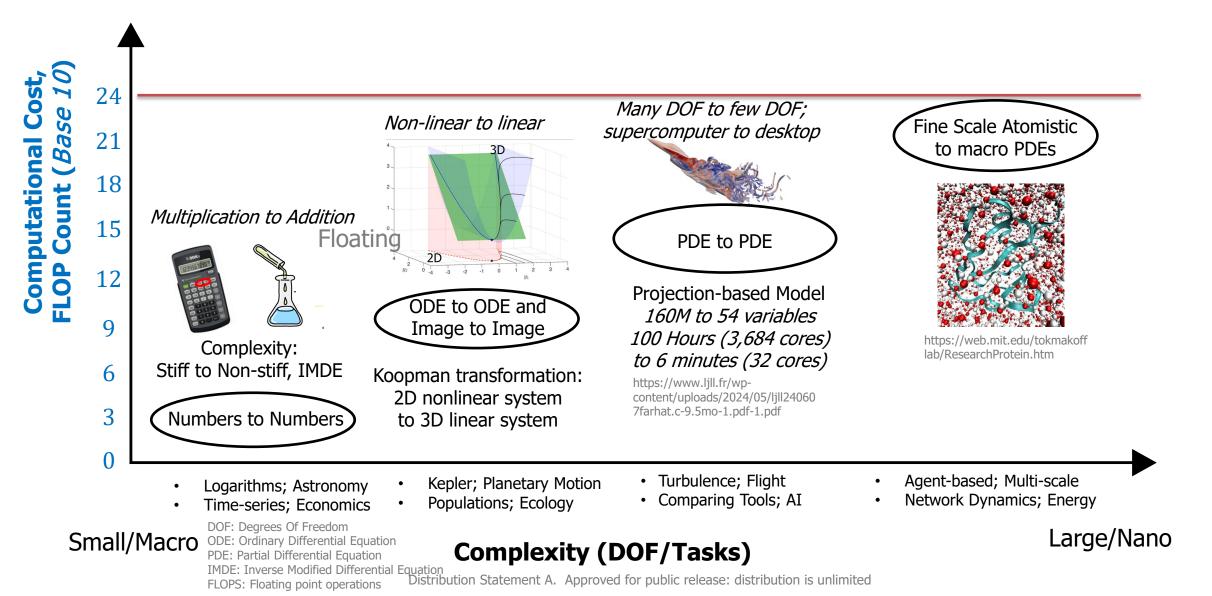




DOF: Degrees Of Freedom SARS: Severe Acute Respiratory Syndrome

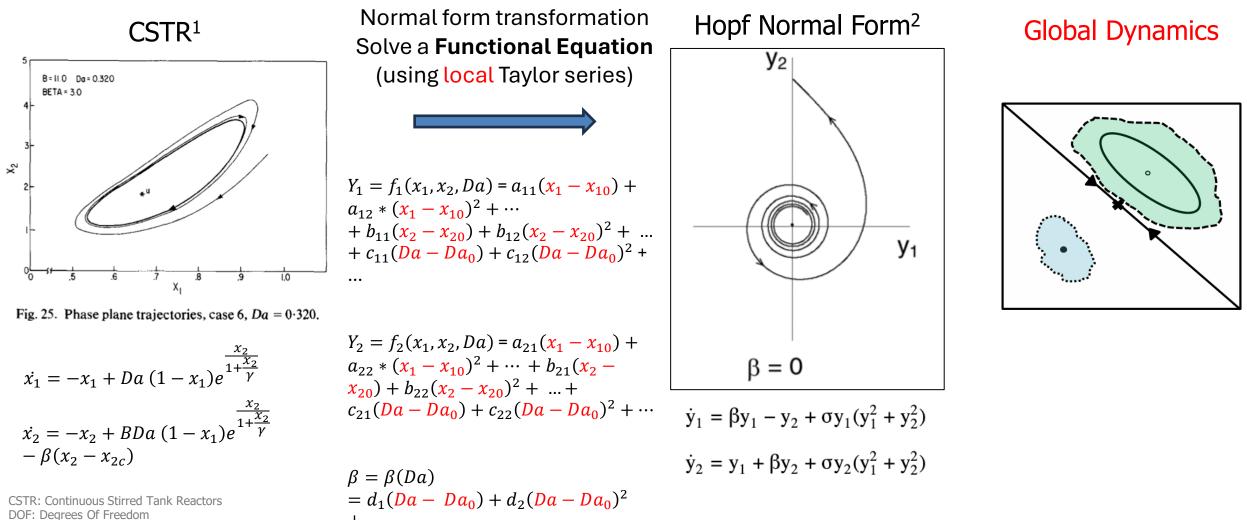












Simplification methods are very local/few DOF/unwieldy and

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





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 <u>Dimension</u> 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

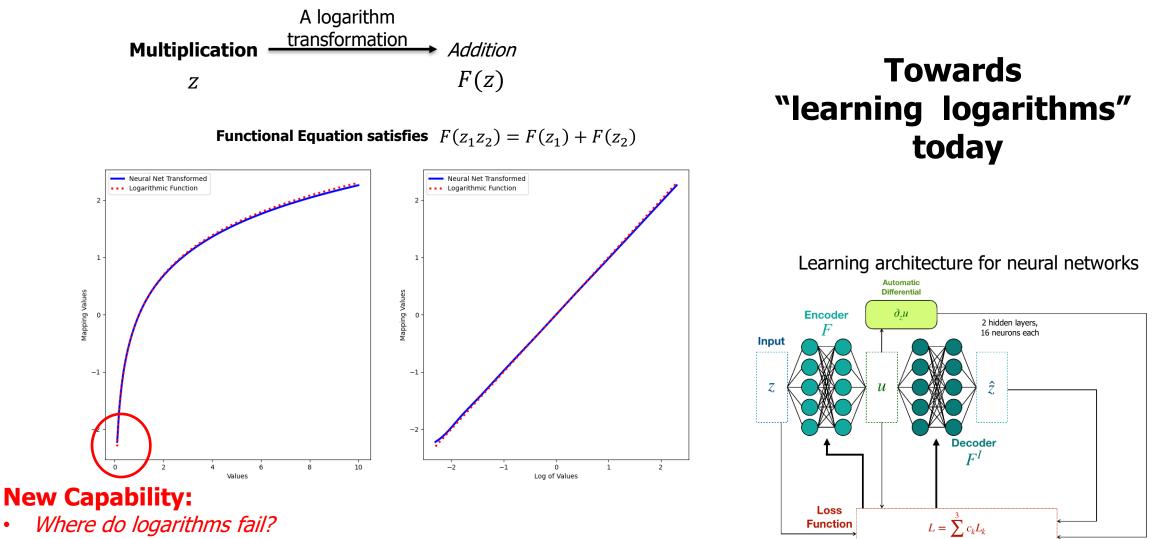
Insight 3: Flow-Box Theorem; singularities bound transformation validity; calibration IS a transformation

• e.g., neural network activations for singular function approximation

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







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





Disruption Opportunity Description





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





- 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





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 discoveryExtendable:Expected limits of validity and their detection/mitigationGeneralizable:Expected generalizability across problem classesUseful:Expected computational acceleration

Work with IV&V team





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)
-					(c) Discover transformation in a new class and identify its limits (d) Enable 100-1000x reduction and attempt to mitigate failures			
Phase Kicko				TRS + Governmer Simulation Commu	5	Progra Comple		

FLOP: Floating point operation CFD: Computational Fluid Dynamics





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"





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.





- 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.





- 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.





- 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.





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.





Administrative





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





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

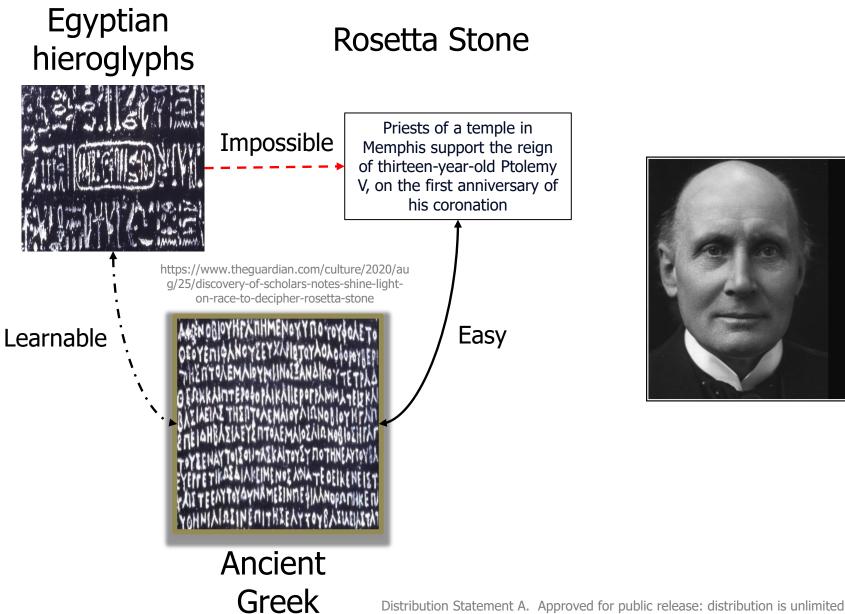
Assumed Start Date of Successful Proposals: 06/30/2025

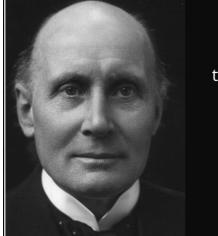


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Civilization advances by extending the number of important operations which we can perform without thinking of them.

— Alfred North Whitehead —